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THE CONTROL OF OXIDES OF NITROGEN EMISSIONS FROM AIRCRAFT GAS TURBINE ENGINES

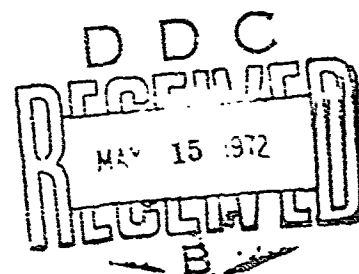
Volume 2: The NO_x Formation Process

Ronald S. Fletcher Richard D. Siegel
Northern Research and Engineering Corporation
219 Vassar Street
Cambridge, Massachusetts 02139



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16. Abstract The objective of this study was to develop criteria for use in the design of aircraft gas turbine combustion chambers to minimize nitrogen oxide emissions. The approach adopted involved the development of a mathematical model of NO_x emission from aircraft engine combustors; a parametric analysis, using the model, to determine the sensitivity of NO_x emissions to variations of model parameters and engine design variables; evaluation of critical model parameters by means of experimental measurements; and the incorporation of the model into combustor design methods to provide guidelines for minimizing NO_x emission while maintaining other performance and emission characteristics. The results of the study and the NO_x emission control criteria are described in Volume 1 (FAA-RD-71-111-1). Volume 2 (FAA-RD-71-111-2) describes the nitric oxide formation process and a computer program (NOXRAT) for calculating thermodynamic data. The program is based upon a six-reaction model of NO formation. Volume 3 (FAA-RD-71-111-3) describes combustion and flow processes in gas turbine combustors and a computer program (GASNOX) for calculating gas properties and NO concentrations throughout a combustor. This program is based upon a three-zone, heterogeneous model of gas turbine combustor operation. Program GASNOX is used with input data from Program NOXRAT to calculate NO emission rates.					
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The study reported here was carried out under the technical direction of Dr. D. M. Dix with Dr. Ronald S. Fletcher assuming project responsibilities. Other participants in the program were Dr. R. D. Siegel, Dr. E. K. Bastress, and Mr. R. J. Murad; Professors J. B. Heywood, A. H. Lefebvre, and Mr. E. R. Norster served in a consulting capacity during the course of the study.

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1. INTRODUCTION

Volume 1 of this report carries a full description of the complete program but omits mathematical details of the model developed to predict the nitric oxide (NO_x) emissions from aircraft gas turbine combustors and also the details of two computer programs developed as part of the study for obtaining predictions from the model. It is the purpose of Volumes 2 and 3 of the report to present full descriptions of both the model and the computer programs.

It is convenient to consider the model in two parts, one part being concerned with the NO_x formation process and the other with modeling the flow behavior within gas turbine combustors. The convenience arises not only due to the basic difference in the studies of these two parts, but also due to the fact that a separate computer program has been developed for each part. This approach has been adopted in the interests of economy of computation as calculation of the necessary data for the determination of the NO_x formation process requires appreciable computer time, but, of course, the data once collected can be applied to any combustor calculation with the same reference conditions (in this case, combustor inlet conditions) of pressure and temperature. The computer program developed for this task has the name NOXRAT, and its function is to compute the rate terms of the NO_x formation process and all relevant thermodynamic data for a series of fuel-to-air ratios with a common reference state.

Volume 2 of this report is solely concerned with the nitric oxide formation process. It presents a mathematical description of the process, a full description of the program NOXRAT, and also includes a section which is essentially a user's manual for the program. Volume 3 produces the same details for the flow model developed to describe the flow conditions in a gas turbine combustor. The corresponding computer program is named GASNOX and it is so arranged that the rate terms and all relevant thermodynamic data computed in NOXRAT are punched onto a deck of computer cards which serves as input data to the main program GASNOX.

The objective of this volume of the report, therefore, is to present the theory behind the NO_x formation process and details of the computer program developed for its application.

2. THE NO_x FORMATION PROCESS

While engine exhaust emissions are often expressed as nitrogen oxides (NO_x), or as nitrogen dioxide (NO₂), the pollutant present in the exhaust gas as it leaves the engine is almost completely nitric oxide, NO, with only a few per cent of NO₂ (Ref 1). The conversion to NO_x or NO₂ is made because many of the techniques used to measure nitric oxide require first that it be oxidized to nitrogen dioxide. Thus, inside the engine, the important oxide of nitrogen to consider is nitric oxide, NO.

Several authors have proposed reaction schemes for nitric oxide formation, e.g., Caretto, Sawyer, and Starkman (Ref 1), Bartok, et al (Ref 2), Newhall (Ref 3), Lavoie, Heywood, and Keck (Ref 4). The set of reactions proposed by Lavoie, et al (Ref 4) is the most complete for predicting nitric oxide formation, and it has been evaluated experimentally for a range of equivalence ratios (0.9-1.2), pressures (10-30 atm), and temperatures (2200-2800 deg K) in a spark-ignition engine (Refs 4 and 5). These conditions are directly comparable to those occurring in the gas turbine combustor primary zone as shown by Heywood et al (Ref 6), and the reaction scheme does predict NO emission levels which are in good agreement with measurements made on such combustion systems.

The set of reactions included in the analyses of References 4, 5, and 6 are incorporated in the model and are shown below.



Note that the reaction $2\text{NO} \rightleftharpoons \text{N}_2 + \text{O}_2$ has been omitted from this scheme as it is very slow and does not proceed directly. In References 4 through 6 the rate constants selected for these reactions were taken from Schofield (Ref 7) except for reaction 3 which was taken from

Campbell and Thrush (Ref 8). These constants are,

$$k_1 = 2 \times 10^{-11}$$

$$k_2 = 2 \times 10^{-11} \exp(-7.1/RT)$$

$$k_3 = 7 \times 10^{-11}$$

$$k_4 = 5 \times 10^{-11} \exp(-10.8/RT)$$

$$k_5 = 6 \times 10^{-11} \exp(-24.0/RT)$$

$$k_6 = 8 \times 10^{-11} \exp(-24.0/RT)$$

and are in $\text{cm}^3/\text{sec-molecule}$. R is in $\text{kcal/gm-mole-deg K}$. Since the equilibrium constants for these reactions are known, the kinetic scheme is thus completely defined.

Recently completed analyses of data and correlations available in the latest literature have raised some question as to the reliability of the above constants. A group at Leeds University (Ref 9) reports k_1 better correlated in the form $A \exp(-E/RT)$ while both Leeds and Newhall (Ref 3) show reaction 2 to be correlated more satisfactorily in the form $AT \exp(-E/RT)$. Newhall also correlated reaction 6 with a pre-exponential factor 3.6 times greater, and an activation energy 1.16 times greater, than the corresponding values determined by Schofield.

With this lack of agreement of the rate constants, it was decided to represent all six reactions in the reaction scheme in the general form,

$$k_i = A_i T_i^n \exp(-E_i/RT) \quad (7)$$

This format allows maximum flexibility in comparing the different fits of the kinetic rate data for each of the expressions. Further, as new data and correlations become available, it will be a simple matter to adjust the three constants to correspond accordingly to those correlations and data.

Not all of the above reactions are equally important over the equivalence ratio and temperature range of interest. The first two reactions, the Zeldovich chain mechanism, are the two most important reactions at high temperatures (greater than 2200 deg K) in fuel-lean mixtures. The importance of this pair of reactions is well established. The third reaction becomes important in fuel-rich mixtures. Reactions

4, 5, and 6 involving N_2O as an intermediary become important at temperatures about 2000 deg K. It can be shown that the small amount of NO_2 present is in equilibrium with the NO and other reactions with NO_2 need not be included (Ref 5).

Conditions in gas turbine combustors fall into all of these regimes, but calculations indicate that the reactions 4, 5, and 6 do not contribute greatly to the nitric oxide formation rate. In fact, if one accepts the probable limits of accuracy for any such kinetic scheme, a case may be made for their exclusion. However, these reactions are included in the reaction scheme for the sake of completeness.

In order to apply this reaction scheme to gas turbine combustors, it is necessary to be able to predict the concentration levels of all species active in the set of six reactions specified above at all thermodynamic states typical of the combustor. At the pressure and temperature levels that exist in such combustors during high thrust, low altitude operation, the hydrocarbon oxidation reactions go rapidly to completion compared with the nitric oxide formation processes. In order to predict these species concentrations therefore, the following assumptions are made:

- a. Combustion is mixing controlled and not rate-limited, and therefore, in the combustor, N_2 , O_2 , O, OH, H, and H_2 concentrations are the equilibrium concentrations corresponding to the combustor inlet temperature and pressure, and to the equivalence ratio. This assumption limits the usefulness of the model to high pressure, high temperature operating conditions, but it is precisely these conditions at which most nitric oxide is produced and are therefore of most interest to this study.
- b. N and N_2O concentrations are given by the steady-state assumption; That these concentrations are not in equilibrium but are in steady-state with NO can be shown by deriving rate equations for N and N_2O which have relaxation times short compared with the NO rate equation.

If these assumptions are applied to Equations 1 through 7, then the change, $\dot{r}$, in total nitric oxide per unit time per unit volume,

that results from chemical reaction over a fixed element can be written as

$$\dot{r} = 2M_{NO} (1 - \alpha^2) \left[\frac{R_1}{1 + \alpha K_1} + \frac{R_6}{1 + K_2} \right] \quad (8)$$

where M_{NO} is the molecular weight of NO, $\alpha = [NO]/[NO]_e$ is the local nitric oxide concentration divided by the equilibrium nitric oxide concentration, R_1 is the "one-way" equilibrium rate of reaction 1, i.e., $R_1 = k_1 [N]_e [NO]_e$; $K_1 = R_1/(R_2 + R_3)$ with R_2 and R_3 defined analogously to R_1 but for reactions 2 and 3; and $R_6 = k_6 [O]_e [N_2O]_e$ and $K_2 = R_6/(R_4 + R_5)$.

It is interesting to consider the form of the equation above when applied to the gas turbine combustor. In this case the thermodynamic base state is represented by the combustor inlet pressure and temperature, both of which are nonvariable with time for a fixed operating condition. If the fuel-to-air ratio is specified, therefore, the terms R_1 , R_6 , K_1 and K_2 all become constants as a consequence of assumptions a and b above. The molecular weight M_{NO} is a constant, hence the only variable is α and the equation reduces to the simple form,

$$dNO/dt = f(NO)$$

which may readily be integrated to follow the nitric oxide concentration levels through the combustor.

Maximum utility has been made of this simplicity, chiefly in the interests of reducing the computer operating costs for each sample case tested in the flow model. The computational procedure, as previously explained in the introduction, was separated into two tasks; the first task primarily determines the rate terms R_1 , R_6 , K_1 , and K_2 for a specified combustor inlet temperature and pressure over the complete range of fuel-to-air ratios that cause sufficiently high temperatures to form nitric oxide, and the second task computes the flow conditions throughout the combustor and uses the data collected from task one to predict nitric oxide emission levels.

A computer program has been developed for each task and the program for Task 1 will be described in the next section.

3. PROGRAM NOXRAT

3.1 INTRODUCTION

3.1.1 Program Function and Capabilities

Program NOXRAT is a modified version of CEC, a NASA developed digital computer program written in Fortran IV (Refs 10, 11 and 12). NOXRAT is designed to evaluate the chemical equilibrium products, the adiabatic flame temperature, and the kinetic properties used in the nitric oxide formation model (previously described) for the combustion of a reactive fuel, or a fuel mixture with an oxidant or mixture of oxidants. NOXRAT iteratively calculates the equilibrium properties of the combustion products based on a minimized Gibbs free energy. In a typical equilibrium computation NOXRAT prints the following properties for each assigned fuel-to-air ratio:

- a. The equilibrium temperature and pressure; the sonic velocity, the enthalpy, entropy, mean molecular weight, $(\partial V / \partial P)_T$, the heat capacity, and the heat capacity ratio (C_p / C_v) , of the combustion stream.*
- b. The mole fraction of each of the combustion products present at equilibrium at concentrations greater than 5×10^{-6} .*
- c. The chemical formula, weight fraction in the total fuel or oxidant, and the base enthalpy, temperature, density, and physical state of each of the specified reactants.*
- d. The total oxidant to total fuel weight ratio, the per cent fuel, the equivalence ratio, and the average density of the reaction mixture.*
- e. The equilibrium mole fraction of each of the species of interest in the nitric oxide kinetic scheme (Ref 18) and the equilibrium mole fractions of $C(s)$, CO, and CO_2 .
- f. The molecular weight and the adiabatic flame temperature of the combustion products; the assigned inlet pressure; the

*. Normal output of CEC.

fuel-to-air ratio; and the atomic composition, inlet temperature, and enthalpy of both the fuel(s) and the oxidant(s).

For each assigned pressure the program also prints and punches:

- a. The atomic composition of the fuel (C_xH_y); the inlet air temperature; a code number identifying the set of kinetic constants used in the NO rate formation calculations; the assigned pressure; and the stoichiometric equivalence ratio.
- b. For each specified fuel-to-air ratio: the mixture ratio (mass of fuel to mass of fuel and air); the equivalence ratio; the density and adiabatic flame temperature of the combustion products; the equilibrium concentration of NO, CO, $C(s)$, and CH_2 (unburned fuel); and the kinetic parameters* R_1 , R_6 , K_1 , and K_2 where R_1 and R_6 are forward reaction rates for reactions 1 and 6 and K_1 and K_2 are ratios of forward reaction rates used in the kinetic scheme (see Appendix V).

NOXRAT also permits calculation of:

- a. Chemical equilibrium for assigned temperatures and pressures.
- b. Theoretical rocket performances for both frozen and equilibrium compositions during expansion.
- c. Chapman-Jouguet detonation properties.

The latter two options were not exercised in this study.

3.1.2 Analysis Procedures

The analytical procedures on which NOXRAT is based are described in Section 2. A detailed description of the changes that have been incorporated into these procedures to permit calculation of the reaction rate constants and the thermal properties used in the chemical

* These parameters are used to compute the rate of change of the NO mass fraction due to chemical reaction by:

$$\frac{d\{NO\}}{dt} = \frac{2M_{NO}}{\rho}(1-\alpha^2)\left[\frac{R_1}{1+\alpha K_1} + \frac{R_6}{1+K_2}\right]$$

where M_{NO} is the molecular weight of NO, ρ is the gas density, $\{NO\}$ is the mass fraction concentration of NO and α is the ratio of NO concentration to the NO concentration at equilibrium.

reaction scheme for the formation of nitric oxide are presented in the appendices of this report. Reference to any of these procedures is unnecessary for operation of the computer program.

3.1.3 Report Arrangement

The main body of the report begins with a section in which the input data necessary for the solution of any case are described in detail; this includes instructions for preparing and supplying these data to the program and a sample case in the appropriate format. The next section contains a discussion of the various types of output data which are obtained from the program and also the output data from the sample case. Following that is a section containing miscellaneous information regarding the operation of the program with the CDC 6600 computing system. The next section is a description of the error messages printed by the program.

The first appendix consists of a general discussion of the overall logic structure of the program. The next appendix gives the Fortran nomenclature for the major new variables incorporated into the original CEC program. The remaining appendices, except the last two, provide detailed description of the changes made to existing routines and of the subroutines which have been developed and incorporated into the program, one appendix for each routine. The appendix for each new subroutine contains a presentation of the input and output variables, an internal Fortran nomenclature, a description of the step-by-step calculation procedure, and a Fortran listing of the subroutine. The last two appendices are respectively a listing of the program in its entirety and a listing of the THERMO data.

3.2 INPUT DATA

3.2.1 General Description

The input data to Program NOXRAT is nearly identical with that of NASA's Program CEC. Although the input format for CEC has been described in a preliminary guide (Ref 13) and detailed in a NASA report (Ref 14), NREC has elected to present here

a description of NOXRAT input (and output) data. This description is suitable to allow the reader to understand the mechanics of how to operate the program. Much of this information is taken directly from Reference 13.

Program input data will be discussed under four categories. Three of the categories are required and one is optional. The three required categories and the code names by which they will be referred are as follows:

- a. Library of thermodynamic data for reaction products (THERMO data).
- b. Data pertaining to reactants (REACTANTS cards).
- c. Namelist data which includes the type of problem, required schedules, and options (NAMELISTS Input).
- d. The optional category of data are chemical formulas of species which are singled out for special purposes (OMIT and INSERT cards).

THERMO Data

The thermodynamic data are in the form of 7 least squares coefficients (a_i) for the following equations:

$$\frac{G_T^\circ}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad (1)$$

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

$$\frac{S_T^\circ}{RT} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \quad (3)$$

$$\frac{G_T^\circ}{RT} = \frac{H_T^\circ}{RT} - \frac{S_T^\circ}{R} \quad (4)$$

For each species, two sets of coefficients are included for two adjacent temperature intervals. The data provided cover the temperature intervals 300 deg K to 1000 deg K and 1000 deg K to 5000 deg K.

The supplied data for each species were made by the PAC program described in NASA TN D-4097 (Ref 15). For the gases, the PAC program calculated the thermodynamic functions from the molecular data given in JANAF (Ref 16). For the condensed species, the thermodynamic functions were taken directly from JANAF. However, NASA added the functions at the transition points since they were not included in the JANAF data. The PAC program does a least squares fit of the functions for the two specified temperature intervals. The fits are constrained to give consistent data at transition points and at the common interval temperature (1000 deg K).

Heats of formation and transition were also taken from JANAF. They were combined with sensible heats to give assigned enthalpies H_T^0 . By definition,

$$H_T^0 \equiv H_{298.15}^0 + [H_T^0 - H_{298.15}^0] \quad (5)$$

It has been arbitrarily assumed that $H_{298.15}^0 = (\Delta H_f^0)_{298.15}$. Equation 5 then becomes

$$H_T^0 \equiv (\Delta H_f^0)_{298.15} + [H_T^0 - H_{298.15}^0] \quad (6)$$

For the JANAF reference elements, $H_{298.15}^0 = 0$. In general, $H_T^0 \neq (\Delta H_f^0)_T$ for $T \neq 298.15^\circ\text{K}$.

REACTANTS Data

Reactants data consists of the following physical data for each of the reaction species in the combustion stream.

- Atomic symbols and formula numbers.
- Relative weights or number of moles (for fuel in total fuels or oxidant in total oxidants).
- Enthalpy.
- Physical state (solid, liquid, gas).
- Temperature associated with enthalpy in item c above.
- Density.

NAMELISTS Data

NAMELISTS data is specified on two input NAMELISTS; only the first is necessary for generation of the chemical equilibrium and kinetic rate data of interest. The second NAMELIST is associated with the rocket performance option of NOXRAT described in the introduction to this report. This latter option was not exercised in this study but will be described in the following subsection. The information required in the first NAMELIST is:

- a. The type of problem.
- b. One or more pressures.
- c. One or more temperatures for assigned temperature problems (e.g., rocket problems with an assigned chamber temperature).
- d. The relative amount of fuel(s) and oxidant(s).

The information required in the second NAMELIST is:

- a. The pressure ratio schedule.
- b. The subsonic area ratio values (optional).
- c. The supersonic area ratio values (optional).
- d. Whether only frozen or equilibrium performance is to be calculated (optional).

OMIT and INSERT Data

OMIT and INSERT cards are optional. They contain the names of particular species in the library of thermodynamic data for the specific purposes stated below.

OMIT Cards. These cards list species to be omitted from the THERMO data.

INSERT Cards. These cards contain the names of condensed species only.

3.2.2 Detailed Description of Input Data

The information required to prepare the input data for a case is furnished in the table given below. This information contains a description of each input item as well as a description of the form in

which these items are written on input data sheets. The descriptions of the input items refer frequently to several points, relevant to the selection of input values, which are discussed in the subsequent subsection. The discussions of these points provide additional detailed information useful in preparing the input data for any case.

The first input item read by Program NOXRAT is the code word THERMO. The second input line contains the three temperature values 300, 1000, 5000. This input is followed by the thermodynamic data for any number of species. The last line of the THERMO input contains the code word END and follows the last set of species data (see point a).

<u>Line</u>	<u>Location</u>	<u>Input Item</u>	<u>Type of Number</u>	<u>Fortran Symbol</u>	<u>Description</u>
1	1-6		A		This is the code word "THERMO" that identifies the beginning of the thermodynamic data
2	1-10		FP	TLOW	Low temperature for lowest temperature interval of thermodynamic data
2	11-20		FP	TMID	Common temperature for the two temperature intervals of the thermodynamic data
2	21-30		FP	THIGH	High temperature for highest temperature interval of thermodynamic data
3	1-12		A	DATA	Species name
3	19-24		A	DATA	Date
3	25-26		A	DATA	Atomic symbol
3	27-29		FP	DATA	Atomic formula number
3	30-31		A	DATA	Atomic symbol
3	32-34		FP	DATA	Atomic formula number

<u>Line</u>	<u>Location</u>	<u>Input Item</u>	<u>Type of Number</u>	<u>Fortran Symbol</u>	<u>Description</u>
3	35-36		A	DATA	Atomic symbol
3	37-39		FP	DATA	Atomic formula number
3	40-41		A	DATA	Atomic symbol
3	42-44		FP	DATA	Atomic formula number
3	45		A	DATA	Species phase (S = solid; L = liquid; G = gas)
3	46-55		FP	DATA	Low temperature of temperature interval
3	56-65		FP	DATA	High temperature of temperature interval
3	80		Int	NCD	Integer 1 to identify card
4	1-15	a_1	FP	DATA	Coefficient in equations 1-4 for upper tempera- ture interval
4	16-30	a_2	FP	DATA	Coefficient in equations 1-4 for upper temperature interval
4	31-45	a_3	FP	DATA	Coefficient in equations 1-4 for upper temperature interval
4	46-60	a_4	FP	DATA	Coefficient in equations 1-4 for upper tempera- ture interval
4	61-75	a_5	FP	DATA	Coefficient in equations 1-4 for upper temperature interval

<u>Line</u>	<u>Location</u>	<u>Input Item</u>	<u>Type of Number</u>	<u>Fortran Symbol</u>	<u>Description</u>
4	80		Int	NCD	Integer 2 to identify card
5	1-15	a_6	FP	DATA	Coefficient in equations 1-4 for upper temperature interval
5	16-30	a_7	FP	DATA	Coefficient in equations 1-4 for upper temperature interval
5	31-45	a_1	FP	DATA	Coefficient in equations 1-4 for lower temperature interval
5	46-60	a_2	FP	DATA	Coefficient in equations 1-4 for lower temperature interval
5	61-75	a_3	FP	DATA	Coefficient in equations 1-4 for lower temperature interval
5	80		Int	NCD	Integer 3 to identify card
6	1-15	a_4	FP	DATA	Coefficient in equations 1-4 for lower temperature interval
6	16-30	a_5	FP	DATA	Coefficient in equations 1-4 for lower temperature interval
6	31-45	a_6	FP	DATA	Coefficient in equations 1-4 for lower temperature interval

<u>Line</u>	<u>Location</u>	<u>Input Item</u>	<u>Type of Number</u>	<u>Fortran Symbol</u>	<u>Description</u>
5	46-60	a ₇	FP	DATA	Coefficient in equations 1-4 for lower temperature interval
6	80		Int	NCD	Integer 4 to identify card

Lines 3-6 are repeated for each species in the thermodynamic data. The last line of the thermodynamic data, designated as line N below, contains the word END. This word is a signal to the computer that it has reached the end of the thermodynamic data.

N	1-3		A		This is the code word "END" that identifies the end of the thermodynamic data
---	-----	--	---	--	---

The next set of input data read by Program NOXRAT are reactants cards (see point b). These cards are required for all problems; they contain specific data on the reactants to be combusted. The first item in the set contains the code word REACTANTS; the last card in the set is blank. In between the first and last cards may be any number of cards up to a maximum of 15, one for each reactant species being considered. There is no limit to the number of sets of reactants to be considered by the program; each must, however, be followed by appropriate data from input categories (3) and (4). The input for each series or set of reactants begins with a new data line N+1 and concludes with data line M.

<u>Line</u>	<u>Location</u>	<u>Input Item</u>	<u>Type of Number</u>	<u>Fortran Symbol</u>	<u>Description</u>
N+1	1-9		A		This is the code word "REACTANTS" that identifies the beginning of reactants data
N+2	1-2		A	NAME	Atomic symbol
N+2	3-9		FP	ANUM	Atomic formula number
N+2	10-11		A	NAME	Atomic symbol

<u>Line</u>	<u>Location</u>	<u>Input Item</u>	<u>Type of Number</u>	<u>Fortran Symbol</u>	<u>Description</u>
N+2	13-18		FP	ANUM	Atomic formula number
N+2	19-20		A	NAME	Atomic symbol
N+2	21-27		FP	ANUM	Atomic formula number
N+2	28-29		A	NAME	Atomic symbol
N+2	30-36		FP	ANUM	Atomic formula number
N+2	37-38		A	NAME	Atomic symbol
N+2	39-45		FP	ANUM	Atomic formula number
N+2	46-52		FP	PECWT	Relative weight (or number of moles) of fuel in total fuel or oxidant in total oxidant*
N+2	53		A	MOLE	Symbol to identify if PECWT is relative weight or number of moles = blank if relative weights = M if number of moles
N+2	54-62		FP	ENTH	Enthalpy in calories/gm mole (see point c.)
N+2	63		A	FAZ	State = S for solid = L for liquid = G for gas
N+2	64-71		FP	RTEMP	Temperature in deg K associated with enthalpy in columns 54-62
N+2	72		A	FOX	Symbol to identify if reactant is an oxidant or a fuel = F if fuel = 0 if oxidant
N+2	73-80		FP	DENS	Density in gm/cc (optional)

* A fuel (or oxidant) may be composed of more than one fuel (or oxidant).

Line N+2 is repeated for each reactant in the set up to a maximum of 15 reactant species. The last line in this sequence (M) is blank.

M

1-80

Blank card

The next input items are read into Program NOXRAT using a NAMELIST statement. Input data referring to a NAMELIST statement begins with a \$ in the second location on a new line, immediately followed by the NAMELIST name, immediately followed by one or more blank characters. Any combination of three types of data items may then follow. The data items must be separated by commas. If more than one line is needed for the input data, the last item on each line, except the last line, must be a number followed by a comma. The first location on each line should always be left blank since it is ignored. The end of a group of data is signaled by a \$ immediately after the last item of data. The form that data items may take is:

- a. Variable name = constant, where the variable name may be an array element or a simple variable name. Subscripts must be integer constants.
- b. Array name = set of constants separated by commas where k* constant may be used to represent k consecutive values of a constant. The number of constants must be equal to the number of elements in the array.
- c. Subscripted variable = set of constants separated by commas where, again, k* constant may be used to represent k consecutive values of a constant. This results in the set of constants being placed in consecutive array elements, starting with the element designated by the subscripted variable.

The first input NAMELIST is necessary for all of the options associated with Program NOXRAT. The items in this NAMELIST, INPT2 are:

<u>Fortran</u> <u>Symbol</u>	<u>Input</u> <u>Item</u>	<u>Description</u>
KASE		Optional assigned number associated with the case

<u>Fortran Symbol</u>	<u>Input Item</u>	<u>Description</u>
P	P	Assigned pressures (maximum of 26) Chamber pressure (one value) for rocket problems. Values in atm unless PSIA or MMHG are set TRUE (see below)
T	T	Assigned temperature in deg K (maximum of 26) (see point d)
MIX		Value of fuel-to-oxidant air weight ratios if FA is set TRUE (maximum of 40). For rocket problems (RKT is set TRUE) there must be as many sets of RKTINP NAMELIST inputs as there are MIX values (see point e)
FA		If variable is set TRUE, fuel-to-air weight ratios given in MIX. Value before read: FALSE
TP		If variable is set TRUE, problem type is assigned temperature and pressure Value before read: FALSE (see point f)
HP		If variable is set TRUE, problem type is assigned enthalpy and pressure. Value before read: FALSE (see point g)
RKT		If variable is set TRUE, problem type is rocket. Value before read: FALSE (see point h)
DETN		If variable is set TRUE, problem type is detonation. Value before read: FALSE (see point i)
PSIA	P	If set TRUE, pressure is in psia units Values are converted to atm internally Value before read: FALSE
MMHG	P	If set TRUE, pressure is in mmHg. Values are converted to atm internally. Value before read: FALSE
IONS		If set TRUE, ionic species are considered in the combustion products. Value before read: FALSE

<u>Fortran</u> <u>Symbol</u>	<u>Input</u> <u>Item</u>	<u>Description</u>
IDEBUG		if set TRUE, intermediate output is printed. Value before read: FALSE.

The second NAMELIST, RKTINP, is required only for rocket (RKT) problems. It follows the INPT2 namelist. The items in this NAMELIST are

PCP		Ratio of chamber pressure to exit pressure (maximum of 22 values). See point j.
EQL		If set FALSE, program will not calculate rocket performance assuming equilibrium composition during expansion. Value before read: TRUE. This is an optional input. See point k.
FROZ		If set FALSE, program will not calculate rocket performance assuming frozen composition during expansion. Value before read: TRUE. This is an optional input. See point k.
SUBAR		Subsonic area ratio. This is an optional input. See point l.
SUPAR		Supersonic area ratio. This is an optional input. See point l.

The remaining input items to Program NOXRAT are optional. These are OMIT and INSERT cards. Each card contains the word OMIT (in card columns 1 through 4) or INSERT (in card columns 1 through 6) and the names of from 1 to 4 species starting in columns 16, 31, 46, and 61. The names must be exactly the same as they appear in the THERMO data. See point m for further discussion of these input items.

3.2.3 Discussion of Input Data

Some important aspects to be considered in appropriately specifying the input data are discussed below. Reference to these discussions has been made in the preceding subsection in which the input format was described. The points referred to are as follows:

- a. The library of thermodynamic data for reaction products may be read either from cards or from tape. If the data are read in from cards, the program will write these data on tape 4. During a computer run, the appropriate reaction product data for each new set of REACTANTS cards will be selected from tape 4 and stored.

THERMO data may be read in from cards for each run. However, a permanent tape or disc containing the data may be made during any run by using the required type of control cards preceding the operating deck. Two advantages of using a permanent tape or disc are that the scratch tape will not be made for each run and handling the cards is eliminated.

- b. The fuel specification card(s) must precede the oxidant card(s) in the input deck. Further, the oxygen must be the second specie specified in the oxidant air atomic formula; the atomic formula of the fuel must be specified in the order: carbon, hydrogen.

For gaseous mixtures (such as air) specify equivalent formula numbers on an atomic basis-- e.g., air is 78.03 per cent N_2 , 20.99 per cent O_2 , 0.98 per cent Ar. Air's equivalent formula is then $N_{0.7803}^{0.2099}Ar_{0.0049}$ where the sum of the relative weights is as close to 1.0 as possible.

- c. This enthalpy is not required for assigned temperature problems, i.e., TP.
- d. If no T value is given the program uses the temperature and enthalpies on the reactant cards. When T values are assigned in the INPT2 NAMELIST, the program calculates the enthalpy from the library of THERMO data if the following two conditions are satisfied:
 - i. The reactant card has zeros punched in card columns 37 and 38.
 - ii. The reactant is a species in the library of THERMO data.
- e. Relative amounts of fuel(s) and oxidizer(s). These quantities

may be specified by assigning 1 and 40 values for FA if no value is assigned for any of these, the program assumes the relative amounts of fuel(s) and oxidizer(s) to be those specified on the reactants cards.

- f. TP Problem. Thermodynamic properties will be calculated for all combinations of assigned values for pressure P and temperature T in the NAMELIST. Thus, if 26T values and 26P values are included in the INPT2 lists, properties will be calculated for 676 P and T combinations.
- g. HP Problem. Combustion temperature and corresponding properties will be calculated for each pressure specified.
- h. RKT Problem. One pressure value P is required for the chamber pressure. The T schedule is used only if expansion from an assigned chamber temperature is desired (such as for a nuclear rocket). Otherwise it should be omitted.

The RKT problem requires a second namelist for input (RKTINP) discussed in the previous subsection.

- i. DETN Problem. The temperature and pressures in the T and P input refer to the unburned gas.
- j. The list of pressure ratios should not include values for the chamber and the throat. Values should be in increasing order.
- k. The program will calculate both equilibrium and frozen performance unless RKTINP contains FROZ = F or EQL = F. If FROZ = F, only equilibrium performance will be calculated. If EQL = F, only frozen performance will be calculated.*
- l. The subsonic area ratio values (SUBAR) and/or the supersonic area ratio values (SUPAR) are optional. When assigned area ratios are included, the PCP input should contain values of pressure ratios whose corresponding area ratios will be in the range of the assigned area ratios.
- m. If OMIT cards are not used, the program will consider as possible species all those species in the THERMO data which are consistent with the chemical system being considered.

* F is the symbol for FALSE.

Occasionally, it may be desired to specifically omit one or more species from consideration as possible species. This may be accomplished by means of OMIT cards.

INSERT cards have been included as options for two reasons. The first and less important reason is that if one knows that one or several particular condensed species will be present among the final equilibrium compositions for the first assigned point, then a small amount of computer time can be saved by using an INSERT card. Those condensed species whose chemical formulas are included on an INSERT card will be considered by the program during the initial iterations for the first assigned point. If the INSERT card were not used, only gaseous species would be considered during the initial iterations. However, after convergence, the program would automatically insert the appropriate condensed species and reconverge. Therefore, it usually is immaterial whether or not INSERT cards are used. For all other assigned points the inclusion of condensed species is handled automatically by the program.

The second and more important reason for including the INSERT card option is that, in rare instances, it is impossible to obtain convergence for assigned enthalpy problems (HP or RKT) without the use of an INSERT card. This occurs when, by considering gases only, the temperature becomes extremely low (say several deg K). In these rare cases, the use of an INSERT card containing the name of the required condensed species will eliminate this kind of convergence difficulty. When this difficulty occurs, an error message is generated. This message is described in the subsection Description of Error Messages.

3.2.4 Description of Sample Case Input

A completed input data sheet is shown on page 29 for an assigned enthalpy pressure problem (HP). In this table, lines 1 through 6 identify

the start of the thermodynamic data and include, as examples, data for solid phase aluminum. Lines 10 through 13 identify that the reactant components for this problem are kerosene ($C_{12}H_{19.9423}$) and air ($NO_{0.7803}O_{0.2099}Ar_{0.0049}$). The kerosene (fuel) is supplied as liquid at 298.15 deg K with an enthalpy of -5430 cal/gm-mole. The air (oxidant) is gaseous at 350 deg K with an enthalpy of 195.0 cal/gm-mole. The density of the kerosene is specified as 0.773 gm/cc while that of the air is omitted. Lines 15 through 18 are the NAMELISTS \$INPT2 input. Here the case is given the code number 1, HP is identified as the problem type, the combustor pressure is set at 1.80 atm, and the MIX matrix is assigned 35 fuel-to-air ratios for test.

3.3 OUTPUT DATA

The output of Program NOXRAT consists of both printed and punched data. The data falls into two main categories: normal output and error messages. The normal output consists of the printed and punched results usually obtained with each run of the program. If any difficulties are encountered in the solution of a case, one or more error messages are printed. These messages are diagnostic statements which describe the nature of the difficulty. They are described in greater detail in subsection 3.3.2.

3.3.1 Normal Output

The normal output from NOXRAT falls into two main categories: printed output for each fuel-to-air ratio for each assigned condition (e.g., pressure); and printed and punched output for each assigned pressure. The normal output from the first category is:

- * a. The chemical formula of each reactant specie.
- * b. The weight fraction of each reactant specie in the total fuel or oxidant.
- * c. The base enthalpy of each reactant in cal/gm-mole.
- * d. The input temperature of each reactant in deg-K.

* Also normal output of CEC.

- *e. The density of each reactant (if specified in the input) in gm/cc.
- *f. The physical state of each of the specified reactants.
- *g. The total oxidant to fuel weights ratio.
- *h. The per cent fuel in the reactant mixture.
- *i. The equivalence ratio of the reactants.
- *j. The weight average density of the reaction mixture in gm/cc (printed as zero if the density of any specie is omitted from the input).
- *k. The equilibrium pressure in atm.
- *l. The equilibrium temperature in deg K.
- *m. The sonic velocity of the combustion production mixture in meters/sec.
- *n. The mean enthalpy of the combustion products in cal/gram.
- *o. The mean entropy of the combustion products in cal/gram-deg K.
- *p. The mean molecular weight of the combustion products in grams.
- *q. The differential $(\partial V / \partial P)_T$ in cc/atm.
- *r. The differential $(\partial V / \partial T)_P$ in cc/deg K.
- *s. The mean heat capacity of the combustion products in cal/gram-deg K.
- *t. The mean heat capacity ratio (C_p/C_v) of the combustion products.
- *u. The mole fraction and chemical formula of each of the combustion products present at equilibrium at a concentration greater than 5×10^{-6} .
- v. The mole fraction of each of the species of interest in the nitric oxide kinetic scheme (Refs 4 through 6) and the mole fractions of $C_{(s)}$, CO, CO_2 .
- w. The mean molecular weight of the combustion products in grams.
- x. The adiabatic flame temperature of the combustion products in deg K.
- y. The assigned inlet pressure in atm.
- z. The fuel-to-air weight ratio of the reactants.
- zl. The atomic composition, inlet temperature (in deg K) and enthalpy (cal/gm-mole) of both the fuel(s) and the oxidant(s).

* Also normal output of CEC.

With the exception of the descriptive characteristics of the fuel(s) and oxidant(s) (output #21), the output from this category is clearly labeled and requires no further discussion.

The fuel and oxidant are described by seven characteristic numbers, the first five of which give the atomic composition while the sixth and seventh are the enthalpy in cal/gm-mole at the inlet temperature in deg K. These two lines of output appear directly below the fuel-to-air ratio with the first line always referring to the fuel and the second to the oxidant. Since the fuel used in this analysis has been assumed to be of the form C_xH_y , the first two figures printed describing the fuel are "x" and "y" while the third, fourth, and fifth figures are printed as zero. In this analysis, the oxidant has been taken to be air comprised of nitrogen, oxygen, and argon with the equivalent chemical formula $N_AO_BAr_C$. Hence, the first three numerals printed describing the oxidant are "A", "B", and "C" respectively. The fourth and fifth figures are printed as zero; inclusion of other trace components in the air will change these latter digits accordingly. Further description of this output is included in Appendix IV. The output for the sample data case corresponding to this category of the output is shown on pages 30 and 31.

The normal output for the second category is:

- a. The atomic composition of the fuel (C_xH_y).
- b. The inlet air temperature in deg ...
- c. A code number identifying the set of kinetic constants used in the NO rate formation calculations (see Appendix V).
- d. The assigned pressure in atm.
- e. The stoichiometric fuel-to-air ratio.
- f. For each fuel-to-air ratio specified, the program prints and punches two lines of output containing twelve items of data. This data is (consecutively): the mixture ratio (mass fuel to mass fuel and air); the equivalence ratio; the density of the combustion products in gm/cm^3 ; the adiabatic flame temperature of the combustion products in deg K; the equilibrium mole fraction of NO, CO,

$C(s)$, and CH_2 (unburned hydrocarbons). and the kinetic parameters R_1 , R_6 (in gm-moles/cm³-sec), K_1 , and K_2 (dimensionless). The output for the sample data case corresponding to this category of the output is shown on page 32.

Program NOXRAT prints intermediate output for each input set of REACTANT cards and for each fuel-to-air ratio. The former consists of a listing of the input data for the case and a listing of the species being considered as products of the combustion process. The latter data is the result of intermediate calculations within NOXRAT and is not described here. It is generally not of any interest to the user; however, the output for one fuel-to-air ratio for the sample data case is shown on page 33.

3.3.2 Description of Error Messages

The known error messages in Program NOXRAT* are:

- a. In rare instances, it is impossible to obtain convergence for assigned enthalpy problems (HP or RKT) without the use of an INSERT card. This occurs when, by considering gases only, the temperature becomes extremely low (say several deg K). In these rare cases, the use of an INSERT card containing the name of the required condensed species will eliminate this kind of convergence difficulty. When this difficulty occurs, the following message is printed by the program: "LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE BEEN INCLUDED ON AN INSERT CARD".
- b. If the user mixes the order of the cards for a particular species in the thermodynamic data file, the program will print: "ERROR IN ORDER OF DATA CARDS FOR -----(specie name)". This is a nonfatal error and the program will continue to execute, however, the specie in error will be deleted from the thermodynamic inventory.
- c. If there are cards in the input data deck that do not belong, the program will write the card and: "ERROR IN ABOVE CARD: IGNORE CONTENTS". This is a nonfatal error to the program, but causes it to skip to the next data set.

* These are as those for CEC.

- d. If there are errors in the REACTANTS data cards the program will write: "ERROR IN REACTANT CARDS". This is a nonfatal error to the program but causes it to skip to the next data set.
- e. If the convergence tests are not satisfied for the equilibrium products the program will print: "ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS FOR THE POINT ____".
- f. If the temperature calculated for the combustion is out of the range of the thermodynamic data the program will print: "THE TEMPERATURE = ____ IS OUT OF RANGE FOR POINT ____".
- g. If the phases of a condensed specie are out of order, the program will print: "PHASES OF A CONDENSED SPECIE ARE OUT OF ORDER".

3.4 MISCELLANEOUS OPERATIONAL INFORMATION

Program NOXRAT occupies approximately 71,000 core locations during loading and approximately 63,000 core locations during execution on the CDC 6600 computer. Actual program length is approximately 38,000 core locations. Hence, the total storage requirement for this program is comfortably within the CDC 6600 core capacity of 131,000 locations.

The execution time of Program NOXRAT depends primarily upon the number of assigned pressure levels and upon the number of fuel-to-air ratios at each of the pressure levels to be tested. A typical operating condition of one assigned pressure and 35 fuel-to-air ratios requires approximately 66 systems seconds (central processor time is approximately 52 secs) for execution. Each succeeding point at any given pressure and any selected fuel-to-air ratio will require approximately one second of over-all machine time.

A "scratch" tape is required by the program. This scratch tape number is not assigned a Fortran name but is given the value of 4 by the program. The instructions necessary for mounting this tape must be supplied to the computer/computer operator upon submission of a run.

29

ENGINEER: RDS PROJECT: NOx from Gas Turbine Combustors PROJECT NO. 1152
TITLE: Sample to Illustrate the Use of Program NOXRAT SHEET: 1 OF 1

[illegible]

3.6 SAMPLE CASE OUTPUT

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 1

CHEMICAL FORMULA

FUEL C 1.00000 H 1.94230

OXYDANT N .78030 O .20990 AR .00490

O/F= 5.2549 PERCENT FUEL= 15.9876 EQUIVALENCE RATIO= 2.7929 DENSITY= 0.0000

WT FRACTION ENTHALPY STATE TEMP DENSITY

(SEE NOTE) CAL/MOL DEG K O/CC

1.00000 -5430.000 L 298.15 .7730

1.00000 195.000 0 350.00 -0.0000

THERMODYNAMIC PROPERTIES

P= ATM 1.8000

T= DEG K 1184

M= CAL/O -50.8

S= CAL/O 2.4405

M= MOL WT 22.018

(DLV/DLP)T -1.00236

(DLV/DLP)P 1.4288

CP= CAL/(O) (K) .3974

GAHWA (S) 1.3123

SON VEL= M/SEC 766.1

MOLE FRACTIONS

AR .00626

CH4 .00651

CO .24395

CO2 .00742

HCN .00001

H2 .23416

H2O .00429

NH3 .00003

N2 .49827

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

C(S)	C2H4	H2O(L)	O	C	C2N	N	OH	CH	C2H2	C2O	NH2	CH3	C3	NO	CH	C3O2	NO2	UN2	H	N2C	C2	HCO	N2H4	C2H	H2O2	N2O	C2H2	H2O(S)	N2O4

NOTE: WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXYDANT IN TOTAL OXYDANTS

OUTPUT FROM OUT3

```

C(S)      0.
CO         2.4395461E-01
CO2        7.41718910E-03
H          5.26478295E-08
N          0.
NO         0.
N2O        0.
C          0.
O2         0.
OH         0.
MOLEC. WT. 2.20178947E-01
TEMP.(K)   1.14428579E+03
PRESS.(ATM) 1.80000000E+00
FUEL AIR RATIO 1.90300000E-01
1.90000000E+00 1.94230000E+00-0.0.
7.80300000E-01 2.09900000E-01 4.90000000E-03-0.0.
-5.43000000E+03 2.98150000E+02
1.95000000E+02 3.50000000E+02
-0.
-0.

```

OUTPUT FROM RATES

```

FUELS C 1.00000000E+00H 1.94230000E+00 INLET AIR T.(K)= 3.50000000E+02
PRESS.(ATM)= 1.80000000E+00ICNOE= IPHI STOICH.= 6.79522849E-02
-8.48679E-04 1.24999E-02 1.62731E-03 3.90469E-02 0.
0. 3.36136E-06 0. 0. 1.00000E+35 1.00000E+35
6.7491E-03 9.9996E-02 1.00034E-03 6.35172E-02 0.40730E-08 0.
1.67062E-02 2.50028E-01 6.27463E-04 1.01256E+03 1.00000E+35 1.00000E+35
0. 6.61614E-05 0. 0. 1.00000E+35 1.00000E+35
2.64608E-02 3.99987E-01 4.71210E-04 1.34823E+03 4.38710E-04 4.47846E-08
0. 1.04765E-04 0. 5.68904E-15 1.00000E+35 1.33333E+00
3.28433E-02 5.00057E-01 4.08777E-04 1.55405E+03 1.15681E-03 1.69756E-06
0. 1.30132E-04 0. 6.35516E-13 1.00000E+35 8.44145E-01
3.00239E-02 5.49945E-01 3.84573E-04 1.65178E+03 1.45294E-03 7.04703E-06
0. 1.42640E-04 0. 3.76222E-12 1.00000E+35 1.42708E-01
3.91729E-02 5.99980E-01 3.43656E-04 1.74667E+03 2.21655E-03 2.46379E-05
0. 1.55097E-04 0. 1.70770E-11 1.00000E+35 6.43491E-01
4.23013E-02 6.50015E-01 3.45472E-04 1.83338E+03 2.81087E-03 7.44642E-05
0. 1.67465E-04 0. 6.09179E-11 1.00000E+35 5.48862E-01
4.54099E-02 7.00050E-01 3.24566E-04 1.92073E+03 3.38846E-03 1.99926E-04
0. 1.79235E-04 0. 1.77669E-10 1.00000E+35 4.60009E-01
4.44490E-02 7.49978E-01 3.15653E-04 2.01049E+03 1.48817E-03 4.85744E-04
0. 1.91859E-04 0. 4.25701E-10 1.00000E+35 3.77729E-01
5.15573E-02 7.99973E-01 3.03440E-04 2.09074E+03 4.24244E-03 1.06627E-03
0. 2.03845E-04 0. 8.56118E-10 1.00000E+35 3.01751E-01
5.46060E-02 8.50000E-01 2.92843E-04 2.16427E+03 4.37220E-03 2.26136E-03

```


FUEL OXIDANT MIXTURE

HCAL/O -3.88719820E+02 1.34636455E+01 -5.08357020E+01

V+ 4.25394067E-01 0. 6.80101579E-02

V- 0. -2.89848123E-02 -2.43808462E-02

ATOMS/O
C 7.15074437E-02 0. 3.14450899E-02

H 1.39044292E-01 0. 2.22297982E-02

N 0. 5.38752954E-02 4.52619469E-02

O 0. 1.44924061E-02 1.21754231E-02

AR 0. 3.38317246E-04 2.84228553E-04

PT °C H N O AR
1 -2.832 -0.000 -9.396 -0.000 -12.706 -0.000 -35.262 -0.000 -24.674 -0.000 15.000

4. REFERENCES

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5. TABLES

TABLE I
KINETIC DATA FOR THE NITRIC OXIDE REACTION SCHEME

	Reaction No.	A_i (cm ³ /sec gm-mole deg K)	n_i	E_i (kcal/gm-mole)
ICODE = 1 (from Refs 4, 5)	1	1.2046×10^{13}	0.0	0.0
	2	1.2046×10^{13}	0.0	7.1
	3	4.2161×10^{13}	0.0	0.0
	4	3.0115×10^{13}	0.0	10.8
	5	3.6138×10^{13}	0.0	24.0
	6	4.8184×10^{13}	0.0	24.0
ICODE = 2 (from Refs 9, 17)	1	3.1×10^{13}	0.0	0.334
	2	6.4×10^9	1.0	6.25
	3	4.1×10^{13}	0.0	0.0
	4	2.9513×10^{13}	0.0	10.77
	5	3.8146×10^{13}	0.0	24.1
	6	4.5775×10^{13}	0.0	24.1
ICODE = 3 (from Ref 18)	1	3.0717×10^{13}	0.0	0.33
	2	1.3251×10^{10}	1.0	7.1
	3	4.2161×10^{13}	0.0	0.0
	4	2.9513×10^{13}	0.0	10.77
	5	3.8146×10^{13}	0.0	24.1
	6	4.5775×10^{13}	0.0	24.1
ICODE = 4 (from Ref 18)	1	1.0239×10^{13}	0.0	0.0
	2	3.7945×10^{12}	0.0	7.0
	3	4.1559×10^{13}	0.0	0.0
	4	2.9513×10^{13}	0.0	10.77
	5	3.8146×10^{13}	0.0	24.1
	6	4.5775×10^{13}	0.0	24.1

where

$$k = A_i T^{n_i} \exp(-E_i/RT)$$

T = Temperature in deg K

$$R = 1.987 \times 10^{-3} \text{ kcal/gm-mole deg K}$$

TABLE 2 - PROGRAM OR SUBPROGRAM FUNCTION

<u>Program or Subprogram</u>	<u>Description</u>
NOXRAT	Main program to calculate chemical equilibrium compositions with applications; the main program controls the calculation and directs the input and output
REACT	Subroutine to read and convert reaction input data
SEARCH	Subroutine to search tape for thermodynamic data for species to be considered
EQLBRM	Subroutine to calculate equilibrium composition and properties
CPHS	Subroutine to calculate thermodynamic properties for individual species
MATRIX	Subroutine to perform matrix inversion
MGAUSD	Subroutine to solve any linear set of up to 20 equations
VARFMT	Subroutine to set variable formats
OUT1	Subroutine to write output
OUT2	Subroutine to write output
OUT3	Subroutine to write output
HCALC	Subroutine to calculate enthalpy for propellant using coefficients
MOLIER	Subroutine to calculate thermodynamic equilibrium properties at assigned temperatures and pressures
CMBSTN	Subroutine to calculate theoretical thermodynamic combustion properties
DETON	Subroutine to calculate Chapman-Jouguet detonations
SHCK	Subroutine to terminate program if a shock occurs
ROCKET	Subroutine to calculate rocket performance

TABLE 2 - PROGRAM OR SUBPROGRAM FUNCTION (CONTINUED)

<u>Program or Subprogram</u>	<u>Description</u>
RKTOUT	Subroutine to write output for rocket performance
RATIO	Subroutine to interpolate area ratio
SET	Subroutine to interpolate area ratio
FROZEN	Subroutine to calculate frozen composition expansion only
RATES	Subroutine to calculate rate constants for the NO reaction scheme

6. FIGURES

7. NOMENCLATURE

<u>Symbol</u>	<u>Description</u>	<u>Units</u>
C_p	Specific heat at constant pressure	cal/gm-deg K
C_v	Specific heat at constant volume	cal/gm-deg K
P	Pressure	atm
T	Temperature	deg K
V	V	cc

8. APPENDICES

APPENDIX 1 - OVER-ALL PROGRAM LOGIC

The over-all computer flow of NOXRAT is identical to that of CEC excepting the additional CALL to Subroutine RATES by Subroutine OUT3. The other modifications to OUT3 and to the main program (NOXRAT) do not affect the over-all program logic. A complete description of the program logic is available in References 11, 13, 14, and 15. A modular diagram of NOXRAT is provided as Figure 1 (Ref 13). Table 2 contains a brief statement as to the role of each routine in the program.

APPENDIX II - COMMON FORTRAN NOMENCLATURE

The following tables contain the COMMON Fortran nomenclature for Program NOXRAT that was added to that of Program CEC. COMMON consists of labeled blocks; the nomenclature is arranged in alphabetical order for each block. The metric system of units is included in the nomenclature.

Nomenclature for COMMON/SNEW

<u>Fortran Symbol</u>	<u>Symbol</u>	<u>Description</u>	<u>Units</u>
INDFA		Index of equivalence ratios	
RON	F/A	Fuel-to-air mass ratio	

Nomenclature for COMMON/DICK

<u>Fortran Symbol</u>	<u>Symbol</u>	<u>Description</u>	<u>Units</u>
ATT(J,I)	T_j	jth value of the adiabatic flame temperature (in the combustor) at a particular fuel-to-air mass ratio i	deg K
BCON1(J,I)	$y_{C(s)j}$	Equilibrium mole fraction of carbon at the jth pressure level at a particular fuel-to-air mass ratio i	
BCON2(J,I)	y_{COj}	Equilibrium mole fraction of carbon monoxide at the jth pressure level at a particular fuel-to-air mass ratio i	
BCON6(J,i)	y_{NOj}	Equilibrium mole fraction of nitric oxide at the jth pressure level at a particular fuel-to-air mass ratio i	
CH2(J,I)	y_{CH_2j}	Equilibrium mole fraction of unburned hydrocarbons in the combustion products (excluding $C_{(s)}$ and CO) expressed as CH2 at the jth pressure level at a particular fuel-to-air mass ratio i	

<u>Fortran Symbol</u>	<u>Symbol</u>	<u>Description</u>	<u>Units</u>
EK1(J,I)	$(K_1)_j$	Ratio of forward reaction rate at the ith pressure level for a particular fuel-to-air mass ratio i	
EK2(J,i)	$(K_2)_j$	Ratio of forward reaction rate at the jth pressure level for a particular fuel-to-air mass ratio i	
F(I)	F	Mixture ratio	
MIX(I)		Matrix of specified fuel-to-air mass ratios	
PHI(I)	Φ	Equivalence ratio	
ROH(J,I)	ρ_j	Equilibrium density at the jth pressure level at a particular fuel-to-air mass ratio i	gm/cm ³
R1(J,I)	$(R_1)_j$	Forward reaction rate for the first reaction at the jth pressure level at a particular fuel-to-air mass ratio i	gm-mole/cm ³ -sec
R6(J,I)	$(R_6)_j$	Forward reaction rate for the sixth reaction at the jth pressure level at a particular fuel-to-air mass ratio i	gm-mole/cm ³ -sec

APPENDIX III - MAIN ROUTINE - NOXRAT

The changes to the main routine of CEC are as follows:

- a. The main program was renamed NOXRAT, thus replacing the CEC name "MAIN".
- b. The subscripted variable MIX was expanded from 15 to 50. MIX is the matrix of specified fuel-to-air ratios.
- c. Labeled COMMON blocks SNEW, DICK, and EQNEW were added. Definitions of the variables contained in these blocks are provided in Appendix II.
- d. The statement `DO 303 I = 1, 15` was modified to `DO 303 I = 1, 50`. This is consistent with the expansion of the MIX matrix from 15 to 50.
- e. Statement number 322: `DO 625 IST = 1, 15` was modified to read `DO 625 IST = 1, 40`. This is consistent with the decision to limit each set of specified fuel-to-air ratios to between 35 and 40 entries.
- f. The statement `INDFA = IST` was inserted directly after the statement numbered 322. The statement `RON = MIX(IST)` was inserted directly after the statement numbered 323. Both of these new variables are part of the new labeled COMMON blocks and are used only in Subroutine RATES.

APPENDIX IV - SUBROUTINE OUT3

Subroutine OUT3 is an entry point to Subroutine OUT1. The main purpose of this subroutine had been to provide the written output for the CEC program. The modifications incorporated into OUT3 permit identification of the species of interest in the kinetic scheme (previously described). Once identified, these variables are transmitted to Subroutine RATES by means of COMMON and a call statement from OUT3. The specific changes to OUT3 are as follows:

- a. The subscripted variable MIX was expanded from 15 to 50. MIX is the matrix of specified fuel-to-air ratios.
- b. A dimension statement was added for the variables "SIEGEL" and "CONCKI". "SIEGEL" is a singly-subscripted variable containing the alphanumeric characters used in the identification of the chemical species of interest in the kinetic scheme. The variable "CONCKI" is a doubly-subscripted array representing the equilibrium mole fraction of a given species for a particular pressure level at a specified fuel-to-air ratio.
- c. Labeled COMMON blocks SNEW, DICK, and EQNEW were added. Definitions of the variables contained in these blocks are provided in Appendix II.
- d. The elements of the "SIEGEL" array were entered into the program via a DATA statement.
- e. Statement number 1000 was changed from a RETURN statement to a CONTINUE statement.
- f. 34 statements were added to the program after statement number 1000 in order to identify which elements of the CLC array EN (containing the moles of a given species present in a particular reaction mixture) were the ones of interest in the kinetic analysis. This problem was created by the storage of the alphanumeric characters identifying reaction species in the CEC generated array

"SUB". This array was created in such a manner that determination of the specific elements of interest to NREC had to be accomplished by a direct comparison of the alphanumeric data in the "SUB" array with the specific names in the input "SIEGEL" array. This comparison and the calculation of the equilibrium mole fractions was accomplished in the DO 3000 loop of OUT3. The remaining statements added to OUT3 allow the equilibrium mole fractions and names of the species of interest, the molecular weight and adiabatic flame temperature of the combustion products, the assigned pressure, the fuel-to-air ratio, and the atomic and thermal characteristics of the fuel and oxidant to be printed for each specified fuel-to-air ratio. This output appears directly beneath the "normal" output (i.e., regular CEC type) generated by OUT3. The final cards added to OUT3 are the CALL statement to Subroutine RATES and the Subroutine RETURN statement.

APPENDIX V - SUBROUTINE RATES

The primary function Subroutine RATES is to produce data, in the form of a deck of cards, which specify all of the kinetic properties required by Program GASNOX* at the equilibrium combustor conditions.

Subroutine RATES is called by Subroutine OUT3 of Program NOXRAT; it does not call any other subroutines. Subroutine RATES does not require external input but does provide external output in the form of punch cards and paper. Internal input and output are transmitted as arguments of the subroutine and through COMMON. The internal input consists of:

A	ANUM	CONCKI	E	EN
ENTH	ICODE	INDFA	MIX	NPT
NREAC	PPP	RON	RTEMP	TTT
WM				

The internal output consists of:

ATT	BCON1	BCON2	BCON6	CH2
EK1	EK2	F	PHI	RON
R1	R6			

The external output consists of:

ANUM	ATT	BCON1	BCON2	BCON6
CH2	EKS	EK1	EK2	F
ICODE	PHI	PPP	RON	RTEMP
A1	R6			

Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols used in Subroutine RATES which are not included in COMMON.

<u>Fortran</u> <u>Symbol</u>	<u>Symbol</u>	<u>Description</u>	<u>Units</u>
A(I)	A _i	Pre-exponential factors in the kinetic equations	cm ³ /sec-gm mole deg K
ANUM(I,J)	a _{i,j}	Atomic number a _{1,1} = carbon a _{1,2} = hydrogen a _{2,2} = oxygen	

* See Volume 3.

<u>Fortran</u> <u>Symbol</u>	<u>Symbol</u>	<u>Description</u>	<u>Units</u>
CONCKI(J,I)	$y_{i,j}$	Equilibrium mole fraction of the i th species for the j th pressure at a particular fuel-to-air mass ratio i	
CONMCM(K,J,I)	$(y_i)_j$	Equilibrium concentration of the k th species for the j th pressure at a particular fuel-to-air mass ratio i	gm moles/cm ³
E(I)	E_i	Activation energies for the kinetic equations	kcal/gm-mole
EKS	k_s	Fuel-to-air mass ratio at stoichiometric conditions	
EN(I)	n_i	Temperature exponent for the kinetic equations	
ENTH(N)	H_n	Enthalpy of reactant n	cal/gm-mole
ICODE		Indicator ICODE = 1 if kinetic rate constants of Lavoie are employed (Refs 4, 5) ICODE = 2 if "best" kinetic data are employed (Refs 9, 17) ICODE = 3 if "high" kinetic data selected from Reference 18 are employed ICODE = 4 if "low" kinetic data selected from Reference 18 are employed	
IPRINT		Indicator IPRINT = 0 if data is not to be printed and punched IPRINT = 1 if data is to be printed and punched	
IST		Index of equivalence ratios	
NPT		Index of pressures	
NREAC	n_{react}	Number of the n th reactant species	
PPF(J)	P_j	j th value of the pressure in the combustor	atm

<u>Fortran</u> <u>Symbol</u>	<u>Symbol</u>	<u>Description</u>	<u>Units</u>
RATEK(K,J,I) (k_k) _j		jth value of the reaction rate for the kth kinetic equation at a particular fuel-to-air mass ratio i	cm ³ /sec-gm mole
RATWTS		Ratio of atomic numbers	
RTEMP(N)	T _n	Inlet temperature of reactant n	deg K
R2(J,I)	(R ₂) _j	Forward Reaction rate for the second reaction at the jth pressure level at a particular fuel-to-air mass ratio i	gm-mole/cm ³ -sec
R3(J,I)	(R ₃) _j	Forward reaction rate for the third reaction at the jth pressure level at a particular fuel-to-air mass ratio i	gm-mole/cm ³ -sec
R4(J,I)	(R ₄) _j	Forward reaction rate for the fourth reaction at the jth pressure level at a particular fuel-to-air mass ratio i	gm-mole/cm ³ -sec
R5(J,I)	(R ₅) _j	Forward reaction rate for the fifth reaction at the jth pressure level at a particular fuel-to-air mass ratio i	gm-mole/cm ³ -sec
TTT(J)	T _j	jth value of the temperature (in the combustor) at a particular fuel-to-air mass ratio	deg K
WM(J,I)	MW _j	jth value of the molecular weight of the reaction products at a particular fuel-to-air mass ratio	gm/gm-mole

Analysis Procedure

The step-by-step procedure of Subroutine RATES is given below. At the conclusion of the step-by-step procedure, the Fortran listing of the subroutine appears:

- Establish the printing and punching control.
- Convert equilibrium mole fractions of C_(s), CO, CO₂, H₂, N, NO, N₂O, O, O₂ to moles/cm³ by the relationship

$$(y_i)_j = [y_{i,j}] [P_j / 82.057 T_j]$$

- c. Compute the forward reaction rate constants as

$$(k_i)_j = A_i T_j^n \exp[-E_i/RT_j]$$

- d. Calculate $(R_1)_j$, $(R_2)_j$, $(R_3)_j$, $(R_4)_j$, $(R_5)_j$, and $(R_6)_j$

$$(R_1)_j = (k_1)_j (N_e)_j (NO_e)_j$$

$$(R_2)_j = (k_2)_j (N_e)_j (O_{2e})_j$$

$$(R_3)_j = (k_3)_j (N_e)_j (OH_e)_j$$

$$(R_4)_j = (k_4)_j (H_e)_j (N_2O_e)_j$$

$$(R_5)_j = (k_5)_j (O_e)_j (N_2O_e)_j$$

$$(R_6)_j = (k_6)_j (O_e)_j (N_2O_e)_j$$

- e. Compute $(K_1)_j$ and $(K_2)_j$

$$(K_1)_j = (R_1)_j / [(R_2)_j + (R_3)_j]$$

$$(K_2)_j = (R_6)_j / [(R_4)_j + (R_5)_j]$$

If $(R_2)_j$ and $(R_3)_j$ equal zero, $(K_1)_j = 10^{35}$

If $(R_4)_j$ and $(R_5)_j$ equal zero, $(K_2)_j = 10^{35}$

- f. Compute ρ_j as

$$\rho_j = P_j \text{ MW}_j / 82.057 T_j$$

- g. Compute k_s as

$$k_s = \frac{(12 a_{1,1} + 1 a_{1,2}) a_{2,2}}{28.99 (a_{1,1} + \frac{a_{1,2}}{4})}$$

- h. Compute ϕ as

$$\phi = \frac{F/A}{k_s}$$

- i. Compute F as

$$F = \phi k_s / (1 + \phi k_s)$$

- j. Compute $y_{CH_2}_j$

$$y_{CH_2}_j = 1 \left\{ \left[\frac{a_{1,1}/a_{1,2}}{1 + \frac{12a_{1,1}}{a_{1,2}}} \right] \left[\frac{\text{MW}_j (F/A)}{(F/A) + 1} \right] - y_{CO_j} - y_{CO_2_j} - y_{C(s)_j} \right\}$$

- k. Repeat steps a through j for each of the specified pressure levels.

- l. If all of the input fuel-to-air mass ratios have been examined, proceed to step m. If not, return to Subroutine OUT3 of Program NOXRAT and repeat the set of calculations in NOXRAT leading up to the calling of Subroutine RATES.
- m. If this is the first fuel-to-air mass ratio at the particular pressure in question, write and punch a heading card. If not, go to step n.
- n. Write and punch the required output data at the jth pressure level (for each fuel-to-air mass ratio at that pressure level). This data is: $F; \phi; \rho_j; T_j; y_{NO,j}; y_{CO,j}; y_{C(s),j}; y_{CH_2,j}; (R_1)_j, (R_6)_j, (K_1)_j$ and $(K_2)_j$.
- o. If this is the last fuel-to-air mass ratio at the jth pressure level, proceed to step p. If not, return to step m at the next ratio.
- p. If this is the last pressure specified, proceed to step q. If not, return to step m.
- q. Return.

```

SUBROUTINE RATES(CONCKI,WM,TTT,PPP,ANUM,ENTH,RTEMP,NPT,NREAC)  RAT*0000
REAL MIX(50)  RAT*0010
DIMENSION CONCKI(10,30),TTT(13),PPP(13),WM(13),ANUM(15,5),ENTH(15)  RAT*0020
1,RTEMP(15)  RAT*0030
DIMENSION R2(30,40),R3(30,40),R4(30,40),R5(30,40),RATEK(6,30,40),CRAT*0040
10RMCM(10,30,40),A(6),EN(6),F(6)  RAT*0050
COMMON/SNEW/ROH,INDFA  RAT*0060
COMMON/DICK/MIX  RAT*0070
COMMON/EGNEW,R1(30,40),R6(30,40),EK1(30,40),EK2(30,40),ROH(30,40),RAT*0080
1CH2(30,40),ATT(13,40),F(40),PHI(40),BCON1(30,40),RCON2(30,40),BCONRAT*0090
20(30,40)  RAT*0100
DATA(A(I),I=1,6)/3.,1E+13,6.4E+02,4.,1E+13,2.9513E+13,3.8146E+13,4.5RAT*0110
1775E+13/(EN(I),I=1,6)/0.,1.,0.,0.,0.,0.,/(E(I),I=1,6)/0.334E+00,6RAT*0120
2.250E+00,0.0E+00,10.77E+00,24.1E+00,24.1E+00/,ICODE/2/  RAT*0130
C****  RAT*0140
C**** TEST FOR WRITE CONTROL  RAT*0150
C****  RAT*0160
IST = INDFA  RAT*0170
IPRINT = 0  RAT*0180
IF(MIX(IST+1).EQ.0.0) IPRINT = 1  RAT*0190
C****  RAT*0200
C**** SET PRESSURE LOOP  RAT*0210
C****  RAT*0220
DO 6000 J = 1,NPT  RAT*0230
C****  RAT*0240
C**** CALCULATE CONCENTRATIONS  RAT*0250
C****  RAT*0260
HCON1(J,IST) = CONCKI(1,J)  RAT*0270
BCON2(J,IST) = CONCKI(2,J)  RAT*0280
CON6(J,IST) = CONCKI(6,J)  RAT*0290
GO 1000 I = 1,10  RAT*0300
CONVCM(I,J,IST) = (CONCKI(I,J)*PPP(J))/(82.057*TTT(J))  RAT*0310
1000 CONTINUE  RAT*0320
C****  RAT*0330
C**** COMPUTE RATE CONSTANTS  RAT*0340
C****  RAT*0350
DO 2000 I = 1,6  RAT*0360
RATEK(I,J,IST) = A(I)*(TTT(J)**EN(I))*EXP(-E(I)/(1.987E-03*TTT(J)))  RAT*0370
1)  RAT*0380
2000 CONTINUE  RAT*0390
C****  RAT*0400
C**** CALCULATE FORWARD REACTION CONSTANTS  RAT*0410
C****  RAT*0420
R1(J,IST) = (RATEK(1,J,IST)*CONVCM(5,J,IST)*CONVCM(6,J,IST))  RAT*0430
R2(J,IST) = (RATEK(2,J,IST)*CONVCM(5,J,IST)*CONVCM(9,J,IST))  RAT*0440
R3(J,IST) = (RATEK(3,J,IST)*CONVCM(5,J,IST)*CONVCM(10,J,IST))  RAT*0450
R4(J,IST) = (RATEK(4,J,IST)*CONVCM(4,J,IST)*CONVCM(7,J,IST))  RAT*0460
R5(J,IST) = (RATEK(5,J,IST)*CONVCM(8,J,IST)*CONVCM(7,J,IST))  RAT*0470
R6(J,IST) = (RATEK(6,J,IST)*CONVCM(8,J,IST)*CONVCM(7,J,IST))  RAT*0480
C****  RAT*0490
C**** CALCULATE K1,K2,RHO,KS, AND PHI  RAT*0500
C****  RAT*0510
IF(R2(J,IST).EQ.0.0.AND.R3(J,IST).EQ.0.0) EK1(J,IST) = 1.0E+35  RAT*0520
IF(R2(J,IST).EQ.0.0.AND.R3(J,IST).EQ.0.0) GO TO 2500  RAT*0530
EK1(J,IST) = (R1(J,IST)/(R2(J,IST)+R3(J,IST)))  RAT*0540
2500 IF(R4(J,IST).EQ.0.0.AND.R5(J,IST).EQ.0.0) EK2(J,IST) = 1.0E+35  RAT*0550
IF(R4(J,IST).EQ.0.0.AND.R5(J,IST).EQ.0.0) GO TO 2750  RAT*0560
EK2(J,IST) = (R6(J,IST)/(R4(J,IST)+R5(J,IST)))  RAT*0570
2750 ROH(J,IST) = (PPP(J)*WM(J))/(82.057*TTT(J))  RAT*0580
C****  RAT*0590

```

```

C**** NOTE...FUEL CARD IS PHYSICALLY BEFORE OXIDANT CARD IN INPUT, OXYGENRAT*0600
C**** IS SECOND SPECIE SPECIFIED IN OXIDANT AIR, FUEL IS SPECIFIED C-A, RAT*0610
C**** N=B RAT*0620
C**** RAT*0630
      EKS = ((12.*ANUM(1,1)+1.*ANUM(1,2))*ANUM(2,2))/(28.99*(ANUM(1,1)+(RAT*0640
1ANUM(1,2)/4.))) RAT*0650
      PHI(IST) = RON/EKS RAT*0660
      F(IST) = PHI(IST)*EKS/(1.+(PHI(IST)*EKS)) RAT*0670
C**** RAT*0680
C**** CALCULATE CONCENTRATION OF CH2 RAT*0690
C**** RAT*0700
      RATWTS = ANUM(1,1)/ANUM(1,2) RAT*0710
      CH2(J,IST) = (((RATWTS/(1.+12.*RATWTS))* (WH(J)*RON/(RON+1.)))-CONCRAT*0720
1KI(2,J)-GCNCKI(3,J)-CONCKI(1,J)) RAT*0730
C**** RAT*0740
C**** STORE VALUES OF T RAT*0750
C**** RAT*0760
      ATT(J,IST) = TTI(J) RAT*0770
      8000 CONTINUE RAT*0780
C**** RAT*0790
C**** PRINT AND PUNCH OUTPUT RAT*0800
C**** RAT*0810
      IF(IPRINT.EQ.0) GO TO 9999 RAT*0820
      DO 9500 J = 1,NPT RAT*0830
      DO 9000 I = 1,IST RAT*0840
      IF(I.NE.1) GO TO 8500 RAT*0850
      WRITE(6,8100) ANUM(1,1),ANUM(1,2),RTEMP(2),PPP(J),ICODE,EKS RAT*0860
      WRITE(7,8100) ANUM(1,1),ANUM(1,2),RTEMP(2),PPP(J),ICODE,EKS RAT*0870
8100 FORMAT(1X,7HFUEL= C,E15.8,1WH,E15.8,18H INLET AIR T.(K)= ,E15.8/1XRAT*0880
1,13HPRESS.(ATM)= ,E15.8,7HICODE= ,I2,13HPHI STOICH.= ,E15.8) RAT*0890
8500 WRITE(5,8200) F(I),PHI(I),RON(J,I),ATT(J,I),RCON6(J,I),BCON2(J,I),RAT*0900
1-CON1(J,I),CH2(J,I),R1(J,I),R6(J,I),EK1(J,I),EK2(J,I) RAT*0910
8200 FORMAT(1X,6E12.5/1X,6E12.5) RAT*0920
      WRITE(7,8250) F(I),PHI(I),RON(J,I),ATT(J,I),RCON6(J,I),BCON2(J,I),RAT*0930
1-CON1(J,I),CH2(J,I),R1(J,I),R6(J,I),EK1(J,I),EK2(J,I) RAT*0940
8250 FORMAT(6E12.5/6E12.5) RAT*0950
9000 CONTINUE RAT*0960
9500 CONTINUE RAT*0970
9999 RETURN RAT*0980
      END RAT*0990

```

APPENDIX VI - LISTING OF PROGRAM NOXRAT

PROGRAM NOXRAT(INPUT,OUTPUT,PUNCH,TAPE 5 = INPJT,TAPE 6 = OUTPUT,TNOX*0000
TAPE 7 = PUNCH,TAPE 4)

```

C
C MAIN PROGRAM
C
DOUBLE PRECISION G,X
REAL MIX(50)
INTEGER DATA, OMIT, INSERT, REAC, BLANK, THRM, END, SUB
LOGICAL HP, SP, TP, IDEBUG, NEWR, IONS, MOLES, FROZ, EQL, PSIA, RKT
LOGICAL SHOCK, MMHG, PASCAL, EV, IC, DETN, CPCVFR, CPCVEQ, SIUNIT, EUNITS
LOGICAL FA, OF, ERATIO, FPCT
C
DIMENSION OMIT(3,3), NCD(4), INSERT(3,3), LH(2), LVP(2), LVM(2)
COMMON/POINTS/MSUM(13), SSUM(13), CPR(13), DLVTP(13), DLVPT(13)
1  ,SAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
2  ,TOTN(13)
COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),MO(150)
1  ,DELN(150),A(15,150),SUR(150,3),IUSE(150),TEMP(50,2)
COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),BOP(15,2)
1  ,T4,TLOW,TMTN,THIGH,PP,CPSUM,OF,EORAT,FPCT,R,RR,HSUR0,AC(2),AM(2)
2  ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
3  ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FCX(15),DENS(15)
4  ,RHOP,RMW(15),TLN
COMMON/DOUBLE/G(20,21),X(20)
COMMON/INDX/IDEBUG,CONVG,TP,HP,SF,HPSP,TPSP,MOLES,NP,NT,NPT,NL4
1  ,NS,KKAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
2  ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JSI,VOL,SHOCK
COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SURR(13)
1  ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSO
COMMON/GNEW/RON,INDFA
COMMON/DICK/MIX
COMMON/ERNEW/R1(30,40),R6(30,40),EK1(30,40),EK2(30,40),ROH(30,40),
1CH2(30,40),ATT(13,40),F(40),PHI(40),BCON1(30,40),BCON2(30,40),BCON
26(30,40)
C
EQUIVALENCE (OMIT,ENLN),(INSERT,EN(1,3)),(NLM,L),(OF,OXFL)
C
DATA MIT/4HOMIT/,BLANK/1H/,PSIA/4HPSIA/,REAC/4HREAC/,IZ/2H00/
1  ,INPUT/4HINPU/,IF/1HE/,INSERT/4HINSE/,THRM/4HTHER/,END/3HEND/
DATA LH/4HL,CA,4HL/G/,LVP/2HV,1H/,LVM/2HV,1H/,NMLT/4HNAME/
C
NAMELIST/INPT2/KASE,P,T,ERATIO,OF,FPCT,FA,TP,HP,SP,RKT
1,PSIA,MMHG,SHOCK,IONS,EV,V,DETN,CPCVFR,CPCVEQ,IDEBUG
2,SIUNIT,EUNITS,MIX
C
TLOW = 0.
NEWR = .FALSE.
C
1 WRITE(6,400)
400 FORMAT(1H1)
203 READ(5,204) (DATA(I),I=1,15)
204 FORMAT(5(3A4,3X))
WRITE(6,2045) (DATA(I),I=1,15)
2045 FORMAT(1X,5(3A4,3X))
IF(DATA(1).EQ.THRM) GO TO 90
IF(DATA(1).EQ.REAC) GO TO 11
IF(DATA(1).EQ.MIT) GO TO 205
IF(DATA(1).EQ.INSERT) GO TO 180
IF(DATA(1).EQ.INPUT.OR.DATA(1).EQ.NMLT) GO TO 210
IF(DATA(1).EQ.BLANK) GO TO 203

```

```

1023 WRITE(6,1024)
1024 FORMAT(40H0ERROR IN ABOVE CARD. IGNORE CONTENTS.
      GO TO 203
      I1 NOMIT = 0
      NSERT = 0
      MOLES = .FALSE.
      CALL REACT
      IF(L.EQ.0) WRITE(6,52)
52  FORMAT(24H0ERROR IN REACTANT CARDS)
      GO TO 203
C
C  READ THERMO DATA FROM CARDS AND STORE ON TAPE 4
C
90  NEWR = .TRUE.
      REWIND 4
      READ(5,5) TLOW,TMIN,THIGH
5  FORMAT(3F10.3)
      WRITE(4,5) TLOW,TMIN,THIGH
97  READ(5,10) (DATA(I),I=1,16),NCD(1)
10  FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3,I15)
      IF(DATA(1).EQ.BLANK) DATA(1)=END
      WRITE(4,10) (DATA(I),I=1,16)
      IF(DATA(1).EQ.END) GO TO 203
      READ(5,20) (DATA(I),I=1,5),NCD(2), (DATA(J),J=6,10),NCD(3), (DATA(K),
      K=11,14),NCD(4)
20  FORMAT(5E15.8,I5/5E15.8,I5/4E15.8,I20)
      WRITE(4,21) (DATA(I),I=1,14)
21  FORMAT(5E15.8/5E15.8/4E15.8)
      DO 25 I=1,4
      IF(NCD(I).EQ.I) GO TO 25
      WRITE(6,22) (DATA(J),J=1,3)
22  FORMAT(28H0ERROR IN ORDER OF CARDS FOR ,3A4)
25  CONTINUE
      GO TO 97
C
C  CHECK INSERT CARDS
C
180 DO 185 I=4,15,3
      IF (DATA(I).EQ.BLANK) GO TO 185
      NSERT = NSERT+1
      ENSERT(1,NSERT) = DATA(I)
      ENSERT(2,NSERT) = DATA(I+1)
      ENSERT(3,NSERT) = DATA(I+2)
185 CONTINUE
      GO TO 203
C
C  CHECK OMIT CARDS
C
205 DO 208 I=4,15,3
      IF (DATA(I).EQ.BLANK) GO TO 208
      NOMIT = NOMIT+1
      OMIT(1,NOMIT) = DATA(I)
      OMIT(2,NOMIT) = DATA(I+1)
      OMIT(3,NOMIT) = DATA(I+2)
208 CONTINUE
      NEWR = .TRUE.
      GO TO 203
C
C  BEGIN NAMELIST INPT2
C

```

```

NOX*0600
NOX*0610
NOX*0620
NOX*0630
NOX*0640
NOX*0650
NOX*0660
NOX*0670
NOX*0680
NOX*0690
NOX*0700
NOX*0710
NOX*0720
NOX*0730
NOX*0740
NOX*0750
NOX*0760
NOX*0770
NOX*0780
NOX*0790
NOX*0800
NOX*0810
NOX*0820
NOX*0830
NOX*0840
NOX*0850
NOX*0860
NOX*0870
NOX*0880
NOX*0890
NOX*0900
NOX*0910
NOX*0920
NOX*0930
NOX*0940
NOX*0950
NOX*0960
NOX*0970
NOX*0980
NOX*0990
NOX*1000
NOX*1010
NOX*1020
NOX*1030
NOX*1040
NOX*1050
NOX*1060
NOX*1070
NOX*1080
NOX*1090
NOX*1100
NOX*1110
NOX*1120
NOX*1130
NOX*1140
NOX*1150
NOX*1160
NOX*1170
NOX*1180
NOX*1190

```

```

210 DO 300 I=1,26
    PCP(I) = 0.
    P(I) = 0.
    T(I) = 0.
    V(I) = 0.
300 CONTINUE
    V1 = 0.
    V2 = 0.
    RHOP = 0.
    KASE = 0
    TP = .FALSE.
    WP = .FALSE.
    SP = .FALSE.
    RKT = .FALSE.
    CPCVFR = .FALSE.
    CPCVEQ = .FALSE.
    SHOCK = .FALSE.
    DETN = .FALSE.
    EV = .FALSE.
    PASCAL = .FALSE.
    MMHG = .FALSE.
    PSIA = .FALSE.
    R = 1.987165
    RR = 4184.*R
    SIUNIT = .FALSE.
    EUNITS = .FALSE.
    IONS = .FALSE.
    IDERUG = .FALSE.
    FA = .FALSE.
    OF = .FALSE.
    ERATIO = .FALSE.
    FPCT = .FALSE.
    DO 303 I = 1,50
    MIX(I) = 0.
303 CONTINUE
    EQL = .TRUE.
    READ(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 (PSIA) P(NP) = P(NP)/14.696006
315 CONTINUE
322 DO 625 IST = 1,40
    INDFA = IST
    IF(IST.NE.1) WRITE(6,400)
    IF(MIX(IST).NE.0.) GO TO 323
    IF(IST.NE.1) GO TO 1
    WRITE(6,724)
724 FORMAT(48HONO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT
    IF (WP(2).NE.0.) OXFL = WP(1)/WP(2)
    GO TO 333
323 OXFL = MIX(IST)
    RON = MIX(IST)
    IF(FA) OXFL = 1./ MIX(IST)
    IF(FPCT) OXFL = (100.- MIX(IST))/ MIX(IST)
    IF(.NOT.ERATIO) GO TO 333
    EQRAT = MIX(IST)
    IF(EQRAT.EQ.1.) EQRAT = 1.000005

```

```

NOX*1200
NOX*1210
NOX*1220
NOX*1230
NOX*1240
NOX*1250
NOX*1260
NOX*1270
NOX*1280
NOX*1290
NOX*1300
NOX*1310
NOX*1320
NOX*1330
NOX*1340
NOX*1350
NOX*1360
NOX*1370
NOX*1380
NOX*1390
NOX*1400
NOX*1410
NOX*1420
NOX*1430
NOX*1440
NOX*1450
NOX*1460
NOX*1470
NOX*1480
NOX*1490
NOX*1500
NOX*1510
NOX*1520
NOX*1530
NOX*1540
NOX*1550
NOX*1560
NOX*1570
NOX*1580
NOX*1590
NOX*1600
NOX*1610
NOX*1620
NOX*1630
NOX*1640
NOX*1650
NOX*1660
NOX*1670
NOX*1680
NOX*1690
NOX*1700
NOX*1710
NOX*1720
NOX*1730
NOX*1740
NOX*1750
NOX*1760
NOX*1770
NOX*1780
NOX*1790

```

```

      OXFL = (-EQRAT*VMIN(2)-VPLS(2))/(VPLS(1)+EQRAT*VMIN(1))
333 SUM = OXFL + 1.
      V2 = (OXFL*VMIN(1)+VMIN(2))/SUM
      V1 = (OXFL*VPLS(1)+VPLS(2))/SUM
      IF (V2.NE.0.) EQRAT=ABS(V1/V2)
      IF (RHO(1).NE.0. .AND. RHO(2).NE.0.) GO TO 744
      RHOP = RHO(2)
      IF (RHOP.EQ.0.) RHOP = RHO(1)
      GO TO 745
744 RHOP = (OXFL+1.)*RHO(1)*RHO(2)/(RHO(1)+OXFL*RHO(2))
745 LL = L
      IF (.NOT.IONS) GO TO 746
      LL = L-1
      IF (LLMT(LL).EQ.IE) GO TO 746
      LL = L
      L = L+1
      LLMT(L) = IE
      B0(L) = 0.
746 DO 747 I=1,LL
      B0(I) = (OXFL*B0P(I,1)+      B0P(I,2))/SUM
747 CONTINUE
      NPT = 1
      HSUB0 = (OXFL*HPP(1) + HPP(2))/SUM
      IF (.NOT.NEWR) GO TO 786
      CALL SEARCH
      IF (SHOCK.OR.DETN) GO TO 760
      DO 755 N=1,NREAC
      IF (NAME(N,5).NE.IZ) GO TO 755
      IT = RTEMP(N)
      CALL HCALC
      GO TO 760
755 CONTINUE
760 WRITE(6,INPT2)
786 ENN = .1
      SUMV = ENN
      XI = NS - NC
      XI = ENN/XI
      XLN = ALOG(XI)
      DO 432 J=1,NS
      IF (IUSE(J).EQ.-10000) IUSE(J)=0
      IF (IUSE(J).NE.0) GO TO 432
      EV(J,1) = XI
      EVLN(J) = XLN
432 CONTINUE
      WRITE(6,770)
770 FORMAT (1H0,17X,4HFUEL,13X,7HOXIDANT,12X,7H4MIXTURE //)
780 FORMAT (1H 2A4,3E18.8/)
      DO 780 LH,HPP(2),HPP(1),HSUB0,LVP,VPLS(2),VPLS(1),V1,
      1V2,VMIN(2),VMIN(1),V2
      HSUB0 = HSUB0/R
      WRITE(6,785)
785 FORMAT (8H ATOMS/G )
      WRITE(6,780) (LLMT(I),BLANK,B0P(I,2),B0P(I,1),B0(I),I=1,L)
      IGL = L+1
      IF (NC.EQ.0) GO TO 790
      DO 302 J=1,NS
      IF (IUSE(J).EQ.0) GO TO 302
      IF (IUSE(J).GT.0) IUSE(J) = -IUSE(J)
      EV(J,1) = 0.
      EVLN(J) = 0.

```

NOX*1800
 NOX*1810
 NOX*1820
 NOX*1830
 NOX*1840
 NOX*1850
 NOX*1860
 NOX*1870
 NOX*1880
 NOX*1890
 NOX*1900
 NOX*1910
 NOX*1920
 NOX*1930
 NOX*1940
 NOX*1950
 NOX*1950
 NOX*1950
 NOX*1970
 NOX*1980
 NOX*1990
 NOX*2000
 NOX*2010
 NOX*2020
 NOX*2030
 NOX*2040
 NOX*2050
 NOX*2060
 NOX*2070
 NOX*2080
 NOX*2090
 NOX*2100
 NOX*2110
 NOX*2120
 NOX*2130
 NOX*2140
 NOX*2150
 NOX*2160
 NOX*2170
 NOX*2180
 NOX*2190
 NOX*2200
 NOX*2210
 NOX*2220
 NOX*2230
 NOX*2240
 NOX*2250
 NOX*2260
 NOX*2270
 NOX*2280
 NOX*2290
 NOX*2300
 NOX*2310
 NOX*2320
 NOX*2330
 NOX*2340
 NOX*2350
 NOX*2360
 NOX*2370
 NOX*2380
 NOX*2390


```

IF(NSERT.EQ.0) GO TO 302
DO 301 I=1,NSERT
IF(SUB(J,1).NE.ENSERT(1,I)) GO TO 301
IF(SUB(J,2).NE.ENSERT(2,I)) GO TO 301
IF(SUB(J,3).NE.ENSERT(3,I)) GO TO 301
ENSERT(1,I) = 0.
IQ1= IQ1+1
IUSE(J) = -IUSE(J)
301 CONTINUE
302 CONTINUE
790 ITN= 35
IC = .FALSE.
JSOL = 0
JLIQ = 0
IF(DETN) CALL DETON
IF(RKT) CALL ROCKET
IF(TP) CALL MOLIER
IF(HP) CALL CMRSTN
IF(SHOCK) CALL SHCK
625 CONTINUE
NSERT = 0
GO TO 1
END

```

```

NOX*2400
NOX*2410
NOX*2420
NOX*2430
NOX*2440
NOX*2450
NOX*2460
NOX*2470
NOX*2480
NOX*2490
NOX*2500
NOX*2510
NOX*2520
NOX*2530
NOX*2540
NOX*2550
NOX*2560
NOX*2570
NOX*2580
NOX*2590
NOX*2600
NOX*2610
NOX*2620

```

```

SUBROUTINE REACT
C
DOUBLE PRECISION G,X
LOGICAL HP,SP,TP,INEL,UG,CONVG,NEW,IONS,MOLES,EOL,FROZ
C
DIMENSION ANAME(15,5),V(15)
C
COMMON/MISC/ FNN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
1  ,T4,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUR0,AC(2),AM(2)
2  ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
3  ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTMP(15),FOX(15),DENS(15)
4  ,RMUP,RMW(15),TLV
COMMON/INDX/ I0F,UG,CONVG,TP,HP,SP,HSP,TPSP,MOLES,NP,NT,NPT,NLM
1  ,NS,KMAT,IMAT,101,IQ2,NOMIT,IP,NEW,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
2  ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
C
EQUIVALENCE (NAME,ANAME),(NLM,L)
C
DATA MOL/1HM/.OX/1H0/.LANK/1H /.IZERO/2H00/
C
DO 10 K=1,2
  WP(K)=0.
  HPP(K)=0.
  RHO(K)=0.
  VPLS(K)=0.
  VMIN(K)=0.
  AC(K)=0.
  AM(K)=0.
  DO 8 J=1,15
    LLMT(J)=0
    B0P(J,K)=0.
8  CONTINUE
10 CONTINUE
  N=1
  L=1
20 READ(5,21) (NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ(N)
1  ,RTMP(N),FOX(N),DENS(N)
21 FORMAT(5(A2,F7.3),F7.5,A1,F9.5,A1,F8.5,A1,F8.5)
  IF (NAME(N,1).EQ.LANK) GO TO 200
  IF (L.EQ.0) GO TO 20
  WRITE(6,31) (NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ
1  (N),RTMP(N),FOX(N),DENS(N)
31 FORMAT(1X,5(A2,1X,F7.4,2X),F8.4,2X,A1,F11.2,2X,A1,2X,F8.3,2X,
1  ,1,3X,F8.5)
35 IF (MOLE.EQ.MOL) MOLES=.TRUE.
  K=2
  IF (FOX(N).EQ.OX) K=1
  DO 38 J=1,15
    DATA(J) = 0.
38 CONTINUE
  RM=0.
  DO 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
    LLMT(J)=NAME(N,JJ)

```

RCT*0000
 RCT*0010
 RCT*0020
 RCT*0030
 RCT*0040
 RCT*0050
 RCT*0060
 RCT*0070
 RCT*0080
 RCT*0090
 RCT*0100
 RCT*0110
 RCT*0120
 RCT*0130
 RCT*0140
 RCT*0150
 RCT*0160
 RCT*0170
 RCT*0180
 RCT*0190
 RCT*0200
 RCT*0210
 RCT*0220
 RCT*0230
 RCT*0240
 RCT*0250
 RCT*0260
 RCT*0270
 RCT*0280
 RCT*0290
 RCT*0300
 RCT*0310
 RCT*0320
 RCT*0330
 RCT*0340
 RCT*0350
 RCT*0360
 RCT*0370
 RCT*0380
 RCT*0390
 RCT*0400
 RCT*0410
 RCT*0420
 RCT*0430
 RCT*0440
 RCT*0450
 RCT*0460
 RCT*0470
 RCT*0480
 RCT*0490
 RCT*0500
 RCT*0510
 RCT*0520
 RCT*0530
 RCT*0540
 RCT*0550
 RCT*0560
 RCT*0570
 RCT*0580
 RCT*0590

```

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+ANUM(N, JJ)*ATOM(2, KK)
   V(J)=ATOM(3, KK)
   DATA(J)=ANUM(N, JJ)
100 CONTINUE
101 PCWT=PECWT(N)
   IF (MOLES) PCWT=PCWT*RM
   WP(K)=WP(K) + PCWT
   IF (NAME(N, 5).NE.IZERO) HPP(K)=HPP(K)+ENTH(N)*PCWT/RM
   AM(K)=AM(K)+PCWT/RM
   DO 110 J=1, L
     BOP(J, K)=DATA(J)*PCWT/RM +BOP(J, K)
110 CONTINUE
   IF (DENS(N).NE.0.) GO TO 115
   GO TO 117
115 RHO(K)=RHO(K)+PCWT/DENS(N)
117 RMW(N) = RM
   N = N+1
   IF (N.NE.16) GO TO 20
200 NREAC =N-1
   IF (L.EQ.0) GO TO 1000
   DO 220 K=1, 2
     IF (WP(K).EQ.0.) GO TO 220
     HPP(K)=HPP(K)/WP(K)
     AM(K) = WP(K)/AM(K)
     IF (RHO(K).NE.0.) RHO(K)=WP(K)/RHO(K)
     DO 215 J=1, L
       BOP(J, K)=BOP(J, K)/WP(K)
       IF (V(J).LT.0.) VMIN(K)= VMIN(K)+BOP(J, K)*V(J)
       IF (V(J).GT.0.) VPLS(K)=VPLS(K)+BOP(J, K)*V(J)
215 CONTINUE
     IF (MOLES) GO TO 220
     DO 218 N=1, NREAC
       IF (FOX(N).EQ.OX.AND.K.EQ.2) GO TO 218
       IF (FOX(N).NE.OX.AND.K.EQ.1) GO TO 218
       PECWT(N) = PECWT(N)/WP(K)
218 CONTINUE
220 CONTINUE
   VEMR=.TRUE.
   DO 230 N = 1, NREAC
     IF (DENS(N).NE.0.) GO TO 230
     RHO(1) = 0.
     RHO(2) = 0.
     GO TO 1000
230 CONTINUE
1000 RETURN
END

```

```

RCT*0600
RCT*0610
RCT*0620
RCT*0630
RCT*0640
RCT*0650
RCT*0660
RCT*0670
RCT*0680
RCT*0690
RCT*0700
RCT*0710
RCT*0720
RCT*0730
RCT*0740
RCT*0750
RCT*0760
RCT*0770
RCT*0780
RCT*0790
RCT*0800
RCT*0810
RCT*0820
RCT*0830
RCT*0840
RCT*0850
RCT*0860
RCT*0870
RCT*0880
RCT*0890
RCT*0900
RCT*0910
RCT*0920
RCT*0930
RCT*0940
RCT*0950
RCT*0960
RCT*0970
RCT*0980
RCT*0990
RCT*1000
RCT*1010
RCT*1020
RCT*1030
RCT*1040
RCT*1050
RCT*1060
RCT*1070
RCT*1080
RCT*1090
RCT*1100

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```

SUBROUTINE SEARCH
C SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED
  INTEGER SUR, OMIT, END
C LOGICAL NFWR
C DIMENSION DATE(2,3), MT(4), B(4), OMIT(3,3)
C COMMON/SPECES/ COEF(2,7,150), S(150), EN(150,13), ENLN(150), MO(150)
  1 .DELN(150), A(15,150), SUR(150,3), IUSE(150), TEMP(50,2)
  COMMON/MISC/ ENN, SUMN, TT, S0, ATOM(3,101), LLMT(15), B0(15), B0P(15,2)
  1 .T, TLOW, TMID, THIGH, PP, CPSUM, OF, EQRAT, FPCT, R, RR, HSUB0, AC(2), AM(2)
  2 .HPP(2), RHG(2), VMTN(2), VPLS(2), WP(2), DATA(22), NAME(15,5)
  3 .ANUM(15,5), PECWT(15), ENTH(15), FAZ(15), RTEMP(15), FOX(15), DENS(15)
  4 .RHOP, RMW(15), TLN
  COMMON/INPX/ INDEBUG, CONVG, TP, HP, SP, HPSP, TPSP, MOLES, NP, NT, NPT, NLN
  1 .NS, KMA7, IMAT, IQ1, IQ2, NOMIT, IP, NEWR, NSUB, NSUP, ITN, CPCVFR, CPCVEO
  2 .IONS, NC, NSERT, JSOL, JLIQ, KASE, NREAC, IC, JS1, VOL, SHOCK
C EQUIVALENCE (DATE, EN), (OMIT, ENLN), (ENDD, END), (L, NLN)
C DATA GAS/1HG/, END/3HEND/
C NC= 0
  IX= 0
  COEF(1,1,1) = ENDD
  I = 1
  DO 3 I=1,150
    IF(A(1,I).EQ.ENDD) GO TO 4
    DO 3 J=1,L
      A(J,I) = 0.
  3 CONTINUE
  4 MAXNS = I
  REWIND 4
  READ(4,5) TLOW, TMID, THIGH
  5 FORMAT (3F10,3)
  NS = 1
  7 READ (4,10) (SUR(NS,I), I=1,3), DATE(1,NS), DATE(2,NS), (MT(J), B(J),
  1 J=1,4), PHAZ, T1, T2
  10 FORMAT (3A4,6X,2A3,4(A2,F3,0),A1,2F10,3)
  IF(SUR(NS,1).EQ.END) GO TO 171
  READ (4,20) ((COEF(I,J,NS), J=1,7), I=1,2)
  20 FORMAT (5E15,8)
  IF(NOMIT.FQ.0) GO TO 810
  DO 805 I=1,NOMIT
    DO 804 J=1,3
      IF(OMIT(J,I).NE.SUR(NS,J)) GO TO 805
  804 CONTINUE
  GO TO 7
  805 CONTINUE
  810 DO 820 K=1,4
    IF(B(K).EQ.0.) GO TO 825
    DO 168 I=1,L
      IF(LLMT(I).EQ.MT(K)) GO TO 820
  168 CONTINUE
  DO 819 J=1,L
    A(J,NS) = 0.
  GO TO 7
  820 A(I,NS) = B(K)

```

```

SEA*0000
SEA*0010
SEA*0020
SFA*0030
SEA*0040
SEA*0050
SEA*0060
SEA*0070
SEA*0080
SFA*0090
SEA*0100
SEA*0110
SFA*0120
SEA*0130
SEA*0140
SFA*0150
SEA*0160
SEA*0170
SFA*0180
SEA*0190
SFA*0200
SEA*0210
SEA*0220
SFA*0230
SEA*0240
SEA*0250
SFA*0260
SEA*0270
SEA*0280
SEA*0290
SEA*0300
SEA*0310
SFA*0320
SEA*0330
SEA*0340
SFA*0350
SEA*0360
SEA*0370
SEA*0380
SEA*0390
SEA*0400
SEA*0410
SEA*0420
SEA*0430
SEA*0440
SEA*0450
SEA*0460
SEA*0470
SEA*0480
SEA*0490
SEA*0500
SFA*0510
SEA*0520
SFA*0530
SEA*0540
SEA*0550
SFA*0560
SEA*0570
SEA*0580
SEA*0590

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```

825 IF(NS.EQ.MAXNS) 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
      IF(A(I,NS).NE.A(I,NS-1)) GO TO 145
830 CONTINUE
      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/SPECES/TOO SMALL 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
      IS= I+4
      IF(NS.LT.IS) IS=NS
174 WRITE (6,176) (DATE(I,J),DATE(2,J),SUB(J,1),SUB(J,2),SUB(J,3),J=I,
1 IS)
176 FORMAT(5(5X,2A3,2X,3A4))
      RETURN
      END

```

```

SEA*0600
SEA*0610
SFA*0620
SEA*0630
SEA*0640
SEA*0650
SEA*0660
SEA*0670
SEA*0680
SFA*0690
SEA*0700
SFA*0710
SEA*0720
SEA*0730
SFA*0740
SEA*0750
SFA*0760
SEA*0770
SEA*0780
SEA*0790
SEA*0800
SEA*0810
SFA*0820
SEA*0830
SEA*0840
SEA*0850
SEA*0860
SEA*0870
SEA*0880
SEA*0890

```

```

SUBROUTINE EQLARM
C ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES
C
C   DOUBLE PRECISION X,G
C   LOGICAL HP,SP,TP,INDBG,CONVG,IONS,MOLES,FROZ,EQL,LOGV,HPSP,TPSP
C   LOGICAL ISING,IC,SHOCK
C
C   DIMENSION PROW(18)
C
C   COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
C   1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SDNVEL(13),TTT(12)
C   2,TOTN(13)
C   COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
C   1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
C   COMMON/MISC/ENN,SUM,TT,S0,ATOM(3,101),LLMT(15),B0(15),ROP(15,2)
C   1 ,TM,TLOW,TMIN,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
C   2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
C   3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
C   4 ,RHOP,RMW(15),TLN
C   COMMON /DOUBLE/ G(20,21), X(20)
C   COMMON/IN/X/ INDBG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
C   1 ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEW,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
C   2 ,IONS,NC,NSERT,JSOL,JLID,KASE,NREAC,IC,JS1,VOL,SHOCK
C   COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
C   1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SS0
C
C   EQUIVALENCE (NLM,L)
C
C   DATA IE/IHE/,SMALNO/1.E-6/,SMNOL/-13.815511/
C
C   SIZE= 18.5
C   SIZEFF = 0.
C   ISING = .FALSE.
C   ENNL = ALOG(ENN)
C   LOGV = .FALSE.
C   PPLN = ALOG(PP)
C   TLN = ALOG(TT)
C   CONVG = .FALSE.
C   ITNUMB = ITN
C   JS1 = 1
C   CALL CPM5
C   TM = PPLN - FNNL
C
C   IF(IC) PREVIOUS POINT HAD SINGULAR MATRIX
C
C   IF(IC) GO TO 966
C   IF (.NOT.IONS.OR.IE.EQ.LLMT(L)) GO TO 33
C   L = L+1
C   ICI = IC+1
C   DO 499 J = 1,NS
C   IF (A(L,J).EQ.0.) GO TO 499
C   EN(J,NPT) = SMALNO
C   ENLN(J) = SMNOL
C   IUSE(J) = 0
C   499 CONTINUE
C   33 IF(NPT.EQ.)AND(.NOT.SHOCK) WRITE(6,244) (LLMT(I),I=1,L)
C   244 FORMAT (4H0PT,14(5X,A4))
C
C   BEGIN ITERATION
C

```

```

EQL*0000
EQL*0010
EQL*0020
EQL*0030
EQL*0040
EQL*0050
EQL*0060
EQL*0070
EQL*0080
EQL*0090
EQL*0100
EQL*0110
EQL*0120
EQL*0130
EQL*0140
EQL*0150
EQL*0160
EQL*0170
EQL*0180
EQL*0190
EQL*0200
EQL*0210
EQL*0220
EQL*0230
EQL*0240
EQL*0250
EQL*0260
EQL*0270
EQL*0280
EQL*0290
EQL*0300
EQL*0310
EQL*0320
EQL*0330
EQL*0340
EQL*0350
EQL*0360
EQL*0370
EQL*0380
EQL*0390
EQL*0400
EQL*0410
EQL*0420
EQL*0430
EQL*0440
EQL*0450
EQL*0460
EQL*0470
EQL*0480
EQL*0490
EQL*0500
EQL*0510
EQL*0520
EQL*0530
EQL*0540
EQL*0550
EQL*0560
EQL*0570
EQL*0580
EQL*0590

```

```

43 CONTINUE
  IF(IC) GO TO 1171
  IF (.NOT.CONVG.OR.JSOL.EQ.0) GO TO 62
  ENSOL = EN(JSOL,NPT)
  EV(JSOL,NPT) = EN(JSOL,NPT)*EN(JLIQ,NPT)
  IUSE(JLIQ) = -IUSE(JLIQ)
  IQ1 = IQ1-1
  DLVTP(NPT) = 0.
  CPR(NPT) = 0.
  GAMMAS(NPT) = 0.
  LOGV = .TRUE.
62 CALL MATRIX
  NUMB = ITN-ITNUMB+1
  IF(.NOT.CONVG) GO TO 67
  IF (LOGV.AND.JSOL.EQ.0) GO TO 63
  DO 182 I=1,L
    PROW(I) = G(IQ1,I)
182 CONTINUE
  IF (.NOT.LOGV) GO TO 67
C
C   LOGV = .TRUE.-- SET UP MATRIX TO SOLVE FOR DLVPT
C
63 G(IQ1,IQ2) = ENN
  IQ = IQ1 - 1
  DO 777 I = 1,IQ
    G(I,IQ2) = G(I,IQ1)
777 CONTINUE
  A7 IF (.NOT.IDERUG) GO TO 72
  WRITE(6,772) NUMB
772 FORMAT (11HITERATION ,I3,6X,7HMATRIX //)
  DO 911 I=1,IMAT
911 WRITE (6,73) (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.IDERUG.OR.CONVG) GO TO 773
  WRITE (6,373) (LLMT(I),I=1,L)
373 FORMAT (7HOP1 ,9(A4,10X))
  WRITE (6,73) (X(I),I=1,IMAT)
  73 FORMAT (9F14.6)
773 IF(.NOT.CONVG) GO TO 85
  IF(.NOT.LOGV) GO TO 174
  IF(JLIQ.NE.0) EN(JSOL,NPT)=ENSOL
  GO TO 171
174 SUM = 0.
  DO 175 J=1,L
    SUM = SUM+PROW(J)*X(J)
175 CONTINUE
  DLVTP(NPT) = 1.+G(IQ2,IQ1)/ENN-SUM/ENN - X(IQ1)
  CPR(NPT) = G(IQ2,IQ2)
  DO 176 J=1,IQ1
    CPR(NPT) = CPR(NPT)-G(IQ2,J)*X(J)
176 CONTINUE
  LOGV = .TRUE.
  GO TO 62
C
C   SINGULAR MATRIX
C
C   IF(ISING) SINGULAR ONCE

```

```

EQL*0600
EQL*0610
EQL*0620
EQL*0630
EQL*0640
EQL*0650
EQL*0660
EQL*0670
EQL*0680
EQL*0690
EQL*0700
EQL*0710
EQL*0720
EQL*0730
EQL*0740
EQL*0750
EQL*0760
EQL*0770
EQL*0780
EQL*0790
EQL*0800
EQL*0810
EQL*0820
EQL*0830
EQL*0840
EQL*0850
EQL*0860
EQL*0870
EQL*0880
EQL*0890
EQL*0900
EQL*0910
EQL*0920
EQL*0930
EQL*0940
EQL*0950
EQL*0960
EQL*0970
EQL*0980
EQL*0990
EQL*1000
EQL*1010
EQL*1020
EQL*1030
EQL*1040
EQL*1050
EQL*1060
EQL*1070
EQL*1080
EQL*1090
EQL*1100
EQL*1110
EQL*1120
EQL*1130
EQL*1140
EQL*1150
EQL*1160
EQL*1170
EQL*1180
EQL*1190

```

```

C      IF(IC)      SINGULAR TWICE
C
774 IF(.NOT.CONVG) GO TO 775
    WRITE(6,172)
172 FORMAT(28H0DERIVATIVE MATRIX SINGULAR )
    IC = .TRUE.
    GO TO 1171
775 IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.) GO TO 871
    WRITE(6,874)
874 FORMAT(96H0LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE
18EEN INCLUDED ON AN INSERT CARD. RESTART )
    GO TO 873
871 WRITE (6,74)
    74 FORMAT(16H0SINGULAR MATRIX)
    IF(IC) GO TO 873
    IF (ISING) GO TO 997
    NTZERO = 0
966 DO 970 JJ = 1, NS
    IF(IUSE(JJ)) 970,968,967
967 IF(EN(JJ,NPT).EQ.0.) GO TO 873
    GO TO 969
968 IF(EN(JJ,NPT).NE.0.) GO TO 969
    EN(JJ,NPT) = SMALNO
    ENLN(JJ) = SMNOL
    GO TO 970
969 NTZERO = NTZERO+1
970 CONTINUE
    IF(.NOT.IC) GO TO 971
    IC = .FALSE.
    GO TO 43
971 ISING = .TRUE.
    WRITE (6,776)
776 FORMAT (8H0RESTART)
    GO TO 43
997 IF(NTZERO.NE.(L-1)) GO TO 873
    IF(EQRAT.GT.1.00001.OR.EQRAT.LT.0.99999) GO TO 873
    ENN=0.
    NEN = 0
    DO 83 I=1,L
    JEN=0
    DO 80 J=1,NS
    IF(EN(J,NPT).EQ.0.) GO TO 80
    IF(EN(I,J).EQ.0.) GO TO 80
    IF(JEN.NE.0) GO TO 83
    JEN = J
80 CONTINUE
    NEN = NEN+1
    EN(JEN,NPT) = EN(I)/A(I,JEN)
83 CONTINUE
    IF(NEN.LT.NTZERO) GO TO 873
    CONVG = .TRUE.
    IC = .TRUE.
    HSUM(NPT) = 0.
    DO 84 J=1,NS
    IF(EN(J,NPT).EQ.0.) GO TO 84
    ENN = EN(J,NPT)*ENN
    TEM = EN(J,NPT)
    ENLN(J) = ALOG(TEM)
    HSUM(NPT) = HSUM(NPT) + EN(J,NPT)*H0(J)
84 CONTINUE

```

69

```

EQL*1200
EQL*1210
EQL*1220
EQL*1230
EQL*1240
EQL*1250
EQL*1260
EQL*1270
EQL*1280
EQL*1290
EQL*1300
EQL*1310
EQL*1320
EQL*1330
EQL*1340
EQL*1350
EQL*1360
EQL*1370
EQL*1380
EQL*1390
EQL*1400
EQL*1410
EQL*1420
EQL*1430
EQL*1440
EQL*1450
EQL*1460
EQL*1470
EQL*1480
EQL*1490
EQL*1500
EQL*1510
EQL*1520
EQL*1530
EQL*1540
EQL*1550
EQL*1560
EQL*1570
EQL*1580
EQL*1590
EQL*1600
EQL*1610
EQL*1620
EQL*1630
EQL*1640
EQL*1650
EQL*1660
EQL*1670
EQL*1680
EQL*1690
EQL*1700
EQL*1710
EQL*1720
EQL*1730
EQL*1740
EQL*1750
EQL*1760
EQL*1770
EQL*1780
EQL*1790

```



```

      TM = ALOG(PP/ENN)
      GO TO 43
R5 ITNUMB= ITNUMB-1
C
C      OBTAIN CORRECTIONS TO THE ESTIMATES
C
      KK = L + 1
      DLNT= X(IQ2)
      IF (IP) DLNT=0.
      DO 101 J=1,NS
      IF (IUSE(J)) 101,99,100
98 DELN(J) = H0(J)*DLNT-H0(J)+S(J)-ENLN(J)-TM*X(IQ1)
      DO 99 K=1,L
      DELN(J)= DELN(J)+A(K,J)*X(K)
99 CONTINUE
      GO TO 101
100 DELN(J) = X(KK)
      KK = KK + 1
101 CONTINUE
      AMBDA= 1.
      AMBDA1= 1.
      SUM = X(IQ1)
      IF(SUM.LT.0.) SUM=-SUM
      IF(DLNT.GT.SUM) SUM=DLNT
      IF(-DLNT.GT.SUM) SUM=-DLNT
      DO 917 J=1,NS
      IF (IUSE(J).NE.0) GO TO 917
      IF((EN(J,NPT).GT.0.) .AND. DELN(J).GT.SUM) SUM = DELN(J)
      IF((EN(J,NPT).NE.0.) .OR. DELN(J).LE.0.) GO TO 917
      SUM1 = (-9.212-ENLN(J)+ENNL)/(DELN(J)-X(IQ1))
      IF(SUM1.LT.0.) SUM1=-SUM1
      IF (SUM1.LT.AMBDA1) AMBDA1 = SUM1
917 CONTINUE
      IF(SUM.GT.2.) AMBDA=2./SUM
      IF (AMBDA1.LT.AMBDA) AMBDA = AMBDA1
      IF (.NOT.IDERUG) GO TO 111
      WRITE(6,923) TT,ENN,ENNL,PP,PPLN,AMBDA
923 FORMAT(3H0T=,F15.8,6H ENN=,E15.8,7H ENNL=E15.8,5H PP=,E15.8,
1 7H PPLN=E15.8,8H AMBDA=E15.8 )
      WRITE(6,924)
924 FORMAT(1H0,18X,2HNT,12X,5HLN NI,8X,9HDEL LN NI,10X,4HH/RT,9X,4HS0,
12X,6H-G/RT,9X,5H-G/RT )
      DO 926 J=1,NS
      FNEG1 = S(J)-H0(J)
      FNEG2 = FNEG1
      IF(IUSE(J).EQ.0) FNEG2=FNEG2-ENLN(J)-TM
      WRITE(6,925) SUB(J,1),SUB(J,2),
1 SUB(J,3),EN(J,NPT),ENLN(J),DELN(J),H0(J),S(J),FNEG1,FNEG2
925 FORMAT(1X,3A4,7E15.6)
926 CONTINUE
      WRITE(6,110)
110 FORMAT(1H0)
C
C      APPLY CORRECTIONS TO ESTIMATES
C
111 SU4 = 0.
      ENNL = ENNL+AMBDA*X(IQ1)
      FNN = EXP(ENNL)
      TM = PPLN - FNNL
      DO 113 J=1,NS
      EQL*1800
      EQL*1810
      EQL*1820
      EQL*1830
      EQL*1840
      EQL*1850
      EQL*1860
      EQL*1870
      EQL*1880
      EQL*1890
      EQL*1900
      EQL*1910
      EQL*1920
      EQL*1930
      EQL*1940
      EQL*1950
      EQL*1960
      EQL*1970
      EQL*1980
      EQL*1990
      EQL*2000
      EQL*2010
      EQL*2020
      EQL*2030
      EQL*2040
      EQL*2050
      EQL*2060
      EQL*2070
      EQL*2080
      EQL*2090
      EQL*2100
      EQL*2110
      EQL*2120
      EQL*2130
      EQL*2140
      EQL*2150
      EQL*2160
      EQL*2170
      EQL*2180
      EQL*2190
      EQL*2200
      EQL*2210
      EQL*2220
      EQL*2230
      EQL*2240
      EQL*2250
      EQL*2260
      EQL*2270
      EQL*2280
      EQL*2290
      EQL*2300
      EQL*2310
      EQL*2320
      EQL*2330
      EQL*2340
      EQL*2350
      EQL*2360
      EQL*2370
      EQL*2380
      EQL*2390

```

```

      IF (IUSE(J)) 113*112*114
112 ENLN(J)=ENLN(J)+AMRDA*DELN(J)
      EN(J,NPT) = 0.
      IF((ENLN(J)-ENNL*SIZE).LE.0.) GO TO 113
      EN(J,NPT) = EXP(ENLN(J))
      SUM = SUM+EN(J,NPT)
      GO TO 113
114 EN(J,NPT) = EN(J,NPT) + AMBDA * DELN(J)
113 CONTINUE
      SUMN = SUM
      IF (TP) GO TO 115
      TLN= TLN+AMRDA*DLNT
      TT = EXP(TLN)
      JS1 = 1
      CALL CPHS
115 IF (LLMT(L).NE.IE) GO TO 116
C
C   CHECK ON REMOVING IONS
C
      DO 1116 J = 1,NS
      IF (A(L,J).EQ.0.) GO TO 1116
      IF (EN(J,NPT).GT.0.) GO TO 116
1116 CONTINUE
      DO 1118 J=1,NS
      IF(A(L,J).NE.0.) IUSE(J) = -10000
1118 CONTINUE
      L = L-1
      IQ1 = IQ1-1
      GO TO 43
C
C   TEST FOR CONVERGENCE
C
116 IF (ITNUMB.EQ.0) GO TO 13
      IF (AMRDA.LT.1.) GO TO 43
      SUM = (ENN-SUMN)/ENN
      IF (SUM.LT.0.) SUM = -SUM
      IF (SUM.GT.0.5E-5) GO TO 43
      DO 130 J=1,NS
      IF (IUSE(J).LT.0) GO TO 130
      AA= DELN(J)/SUMN
      IF(A.LT.0.) AA=-AA
      IF (IUSE(J).EQ.0) AA = AA*EN(J,NPT)
129 IF(AA.GT.0.5E-5) GO TO 43
130 CONTINUE
C
C   CALCULATE ENTROPY, CHECK ON DELTA S FOR SP PROBLEMS
C
      SSUM(NPT) = 0.
      DO 183 J=1,NS
      IF (NPT.EQ.1) SS0 = SS0 + EN(J,1)*S(J)
      SS = S(J)
      IF(IUSE(J).EQ.0) SS=SS-ENLN(J)-TM
      SSUM(NPT) = SSUM(NPT)+SS*EN(J,NPT)
183 CONTINUE
      IF(.NOT.SP.OR.NPT.EQ.1) GO TO 13
      SS = SSUM(NPT) -S0
      IF(SS.LT.(-0.00005).OR.SS.GT.0.00005) GO TO 43
      IF(IDEBUG) WRITE(6,1183) SS
1183 FORMAT(12HDELTA S/R =,E15.8)
      13 CONVG= .TRUE.

```

EQL*2400
 EQL*2410
 EQL*2420
 EQL*2430
 EQL*2440
 EQL*2450
 EQL*2460
 EQL*2470
 EQL*2480
 EQL*2490
 EQL*2500
 EQL*2510
 EQL*2520
 EQL*2530
 EQL*2540
 EQL*2550
 EQL*2560
 EQL*2570
 EQL*2580
 EQL*2590
 EQL*2600
 EQL*2610
 EQL*2620
 EQL*2630
 EQL*2640
 EQL*2650
 EQL*2660
 EQL*2670
 EQL*2680
 EQL*2690
 EQL*2700
 EQL*2710
 EQL*2720
 EQL*2730
 EQL*2740
 EQL*2750
 EQL*2760
 EQL*2770
 EQL*2780
 EQL*2790
 EQL*2800
 EQL*2810
 EQL*2820
 EQL*2830
 EQL*2840
 EQL*2850
 EQL*2860
 EQL*2870
 EQL*2880
 EQL*2890
 EQL*2900
 EQL*2910
 EQL*2920
 EQL*2930
 EQL*2940
 EQL*2950
 EQL*2960
 EQL*2970
 EQL*2980
 EQL*2990

```

IF(TT .LT.TLOW.OR.TT .GT.THIGH)WRITE (6,306)TT ,NPT EQL*3000
306 FORMAT(17H0THE TEMPERATURE=E12.4*26H IS OUT OF RANGE FOR POINT,15)EQL*3010
IF(ITNUMB.NE.0) GO TO 160 EQL*3020
WRITE(6,973) ITN,NPT EQL*3030
973 FORMAT(1HL,I2.69H ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREME EQL*3040
ENTS FOR THE POINT 15) EQL*3050
IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.IT.GT.100.) GO TO 873 EQL*3060
WRITE(6,874) EQL*3070
TT = T(1) EQL*3080
RETURN EQL*3090
C EQL*3100
C CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES. EQL*3110
C EQL*3120
160 IF(NC.EQ.0) GO TO 143 EQL*3130
SIZEF = 0. EQL*3140
INC = 0 EQL*3150
DO 170 J = 1,NS EQL*3160
IF (IUSE(J).EQ.0 .OR. IUSE(J).EQ.-10000) GO TO 170 EQL*3170
INC = INC + 1 EQL*3180
IF(IDERUG) WRITE(6,144) (SUB(J,I),I=1,3) *TEMP(INC,1) *TEMP(INC,2), EQL*3190
IUSE(J),EN(J,NPT) EQL*3200
144 FORMAT (1H0,3A4,2F10.3,3X,5HIUSE=,I4,E15.7) EQL*3210
IF (EN(J,NPT)) 146,148,169 EQL*3220
146 IF (J.NE.JSOL .AND. J.NE.JLIQ) GO TO 147 EQL*3230
JSOL = 0 EQL*3240
JLIQ = 0 EQL*3250
147 IQ1 = IQ1 - 1 EQL*3260
EN(J,NPT) = 0. EQL*3270
GO TO 166 EQL*3280
148 KG = 1 EQL*3290
IF(IUSE(J).EQ.-IUSE(J+1)) GO TO 154 EQL*3300
151 IF(J.EQ.1.OR.IUSE(J).NE.-IUSE(J-1)) GO TO 153 EQL*3310
KG = -1 EQL*3320
154 JKG = J + KG EQL*3330
IF (EN(JKG,NPT).LT.0.) GO TO 170 EQL*3340
TMELT = TEMP(INC,1) EQL*3350
IMP = INC + KG EQL*3360
IF(TMELT.EQ.TEMP(IMP,2 )) GO TO 158 EQL*3370
TMELT = TEMP(INC,2) EQL*3380
IF (TMELT.EQ.TEMP(IMP,1)) GO TO 157 EQL*3390
WRITE (6,156) EQL*3400
156 FORMAT (50H03 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER ) EQL*3410
C EQL*3420
C JTH SPECIES A SOLID (EN=0), (J*KG)TH SPECIES A LIQUID (EN IS + EQL*3430
C EQL*3440
157 IF(TT.GT.TMELT) GO TO 169 EQL*3450
IF (TP.AND.TT.EQ.TMELT) GO TO 169 EQL*3460
IF (TP) GO TO 1165 EQL*3470
IF (TT.LE.TMELT-150.) GO TO 1165 EQL*3480
JSOL = J EQL*3490
JLIQ = JKG EQL*3500
GO TO 159 EQL*3510
C EQL*3520
C JTH SPECIES A LIQUID (EN=0), (J*KG)TH SPECIES A SOLID (EN IS +) EQL*3530
C EQL*3540
158 IF (TT.LT.TMELT) GO TO 169 EQL*3550
IF (TP.AND.TT.EQ.TMELT) GO TO 169 EQL*3560
IF (TP) GO TO 1165 EQL*3570
IF (TT.GE.TMELT+150.) GO TO 1165 EQL*3580
JSOL = JKG EQL*3590

```

```

      JLIQ = J
159 TLN = ALOG (TMELT)
      IT = TMELT
      EN(JKG,NPT) = .5 * EN(JKG,NPT)
      EN(J,NPT) = EN(JKG,NPT)
      GO TO 165
C
C   WRONG PHASE INCLUDED FOR T INTERVAL. SWITCH EN
C
1145 EN(J,NPT) = EN (JKG, NPT)
      IUSE(J) = -IUSE(J)
      IUSE (JKG) = -IUSE(JKG)
      EN(JKG,NPT) = 0.
      GO TO 40
153 IF (IT.LT.TEMP(INC,1) .AND. TEMP(INC,1).NE.TLOW) GO TO 169
      IF (IT.GT.TEMP(INC,2)) GO TO 169
C
C
      SUM = 0.
      DO 167 I = 1,L
      SUM = SUM + A(I,J)*X(I)
167 CONTINUE
      DELF = H0(J)-S(J)-SUM
      IF (IDEBUG) WRITE(6,168)DELF,SIZEF
168 FORMAT (17H G0-SUM(AIJ*PI) =E15.7,10X,18HPREVIOUS DELTA G =E15.7)
      IF (DELF.GE.SIZEF .OR. DELF.GE.0.) GO TO 169
      SIZEF = DELF
      JDELF = J
169 IF (INC.EQ.NC) GO TO 1160
170 CONTINUE
1160 IF (SIZEF.EQ.0.) GO TO 143
      J = JDELF
165 IQ1 = IQ1 + 1
166 IUSE(J) = - IUSE(J)
      40 CONVG = .FALSE.
      IF (NPT.EQ.1) SS0 = 0.
      JS1 = 1
      CALL CPHS
143 TN = NUMB
      IF (.NOT.SHOCK) WRITE(6,771)NPT,(X(IL),IL=1,L),TN
771 FORMAT (13,14F9.3)
      ITNUMB = ITN
      JS1 = 1
      IF (TP.AND.CONVG) CALL CPHS
      GO TO 43
C
C   CALCULATE EQUILIBRIUM PROPERTIES
C
1171 DLVPT(NPT) = -1.
      DLVTP(NPT) = 1.
      CPR(NPT) = CPSUM
      GO TO 199
171 SUM = 0.
      DO 179 J = 1,L
      SUM = SUM + PROW(J)*X(J)
179 CONTINUE
      DLVPT(NPT) = -2.*SUM/ENN+ X(IQ1)
184 IF (JLIQ.EQ.0) GO TO 199
      IUSE(JLIQ) = -IUSE(JLIQ)
      HSUM(NPT) = HSUM(NPT)+EN(JLIQ,NPT)*(H0(JLIQ)-H0(JSOL))

```

EQL*3600
 EQL*3610
 EQL*3620
 EQL*3630
 EQL*3640
 EQL*3650
 EQL*3660
 EQL*3670
 EQL*3680
 EQL*3690
 EQL*3700
 EQL*3710
 EQL*3720
 EQL*3730
 EQL*3740
 EQL*3750
 EQL*3760
 EQL*3770
 EQL*3780
 EQL*3790
 EQL*3800
 EQL*3810
 EQL*3820
 EQL*3830
 EQL*3840
 EQL*3850
 EQL*3860
 EQL*3870
 EQL*3880
 EQL*3890
 EQL*3900
 EQL*3910
 EQL*3920
 EQL*3930
 EQL*3940
 EQL*3950
 EQL*3960
 EQL*3970
 EQL*3980
 EQL*3990
 EQL*4000
 EQL*4010
 EQL*4020
 EQL*4030
 EQL*4040
 EQL*4050
 EQL*4060
 EQL*4070
 EQL*4080
 EQL*4090
 EQL*4100
 EQL*4110
 EQL*4120
 EQL*4130
 EQL*4140
 EQL*4150
 EQL*4160
 EQL*4170
 EQL*4180
 EQL*4190

131 = 131+1	EQL*4200
GAMMAS(NPT) = -1./DLVPT(NPT)	EQL*4210
GO TO 186	EQL*4220
109 GAMMAS(NPT) = -1./ (DLVPT(NPT) + (DLVTP(NPT)**2)*ENN/CPR(NPT))	EQL*4230
186 TTT(NPT) = TT	EQL*4240
OPP(NPT) = PP	EQL*4250
CPRF(NPT) = CPSUM	EQL*4260
HSUM(NPT) = HSUM(NPT)*TT	EQL*4270
WM(NPT) = 1./ENN	EQL*4280
200 IF (.NOT.IDEBUG) RETURN	EQL*4290
PRATIO = 1.	EQL*4300
IF (SP) PRATIO=PP/P(1)	EQL*4310
WRITE(6,201) NPT,PRATIO, PP,TT,HSUM(NPT),SSUM(NPT),WM(NPT),CPR(NPT)	EQL*4320
1T=DLVPT(NPT)*DLVTP(NPT),GAMMAS(NPT)	EQL*4330
201 FORMAT (7H0POINT=I3,3X,4HPCP=E13.6,3X,2HP=E13.6,3X,2HT=E13.6,3X,4HEQL*4340	
1H/R=E13.6,3X,4HS/R=E13.6//3X,3HWW=E13.6,3X,5HCP/R=E13.6,3X,6HDLVPT	EQL*4350
2=E13.6,3X,6HDLVTP=E13.6,3X,9HGAMMA(S)=E13.6)	EQL*4360
GO TO 1000	EQL*4370
	EQL*4380
C	EQL*4390
C ERROR. SET TT=0	EQL*4400
C	EQL*4410
873 TT=0.	EQL*4420
NPT = NPT-1	EQL*4430
1000 RETURN	EQL*4440
END	

```

SUBROUTINE CPHS
CALCULATES THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES
COMMON/SPECES/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(150,2)
COMMON/MISC/FNN,SUMN,TT,S0,ATOM(3,101),LLMT(15),Z0(15),R0P(15,2)
1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EORAT,FPCT,R,RR,HSUR0,AC(2),AM(2)
2 ,HOP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
4 ,R0P,RMW(15),TLN
COMMON/INDX/ INDEBUG,CONVG,TP,HP,SP,H0SP,TPSP,M0LES,NP,NT,NPT,NLM
1 ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEW,NSUR,NSUP,ITN,CPCVFR,CPCVEQ
2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
EQUIVALENCE (J,JS1)
K = 1
IF (TT.LE.TMID) 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 S(J) = (((COEF(K,5,J)/4.)*TT + COEF(K,4,J)/3.)*TT + COEF(K,3,J)/2.
1)*TT + COEF(K,2,J))*TT + COEF(K,1,J)*TLN + COEF(K,7,J)
H0(J) = (((COEF(K,5,J)/5.)*TT + COEF(K,4,J)/4.)*TT + COEF(K,3,J)/3.
1)*TT + COEF(K,2,J)/2.)*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)
IF (KK.EQ.0) GO TO 100
K = KK
KK = 0
100 IF (J.EQ.NS) GO TO 200
J=J+1
GO TO 90
200 RETURN
END

```

CPH*0000

CPH*0010

CPH*0020

CPH*0030

CPH*0040

CPH*0050

CPH*0060

CPH*0070

CPH*0080

CPH*0090

CPH*0100

CPH*0110

CPH*0120

CPH*0130

CPH*0140

CPH*0150

CPH*0160

CPH*0170

CPH*0180

CPH*0190

CPH*0200

CPH*0210

CPH*0220

CPH*0230

CPH*0240

CPH*0250

CPH*0260

CPH*0270

CPH*0280

CPH*0290

CPH*0300

CPH*0310

CPH*0320

CPH*0330

CPH*0340

CPH*0350

CPH*0360

CPH*0370

CPH*0380

SUBROUTINE MATRIX

```

C
C
C      DOUBLE PRECISION G,X
C      LOGICAL HP,SP,TP,IDEBUG,CONVG,NEWK
C
COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
1  ,GAMMAS(13),P(26),T(26),V(13),FDP(13),WM(13),SONVEL(13),TTT(13)
2  ,TOTN(13)
COMMON/SPECES/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)
COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,10),LLMT(15),B0(15),B0P(15,2)
1  ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAF,CPCT,R,RR,HSUB0,AC(2),AM(2)
2  ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
3  ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
4  ,R4OP,RMW(15),TLN
COMMON/DOUBLE/ G(20,21), X(20)
COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,T,SP,M0,ES,NP,NT,NPT,NLM
1  ,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWK,NSUB,NSUP,ITN,CPVVFH,CPVVD
2  ,IONS,NC,NSERT,JSOL,JLIO,KASE,NREAC,IC,JS1,VOL,SHOCK
C
C      EQUIVALENCE (L,NLM)
C
      IQ2 = IQ1 + 1
      IQ3 = IQ2 + 1
      KMAT = IQ3
      IF(.NOT.CONVG.AND.TP) KMAT = IQ2
      IMAT = KMAT - 1
C
C      CLEAR MATRIX STORAGES TO ZERO
C
      DO 211 I=1,IMAT
      DO 211 K=1,KMAT
        G(I,K) = 0.000
211 CONTINUE
      SSS = 0.
      HSUM(NPT) = 0.
C
C      BEGIN SET UP OF ITERATION MATRIX
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)+TM)*EN(J,NPT)
        SS = H-F
        TERM1 = H
        IF (KMAT.EQ. IQ2) TERM1 = F
        DO 55 I = 1, L
C
C      CALCULATE THE ELEMENTS P(I,K)
C
        IF (A(I,J).EQ. 0.) GO TO 55
        TERM = A(I,J)*EN(J,NPT)
        DO 35 K=1, L
          S(I,K) = G(I,K) + A(K,J)*TERM
15 CONTINUE
C
          S(I,IQ1) = G(I,IQ1) + TERM
          S(I,IQ2) = G(I,IQ2) + A(I,J)*TERM1

```

```

IF (CONVG .OR. TP) GO TO 55
G(I,IQ3) = G(I,IQ3) + A(I,J)*F
IF (SP) G(IQ2,I) = G(IQ2,I) + A(I,J)*SS
55 CONTINUE
IF (KY) .EQ. IQ2) GO TO 64
IF (CONVG .OR. HP) GO TO 59
G(IQ2,IQ1) = G(IQ2,IQ1) + SS
G(IQ2,IQ2) = G(IQ2,IQ2) + H0(J)*S
G(IQ2,IQ3) = G(IQ2,IQ3) + (S(J) - ENLN(J) - TM)*F
GO TO 62
59 G(IQ2,IQ2) = G(IQ2,IQ2) + H0(J)*H
IF (CONVG) GO TO 64
G(IQ2,IQ3) = G(IQ2,IQ3) + H0(J)*F
62 G(IQ1,IQ3) = G(IQ1,IQ3) + F
64 G(IQ1,IQ2) = G(IQ1,IQ2) + TERM1
GO TO 55

C
C CONDENSED SPECIES
C
70 KK = KK + 1
DO 75 I = 1,L
G(I,KK) = A(I,J)
G(I,KMAT) = G(I,KMAT) - A(I,J)*EN(J,NPT)
75 CONTINUE
G(KK,IQ2) = H0(J)
G(KK,KMAT) = H0(J) - S(J)
PSUM(NPT) = HSUM(NPT) + H
IF (.NOT. SP) GO TO 65
SSS = SSS + S(J)*EN(J,NPT)
G(IQ2,KK) = S(J)
65 CONTINUE
SSS = SSS + G(IQ2,IQ1)
HSUM(NPT) = HSUM(NPT) + G(IQ1,IQ2)
G(IQ1,IQ1) = SUMN - ENN

C
C REFLECT SYMMETRIC PORTIONS OF THE MATRIX
C
ISYM = IQ1
IF (HP .OR. CONVG) ISYM = IQ2
DO 102 I = 1, ISYM
DO 102 J = I, ISYM
G(J,I) = G(I,J)
102 CONTINUE

C
C COMPLETE THE RIGHT HAND SIDE
C
IF (CONVG) GO TO 175
DO 145 I = 1,L
X(I) = S0(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. IQ2) GO TO 185
IF (SP) ENERGY = S0 + ENN - SUMN - SSS
IF (HP) ENERGY = HSUB0/TT - HSUM(NPT)
G(IQ2,IQ3) = G(IQ2,IQ3) + ENERGY
175 G(IQ2,IQ2) = G(IQ2,IQ2) + CPSUM

```

```

MAT*0600
MAT*0610
MAT*0620
MAT*0630
MAT*0640
MAT*0650
MAT*0660
MAT*0670
MAT*0680
MAT*0690
MAT*0700
MAT*0710
MAT*0720
MAT*0730
MAT*0740
MAT*0750
MAT*0760
MAT*0770
MAT*0780
MAT*0790
MAT*0800
MAT*0810
MAT*0820
MAT*0830
MAT*0840
MAT*0850
MAT*0860
MAT*0870
MAT*0880
MAT*0890
MAT*0900
MAT*0910
MAT*0920
MAT*0930
MAT*0940
MAT*0950
MAT*0960
MAT*0970
MAT*0980
MAT*0990
MAT*1000
MAT*1010
MAT*1020
MAT*1030
MAT*1040
MAT*1050
MAT*1060
MAT*1070
MAT*1080
MAT*1090
MAT*1100
MAT*1110
MAT*1120
MAT*1130
MAT*1140
MAT*1150
MAT*1160
MAT*1170
MAT*1180
MAT*1190

```


1AS RETURN
END

78

4AT*1200
4AT*1210

```

SUBROUTINE MGAUSD
C
C SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS
C
C DOUBLE PRECISION G,X,COEFX(20),SUM,Z
C
COMMON/DOUBLE/G(20,21),X(20)
COMMON/INDX/ IDEBUG,CONVG,IP,HP,SP,HPSP,TPSP,MOLDS,NP,NT,NPT,NLM
1  ,N3,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
2  ,IONS,NC,NSERT,J5OL,JLIQ,KASE,VREAC,IC,JS1,VO1,SHOCK
C
EQUIVALENCE (IUSE,IMAT)
C
DATA BIGNO/1.E+38/
C
C BEGIN ELIMINATION OF NTH VARIABLE
C
IUSE1=IUSE+1
6 DO 45 NN=1,IUSE
IF (NN-IUSE) 8,83,8
83 IF (G(NN,NN)) 31,23,31
C
C SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW
C
C
8 DO 18 I=NN,IUSE
COEFX(I) = RIGNO
IF (G(I,NN).EQ.0.) GO TO 18
COEFX(I) = 0.
DO 10 J=NN,IUSE1
SUM = G(I,J)
IF (SUM.LT.0.) SUM=-SUM
IF (J.NE.NN) GO TO 9
Z = SUM
GO TO 10
9 IF (SUM.GT.COEFX(I)) COEFX(I)=SUM
10 CONTINUE
COEFX(I) = COEFX(I)/Z
18 CONTINUE
TEMP = RIGNO
I=0
20 DO 22 J=NN,IUSE
IF (COEFX(J)-TEMP) .87,22,22
87 TEMP=COEFX(J)
I=J
22 CONTINUE
IF (I) 28,23,28
C
C INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH
C VARIABLE FROM THE REMAINING EQUATIONS
C
C INTERCHANGE EQUATIONS I AND NN
C
28 IF (NN-I) 29,31,29
29 DO 30 J=NN,IUSE1
Z=G(I,J)
G(I,J)=G(NN,J)
G(NN,J)=Z
30 CONTINUE
C
C DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH

```

```

GAU*0000
GAU*0010
GAU*0020
GAU*0030
GAU*0040
GAU*0050
GAU*0060
GAU*0070
GAU*0080
GAU*0090
GAU*0100
GAU*0110
GAU*0120
GAU*0130
GAU*0140
GAU*0150
GAU*0160
GAU*0170
GAU*0180
GAU*0190
GAU*0200
GAU*0210
GAU*0220
GAU*0230
GAU*0240
GAU*0250
GAU*0260
GAU*0270
GAU*0280
GAU*0290
GAU*0300
GAU*0310
GAU*0320
GAU*0330
GAU*0340
GAU*0350
GAU*0360
GAU*0370
GAU*0380
GAU*0390
GAU*0400
GAU*0410
GAU*0420
GAU*0430
GAU*0440
GAU*0450
GAU*0460
GAU*0470
GAU*0480
GAU*0490
GAU*0500
GAU*0510
GAU*0520
GAU*0530
GAU*0540
GAU*0550
GAU*0560
GAU*0570
GAU*0580
GAU*0590

```

C VARIABLE FROM THE REMAINING EQUATIONS

C
 31 K = NN + 1
 DO 36 J = K, IUSE1
 IF (G(NN,NN).EQ.0.) GO TO 23
 G(NN,J) = G(NN,J) / G(NN,NN)
 36 CONTINUE
 IF (K-IUSE1) 88,45,88
 88 DO 44 I = K, IUSE
 40 DO 44 J = K, IUSE1
 G(I,J) = G(I,J) - G(I,NN)*G(NN,J)
 44 CONTINUE
 45 CONTINUE

C
 C BACKSOLVE FOR THE VARIABLES
 C

K = IUSE
 47 J = K + 1
 X(K) = 0.0D0
 SUM = 0.0
 IF (IUSE = J) 51,48,48
 48 DO 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

GAU*0600
 GAU*0610
 GAU*0620
 GAU*0630
 GAU*0640
 GAU*0650
 GAU*0660
 GAU*0670
 GAU*0680
 GAU*0690
 GAU*0700
 GAU*0710
 GAU*0720
 GAU*0730
 GAU*0740
 GAU*0750
 GAU*0760
 GAU*0770
 GAU*0780
 GAU*0790
 GAU*0800
 GAU*0810
 GAU*0820
 GAU*0830
 GAU*0840
 GAU*0850
 GAU*0860
 GAU*0870
 GAU*0880
 GAU*0890

	SUBROUTINE VARFMT(V,NPT)	VAR*0000
C		VAR*0010
	DIMENSION V(13)	VAR*0020
		VAR*0030
	COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FC(4)	VAR*0040
	1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2	VAR*0050
	2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0	VAR*0060
C		VAR*0070
	DO 45 I=1,NPT	VAR*0080
	K= 2*I+3	VAR*0090
	FMT(K) = F4	VAR*0100
	IF (V(I).GE.10.) FMT(K) = F3	VAR*0110
	IF (V(I).GE.100.) FMT(K) = F2	VAR*0120
	IF (V(I).GE.10000.) FMT(K) = F1	VAR*0130
	IF (V(I).GE.1000000.) FMT(K) = F0	VAR*0140
45	CONTINUE	VAR*0150
	RETURN	VAR*0160
	END	VAR*0170

```

SUBROUTINE OUTJ
C
DOUBLE PRECISION G,X
REAL MIX(50)
LOGICAL EQL,FKNZ,TP,HP,SP,HPSP,TPSP,MOLES
C
DIMENSION NV(13),Z(10,3),HEAD(15),YX(5),YN(5)
DIMENSION SIEGEL(30),CONCKI(10,30)
C
COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
1 GAMMAS(13),P(26),T(26),V(13),PPF(13),WM(13),SONVEL(13),TTT(13)
2 TOTN(13)
COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)
1 DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),BO(15),BOP(15,2)
1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,R,HSUBO,AC(2),AM(2)
2 HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
4 RHOP,RMW(15),TLN
COMMON/DOUBLE/G(20,21),X(20)
COMMON/INDX/IDERUG,CUNVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
1 NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEW,NSUB,NSU2,ITN,CPCVFR,CPCVEQ
2 IONS,NC,NSERT,JSOL,CLIO,KASE,NREAC,IC,JS1,VOL,SHOCK
COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
1 CPRF(13),AEAT(13),CSTR,EGL,FROZ,SSO
COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)
1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2
2 FRI,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
COMMON/SNEW/RON,INDFA
COMMON/EQNEW/R1(30,40),R6(30,40),EK1(30,40),EK2(30,40),ROH(30,40),
1 CH2(30,40),ATT(13,40),F(40),PHI(40),BCON1(30,40),BCON2(30,40),BCON3(30,40)
26(30,40)
C
EQUIVALENCE (V,NV),(Z,H0),(IB,FB)
C
HEAD=(1H,2A4,5 (42,F8,5,3X),5 X,F7,5,F13,3,4X,A1,F10,2,F9,4;
C
DATA HEAD/4H(1H,4H,2A4,2H,5,4H(A2,,4HF8,5,4H,3X),2H,5,2HX,
1 4HF7,5,4H,F13,4H,3,4,4HX,A1,4H,F10,4H,2,F,4H9,4)/
DATA FUEL/4HFUEL/,OXID/4HOXID/,ANT/3HANT/,OX/1H0/,IZ/2H00/
1 YN/2H,1,2H,2,2H,3,2H,4,2H,5 /,F75/4HF7,5/
2 YX/3H,57,3H,44,3H,31,3H,18,2H,5 /,F73/4HF7,3/
DATA(SIEGEL(I),I=1,30)/4HC(S),4H 4H 4HCO 4H 4H 4H
1 HCO2 4H 4H 4HH 4H 4H 4HN 4H 4H 4HN0
2 4H 4H 4HN20 4H 4H 4H0 4H 4H 4H02
34H 4H 4H0H 4H 4H /
C
IF(KASE.NE.0) WRITE(6,3) KASE
3 FORMAT(9H CASE NO.,I5)
IF(.NOT.MOLES) WRITE(6,5)
5 FORMAT(77X,46HWT FRACTION ENTHALPY STATE TEMP DENSITY/
1 10X,16HCHEMICAL FORMULA,51X,21H(SEE NOTE) CAL/MOL,10X,5HDEG K,
2 4X,4HG/CC)
IF(MOLES) WRITE(6,6)
6 FORMAT(79X,5HMOLES,7X,33HENTHALPY STATE TEMP DENSITY/
1 10X,16HCHEMICAL FORMULA,65X,7HCAL/MOL,10X,13HDEG K
2 15 N=1,NREAC G/CC)
IF(FOX(N).NE.OX)GO TO 10
H01 = OXID
H02 = ANT

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      GO TO 11
10  HD1 = FUEL
      HD2 = FR
11  DO 13 J=1,5
      IF (NAME(N,J).EQ.IZ.OR.NAME(N,J).EQ.IB) GO TO 14
13  CONTINUE
      J=6
14  J=J-1
      HEAD(3)=YN(J)
      HEAD(7)=YX(J)
      HEAD(9) = F75
      IF (PECWT(N).GE.10.) HEAD(9)=F73
      WRITE (6,HEAD)HD1,HD2,(NAME(N,JJ),ANUM(N,JJ),JJ=1,J),PECWT(N),ENTH(
14),FAZ(N),RTMP(N),DENS(N)
15  CONTINUE
      FPC = 100./(1.+OF)
      WRITE(6,20) OF ,FPC,EQRAT,RHOP
20  FORMAT (1H0,15X, 4H0/F=, F9.4,3X,13HPERCENT FUEL=,F8.4,4X,
1 19HEQUIVALENCE RATIO= ,F7.4,4X,9HDENSITY=,F8.4//)

C      4GV = 9.80665
      RETURN

C      ENTRY OUT2

C      PRESSURE

C      FMT(4)= FMT(6)
      CALL VARFMT (PPP ,NPT)
      WRITE (6,FMT) (FP(I),I=1,4), (PPF(J),J=1,NPT)

C      TEMPERATURE

C      DO 65 I=1,NPT
      NV(I)= TTT(I)+.5
65  CONTINUE
      FMT(4)= FMT13
      FMT(5)= FMT19
      WRITE (6,FMT) (FT(I),I=1,4), (NV(J),J=1,NPT)

C      ENTHALPY

C      DO 75 I=1,NPT
      V(I) = HSUM(I) * R
75  CONTINUE
      FMT(5)= F8
      FMT(7)= F1
      WRITE (6,FMT) (FH(I),I=1,4), (V(J),J=1,NPT)

C      ENTROPY

C      FMT(7)=F4
      DO 78 I = 1,NPT
      V(I) = SSUM(I) * R
78  CONTINUE
      WRITE (6,FMT) (FS(I),I=1,4), (V(J),J=1,NPT)
      WRITE (6,R0)
90  FORMAT ( 1H )

C      MOLECULAR WEIGHT

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```

OUT*0600
OUT*0610
OUT*0620
OUT*0630
OUT*0640
OUT*0650
OUT*0660
OUT*0670
OUT*0680
OUT*0690
OUT*0700
OUT*0710
OUT*0720
OUT*0730
OUT*0740
OUT*0750
OUT*0750
OUT*0770
OUT*0780
OUT*0790
OUT*0800
OUT*0810
OUT*0820
OUT*0830
OUT*0840
OUT*0850
OUT*0860
OUT*0870
OUT*0880
OUT*0890
OUT*0900
OUT*0910
OUT*0920
OUT*0930
OUT*0940
OUT*0950
OUT*0960
OUT*0970
OUT*0980
OUT*0990
OUT*1000
OUT*1010
OUT*1020
OUT*1030
OUT*1040
OUT*1050
OUT*1060
OUT*1070
OUT*1080
OUT*1090
OUT*1100
OUT*1110
OUT*1120
OUT*1130
OUT*1140
OUT*1150
OUT*1160
OUT*1170
OUT*1180
OUT*1190

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C      FMT(7) = F3
      WRITE (6,FMT) (FM(I), I=1,4), (WM(J), J=1,NPT)
C
C      (DLV/DLP) T
C
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
C      FMT(7) = F4
      IF (EQL) WRITE (6,FMT) (FD(I), I=1,4), (DLVTP(J), J=1,NPT)
C
C      HEAT CAPACITY
C
C      DO 85 I = 1, NPT
      V(I) = CPR(I) * R
85  CONTINUE
      WRITE (6,FMT) (FC(I), I=1,4), (V(J), J=1,NPT)
C
C      GAMMA(S)
C
C      WRITE (6,FMT) (FG(I), I=1,4), (GAMMAS(J), J=1,NPT)
C
C      SONIC VELOCITY
C
C      FMT(7) = F1
      DO 95 I = 1, NPT
      SONVEL(I) = SQRT(RR * GAMMAS(I) * TTT(I) / WM(I))
95  CONTINUE
      WRITE (6,FMT) (FL(I), I=1,4), (SONVEL(J), J=1,NPT)
      RETURN
C
C      ENTRY OUT3
      IF (.NOT. EQL) GO TO 331
      DO 309 I = 1, NPT
      DATA(I) = 0.
      DO 308 K = 1, NS
      DATA(I) = DATA(I) + EN(K,I)
308  CONTINUE
309  CONTINUE
C
C      MOLE FRACTIONS - EQUILIBRIUM
C
C      WRITE (6,80)
      FMT(7) = F5
      WRITE (6,310)
310  FORMAT(15H0MOLE FRACTIONS //)
      DO 330 K = 1, NS
      DO 315 I = 1, NPT
      V(I) = EN(K,I) / DATA(I)
315  CONTINUE
      DO 316 I = 1, NPT
      IF (V(I) * GE * (5.E-6)) GO TO 320
316  CONTINUE
      GO TO 330
320  WRITE (6,FMT) SUB(K,1), SUB(K,2), SUB(K,3), FB, (V(I), I=1,NPT)
330  CONTINUE
331  WRITE (6,335)

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```

OUT*1200
OUT*1210
OUT*1220
OUT*1230
OUT*1240
OUT*1250
OUT*1260
OUT*1270
OUT*1280
OUT*1290
OUT*1300
OUT*1310
OUT*1320
OUT*1330
OUT*1340
OUT*1350
OUT*1360
OUT*1370
OUT*1380
OUT*1390
OUT*1400
OUT*1410
OUT*1420
OUT*1430
OUT*1440
OUT*1450
OUT*1460
OUT*1470
OUT*1480
OUT*1490
OUT*1500
OUT*1510
OUT*1520
OUT*1530
OUT*1540
OUT*1550
OUT*1560
OUT*1570
OUT*1580
OUT*1590
OUT*1600
OUT*1610
OUT*1620
OUT*1630
OUT*1640
OUT*1650
OUT*1660
OUT*1670
OUT*1680
OUT*1690
OUT*1700
OUT*1710
OUT*1720
OUT*1730
OUT*1740
OUT*1750
OUT*1760
OUT*1770
OUT*1780
OUT*1790

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335 FORMAT(118H0ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOOUT*1800
    LE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS//)OUT*1810
    LINE= 0OUT*1820
    NN = 1OUT*1830
    IF(FQL) NN=NPTOUT*1840
    DO 350 K=1,NSOUT*1850
    DO 340 I=1,NNOUT*1860
    IF ((EN(K,I)/DATA(I)).GE.(5.E-6)) GO TO 343OUT*1870
340 CONTINUEOUT*1880
    LINE= LINE+1OUT*1890
    Z(LINE,1)= SUR(K,1)OUT*1900
    Z(LINE,2)= SUR(K,2)OUT*1910
    Z(LINE,3)= SUR(K,3)OUT*1920
343 IF ((LINE.NE.3) .AND. K.NE.NS) GO TO 350OUT*1930
    IF (LINE.EQ.0) GO TO 1000OUT*1940
    WRITE(6,345) (Z(LN,1),Z(LN,2),Z(LN,3),LN=1,LINE)OUT*1950
345 FORMAT (10(1X,3A4))OUT*1960
    LINE= 0OUT*1970
350 CONTINUEOUT*1980
    IF(.NOT.MOLES) WRITE(6,360)OUT*1990
360 FORMAT(78H0NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIOUT*2000
    DANT IN TOTAL OXIDANTS )OUT*2010
1000 CONTINUEOUT*2020
    DO 3000 I =1,10OUT*2030
    II = 3*I - 2OUT*2040
    DO 2000 K =1,NSOUT*2050
    IF(SIEGEL(II).NE.SUB(K,1)) GO TO 2000OUT*2060
    IF(SIEGEL(II+1).NE.SUB(K,2)) GO TO 2000OUT*2070
    IF(SIEGEL(II+2).NE.SUB(K,3)) GO TO 2000OUT*2080
    DO 1500 J =1,NPTOUT*2090
1500 CONCKI(I,J) = EN(K,J)/DATA(J)OUT*2100
    GO TO 3000OUT*2110
2000 CONTINUEOUT*2120
3000 CONTINUEOUT*2130
C****OUT*2140
C**** NOTE...FOR MORE THAN NPT=6,THESE PRINT STATEMENTS MUST BE MODIFIEDOUT*2150
C****OUT*2160
    DO 5000 K=1,10OUT*2170
    II = 3*K - 2OUT*2180
    WRITE(6,4000) SIEGEL(II),SIEGEL(II+1),SIEGEL(II+2),(CONCKI(K,J),J=OUT*2190
    11,NPT)OUT*2200
4000 FORMAT(1X,3A4,2X,6(E15.8,1X))OUT*2210
5000 CONTINUEOUT*2220
    WRITE(6,5000) (WM(J),J =1,NPT)OUT*2230
5000 FORMAT(11H MOLEC. WT.,4X,6(E15.8,1X))OUT*2240
    WRITE(6,7000) (TTY(J),J=1,NPT)OUT*2250
7000 FORMAT(9H TEMP.(K),6X,6(E15.8,1X))OUT*2260
    WRITE(6,8000) (PPF(J),J=1,NPT)OUT*2270
8000 FORMAT(12H PRESS.(ATM),3X,6(E15.8,1X))OUT*2280
    WRITE(6,9000) RONOUT*2290
9000 FORMAT(14H FUEL AIR RAT.,1X,E15.8)OUT*2300
    DO 9600 N =1,NREACOUT*2310
    WRITE(6,9500) (ANUM(N,JJ),JJ=1,5),ENTH(N),RTEMP(N)OUT*2320
9500 FORMAT(1X,7E15.8)OUT*2330
9600 CONTINUEOUT*2340
    CALL RATES(CONCKI,WM,TTY,PPP,ANUM,ENTH,RTEMP,NPT,NREAC)OUT*2350
9999 RETURNOUT*2360
    ENDOUT*2370

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SUBROUTINE RATES(CONCKI,WM,TTT,PPP,ANUM,ENTH,RTMP,NPT,NREAC)
REAL MIX(50)
DIMENSION CONCKI(10,30),TTT(13),PPP(13),WM(13),ANUM(15,5),ENTH(15)
1 RTMP(15)
DIMENSION R2(30,40),R3(30,40),R4(30,40),R5(30,40),RATEK(6,30,40),CRAT*0040
10N4CM(10,30,40),A(6),EN(6),E(6)
COMMON/SNEW/ROH,INDFA
COMMON/DICK/MIX
COMMON/EQNEW/R1(30,40),R6(30,40),EK1(30,40),EK2(30,40),ROH(30,40),RAT*0050
1CH2(30,40),ATT(13,40),F(40),PHI(40),BCON1(30,40),BCON2(30,40),BCONRAT*0060
26(30,40)
DATA(A(I),I=1,6)/3.1E+13,6.4E+09,4.1E+13,2.9513E+13,3.8146E+13,4.5RAT*0070
1775E+13/, (EN(I),I=1,6)/0.,1.,0.,0.,0.,0./, (E(I),I=1,6)/0.334E+00,6RAT*0080
2.250E+00,0.0E+00,10.77E+00,24.1E+00,24.1E+00/,ICODE/2/
RAT*0090
C****
C**** TEST FOR WRITE CONTROL
RAT*0100
C****
IST = INDFA
IPRINT = 0
IF(MIX(IST+1).EQ.0.0) IPRINT = 1
RAT*0110
C****
C**** SET PRESSURE LOOP
RAT*0120
C****
DO 8000 J = 1,NPT
RAT*0130
C****
C**** CALCULATE CONCENTRATIONS
RAT*0140
C****
BCON1(J,IST) = CONCKI(1,J)
RAT*0150
BCON2(J,IST) = CONCKI(2,J)
RAT*0160
BCON6(J,IST) = CONCKI(6,J)
RAT*0170
DO 1000 I = 1,10
RAT*0180
CONMCM(I,J,IST) = (CONCKI(I,J)*PPP(J))/(82.057*TTT(J))
RAT*0190
1000 CONTINUE
RAT*0200
C****
C**** COMPUTE RATE CONSTANTS
RAT*0210
C****
DO 2000 I = 1,6
RAT*0220
RATEK(I,J,IST) = A(I)*(TTT(J)**EN(I))*EXP(-E(I)/(1.987E-03*TTT(J)))
RAT*0230
1)
RAT*0240
2000 CONTINUE
RAT*0250
C****
C**** CALCULATE FORWARD REACTION CONSTANTS
RAT*0260
C****
R1(J,IST) = (RATEK(1,J,IST)*CONMCM(5,J,IST)*CONMCM(6,J,IST))
RAT*0270
R2(J,IST) = (RATEK(2,J,IST)*CONMCM(5,J,IST)*CONMCM(9,J,IST))
RAT*0280
R3(J,IST) = (RATEK(3,J,IST)*CONMCM(5,J,IST)*CONMCM(10,J,IST))
RAT*0290
R4(J,IST) = (RATEK(4,J,IST)*CONMCM(4,J,IST)*CONMCM(7,J,IST))
RAT*0300
R5(J,IST) = (RATEK(5,J,IST)*CONMCM(8,J,IST)*CONMCM(7,J,IST))
RAT*0310
R6(J,IST) = (RATEK(6,J,IST)*CONMCM(8,J,IST)*CONMCM(7,J,IST))
RAT*0320
C****
C**** CALCULATE K1,K2,RHO,KS, AND PHI
RAT*0330
C****
IF(R2(J,IST).EQ.0.0.AND.R3(J,IST).EQ.0.0) EK1(J,IST) = 1.0E+35
RAT*0340
IF(R2(J,IST).EQ.0.0.AND.R3(J,IST).EQ.0.0) GO TO 2500
RAT*0350
EK1(J,IST) = (R1(J,IST)/(R2(J,IST)+R3(J,IST)))
RAT*0360
2500 IF(R4(J,IST).EQ.0.0.AND.R5(J,IST).EQ.0.0) EK2(J,IST) = 1.0E+35
RAT*0370
IF(R4(J,IST).EQ.0.0.AND.R5(J,IST).EQ.0.0) GO TO 2750
RAT*0380
EK2(J,IST) = (R6(J,IST)/(R4(J,IST)+R5(J,IST)))
RAT*0390
2750 ROH(J,IST) = (PPP(J)*WM(J))/(82.057*TTT(J))
RAT*0400
C****
RAT*0410
RAT*0420
RAT*0430
RAT*0440
RAT*0450
RAT*0460
RAT*0470
RAT*0480
RAT*0490
RAT*0500
RAT*0510
RAT*0520
RAT*0530
RAT*0540
RAT*0550
RAT*0560
RAT*0570
RAT*0580
RAT*0590

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C**** NOTE...FUEL CARD IS PHYSICALLY BEFORE OXIDANT CARD IN INPUT, OXYGEN RAT=1600
C**** IS SECOND SPECIE SPECIFIED IN OXIDANT AIR, FUEL IS SPECIFIED C-A* RAT*0610
C**** H=8 RAT*0620
C**** EKS = ((12.*ANUM(1,1)+1.*ANUM(1,2))*ANUM(2,2))/(28.99*(ANUM(1,1)+(RAT*0630
ANUM(1,2)/4.))) RAT*0640
PHI(IST) = RON/EKS RAT*0650
F(IST) = PHI(IST)*EKS/(1.+(PHI(IST)*EKS)) RAT*0660
C**** RAT*0670
C**** CALCULATE CONCENTRATION OF CH2 RAT*0680
C**** RAT*0690
RATWTS = ANUM(1,1)/ANUM(1,2) RAT*0700
CH2(J,IST) = (((RATWTS/(1.+12.*RATWTS))*(WM(J)*RON/(RON+1.)))-CONC RAT*0710
KI(2,J)-CONCKI(3,J)-CONCKI(1,J)) RAT*0720
C**** RAT*0730
C**** STOPE VALUES OF T RAT*0740
C**** RAT*0750
ATT(J,IST) = TTT(J) RAT*0760
8000 CONTINUE RAT*0770
C**** RAT*0790
C**** PRINT AND PUNCH OUTPUT RAT*0800
C**** RAT*0810
IF(IPRINT.EQ.0) GO TO 9999 RAT*0820
DO 9500 J = 1,NPT RAT*0830
DO 9000 I = 1,IST RAT*0840
IF(I.NE.1) GO TO 8500 RAT*0850
WRITE(6,8100) ANUM(1,1),ANUM(1,2),RTEMP(2),PPP(J),ICODE,EKS RAT*0860
WRITE(7,8100) ANUM(1,1),ANUM(1,2),RTEMP(2),PPP(J),ICODE,EKS RAT*0870
8100 FORMAT(1X,7HFUEL= C,E15.8,1HH,E15.8,1BH INLET AIR T.(K)= ,E15.8/1XRAT*0880
1,13HPRESS.(ATM)= ,E15.8,7HICODE= ,I2,13HPHI STOICH.= ,E15.8) RAT*0890
8500 WRITE(6,8200) F(I),PHI(I),RON(J,I),ATT(J,I),BCON6(J,I),BCON2(J,I),RAT*0900
BCON1(J,I),CH2(J,I),R1(J,I),R6(J,I),EK1(J,I),EK2(J,I) RAT*0910
8200 FORMAT(1X,6E12.5/1X,6E12.5) RAT*0920
WRITE(7,8250) F(I),PHI(I),RON(J,I),ATT(J,I),BCON6(J,I),BCON2(J,I),RAT*0930
BCON1(J,I),CH2(J,I),R1(J,I),R6(J,I),EK1(J,I),EK2(J,I) RAT*0940
8250 FORMAT(6E12.5/6E12.5) RAT*0950
9000 CONTINUE RAT*0960
9500 CONTINUE RAT*0970
9999 RETURN RAT*0980
END RAT*0990

```

SUBROUTINE HCALC

C		HCA*0000
C	CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS	HCA*0010
C		HCA*0020
	LOGICAL MOLES	HCA*0030
	DIMENSION NUM(15,5)	HCA*0040
C		HCA*0050
	COMMON/SPECES/COEF(2,7,150),S(150),FN(150,13),ENLN(150),H0(150)	HCA*0060
	1,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)	HCA*0070
	COMMON/MISC/FNN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)	HCA*0080
	1,TM,TLOW,TMIN,THIGH,PP,CPSUM,OF,EQRAT,FPCT,P,RR,HSUB0,AC(2),AM(2)	HCA*0090
	2,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)	HCA*0100
	3,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),PTEMP(15),FOX(15),DENS(15)	HCA*0110
	4,RHOP,RMW(15),TLN	HCA*0120
	COMMON/INDX/IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM	HCA*0130
	1,NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEW,NSUB,NSUP,ITN,CPCVFR,CPCVEQ	HCA*0140
	2,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK	HCA*0150
C		HCA*0160
	EQUIVALENCE (ANUM,NUM),(L,NLM),(J,JS1)	HCA*0170
C		HCA*0180
	DATA AG/1HG/,IZERO/2H00/,OX/1HC/,BLK/1H /	HCA*0190
C		HCA*0200
C	IS TT IN RANGE	HCA*0210
C		HCA*0220
	IF(TT.LT.(TLOW-100.)).OR.TT.GT.(THIGH+1000.))GO TO 75	HCA*0230
	HPP(1)=0.	HCA*0240
	HPP(2)=0.	HCA*0250
	AC(1)=0.	HCA*0260
	AC(2)=0.	HCA*0270
	DO 900 N=1,NREAC	HCA*0280
	K=2	HCA*0290
	IF(FOX(N).EQ.OX)K=1	HCA*0300
	PCWT=PECWT(N)	HCA*0310
	IF(MOLES)PCWT=PCWT*RMW(N)	HCA*0320
	IF(NAME(N,5).EQ.IZERO)GO TO 5	HCA*0330
	AC(1)=0.	HCA*0340
	AC(2)=0.	HCA*0350
	GO TO 500	HCA*0360
5	J = NUM(N,5)	HCA*0370
	IF (J.NE.0) GO TO 90	HCA*0380
	DO 10 J=1,L	HCA*0390
	DATA(J)=0.	HCA*0400
10	CONTINUE	HCA*0410
	DO 40 I=1,4	HCA*0420
	IF(ANUM(N,I).EQ.0.)GO TO 50	HCA*0430
	DO 20 J=1,L	HCA*0440
	IF(LLMT(J).EQ.NAME(N,I)) GO TO 30	HCA*0450
20	CONTINUE	HCA*0460
	DATA(J)=ANUM(N,I)	HCA*0470
40	CONTINUE	HCA*0480
50	IS=0	HCA*0490
	DO 70 J=1,NS	HCA*0500
	IF(IUSE(J).EQ.0)GO TO 55	HCA*0510
	IS = IS+1	HCA*0520
	IF(FAZ(N).EQ.AG)GO TO 70	HCA*0530
	IF(TT.GT.TEMP(IS,2).AND.TEMP(IS,2).NE.THIGH) GO TO 70	HCA*0540
	IF(TT.LT.TEMP(IS,1).AND.TEMP(IS,1).NE.TLOW) GO TO 70	HCA*0550
	GO TO 56	HCA*0560
55	IF(FAZ(N).NE.AG.AND.FAZ(N).NE.RLK) GO TO 70	HCA*0570
56	DO 60 I=1,L	HCA*0580
		HCA*0590

```

      IF (A(I,J).NE.DATA(I)) GO TO 70
60  CONTINUE
      NIM(N+5) = J
      GO TO 90
70  CONTINUE
      GO TO 80
90  VSS = NS
      NS = J
      DELN(J) = EN(J,NPT)
      EN(J,NPT) = 1.
      CALL CPHS
      EN(J,NPT) = DELN(J)
      NS = NSS
      IF (H0(J).GT..01 .AND. H0(J).LT..01) H0(J) = 0.
      RTEMP(N) = TT
      ENTH(N) = H0(J)*R*TT
      AC(K) = AC(K) + CPSUM*PCWT/RMW(N)
500  HPP(K) = HPP(K) + ENTH(N)*PCWT/RMW(N)
900  CONTINUE
      IF (.NOT. MOLES) GO TO 951
      DO 950 K=1,2
      IF (WP(K).EQ.0.) GO TO 950
      HPP(K) = HPP(K)/WP(K)
      AC(K) = AC(K)/WP(K)
950  CONTINUE
951  HSUR0 = (OF*HPP(1) + HPP(2))/(OF+1.)
      GO TO 1000
75  WRITE(6,76)
76  FORMAT(50H0 REACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA )
80  WRITE(6,85) N
85  FORMAT(1H0,I2,34H TH REACTANT IS NOT IN THERMO DATA )
1000 RETURN
      END

```

HCA*0600
 HCA*0610
 HCA*0620
 HCA*0630
 HCA*0640
 HCA*0650
 HCA*0660
 HCA*0670
 HCA*0680
 HCA*0690
 HCA*0700
 HCA*0710
 HCA*0720
 HCA*0730
 HCA*0740
 HCA*0750
 HCA*0760
 HCA*0770
 HCA*0780
 HCA*0790
 HCA*0800
 HCA*0810
 HCA*0820
 HCA*0830
 HCA*0840
 HCA*0850
 HCA*0860
 HCA*0870
 HCA*0880
 HCA*0890
 HCA*0900
 HCA*0910
 HCA*0920

SUBROUTINE MOLIER

```

C      COMMON/POINTS/MSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),
1      GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
2      TOTN(13)
C      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),MO(150)
1      DELN(150),A(15,150),SUR(150,3),IUSE(150),TEMP(50,2)
C      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
1      TM,TLOW,TMID,THIGH,FP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
2      HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
3      ANUM(15,5),PECNT(15),ENTH(15),FAZ(15),RTMP(15),FOX(15),DENS(15)
4      RHOP,RHW(15),TLN
C      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,M0LES,NP,NT,NPT,NLM
1      NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVED
2      IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
DO 91 IT = 1,26
IF (T(IT).EQ. 0.) GO TO 95
NT = IT
91 CONTINUE
C      SET ASSIGNED P
C
C      95 DO 902 IP = 1,NP
PF = P(IP)
C      SET ASSIGNED T
C
C      DO 902 IT=1,NT
IT = T(IT)
CALL EQLBRM
IF (TT.NE.0.) GO TO 800
IF (NPT.EQ.0) GO TO 1000
800 K = 0
IF (IP.EQ.NP.AND.IT.EQ.NT.OR.TT.EQ.0.) GO TO 860
K = NPT
IF (NPT.NE.13) GO TO 870
860 WRITE (6,5)
5 FORMAT(1H1,41X,48HTHERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
1      1/53X,28H TEMPERATURES AND PRESSURES /// )
CALL OUT1
WRITE (6,863)
863 FORMAT (25H0THERMODYNAMIC PROPERTIES//)
CALL OUT2
CALL OUT3
865 IF (K.EQ.0) GO TO 1000
WRITE (6,868)
868 FORMAT(1H1)
NPT = 0
870 NPT = NPT + 1
C      SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT
C
C      DO 860 I = 1,NS
EN(I,NPT) = EN(I,K)
890 CONTINUE
902 CONTINUE
1000 RETURN
END

```

```

SUBROUTINE CMRSTN
C
COMMON/POINTS/MSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
1 GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
2 TGTN(13)
COMMON/SPECES/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)
COMMON/MISC/ENH,SUM,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
1 TM,LOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUR0,AC(2),AM(2)
2 HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
4 RHOP,RMW(15),TLN
COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,M0LES,NP,NT,NPT,NLM
1 NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEW,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
2 IONS,NC,NSERT,JSOL,J IQ,KASE,NREAC,IC,JS1,VOL,SHOCK
C
C SET ASSIGNED P
C
TT = 3800.
DO 902 IP = 1,NP
PP = P(IP)
CALL EQLBRM
T(NPT) = TT
IF(TT.NE.0.) GO TO 800
IF(NPT.EQ.0) GO TO 1000
800 K=0
IF(IP.EQ.NP.OR.TT.EQ.0.) GO TO 850
K = NPT
IF(NPT.NE.13) GO TO 870
860 WRITE (6,6)
6 FORMAT (1H1,42X,48HTHEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES
1 //)
CALL OUT1
WRITE (6,863)
863 FORMAT (25HTHERMODYNAMIC PROPERTIES//)
CALL OUT2
CALL OUT3
865 IF(K.EQ.0) GO TO 1000
NPT = 0
870 NPT = NPT + 1
C
C
C SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT
DO 880 I = 1,NS
EN(I,NPT) = EN(I,K)
880 CONTINUE
902 CONTINUE
1000 RETURN
END

```

```

CMR*0000
CMR*0010
CMR*0020
CMR*0030
CMR*0040
CMR*0050
CMR*0060
CMR*0070
CMR*0080
CMR*0090
CMR*0100
CMR*0110
CMR*0120
CMR*0130
CMR*0140
CMR*0150
CMR*0160
CMR*0170
CMR*0180
CMR*0190
CMR*0200
CMR*0210
CMR*0220
CMR*0230
CMR*0240
CMR*0250
CMR*0260
CMR*0270
CMR*0280
CMR*0290
CMR*0300
CMR*0310
CMR*0320
CMR*0330
CMR*0340
CMR*0350
CMR*0360
CMR*0370
CMR*0380
CMR*0390
CMR*0400
CMR*0410
CMR*0420
CMR*0430
CMR*0440
CMR*0450
CMR*0460
CMR*0470
CMR*0480

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SUBROUTINE DETON
C
C   CHAPMAN-JOUQUET DETONATIONS
C
LOGICAL HP,SP,TP,INERUG,NEW,IONS,MOL,FRZ,EQL,PSIA,RKT
LOGICAL CPCVEQ, CPCVFR, CALCH
C
DIMENSION GM(13),CP(13),H(13),PUB(13),TUB(13),GM1(13),RRHO(13)
C
COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
1 GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
2 TOTN(13)
COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)
1 DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),BO(15),BOP(15,2)
1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AC(2),AM(2)
2 HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTMP(15),FOX(15),DENS(15)
4 RHOP,RMW(15),TLN
COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOL,NT,NPT,NLM
1 NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEW,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
COMMON/PERF/PCP(26),VHOC(13),SPIH(13),VACI(13),SUBAR(13),SUPAR(13)
1 CPRF(13),AEAT(13),CSTR,EQL,FRZ,SSO
COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)
1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2
2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
C
EQUIVALENCE(CP,DATA),(GM,SPIH),(H1,VAC1),(PUB,SUBAR),(TUB,SUPAR)
EQUIVALENCE(GM1,AEAT),(PCP(14),RRHO)
C
DATA FT1/4HT1,D/, FP1/4HP1,A/, FH1/4HM1,C/, FM1/4HM1,M/
1 FC1/4HCP1,/, FG1/4HA1 /, FPP/4HP/P1/, FTT/4HT/T1/
2 FUD/4HDET /, FMM/4HM/M1/, FRA/4HRHO//, FR3/4HRHO1/
3 FMA/4HMACH/, FMB/4HND/, IZERO/2H00/
C
D(C)= A11*A22-A21*A12
XX(Y)= (B1*A22-B2*A12)/D(C)
YY(Z)= (B2*A11-B1*A21)/D(C)
C
NT = 1
HSUBO = HSUBO*R
CALCH = .FALSE.
TT = 0.
IF(T(1).EQ.0.) T(1)=RTMP(1)
DO 2 N = 1,NREAC
IF(NAME(N,5).EQ.IZERO) CALCH = .TRUE.
2 CONTINUE
DO 3 IT = 1,26
IF (T(IT).EQ.0.) GO TO 7
NT = IT
3 CONTINUE
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 = (OF+1.)*AM(2)*AM(1)/(AM(1)+OF*AM(2))
9 WRITE (6,11)
11 FORMAT(33H1DETONATION VELOCITY CALCULATIONS)
DO 903 IT=1,NT

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DET*0000
DET*0010
DET*0020
DET*0030
DET*0040
DET*0050
DET*0060
DET*0070
DET*0080
DET*0090
DET*0100
DET*0110
DET*0120
DET*0130
DET*0140
DET*0150
DET*0160
DET*0170
DET*0180
DET*0190
DET*0200
DET*0210
DET*0220
DET*0230
DET*0240
DET*0250
DET*0260
DET*0270
DET*0280
DET*0290
DET*0300
DET*0310
DET*0320
DET*0330
DET*0340
DET*0350
DET*0360
DET*0370
DET*0380
DET*0390
DET*0400
DET*0410
DET*0420
DET*0430
DET*0440
DET*0450
DET*0460
DET*0470
DET*0480
DET*0490
DET*0500
DET*0510
DET*0520
DET*0530
DET*0540
DET*0550
DET*0560
DET*0570
DET*0580
DET*0590

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```

T1= T(IT)
TT = T1
IF (.NOT.CALCH) GO TO 15
CALL MCALC
CALL OUT1
15 CP1 = (OF*AC(1) + AC(2))/(OF+1.)
DO 202 IP=1,NP
P1= P(IP)
H1(NPT) = HSUR0
TUB(NPT)=T1
SUB(NPT)=P1
CP(NPT) = CP1*R
ITR= 0
TT= 3800.
PP1= 15.
PP= PP1*P1
HSUB0 = H1(NPT)/R + .75*T1*PP1/AM1
TP = .FALSE.
HP= .TRUE.
CALL EQLBRM
HSUB0 = H1(NPT)
HP= .FALSE.
IF (TT.EQ.0.) GO TO 1000
GAM= GAMMAS(NPT)
TT1= TT/T1
II= 0
TEX=TT1-.75*PP1/(CPR(NPT)*AM1)
AMM=WM(NPT)/AM1
WRITE(6,190) TT
190 FORMAT(AH0T EST.=,F8.2/11X,4HP/P1,17X,4HT/T1)
WRITE(6,203) II,PP1,TT1
C
200 DO 202 II=1,4
ALFA=AMM/TT1
PP1= (1.+GAM)*(1.+(1.-4.*GAM*ALFA/(1.+GAM)**2)**5)/(2.*GAM*ALFA)
RK=PP1*ALFA
TT1= TEX+.5*PP1*GAM*(RK*RK-1.)/(AM1*CPR(NPT)*RK)
WRITE(6,203) II,PP1,TT1
203 FORMAT (15,2E20.8)
202 CONTINUE
TP= .TRUE.
TT= T1*TT1
RR1 = PP1*AMM/TT1
C
205 ITR= ITR+1
PP= P1*PP1
CALL EQLBRM
IF (NPT.EQ.0) GO TO 1000
IF (TT.EQ.0.) GO TO 860
GAM= GAMMAS(NPT)
IF (CPCVFR) GAM= CPRF(NPT)/(CPRF(NPT)-1./WM(NPT))
C
IF (CPCVEQ) GAM= -GAMMAS(NPT)*DLVPT(NPT)
AMM= WM(NPT)/AM1
RR1= PP1*AMM/TT1
A11= 1./PP1 + GAM*RR1*DLVPT(NPT)
A12= GAM*RR1*DLVTP(NPT)
A21= .5*GAM*(RR1**2-1.-DLVPT(NPT)*(1.+RR1**2))*DLVTP(NPT)-1.
A22=-.5*GAM*DLVTP(NPT)*(RR1**2+1.)-WM(NPT)*CPR(NPT)
B1= 1./PP1-1.+GAM*(RR1-1.)
B2= WM(NPT)*(HSUM(NPT)-H1(NPT)/R)/TT-.5*GAM*(RR1*RR1-1.)
DET*0600
DET*0610
DET*0620
DET*0630
DET*0640
DET*0650
DET*0660
DET*0670
DET*0680
DET*0690
DET*0700
DET*0710
DET*0720
DET*0730
DET*0740
DET*0750
DET*0760
DET*0770
DET*0780
DET*0790
DET*0800
DET*0810
DET*0820
DET*0830
DET*0840
DET*0850
DET*0860
DET*0870
DET*0880
DET*0890
DET*0900
DET*0910
DET*0920
DET*0930
DET*0940
DET*0950
DET*0960
DET*0970
DET*0980
DET*0990
DET*1000
DET*1010
DET*1020
DET*1030
DET*1040
DET*1050
DET*1060
DET*1070
DET*1080
DET*1090
DET*1100
DET*1110
DET*1120
DET*1130
DET*1140
DET*1150
DET*1160
DET*1170
DET*1180
DET*1190

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X1 = XX(Y)
X2 = YY(Z)
ALAM= 1.
TEM = X1
IF(TEM.LT.0.) TEM = -TEM
IF(X2.GT.TEM) TEM=X2
IF (-X2.GT.TEM) TEM = -X2
IF(TEM.GT.0.4) ALAM=.4/TEM
PP1= PP1*EXP(X1*ALAM)
TT1= TT1*EXP(X2*ALAM)
TT = T1*TT1
US = (RR*GAM*TT/WM(NPT))*0.5
UD= RR1*JS
WRITE(6,10) ITR
10 FORMAT (21H0 ITERATION NUMBER=I2 )
WRITE(6,30) PP1,TT1,RR1,X1,X2,US
30 FORMAT(6X,4HP/P1,10X,1H= E20.8/6X,4HT/T1,10X,1H= E20.8/6X,2HRH0/RHDT
101,5X,1H= E20.8/6X,11HDEL LN P/P1,3X,1H=E20.8/6X,11HDEL LN T/T1,3XDEL
2,1H=E20.8/6X,2HUS,12X,1H=E20.8)
C
C
C CONVERGENCE TEST
IF(ITR.LE.10 .AND. TEM.GT.0.5E-04) GO TO 205
RRH0(NPT)=RR1
IF (CP(NPT).EQ.0.) GO TO 40
GM1(NPT) = CP(NPT) / (CP(NPT)-R/AM1)
VMOC(NPT) = UD/(RR*GM1(NPT)*T1/AM1)**.5
GO TO 41
40 GM1(NPT) = 0.
VMOC(NPT) = 0.
GO TO 150
C
C
C DERIVATIVES
41 WRITE(6,55)
55 FORMAT ( 17H0 DERIVATIVE OF,13X,4HLN P,16X,4HLN T
1,16X,2HUD, /9X,2HBY )
B1= 1./PP1-GAM*RR1
B2= GAM*RR1**2
X1 = XX(Y)
X2 = YY(Z)
AA= .5*(1.-DLVPT(NPT))
BB= -.5*DLVTP(NPT)
DUD= UD*(AA*X1+BB*X2-1.)
X1= X1-1.0
WRITE(6,81)X1,X2,DUD
81 FORMAT(6X,13HLNPI AT T1,H1,6X,1H=,3E17.8 )
B1= GAM*RR1
B2= -B1*RR1-WH(NPT)*CP(NPT)/(R*TT1)
X1 = XX(Y)
X2 = YY(Z)
DUD= UD*(AA*X1+BB*X2-1.)
X2= X2-1.
WRITE(6,84)X1,X2,DUD
84 FORMAT(6X,16HLNIT1 AT P1,H1,M1,3X,1H=3E17.8)
B1= 0.
B2= -WM(NPT)/(R*TT)
X1 = XX(Y)*1000.
X2 = YY(Z)*1000.
DUD= UD*(AA*X1+BB*X2)
DET*1200
DET*1210
DET*1220
DET*1230
DET*1240
DET*1250
DET*1260
DET*1270
DET*1280
DET*1290
DET*1300
DET*1310
DET*1320
DET*1330
DET*1340
DET*1350
DET*1360
DET*1370
DET*1380
DET*1390
DET*1400
DET*1410
DET*1420
DET*1430
DET*1440
DET*1450
DET*1460
DET*1470
DET*1480
DET*1490
DET*1500
DET*1510
DET*1520
DET*1530
DET*1540
DET*1550
DET*1560
DET*1570
DET*1580
DET*1590
DET*1600
DET*1610
DET*1620
DET*1630
DET*1640
DET*1650
DET*1660
DET*1670
DET*1680
DET*1690
DET*1700
DET*1710
DET*1720
DET*1730
DET*1740
DET*1750
DET*1760
DET*1770
DET*1780
DET*1790

```

```

      WRITE(6,85) X1,X2,0.0D
      85 FORMAT (6X,20MH) AT T1,P1,M1 =3E17.8)
C
150 K = 0
      IF(IP.EQ.0.AND.IT.EQ.0.OR.TT.EQ.0) GO TO 650
      K = NPT
      IF(NPT.NE.13) GO TO 870
C
      OUTPUT
C
860 WRITE(6,5)
      5 FORMAT(13H1,42X,46HDETONATION PROPERTIES OF AN IDEAL REACTING GAS)
      CALL OUT1
      WRITE(6,46)
      46 FORMAT(13H UNBURNED GAS//)
      FMT(4)=FMT13
      FMT(5)=FB
      FMT(7)=F4
      WRITE(6,FMT) FPI,FP(2),FB,FB*(PUB(J),J=1,NPT)
      FMT(7)=F2
      WRITE(6,FMT) FT,FT(2),FB,FB*(TUB(J),J=1,NPT)
      WRITE(6,FMT) FHI,FH(2),FB,FB*(HI(J),J=1,NPT)
      DO 56 I=1,NPT
      V(I)=AM1
      SONVEL(I)= (RR*GM1(I)*TUB(I)/AM1)**.5
56 CONTINUE
      FMT(7)=F3
      WRITE(6,FMT) FM1,FM(2),FM(3),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),FG(2),FB,FB*(GM1(J),J=1,NPT)
      FMT(7)=F1
      WRITE(6,FMT) (FL(I),I=1,4),*(SONVEL(J),J=1,NPT)
      WRITE(6,58)
      58 FORMAT(11H0BURNED GAS//)
      FMT(4)=FMT(6)
      CALL OUT2
      WRITE(6,68)
      68 FORMAT(12H0DETONATION PARAMETERS //)
      FMT(7)=F3
      DO 70 I=1,NPT
      V(I)= P02(I)/PUB(I)
      PCP(I)=TTT(I)/TUB(I)
      SONVEL(I)=SONVEL(I)*RRHO(I)
70 CONTINUE
      WRITE(6,FMT) FPP,FB,FB,FB*(V(J),J=1,NPT)
      WRITE(6,FMT) FTT,FB,FB,FB*(PCP(J),J=1,NPT)
      DO 73 I=1,NPT
      V(I)=MM(I)/AM1
73 CONTINUE
      FMT(7)=F4
      WRITE(6,FMT) FMM,FB,FB,FB*(V(J),J=1,NPT)
      WRITE(6,FMT) FRA,FRA,FB,FB*(RRHO(J),J=1,NPT)
      WRITE(6,FMT) FMA,FMA,FB,FB*(V4OC(J),J=1,NPT)
      FMT(7)=F1
      WRITE(6,FMT) FUD,FL(2),FL(3),FL(4),*(SONVEL(J),J=1,NPT)
      EOL=.TRUE.
      CALL OUT3
865 IF(K.EQ.0) GO TO 1000
      WRITE(6,868)

```

```

DET*1800
DET*1810
DET*1820
DET*1830
DET*1840
DET*1850
DET*1860
DET*1870
DET*1880
DET*1890
DET*1900
DET*1910
DET*1920
DET*1930
DET*1940
DET*1950
DET*1960
DET*1970
DET*1980
DET*1990
DET*2000
DET*2010
DET*2020
DET*2030
DET*2040
DET*2050
DET*2060
DET*2070
DET*2080
DET*2090
DET*2100
DET*2110
DET*2120
DET*2130
DET*2140
DET*2150
DET*2160
DET*2170
DET*2180
DET*2190
DET*2200
DET*2210
DET*2220
DET*2230
DET*2240
DET*2250
DET*2260
DET*2270
DET*2280
DET*2290
DET*2300
DET*2310
DET*2320
DET*2330
DET*2340
DET*2350
DET*2360
DET*2370
DET*2380
DET*2390

```

DET*2400
 DET*2410
 DET*2420
 DET*2430
 DET*2440
 DET*2450
 DET*2460
 DET*2470
 DET*2480
 DET*2490
 DET*2500
 DET*2510
 DET*2520
 DET*2530
 DET*2540

```

848 FORMAT(1H1)
      NPT = 0
870 NPT = NPT + 1
C
C   SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT
C
      DO 880 I = 1, NS
      EN(I,NPT) = EN(I,K)
880 CONTINUE
      WRITE (6,868)
902 CONTINUE
903 CONTINUE
1000 TP = .FALSE.
      RETURN
      END
  
```

SUBROUTINE SHCK
RETURN
END

97

SHC*0000
SHC*0010
SHC*0020

```

SUBROUTINE ROCKET
C
C      ROCKET PERFORMANCE
C      EITHER HPSP OR TPSP IS TRUE
C
C      LOGICAL HP,SP,TP,IDEBUG,NEWR,IONS,MOLES,FROZ,EQL,LOGV,HPSP,TPSP
C
C      DIMENSION AA(2),BB(2),CC(2)
C
C      COMMON/POINTS/MSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
C      1 GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
C      2 TOTN(13)
C      COMMON/SPECIES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
C      1 DELN(150),V(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
C      COMMON/MISC/CON,SUMN,TT,SG,ATOM(3,101),LLMT(15),BO(15),BOP(15,2)
C      1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
C      2 HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
C      3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTMP(15),FOX(15),DENS(15)
C      4 RMOP,RMW(15),TLN
C      COMMON/INDX/IDEBUG,CONVE,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM
C      1 NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEWR,NSUR,NSUP,ITN,CPCVFR,CPCVEQ
C      2 IONS,NC,NSFRT,JSOL,JLIR,KASE,NREAC,IC,JS1,VOL,SHOCK
C      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
C      1 CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSO
C
C      NAMELIST/RKTINP/EQL,FROZ,SUBAR,SUPAR,PCP
C
C      ITH = 0
210 DO 300 I=1,26
C      PCP(I) = 0.
C      SUBAR(I) = 0.
300 CONTINUE
C      TT = 3800.
C      HPSP = .TRUE.
C      HP = .TRUE.
C      TPSP = .FALSE.
C      EQL = .TRUE.
C      FROZ = .TRUE.
C      READ (5,RKTINP)
C      IF (T(1).EQ.0.) GO TO 303
C      TPSP = .TRUE.
C      TT = T(1)
C      TP = .TRUE.
C      HPSP = .FALSE.
303 IF (PCP(1).NE.0.) GO TO 308
C      DO 305 I=1,NP
C      K = NP-I+2
C      P(K) = P(K-1)
305 CONTINUE
C      GO TO 311
308 NP = 2
C      DO 310 I=1,24
C      IF (I.GT.2) GO TO 309
C      IF ((PCP(I).EQ.0.).OR.PCP(I).EQ.1.) GO TO 310
309 IF (PCP(I).EQ.0.) GO TO 311
C      NP = NP + 1
C      P(NP) = P(1)/PCP(I)
310 CONTINUE
311 VSUR=0
C      VSUP = 0

```

RCK*0000
 RCK*0010
 RCK*0020
 RCK*0030
 RCK*0040
 RCK*0050
 RCK*0060
 RCK*0070
 RCK*0080
 RCK*0090
 RCK*0100
 RCK*0110
 RCK*0120
 RCK*0130
 RCK*0140
 RCK*0150
 RCK*0160
 RCK*0170
 RCK*0180
 RCK*0190
 RCK*0200
 RCK*0210
 RCK*0220
 RCK*0230
 RCK*0240
 RCK*0250
 RCK*0260
 RCK*0270
 RCK*0280
 RCK*0290
 RCK*0300
 RCK*0310
 RCK*0320
 RCK*0330
 RCK*0340
 RCK*0350
 RCK*0360
 RCK*0370
 RCK*0380
 RCK*0390
 RCK*0400
 RCK*0410
 RCK*0420
 RCK*0430
 RCK*0440
 RCK*0450
 RCK*0460
 RCK*0470
 RCK*0480
 RCK*0490
 RCK*0500
 RCK*0510
 RCK*0520
 RCK*0530
 RCK*0540
 RCK*0550
 RCK*0560
 RCK*0570
 RCK*0580
 RCK*0590

```

DO 320 I=1,13
IF (SUBAR(I).NE.0.) NSUB=NSUB+1
IF (SUPAR(I).NE.0.) NSUP=NSUP+1
320 CONTINUE
WRITE (6,RKTINP)
SSO = 0.
ITROT=.3

C
C   SET ASSIGNED P
C
DO 902 IP = 1,NP
PP = P(IP)
CALL EQLBRM
IF (TT.NE.0.) GO TO 333
IF (NPT.EQ.0) GO TO 1000
GO TO 900
333 PCP(NPT) = P(1)/PP
IF (IP.GT.1) GO TO 195

C
C   COMBUSTION CHAMBER
C
TP = .FALSE.
HP = .FALSE.
SP = .TRUE.
SO = SSUM(1)
PCP(2) = ((GAMMAS(1)+1.)/2.)* (GAMMAS(1)/(GAMMAS(1)-1.))
P(2) = P(1)/PCP(2)
TT = 2.*TT/(GAMMAS(1)+1.)
GO TO 900
195 IF (IP.GT.2) GO TO 900

C
C   THROAT
C
190 IF (ITH.NE.2) GO TO 191
ITH = 0
GAMMAS(2) = 0.
GO TO 900
191 DH = HSUM(1)-HSUM(2)
DHSTAR = DH-GAMMAS(2)*TT*ENN/2.
IF (IDERR) WRITE (6,923) DHSTAR,HSUM(1),HSUM(2),PCP(2)
923 FORMAT(4E25.8)
DH = DHSTAR/DH
IF (DH.LT.0.) DH=-DH
IF (DH.LE.0.4E-4.OR.ITROT.EQ.0) GO TO 900
IF (JSOL.NE.0) ITH = 1
IF (JSOL.EQ.0.AND.ITH.EQ.1) ITH=2
IF (ITH.EQ.0) GO TO 192

C
C   SPECIAL THROAT INTERPOLATION IF ITH = 2
C
DLNI = .5*TT*ENN/(HSUM(1)-HSUM(2))
AA(ITH) = .5*DLNI*(2.*DLNI+(GAMMAS(2)-1.)/GAMMAS(2))
XX = ALOG(PCP(2))
BB(ITH) = 1./GAMMAS(2)-DLNI-2.*XX*AA(ITH)
CC(ITH) = ENN*TT/(PP*(HSUM(1)-HSUM(2))*5)
CC(ITH) = ALOG(CC(ITH))-XX*(BB(ITH)+AA(ITH)*XX)
IF (ITH.EQ.1) GO TO 192
BB(1)=BB(1)-BB(2)
AA(1)=AA(1)-AA(2)
PCP(2) = (-BB(1)+(BB(1)*BB(1)-4.*AA(1)*(CC(1)-CC(2)))*5)/(2.*AA(1)

```

RCK*0600
RCK*0610
RCK*0620
RCK*0630
RCK*0640
RCK*0650
RCK*0660
RCK*0670
RCK*0680
RCK*0690
RCK*0700
RCK*0710
RCK*0720
RCK*0730
RCK*0740
RCK*0750
RCK*0760
RCK*0770
RCK*0780
RCK*0790
RCK*0800
RCK*0810
RCK*0820
RCK*0830
RCK*0840
RCK*0850
RCK*0860
RCK*0870
RCK*0880
RCK*0890
RCK*0900
RCK*0910
RCK*0920
RCK*0930
RCK*0940
RCK*0950
RCK*0960
RCK*0970
RCK*0980
RCK*0990
RCK*1000
RCK*1010
RCK*1020
RCK*1030
RCK*1040
RCK*1050
RCK*1060
RCK*1070
RCK*1080
RCK*1090
RCK*1100
RCK*1110
RCK*1120
RCK*1130
RCK*1140
RCK*1150
RCK*1160
RCK*1170
RCK*1180
RCK*1190

```

11  PCP(2)=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)
    ITR0T = ITR0T-.1
    CALL EQLBRM
    IF(TT.EQ.0.) GO TO 1000
    GO TO 190

C
900 K = 0
    IF (.NOT.EQL .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 RKTOUT
    IF ((NSUB + NSUP).NE.0) CALL RATIO
    IF(K.EQ.0) GO TO 990
    WRITE(6,865)
865 FORMAT(1H1)
    NPT = 2
870 NPT = NPT + 1

C
C  SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT
C
    DO 880 I = 1,NS
    EN(I,NPT) = EN(I,K)
880 CONTINUE
982 CONTINUE
990 IF (FROZ) CALL FROZEN
1000 RETURN
    END

```

```

RCK*1200
RCK*1210
RCK*1220
RCK*1230
RCK*1240
RCK*1250
RCK*1260
RCK*1270
RCK*1280
RCK*1290
RCK*1300
RCK*1310
RCK*1320
RCK*1330
RCK*1340
RCK*1350
RCK*1360
RCK*1370
RCK*1380
RCK*1390
RCK*1400
RCK*1410
RCK*1420
RCK*1430
RCK*1440
RCK*1450
RCK*1460
RCK*1470
RCK*1480
RCK*1490
RCK*1500
RCK*1510
RCK*1520

```

```

SUBROUTINE RKTOUT
C
C ROCKET PERFORMANCE PARAMETERS
C
C LOGICAL EQL,FROZ,TP,HP,SP,HPSP,TPSP,SHOCK
C
C DIMENSION NV(13),Z(10,4)
C
C COMMON/POINTS/USUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
1 GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
2 TOTN(13)
C COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
1 UELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
C COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
1 T4,TLOW,TMIN,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
2 HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FGX(15),DENS(15)
4 R4OP,RMW(15),TLN
C COMMON/INDEX/IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,M0LES,NP,NT,NPT,NLM
1 NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEW,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
2 INNS,NC,NSERT,JSOL,JL12,KASE,NREAC,IC,JS1,VOL,SHOCK
C COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
1 CPRF(13),AFAT(13),CSTR,EQL,FROZ,SS0
C COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)
1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),F4TI9,FA1,FA2
2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9A,F0
C
C EQUIVALENCE (V,NV),(Z,H0)
C
C DATA EXIT/4HEXIT/
C
C IF(EQL) WRITE (6,37)
37 FORMAT(1H1,24X,84HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM
COMPOSITION DURING EXPANSION //)
C IF(.NOT.EQL) WRITE (6,38)
38 FORMAT(1H1,26X,78HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN
COMPOSITION DURING EXPANSION //)
C IF(TPSP) WRITE (6,737)
737 FORMAT(52X,28HAT AN ASSIGNED TEMPERATURE
V(1) = PPP(1)*14.696006
WRITE (6,40) V(1)
40 FORMAT(5H PC = ,F8.1,5H PSIA)
CALL OUT1
NEX = NPT - 2
DO 862 I = 1,NEX
862 V(I) = EXIT
WRITE(6,48) (V(I),I=1,NEX)
48 FORMAT(1H0,16X,16HCHAMBER THROAT ,11(5X,A4))
C
C PRESSURE RATIO:
C
C FMT(4) = FMT(6)
CALL VARFMT(PCP,NPT)
WRITE (6,FMT) FR1,FB,FB,FB,(PCP(J),J=1,NPT)
CALL OUT2
C
C AGV = 9.80665
DO 202 K=2,NPT
SPIM(K) = (2.*RR*(HSUM(1)-HSUM(K)))*.5/AGV
C

```

```

RKT*0000
RKT*0010
RKT*0020
RKT*0030
RKT*0040
RKT*0050
RKT*0060
RKT*0070
RKT*0080
RKT*0090
RKT*0100
RKT*0110
RKT*0120
RKT*0130
RKT*0140
RKT*0150
RKT*0160
RKT*0170
RKT*0180
RKT*0190
RKT*0200
RKT*0210
RKT*0220
RKT*0230
RKT*0240
RKT*0250
RKT*0260
RKT*0270
RKT*0280
RKT*0290
RKT*0300
RKT*0310
RKT*0320
RKT*0330
RKT*0340
RKT*0350
RKT*0360
RKT*0370
RKT*0380
RKT*0390
RKT*0400
RKT*0410
RKT*0420
RKT*0430
RKT*0440
RKT*0450
RKT*0460
RKT*0470
RKT*0480
RKT*0490
RKT*0500
RKT*0510
RKT*0520
RKT*0530
RKT*0540
RKT*0550
RKT*0560
RKT*0570
RKT*0580
RKT*0590

```



```

C  AW (A/W) IN UNITS OF SEC/ATM
C
  AW = RR*TTT(K)/(PPP(K)*
  IF (K.NE.2) GO TO 200
  AWT=AW
  CSTR=32.174*P(I)*AWT
200 AEAT(K)=AW/AWT
  VACI(K)=SPIM(K)+PPP(K)*AW
  IF (SONVEL(K).NE.0.) VMOCK(K)=SPIM(K)*AGV/SONVEL(K)
  NV(K)= CSTR + .5
212 CONTINUE
C
C  MACH NUMBER
C
  VMOCK(1)=0.
  IF (GAMMAS(2).EQ.0.) VMOCK(2)=0.
  FMT(7) = F3
  WRITE(6,FMT) (FN(I),I=1,4), (VMOCK(J),J=1,NPT)
  WRITE (6,208)
208 FORMAT (1H )
C
C  C*
C
  FMT(4) = FMTQX
  FMT(5) = FMT13
  FMT(6) = FMT19
  FMT(7) = F8
  WRITE(6,FMT) (FR(I),I=1,4), (NV(J),J=2,NPT)
C
C  CF - THRUST COEFFICIENT
C
  FMT(6) = FMT(8)
  FMT(7) = F3
  DO 212 I=2,NPT
212 V(I)=32.174*SPIM(I)/CSTR
  WRITE(6,FMT) FC1,FB,FB,FB, (V(J),J=2,NPT)
C
C  AREA RATIO
C
  CALL VARFMT (AEAT,NPT)
  FMT(5) = F8
  WRITE(6,FMT) FA1,FA2,FB,FB, (AEAT(J),J=2,NPT)
C
C  VACUUM IMPULSE
C
  FMT(5) = FMT13
  FMT(7) = F1
  WRITE(6,FMT) (FA(I),I=1,4), (VACI(J),J=2,NPT)
C
C  SPECIFIC IMPULSE
C
  WRITE(6,FMT) (FI(I),I=1,4), (SPIM(J),J=2,NPT)
  WRITE (6,208)
  FMT(4) = F8
  FMT(5) = FMT13
  FMT(7) = F5
  IF (EOL) GO TO 312
  WRITE(6,310)
310 FORMAT(15HOMOLE FRACTIONS //)
C

```

102

```

RKT*0600
RKT*0610
RKT*0620
RKT*0630
RKT*0640
RKT*0650
RKT*0660
RKT*0670
RKT*0680
RKT*0690
RKT*0700
RKT*0710
RKT*0720
RKT*0730
RKT*0740
RKT*0750
RKT*0760
RKT*0770
RKT*0780
RKT*0790
RKT*0800
RKT*0810
RKT*0820
RKT*0830
RKT*0840
RKT*0850
RKT*0860
RKT*0870
RKT*0880
RKT*0890
RKT*0900
RKT*0910
RKT*0920
RKT*0930
RKT*0940
RKT*0950
RKT*0960
RKT*0970
RKT*0980
RKT*0990
RKT*1000
RKT*1010
RKT*1020
RKT*1030
RKT*1040
RKT*1050
RKT*1060
RKT*1070
RKT*1080
RKT*1090
RKT*1100
RKT*1110
RKT*1120
RKT*1130
RKT*1140
RKT*1150
RKT*1160
RKT*1170
RKT*1180
RKT*1190

```

C MOLE FRACTIONS - FROZEN

103

```

C
DO 309 I=1,NPT
DATA(I) = 0.
DO 308 K=1,NS
DATA(I) = DATA(I)+EN(K,I)
308 CONTINUE
309 CONTINUE
LINE = 0
DO 430 K=1,NS
V(LINE+1) = EN(K,1)/DATA(I)
IF (V(LINE+1).LT.(5.E-6)) GO TO 424
LINE = LINE+1
Z(LINE,1) = SUR(K,1)
Z(LINE,2) = SUR(K,2)
Z(LINE,3) = SUR(K,3)
Z(LINE,4) = V(LINE)
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)
426 FORMAT (1H,4(3A4,F9.5,7X))
LINE = 0
430 CONTINUE
312 CALL OUT3
1000 RETURN
END

```

```

RKT*1200
RKT*1210
RKT*1220
RKT*1230
RKT*1240
RKT*1250
RKT*1260
RKT*1270
RKT*1280
RKT*1290
RKT*1300
RKT*1310
RKT*1320
RKT*1330
RKT*1340
RKT*1350
RKT*1360
RKT*1370
RKT*1380
RKT*1390
RKT*1400
RKT*1410
RKT*1420
RKT*1430
RKT*1440
RKT*1450

```

SUBROUTINE RATIO

(USED FOR AREA RATIO INTERPOLATION ONLY)

DOUBLE PRECISION G,X
LOGICAL: EQL, FROZ, TPSPDIMENSION PER(2,2),AI(13),APCP(13),AT(13),AMWT(13),RP(2),NV(13)
1 . RP(2)COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
1 . GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
2 . TOTN(13)COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HG(150)
1 . DELN(150),A(15,150),SUR(150,3),IUSE(150),TEMP(50,2)

COMMON/MISC/ENNSUM,TT,S0,ATOR(13,101),LLMT(15),B0(15),R0P(15,2)

1 . TX,TLOW,TMTD,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)

2 . HPP(2),RHO(2),VMIN(2),VPLS(2),NP(2),DATA(22),NAME(15,5)

3 . ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)

4 . R4OP,RMW(15),TLN

COMMON/DOUBLE/ G(20,21), X(20)

COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOL,ES,NP,NT,NPT,NLM

1 . NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEW,NSUB,NSUP,ITN,CPCVFR,CPCVEQ

2 . IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK

COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)

1 . CPRF(13),AEAT(13),CSTR,EQL,FROZ,SS0

COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FG(4)

1 . FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2

2 . FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0

EQUIVALENCE (V,NV)

NBLO = NPT-2

DO 22 J=3,NPT

IF(PCP(J).GT.PCP(2))GO TO 30

22 CONTINUE

GO TO 31

30 NRLO=J-3

31 DO 1200 ISONIC=1,2

LL = 1

IF(ISONIC.EQ.2) GO TO 34

IF(NSUB.EQ.0) GO TO 1200

NAR = NSUB

GO TO 36

34 IF(NSUP.EQ.0) GO TO 1200

NAR = NSUP

36 DO 1100 I=1,NAR

IF(ISONIC.EQ.2) GO TO 40

IF(NBLO.LE.1) GO TO 1100

K=2+NBLO

DO 38 J=4,K

V(LL) = SURAR(I)

IF(V(LL).GE.AEAT(J)) GO TO 56

38 CONTINUE

GO TO 56

40 IF(NPT-NRLO.LE.3) GO TO 1100

V(LL) = SUPAR(I)

K=4+NBLO

DO 42 J=K,NPT

IF(V(LL).LE.AEAT(J)) GO TO 56

R10*0000

R10*0010

R10*0020

R10*0030

R10*0040

R10*0050

R10*0060

R10*0070

R10*0080

R10*0090

R10*0100

R10*0110

R10*0120

R10*0130

R10*0140

R10*0150

R10*0160

R10*0170

R10*0180

R10*0190

R10*0200

R10*0210

R10*0220

R10*0230

R10*0240

R10*0250

R10*0260

R10*0270

R10*0280

R10*0290

R10*0300

R10*0310

R10*0320

R10*0330

R10*0340

R10*0350

R10*0360

R10*0370

R10*0380

R10*0390

R10*0400

R10*0410

R10*0420

R10*0430

R10*0440

R10*0450

R10*0460

R10*0470

R10*0480

R10*0490

R10*0500

R10*0510

R10*0520

R10*0530

R10*0540

R10*0550

R10*0560

R10*0570

R10*0580

R10*0590

```

42 CONTINUE
   IF(V(LL).GE.AEAT(J)+3.) GO TO 85
56 KJ = J-1
   K = KJ
   DO 64 JJ=1,2
     IF(CPR(K).NE.0.) GO TO 63
     *WRITE(6,62)K
62  FORMAT(17H0CANNOT USE POINT,I2,3X,4HCP=0 )
     GO TO 1100
63  PER(JJ,1)=-1./(CPR(K)*WM(K))
     IF (EQL) PER(JJ,1) = PER(JJ,1)*DLVTP(K)
     PER(JJ,2)= TTT(K)/(2.*WM(K)*(HSUM(1)-HSUM(K)))
     RP(JJ) = 1./(1./GAMMAS(K)-PER(JJ,2))
     IF(EQL)RPP(JJ) = 1.+DLVTP(K)*(1.-DLVTP(K))*PER(JJ,1)
     K = KJ + 1
64  CONTINUE
     AMWT(LL) = WM(1)
     CALL SET(PCP(KJ),RP(1),AEAT(KJ),V(LL), APCP(LL))
     CALL SET(TTT(KJ),PER(1,1),PCP(KJ),APCP(LL),AT(LL))
     IF(EQL)CALL SET (WM(KJ),RPP(1),PCP(KJ),APCP(LL),AMWT(LL))
     K = KJ
     DO 74 JJ=1,2
       G(JJ,7)=SPH(K)**2
       G(JJ+2,7)=2.*G(JJ,7)*PER(JJ,2)
       G(JJ+4,7)=(1.-GAMMAS(K))/GAMMAS(K)*G(JJ+2,7)
       G(JJ,1)=1.
       G(JJ+2,1)= 0
       G(JJ+4,1)=0
       G(JJ,2)=ALOG(PCP(K))
       G(JJ+2,2)=1.
       G(JJ+4,2)=0
       DO 70 M=3,6
         G(JJ,M)=G(JJ,2)**(M-1)
         G(JJ+2,M)=G(JJ,2)**(M-2)*FLOAT(M-1)
         G(JJ+4,M)=G(JJ,2,M)/G(JJ,2)*FLOAT(M-2)
70  CONTINUE
       K = KJ + 1
74  CONTINUE
       IMAT = 6
       CALL MGAUSD
       AI(LL)= X (1)
       DO 84 JJ=2,6
         AI(LL)=AI(LL)+ X (JJ)*ALOG(APCP(LL))**(JJ-1)
84  CONTINUE
       IF(AI(LL).LE.0.)GO TO 85
       AI(LL) = AI(LL)**.5
       GO TO 86
85  LL = LL + 1
86  IF(LL.GE.13.OR.I.GE.NAR) GO TO 90
       LL = LL+1
       GO TO 1100

```

C
C
C

OUTPUT

```

90 IF(EQL) WRITE (6,87)
87  FORMAT(1H1,24X,64HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM
      1IUM COMPOSITION DURING EXPANSION //)
     IF (.NOT.EQL) WRITE (6,88)
88  FORMAT(1H1,26X,78HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN CRI-
      1UMPOSITION DURING EXPANSION //)

```

R10*0600
 R10*0610
 R10*0620
 R10*0630
 R10*0640
 R10*0650
 R10*0660
 R10*0670
 R10*0680
 R10*0690
 R10*0700
 R10*0710
 R10*0720
 R10*0730
 R10*0740
 R10*0750
 R10*0760
 R10*0770
 R10*0780
 R10*0790
 R10*0800
 R10*0810
 R10*0820
 R10*0830
 R10*0840
 R10*0850
 R10*0860
 R10*0870
 R10*0880
 R10*0890
 R10*0900
 R10*0910
 R10*0920
 R10*0930
 R10*0940
 R10*0950
 R10*0960
 R10*0970
 R10*0980
 R10*0990
 R10*1000
 R10*1010
 R10*1020
 R10*1030
 R10*1040
 R10*1050
 R10*1060
 R10*1070
 R10*1080
 R10*1090
 R10*1100
 R10*1110
 R10*1120
 R10*1130
 R10*1140
 R10*1150
 R10*1160
 R10*1170
 R10*1180
 R10*1190

```

      IF (TPSP) WRITE (6,99)
99  FORMAT (52X,2RHAT AN ASSIGNED TEMPERATURE
      WRITE (6,91)
91  FORMAT (52X,24HFOR ASSIGNED AREA RATIOS    //)
      PC = P(1)*14.696006
      WRITE(6,191)PC
191  FORMAT(5H PC = ,F8.1,5H PSIA;
      CALL OUT1
      IF (ISONIC.EQ.1) WRITE(6,33)
33  FORMAT(18H0SUBSONIC FLOW    //)
      IF (ISONIC.EQ.2) WRITE (6,35)
35  FORMAT(18H0SUPERSONIC FLOW    //)
C
C      AREA RATIO
C
      FMT(6) = FMT(8)
      FMT(4) = FMT(6)
      CALL VARFMT (V,NPT)
      WRITE(6,FMT) FA1,FA2,FB,FR,(V(M),M=1,LL)
C
C      VACUUM SPECIFIC IMPULSE AND SPECIFIC IMPULSE
C
      DO 93 M=1,LL
      V(M) = AI(M)*CSTR*V(M)/(32.174*APCP(M))
93  CONTINUE
      FMT(4) = FMT13
      FMT(5) = FB
      FMT(7) = F1
      WRITE(6,FMT) (FA(N),N=1,4), (V(M),M=1,LL)
      WRITE(6,FMT) (FI(N),N=1,4), (AI(M),M=1,LL)
C
C      C*
C
      FMT(5) = FMT19
      DO 94 M=1,LL
      NV(M) = CSTR*.5
94  CONTINUE
      WRITE(6,FMT) (FR(N),N=1,4), (NV(M),M=1,LL)
C
C      CF - THRUST COEFFICIENT
C
      DO 95 M=1,LL
      V(M) = AI(M)*32.174/CSTR
95  CONTINUE
      FMT(5) = FR
      FMT(7) = F3
      WRITE(6,FMT) FC1,FR,FB,FB,(V(M),M=1,LL)
      WRITE(6,96)
96  FORMAT(1H )
C
C      PRESSURE RATIO
C
      FMT(4) = FMT(6)
      CALL VARFMT (APCP,NPT)
C
      CALL VARFMT (APCP,NPT)
C
C      PRESSURE
C
      R10*1200
      R10*1210
      R10*1220
      R10*1230
      R10*1240
      R10*1250
      R10*1260
      R10*1270
      R10*1280
      R10*1290
      R10*1300
      R10*1310
      R10*1320
      R10*1330
      R10*1340
      R10*1350
      R10*1360
      R10*1370
      R10*1380
      R10*1390
      R10*1400
      R10*1410
      R10*1420
      R10*1430
      R10*1440
      R10*1450
      R10*1460
      R10*1470
      R10*1480
      R10*1490
      R10*1500
      R10*1510
      R10*1520
      R10*1530
      R10*1540
      R10*1550
      R10*1560
      R10*1570
      R10*1580
      R10*1590
      R10*1600
      R10*1610
      R10*1620
      R10*1630
      R10*1640
      R10*1650
      R10*1660
      R10*1670
      R10*1680
      R10*1690
      R10*1700
      R10*1710
      R10*1720
      R10*1730
      R10*1740
      R10*1750
      R10*1760
      R10*1770
      R10*1780
      R10*1790

```

```

WRITE(6,FMT) FR1,FR,FB,FB,(APCP(M),M=1,LL)
DO 98 M=1,LL
V(M) = P(1)/APCP(M)
98 CONTINUE
CALL VARFMT (V,NPT)
WRITE(6,FMT) (FP(N),N=1,4), (V(M),M=1,LL)

C
C TEMPERATURE
C
DO 101 M=1,LL
NV(M)=AT(M)+.5
101 CONTINUE
FMT(4)=FMT13
FMT(5)=FMT19
WRITE(6,FMT) (FT(N),N=1,4), (NV(M),M=1,LL)

C
C ENTHALPY
C
FMT(5)=F8
FMT(7)=F1
DO 104 M=1,LL
V(M)=HSM(1)*R-1000.*(AI(M)/294.98)**2
104 CONTINUE
WRITE(6,FMT) (FH(N),N=1,4), (V(M),M=1,LL)

C
C ENTROPY
C
FMT(7)=F4
V(1) = SSUM(2)*R
DO 106 M=1,LL
V(M) = V(1)
106 CONTINUE
WRITE(6,FMT) (FS(N),N=1,4), (V(M),M=1,LL)

C
C MOLECULAR WEIGHT
C
FMT(7)=F3
WRITE(6,FMT) (FM(N),N=1,4), (AMWT(M),M=1,LL)
1100 CONTINUE
1200 CONTINUE
RETURN
END

```

```

R10*1800
R10*1810
R10*1820
R10*1830
R10*1840
R10*1850
R10*1860
R10*1870
R10*1880
R10*1890
R10*1900
R10*1910
R10*1920
R10*1930
R10*1940
R10*1950
R10*1960
R10*1970
R10*1980
R10*1990
R10*2000
R10*2010
R10*2020
R10*2030
R10*2040
R10*2050
R10*2060
R10*2070
R10*2080
R10*2090
R10*2100
R10*2110
R10*2120
R10*2130
R10*2140
R10*2150
R10*2160
R10*2170
R10*2180
R10*2190
R10*2200
R10*2210

```

C	SUBROUTINE SET(ONE,TWO,THREE,ARG,HAL)	SET=0000
C	(USED FOR AREA RATIO INTERPOLATION ONLY)	SET=0010
C	SETS UP ALL 4 BY 5 MATRICES	SET=0020
C	DOUBLE PRECISION A,ANS,G,X	SET=0030
C	DIMENSION ANS(6),ONE(2),TWO(2),THREE(2),A(20,21)	SET=0040
C	COMMON /DOUBLE/ G(20,21), X(20)	SET=0050
	COMMON/INHX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,NLM	SET=0060
1	.NS,KMAT,IMAT,IQ1,IQ2,NOMIT,TP,NEW,NSUB,NSUP,ITW,CPCVPR,CPCVED	S=.0070
2	.IONS,NC,NSERT,JSOL,JLIO,KASE,NREAC,IC,JS1,VOL,SHOCK	SET=0080
C	EQUIVALENCE (G,A),(X,ANS)	SET=0090
C	DO 8 J=1,2	SET=0100
	A(J,5)=ALOG(ONE(J))	SET=0110
	A(J,2,5)=TWO(J)	SET=0120
	A(J,2)=ALOG(THREE(J))	SET=0130
8	CONTINUE	SET=0140
	DO 1 I=1,2	SET=0150
	A(I,1)=1.0	SET=0160
	A(I,2,1)=0.0	SET=0170
	A(I,2,2)=1.0	SET=0180
	DO 1 J=2,3	SET=0190
	A(I,J+1)=A(I,2)**J	SET=0200
	A(I,2,J+1)=A(I,2)**(J-1)*FLOAT(J)	SET=0210
1	CONTINUE	SET=0220
	IMAT = 4	SET=0230
	CALL MGAUSD	SET=0240
	HAL=ANS(1)	SET=0250
	SUM=ALOG(ARG)	SET=0260
	DO 10 J=1,3	SET=0270
	HAL=HAL+SUM**J*(ANS(J+1))	SET=0280
10	CONTINUE	SET=0290
	HAL=EXP(HAL)	SET=0300
	RETURN	SET=0310
	END	SET=0320
		SET=0330
		SET=0340
		SET=0350
		SET=0360
		SET=0370
		SET=0380

```

SUBROUTINE FROZEN
C
C (FROZEN COMPOSITION EXPANSION ONLY)
C
C LOGICAL EQL,FROZ,CONVG
C
COMMON/POINTS,MSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
1 GAMMAS(13),P(26),Z(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
2 TOTN(13)
COMMON/SPECES,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)
COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)
1 TM,TLOW,THID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBC,AC(2),AM(2)
2 HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
3 ANUM(15,5),PECKT(15),ENTH(15),FAZ(15),RTMP(15),FOX(15),DENS(15)
4 RHOP,RMX(15),TLN
COMMON/INDEX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLCS,NP,NT,NPT,NLM
1 NS,KMAT,IMAT,IQ1,IQ2,NOMIT,IP,NEW,NSUR,NSUP,ITN,CPCVFR,CPCVEO
2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK
COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)
1 CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSO
COMMON/OUT/ FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)
1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2
2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0
ITROT = 3
EQL = .FALSE.
NPT = 2
TT = TTT(1)
TLN=ALOG(TT)
GAMMAS(1) = CPRF(1)/(CPRF(1)-1./WM(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 402 IP=2,NP
IF(NPT.EQ.2) GO TO 45
PCP(NPT) = P(1)/P(IP)
45 CONVG = .FALSE.
PCPLN= ALOG(PCP(NPT))
S0 = SSO -PCPLN/WM(1)
SUMH = 0.
51 TT=EXP(TLN)
SUMS=0.
JS1 = 1
NNN = NPT
NPT = 1
CALL CPHS
NPT = NNN
DO 60 J=1,NS
IF(EN(J,1).EQ.0.) GO TO 60
SUMS = SUMS + S(J)*EN(J,1)
IF(CONVG) SUMH=SUMH+H0(J)*EN(J,1)
60 CONTINUE
IF (CONVG) GO TO 81
DLNT=(SUMS-S0)/CPSUM
TLN=TLN-DLNT
IF(DLNT.LT.0.) DLNT=-DLNT
IF(DLNT.LT.0.5E-4) CONVG=.TRUE.
GO TO 51
81 TTT(NPT)= TT

```

```

FRZ*0000
FRZ*0010
FRZ*0020
FRZ*0030
FRZ*0040
FRZ*0050
FRZ*0060
FRZ*0070
FRZ*0080
FRZ*0090
FRZ*0100
FRZ*0110
FRZ*0120
FRZ*0130
FRZ*0140
FRZ*0150
FRZ*0160
FRZ*0170
FRZ*0180
FRZ*0190
FRZ*0200
FRZ*0210
FRZ*0220
FRZ*0230
FRZ*0240
FRZ*0250
FRZ*0260
FRZ*0270
FRZ*0280
FRZ*0290
FRZ*0300
FRZ*0310
FRZ*0320
FRZ*0330
FRZ*0340
FRZ*0350
FRZ*0360
FRZ*0370
FRZ*0380
FRZ*0390
FRZ*0400
FRZ*0410
FRZ*0420
FRZ*0430
FRZ*0440
FRZ*0450
FRZ*0460
FRZ*0470
FRZ*0480
FRZ*0490
FRZ*0500
FRZ*0510
FRZ*0520
FRZ*0530
FRZ*0540
FRZ*0550
FRZ*0560
FRZ*0570
FRZ*0580
FRZ*0590

```



```

SSUM(NPT) = SSUM(1)
MSUM(NPT) = TT * SUMH
GAMMAS(NPT) = CPSUM / (CPSUM - 1. / WM(1))
IF (IP.GT.2) GO TO 90

C
C
C
THROAT CALCULATIONS

DH = MSUM(1) - SSUM(2)
DHSTAR = DH - (GAMMAS(2) * TT / (2. * WM(1)))
DH = DHSTAR / DH
IF (DH.LT.0.) DH = -DH
IF (DH.LE.0.4E-4 .OR. ITROT.EQ.0) GO TO 90
PCP(2) = PCP(2) / (1. + 2. * DHSTAR * WM(1) / (TT * (GAMMAS(2) + 1.)))
P(2) = P(1) / PCP(2)
ITROT = ITROT - 1
GO TO 45
90 WM(NPT) = WM(1)
PPP(NPT) = P(IP)
CPR(NPT) = CPSUM
K = 0
IF (TT.LT.(TLOW-150.)) GO TO 903
IF (NC.EQ.0) GO TO 700
INC = 0
DO 901 I = 1, NS
IF (IUSE(I).EQ.0 .OR. IUSE(I).EQ.-10000) GO TO 901
INC = INC + 1
IF (EN(I,1).EQ.0.) GO TO 901
IF (TT.LT.(TEMP(INC,1)-50.) .OR. TT.GT.(TEMP(INC,2)+50.)) GO TO 903
901 CONTINUE
700 IF (IP.EQ.NP) GO TO 863
K = NPT
IF (NPT.NE.13) GO TO 870
GO TO 863
903 NPT = NPT + 1
863 CALL RKTOUT
IF (MSUB*NSUP.NE.0) CALL RATIO
865 IF (K.EQ.0) GO TO 1000
NPT = 2
870 NPT = NPT + 1
902 CONTINUE
1000 RETURN
END

```

```

FRZ*0600
FRZ*0610
FRZ*0620
FRZ*0630
FRZ*0640
FRZ*0650
FRZ*0660
FRZ*0670
FRZ*0680
FRZ*0690
FRZ*0700
FRZ*0710
FRZ*0720
FRZ*0730
FRZ*0740
FRZ*0750
FRZ*0760
FRZ*0770
FRZ*0780
FRZ*0790
FRZ*0800
FRZ*0810
FRZ*0820
FRZ*0830
FRZ*0840
FRZ*0850
FRZ*0860
FRZ*0870
FRZ*0880
FRZ*0890
FRZ*0900
FRZ*0910
FRZ*0920
FRZ*0930
FRZ*0940
FRZ*0950
FRZ*0960
FRZ*0970
FRZ*0980
FRZ*0990
FRZ*1000
FRZ*1010

```


DATA FP/4HP: A:4HTM :2H :1H /
 1.FT/4HT: D:4HEG K:4H :2H /:FH/4HH: C:4HAL/G:2H :1H /
 2.FS/4HS: C:4HAL/(:4HG) (K:2H) /:FH/4HH: M:4HOL W:2HT :1H /
 3.FV/4H(DLV:4H/DLP:4H)T :2H /:FD/4H(DLV:4H/DT:2H)P:1H /
 4.FC/4HCP: :4HCAL/:4H(G) (:2HK) /:FG/4HGAMM:4HA (S:2H) :1H /
 5.FL/4HSON :4HVEL:4HM/SE:2HC /

BLK*0600
 BLK*0610
 BLK*0620
 BLK*0630
 BLK*0640
 BLK*0650
 BLK*0660
 BLK*0670
 BLK*0680
 BLK*0690
 BLK*0700
 BLK*0710
 BLK*0720

C
 C
 C

INFORMATION USED IN PERFORMANCE OUTPUT

DATA FR1/4HPC/P/: FC1/2HCF/: FN/4HMACH:4H NUM:4HBER :1H /
 1.FR/4HCSTA:4HR: F:4HT/SE:2HC /:FI/4HI: L:4HB-SE:4HC/LB:1H /
 2.FA1/4HIVAC:4H:LB-:4HSEC/:2HLB /:FA1/4HAE/A/:FA2/1HT/
 END

APPENDIX VII - LISTING OF THERMO DATA

THEPMD

300.000		1000.000		5000.000		FIRST CARD		
AL(S)	J12/65AL	10	00	00	05	300.000	933.000	1
0.	0.	0.	0.	0.	0.	0.	0.	2
0.	0.	0.22258601E	01	0.25561638E	02	0.25963942E	06	3
-0.44923993E	-03	0.33343536E	-11	-0.77250039E	03	-0.10016767E	02	4
AL(L)	J12/65AL	10	00	00	0L	933.000	5000.000	1
0.38185052E	01	0.	0.	0.	0.	0.	0.	2
-0.95116344E	02	-0.17518952E	02	0.38185052E	01	0.	0.	3
0.	0.	-0.95116844E	02	-0.17518952E	02	0.	0.	4
AL	J12/65AL	100	000	000	0G	300.000	5000.000	1
0.25450650E	01	-0.75157512E	-04	0.48674178E	-07	-0.14045399E	-10	2
8.38438357E	05	0.53100256E	01	0.27964983E	01	-0.12468435E	-02	3
-0.15437769E	-03	0.43185442E	-12	0.39456100E	05	8.41365426E	01	4
AL+	J 6/65AL	1E	-100	000	0G	300.000	5000.000	1
0.25138516E	01	-0.29077490E	-04	0.20604308E	-07	-0.59989578E	-11	2
0.10959636E	06	0.37023323E	01	0.25006758E	01	-0.44314947E	-05	3
-0.97918340E	-11	0.33894328E	-14	0.10860109E	06	0.37744963E	01	4
AL802	J 6/65AL	1E	10	200	05	300.000	5000.000	1
0.71722995E	01	0.29780741E	-02	-0.12431107E	-05	0.23188779E	-09	2
-0.67683562E	05	-0.39949242E	01	0.23087234E	01	0.18350539E	-01	3
0.10251324E	-07	-0.16941283E	-11	-0.66482167E	05	0.14463834E	02	4
ALCL	J 9/64AL	1CL	100	000	0G	300.000	5000.000	1
0.43754335E	01	0.18702767E	-03	-0.49969033E	-07	0.95147171E	-11	2
-0.69880112E	04	0.23323888E	01	0.33327027E	01	0.44047734E	-02	3
0.44387437E	-08	-0.11170643E	-11	-0.67755002E	04	0.73643189E	01	4
ALCL+	J 6/65AL	1CL	1E	-10	05	300.000	5000.000	1
0.43738449E	01	0.19205255E	-03	-0.54247204E	-07	0.85478382E	-11	2
0.10231686E	06	0.31197190E	01	0.33759844E	01	0.42774116E	-02	3
0.43852415E	-08	-0.11166597E	-11	0.10251734E	06	0.79219510E	01	4
ALCLF	J 9/64AL	1CL	1F	100	0G	300.000	5000.000	1
0.64593361E	01	0.59930273E	-03	-0.25682111E	-06	0.43655729E	-10	2
-0.62463694E	05	-0.33724191E	01	0.35819421E	01	0.11405579E	-01	3
0.93913221E	-08	-0.20431534E	-11	-0.61639641E	05	0.10712370E	02	4
ALCLF2	J 9/64AL	1CL	1F	200	05	300.000	5000.000	1
0.89238843E	01	0.11946919E	-02	-0.51514910E	-06	0.94204282E	-10	2
-0.12250084E	06	-0.15879099E	02	0.42219327E	01	0.15187323E	-01	3
0.13307895E	-07	-0.26426994E	-11	-0.12144555E	05	0.73068442E	01	4
ALCL2	J 9/64AL	1CL	200	000	0G	300.000	5000.000	1
0.66933063E	01	0.33723179E	-03	-0.14321882E	-06	0.26838301E	-10	2
-0.39336262E	05	-0.38121908E	01	0.43363468E	01	0.99563726E	-02	3
0.10272735E	-07	-0.26037172E	-11	-0.39361237E	05	0.75382417E	01	4
ALCL2+	J 6/65AL	1CL	2E	-10	0G	300.000	5000.000	1
0.71747698E	01	0.34798442E	-03	-0.14533267E	-06	0.26784431E	-10	2
0.53103955E	05	-0.95391313E	01	0.47027704E	01	0.10475953E	-01	3
0.11009088E	-07	-0.28333967E	-11	-0.53608594E	05	0.23835549E	01	4
ALCL2-	J 6/65AL	1CL	2E	10	0G	300.000	5000.000	1
0.66765684E	01	0.35805640E	-03	-0.15322113E	-06	0.29934079E	-10	2
-0.42352615E	05	-0.44184290E	01	0.42601657E	01	0.10221323E	-01	3
0.10586258E	-07	-0.26976715E	-11	-0.41365193E	05	0.72193011E	01	4
ALCL2F	J 9/64AL	1CL	2F	100	0G	300.000	5000.000	1
0.91351571E	01	0.30569395E	-03	-0.39032127E	-06	0.74305714E	-10	2
-0.97369793E	05	-0.15822927E	02	0.48609210E	01	0.17353741E	-01	3
0.14933444E	-07	-0.34108042E	-11	-0.96939961E	05	0.54911550E	01	4
ALCL3	J 3/64AL	1CL	300	000	0G	300.000	5000.000	1
0.93992905E	01	0.67170780E	-03	-0.29024817E	-06	0.55354910E	-10	2
-0.73294478E	05	-0.16564590E	02	0.53451571E	01	0.16916688E	-01	3
0.16713999E	-07	-0.41452879E	-11	-0.72452471E	05	0.30263715E	01	4
ALCL3(S)	J 3/64AL	1CL	300	000	05	300.000	465.600	1
0.	0.	0.	0.	0.	0.	0.	0.	2
0.	0.	0.14431490E	02	-0.24545071E	-01	0.20035127E	-04	3
0.14508072E	-06	-0.21371474E	-09	-0.99404228E	05	-0.63344394E	02	4
ALCL3(L)	J 3/64AL	1CL	300	000	0L	465.600	5000.000	1

0.13345264E 02 0.	0.	0.	0.	2
-0.84887230E 05-0.54682110E 02 0.13385264E 02 0.	0.	0.	0.	3
0.	-0.84887230E 05-0.54682110E 02	0.	0.	4
ALF	J 9/E4AL 1F 100 000 0G	300.000 5000.000		1
0.41432941E 01 0.43456010E-03-0.16460575E-06	0.30802017E-10-0.21262355E-14			2
-0.32774410E 05 0.19573280E 01 0.24236585E 01	0.44021164E-02-0.53444016E-05			3
0.24433850E-08-0.28283365E-12-0.32462953E 05	0.85613734E 01			4
ALF+	J E/E8AL 1F 1E -10 0G	300.000 5000.000		1
0.41957106E 01 0.38290900E-03-0.13075649E-06	0.22591321E-10-0.13164857E-14			2
0.79682722E 05 0.24475601E 01 0.23575830E 01	0.50617403E-02-0.61248583E-05			3
0.32221532E-09-0.54448503E-12 0.79991210E 05	0.90992312E 01			4
ALF2	J 9/E4AL 1F 200 000 0G	300.000 5000.000		1
0.61804240E 01 0.90488677E-03-0.38832937E-06	0.73713932E-10-0.51591979E-14			2
-0.85071157E 05-0.39592295E 01 0.33301792E 01	0.10295891E-01-0.11444803E-04			3
0.51484409E-08-0.56416237E-12-0.84387796E 05	0.10315035E 02			4
ALF2+	J E/E8AL 1F 2E -10 0G	300.000 5000.000		1
0.68767776E 01 0.68899830E-03-0.29551540E-06	0.56021377E-10-0.39146708E-14			2
0.18916320E 05-0.10625708E 02 0.37787285E 01	0.12332101E-01-0.16840570E-04			3
0.10394906E-07-0.23427979E-11 0.19590891E 05	0.45427075E 01			4
ALF2-	J E/E8AL 1F 2E 10 0G	300.000 5000.000		1
0.61130125E 01 0.97697473E-03-0.41909432E-06	0.79151704E-10-0.55256597E-14			2
-0.90164129E 05-0.46096515E 01 0.30389102E 01	0.11066587E-01-0.12222733E-04			3
0.54253437E-08-0.56268792E-12-0.85365118E 05	0.10795230E 02			4
ALF3(S)	J 9/E5AL 1F 300 000 0S	300.000 713.000		1
0.	0.	0.	0.	2
0.	0.	0.13819544E 01	0.37097544E-01-0.41036006E-04	3
0.60619212E-08 0.13766618E-10-0.18326306E 06	0.91844203E 01			4
ALF3(S)	J 9/E5AL 1F 300 000 0S	718.000 2500.000		1
0.19522523E 02 0.20940523E-02-0.45541742E-06	0.19209506E-09-0.29475093E-13			2
-0.18432520E 06-0.52885029E 02 0.46589212E 01	0.15809473E-01 0.71160071E-06			3
-0.20754789E-07 0.11298614E-10-0.14335719E 06	0.22679313E 02			4
ALF3	J 9/E5AL 1F 300 000 0S	300.000 5000.000		1
0.86545610E 01 0.14919760E-02-0.64334360E-06	0.12269734E-09-0.86255143E-14			2
-0.14863571E 06-0.17064964E 02 0.36893150E 01	0.13593906E-01-0.22267274E-04			3
0.11536770E-07-0.19253509E-11-0.14747858E 06	0.76223622E 01			4
ALH	J E/E3AL 1H 100 000 0G	300.000 5000.000		1
0.33366898E 01 0.12377864E-02-0.49869941E-06	0.92294633E-10-0.63451694E-14			2
0.30091761E 05 0.30823232E 01 0.36576857E 01	0.19744698E-02 0.68663398E-05			3
-0.62041404E-08 0.18663103E-11 0.30146458E 05	0.20753460E 01			4
ALN(S)	J12/E2AL 1N 100 000 0S	300.000 3000.000		1
0.47798460E 01 0.20198156E-02-0.12548670E-05	0.36283351E-09-0.39253241E-13			2
-0.40062784E 05-0.26091961E 02-0.77586359E-01	0.17140061E-01-0.1794725E-04			3
0.72995522E-08-0.55492557E-12-0.38837390E 05	0.15105473E 01			4
ALN	J 3/E7AL 1N 100 000 0G	300.000 5000.000		1
0.40281038E 01 0.56420940E-03-0.22198395E-06	0.42074947E-10-0.29421886E-14			2
0.51028644E 05 0.21456703E 01 0.22442305E 01	0.39470202E-07-0.32513003E-05			3
0.58151994E-09 0.29409153E-12 0.51346866E 05	0.32192666E 01			4
ALC	J 9/E5AL 1C 100 000 0G	300.000 5000.000		1
0.39717174E 01 0.63212200E-03-0.25846015E-06	0.49488774E-10-0.33027940E-14			2
0.95752335E 04 0.32492563E 01 0.29297104E 01	0.31210445E-02-0.13586470E-05			3
-0.11939557E-08 0.89331277E-12 0.98709961E 04	0.85935845E 01			4
ALO+	J E/E8AL 1C 1E -10 0G	300.000 5000.000		1
0.89679966E 01-0.29837240E-02 0.66474433E-06	0.33295343E-10-0.27636991E-14			2
0.11691005E 06-0.27323300E 02 0.52645833E 01	0.14004473E-01 0.38815976E-04			3
-0.29971726E-07 0.55888964E-11 0.11957910E 05	0.15025924E 01			4
ALGCL	J 9/E4AL 1C 100 100 0G	300.000 5000.000		1
0.67395200E 01 0.79662822E-03-0.34233355E-06	0.65922649E-10-0.45519107E-14			2
-0.44030372E 05-0.23132976E 01 0.32444400E 01	0.11117005E-01-0.19322038E-04			3
0.11952798E-07-0.27059180E-11-0.43312343E 05	0.70922149E 01			4
ALCF	J 3/E4AL 1C 1F 100 0G	300.000 5000.000		1
0.64253366E 01 0.11928086E-02-0.51432842E-06	0.98028793E-10-0.68852831E-14			2
-0.72744337E 05-0.23256977E 01 0.17646910E 01	0.17328839E-01-0.22537031E-04			3
0.12459245E-07-0.23292213E-11-0.71691933E 05	0.13607771E 02			4
ALFH	J12/E7AL 1H 10 10 0G	300.000 5000.000		1
0.36350674E 01 0.33365222E-02-0.12466244E-05	0.21392205E-09-0.13898319E-13			2
-0.23046105E 05 0.36769915E 01 0.26132211E 01	0.27716294E-02 0.74157830E-05			3

```

-0.11354602E-07 0.45569559E-11-0.22586797E 05 0.10062166E 02 4
ALOH+ J12/E7AL 10 1H 1F -1G 300.000 5000.000 1
0.41624797E 01 0.28687165E-02-0.10416171E-05 0.17575550E-09-0.11271622E-13 2
-0.15314295E 04 0.25596643E 01 0.19486482E 01 0.80052285E-02-0.25070514E-05 3
-0.37733979E-05 0.24906051E-11-0.50847219E 03 0.14141875E 02 4
ALOH- J12/67AL 10 1H 1E 1G 300.000 5000.000 1
0.43010718E 01 0.21668503F-02-0.73968645E-06 0.11821055E-09-0.72209941E-14 2
-0.29134095E 05 0.3513A246E 01 0.29130204E 01 0.79530715E-02-0.30558054F-05 3
-0.12598709E-08 0.12886094E-11-0.28781827E 05 0.19309284E 02 4
AL02 J E/E9AL 10 20 00 05 300.000 5000.000 1
0.65519349E 01 0.10730596E-02-0.47379153E-06 0.91425195E-10-0.63074266E-14 2
-0.16146809E 03-0.85088553E 01 0.32187326E 01 0.12556176E-01-0.14970696E-04 3
0.76845277E-08-0.12520185E-11 0.61344440E 03 0.89519547E 01 4
AL02- J E/F9AL 10 2E 10 0G 300.000 5000.000 1
0.62810376E 01 0.13358850E-02-0.57146602E-06 0.10935642E-09-0.75932579E-14 2
-0.23262269E 05-0.86956341E 01 0.32378637E 01 0.10596234E-01-0.10216156E-04 3
0.34746059E-08 0.53681451E-13-0.22489188E 05 0.67504624E 01 4
AL02H J 3/E4AL 10 2H 100 05 300.000 5000.000 1
0.64270590E 01 0.32216643F-02-0.12130266F-05 0.21051077E-09-0.13807379E-13 2
-0.33973090E 05-0.74745628E 01 0.24468083E 01 0.16385868E-01-0.16625070E-04 3
0.70661078E-08-0.64131253E-12-0.33025991E 05 0.12433532E 02 4
AL20L6 J 3/E4AL 2CL 600 000 0G 300.000 5000.000 1
0.20530991E 02 0.13027630E-02-0.56153351E-06 0.10690317E-09-0.74906297E-14 2
-0.16217187E 06-0.62572214E 02 0.12171270E 02 0.36713644E-01-0.55603458E-04 3
0.35113797E-07-0.97237068E-11-0.16042879E 06-0.20882840E 02 4
AL20 J 9/E5AL 20 100 000 05 300.000 5000.000 1
0.61309407E 01 0.96280169E-03-0.41516089E-06 0.79211578E-10-0.55717813E-14 2
-0.17829876E 05-0.44030124E 01 0.34117107E 01 0.96963909E-02-0.10306122E-04 3
0.42754762E-08-0.32573380E-12-0.17165738E 05 0.92734405E 01 4
AL20+ J 6/E8AL 20 1E -10 0G 300.000 5000.000 1
0.61392920E 01 0.94849579E-03-0.40671071E-06 0.77111009E-10-0.54019669E-14 2
0.71439805E 05-0.40782213E 01 0.33910609E 01 0.98468013E-02-0.10650036E-04 3
0.46034848E-08-0.43845353E-12 0.72108359E 05 0.97297393E 01 4
AL202 J 9/E5AL 20 200 000 0G 300.000 5000.000 1
0.77227053E 01 0.25161623E-02-0.10830293E-05 0.20637292E-09-0.14502168E-13 2
-0.51613929E 05-0.13589237E 02 0.19995687E 01 0.19382190E-01-0.16555045E-04 3
0.32432492E-08 0.13877467E-11-0.50096135E 05 0.16211774E 02 4
AL202+ J 6/E8AL 20 2E -10 0G 300.000 5000.000 1
0.80829239E 01 0.21259693E-02-0.91683420E-06 0.17488147E-09-0.12295690E-13 2
0.63056018E 05-0.14431880E 02 0.18140836E 01 0.22238435E-01-0.23492898E-04 3
0.94504231E-08-0.55539774E-12 0.64593715E 05 0.17091430F 02 4
AL203(S) J 3/E4AL 20 300 000 05 300.000 2315.000 1
0.12533023E 02 0.26483766E-02-0.11252155E-08-0.25404213E-09 0.50340293E-13 2
-0.20591407E 06-0.67517363E 02-0.25071773E 01 0.62271160E-01-0.89040804E-04 3
0.60690359E-07-0.15530953E-10-0.20281921E 06 0.53456899E 01 4
AL203(L) J 3/E4AL 20 300 000 0L 2315.000 5000.000 1
0.17422481E 02 0. 0. 0. 0. 2
-0.19704127E 06-0.93759984E 02 0. 0. 0. 3
0. 0. 0. 0. 4
AP L 5/E6AR 100 000 000 0G 300.000 5000.000 1
0.25000000F 01 0. 0. 0. 0. 2
-0.74537502E 03 0.43660005E 01 0.25000000F 01 0. 0. 3
0. 0. -0.74537499E 03 0.43660005E 01 4
AR+ L12/6EAR 1E -100 000 0G 300.000 5000.000 1
0.28420672E 01-0.97648603E-04-0.25463209E-07 0.12240311E-10-0.11895130E-14 2
0.13272563E 06 0.36720201F 01 0.24957001F 01-0.55682680E-03 0.33194849E-05 3
-0.39236795E-05 0.14143279E-11 0.19290215E 06 0.53990154E 01 4
E(S) J12/6AR 10 00 00 05 300.000 2456.000 1
0.21353842E 01 0.62384824E-03 0.52269843F-06-0.34412816E-09 0.54070294E-13 2
-0.87167211E 03-0.12048034E 02-0.13181931E 01 0.11950484E-01-0.19999163F-04 3
0.21567584E-08 0.12019863E-11-0.45997194E 02 0.51212201E 01 4
E(L) J12/E4R 10 00 00 0L 2459.000 5000.000 1
0.36735752E 01 0. 0. 0. 0. 2
0.41164170E 03-0.21048345E 02 0. 0. 0. 3
0. 0. 0. 0. 4
E J12/E4R 100 000 000 0G 300.000 5000.000 1

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 0.37549335E 01 0.33439583E-02-0.12505263E-05 0.21556827E-09-0.24114778E-13 2
 0.96194409E 05 0.14057049E 01 0.24619220E 01 0.36977984E-02 0.59446561E-05 3
 -0.10392932E-07 0.43337733E-11 0.96693753E 05 0.88341593E 01 4
 BE02H2 J 3/E7RE 10 2H 200 0G 300.000 5000.000 1
 0.64853231E 01 0.58388339E-02-0.21839203E-05 0.37665248E-09-0.24568934E-13 2
 -0.81124230E 05-0.93680114E 01 0.24681022E 01 0.13712514E-01-0.16655536E-04 3
 0.62752159E-03-0.30697537E-12-0.80137138E 05 0.10955417E 02 4
 BE20 J 9/E3RE 20 100 000 0G 300.000 5000.000 1
 0.54549734E 01 0.21970305E-02-0.92919578E-06 0.17496410E-09-0.12199932E-13 2
 -0.94958985E 04-0.56835860E 01 0.27527897E 01 0.89648699E-02-0.55359247E-05 3
 -0.34769188E-09 0.11015472E-11-0.87174709E 04 0.84387556E 01 4
 BE20F2 J 9/E6RE 20 1F 200 0G 300.000 5000.000 1
 0.10311343E 02 0.29258151E-02-0.12481987E-05 0.23652169E-09-0.16559160E-13 2
 -0.14844623E 06-0.24500846E 02 0.48600026E 01 0.19438982E-01-0.18818760E-04 3
 0.71009503E-08-0.37225258E-12-0.14703959E 06 0.32285704E 01 4
 BE202 J 9/E3RE 20 200 000 0G 300.000 5000.000 1
 0.31783652E 01 0.30796926E-02-0.13162273E-05 0.24970614E-09-0.17496339E-13 2
 -0.51944876E 05-0.12938758E 02 0.17102739E 01 0.13244939E-01-0.14377253E-04 3
 0.21268816E-08 0.14691993E-11-0.50512366E 05 0.15201347E 02 4
 BE303 J 9/E3RE 30 300 000 0G 300.000 5000.000 1
 0.91507322E 01 0.73623701E-02-0.31292729E-05 0.59162569E-09-0.41360194E-13 2
 -0.13631849E 06-0.23330943E 02 0.26002692E 01 0.29085172E-01 0.57517347E-06 3
 -0.17092805E-07 0.84822785E-11-0.12826867E 06 0.15607790E 02 4
 BE404 J 9/E3RE 40 400 000 0G 300.000 5000.000 1
 0.14547030E 02 0.31903730E-02-0.35162789E-05 0.56923457E-09-0.47005963E-13 2
 -0.19704845E 06-0.51509929E 02-0.13813438E 01 0.52384824E-01-0.40893018E-04 3
 0.47379707E-08 0.49954164E-11-0.19278356E 06 0.39399903E 02 4
 C(S) J 3/E1C 10 00 00 0S 300.000 5000.000 1
 0.13604942E 01 0.19182237E-02-0.84040389E-06 0.16443737E-09-0.11672670E-13 2
 -0.55713870E 03-0.80076207E 01-0.44773053E 00 0.57691002E-02-0.39775571E-06 3
 -0.49459298E-08 0.21134939E-11-0.94280684E 02 0.16340791E 01 4
 C J 3/E1C 100 000 000 0G 300.000 5000.000 1
 0.25310663E 01-0.14696202E-03 0.74388084E-07-0.79481079E-11 0.58900977E-16 2
 0.85215294E 05 0.43128879E 01 0.25328705E 01-0.15887641E-03 0.30682082E-06 3
 -0.26770064E-09 0.87488227E-13 0.85240422E 05 0.45062334E 01 4
 C+ L12/E6C 1E -100 000 0G 300.000 5000.000 1
 0.25118274E 01-0.17359784E-04 0.95042678E-08-0.2218518E-11 0.18621892E-15 2
 0.21657721E 06 0.42281293E 01 0.2595340E 01-0.4068884E-03 0.63923669E-06 3
 -0.52654878E-09 0.15083377E-12 0.21666781E 06 0.34957299E 01 4
 C- J 9/E5C 1E 100 000 0G 300.000 5000.000 1

0.24473591E 01 0.11246424E-03-0.78591462E-07 0.19774614E-10-0.11105555E-14 2
 0.64977969E 05 0.42356992E 01 0.24925640E 01 0.53153068E-04-0.13307934E-06 3
 0.13951379E-09-0.52150992E-13 0.69955757E 05 0.39911657E 01 4
 CCL J 3/61C 1CL 100 000 0G 300.000 5000.000 1
 0.41416363E 01 0.40539002E-03-0.16439027E-06 0.30720262E-10-0.21188745E-14 2
 0.65103661E 05 0.31912321E 01 0.32157640E 01 0.24535798E-02-0.14566418E-05 3
 -0.34501102E-09 0.54359252E-12 0.65354358E 05 0.79740016E 01 4
 CCL2 J 3/65C 1CL 200 000 0G 300.000 5000.000 1
 0.61038747E 01 0.98444553E-03-0.42074189E-06 0.79586589E-10-0.55531496E-14 2
 0.35712188E 05-0.34096661E 01 0.33799227E 01 0.94958893E-02-0.95663552E-05 3
 0.34526939E-03-0.20523433E-13 0.36333677E 05 0.10347469E 02 4
 CCL3 J12/67C 1CL 30 00 0G 300.000 5000.000 1
 0.89058150E 01 0.12216951E-02-0.52931166E-06 0.10131824E-09-0.71437484E-14 2
 0.64579494E 04-0.15547647E 02 0.37933250E 01 0.21999101E-01-0.30090668E-04 3
 0.18562205E-07-0.41715884E-11 0.76531895E 04 0.11422041E 02 4
 CCL4 J 3/61C 1CL 400 000 0G 300.000 5000.000 1
 0.11545200E 02 0.16301810E-02-0.70898111E-06 0.13620159E-09-0.9635049E-14 2
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 CF J12/67C 1F 10 00 0G 300.000 5000.000 1
 0.36869679E 01 0.91143491E-03-0.36463855E-06 0.67492854E-10-0.45269596E-14 2
 0.28471666E 05 0.41513468E 01 0.34655143E 01-0.68779805E-03 0.56784765E-05 3
 -0.64582987E-08 0.22988248E-11 0.23649139E 05 0.53621916E 01 4
 CF2 J 9/66C 1F 200 000 0G 300.000 5000.000 1
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 0.71580200E 01 0.30960154E-02-0.13231685E-05 0.25123920E-09-0.17625389E-13 2
 -0.60854305E 05-0.11141522E 02 0.23610822E 01 0.15999621E-01-0.11811474E-04 3
 0.11443435E-08 0.14709076E-11-0.59534051E 05 0.13665263E 02 4
 CF4 J 9/64C 1F 400 000 0G 300.000 5000.000 1
 0.91592519E 01 0.42023641E-02-0.18038973E-05 0.34302737E-09-0.24082193E-13 2
 -0.11442802E 06-0.23264057E 02 0.11839609E 01 0.27053319E-01-0.23009336E-04 3
 0.52459959E-08 0.14077342E-11-0.11231908E 06 0.17592463E 02 4
 CH J12/67C 1H 10 00 0G 300.000 5000.000 1
 0.22673116E 01 0.22043000E-02-0.62250191E-06 0.69649940E-10-0.21274952E-14 2
 0.70338037E 05 0.87829352E 01 0.35632752E 01-0.20031372E-03-0.40129814E-06 3
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 CH2 J12/62C 1H 200 000 0G 300.000 5000.000 1
 0.27710460E 01 0.40693659E-02-0.14683470E-05 0.24552095E-09-0.15593090E-13 2
 0.46787215E 05 0.47848903E 01 0.26950905E 01 0.36051519E-02 0.79977157E-06 3
 -0.27242167E-08 0.12361950E-11 0.46841314E 05 0.53857501E 01 4
 CH3 J12/62C 1H 300 000 0G 300.000 5000.000 1
 0.26916371E 01 0.63035521E-02-0.26088477E-05 0.45775393E-09-0.30236995E-13 2
 0.14915942E 05 0.58225816E 01 0.33479834E 01 0.19909241E-02 0.64982411E-05 3
 -0.63603524E-08 0.17971111E-11 0.14925320E 05 0.30286042E 01 4
 CH4 J 3/61C 1H 400 000 0G 300.000 5000.000 1
 0.15027072E 01 0.10416798E-01-0.39181522E-05 0.67777829E-09-0.44283706E-13 2
 -0.99737073E 04 0.10707143E 02 0.33261932E 01-0.39794581E-02 0.24558340E-04 3
 -0.22732926E-07 0.69626957E-11-0.10144095E 05 0.85690073E 00 4
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 0.36050744E 01 0.73345861E-03 0.14255732E-06-0.16970505E-10-0.30100883E-15 2
 0.54691625E 05 0.35369408E 01 0.37313064E 01-0.18635137E-02 0.45586474E-05 3
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 CN- L 3/67C 1N 1F 100 0G 300.000 5000.000 1
 0.29314417E 01 0.14942613E-02-0.58261650E-06 0.10444145E-09-0.70091727E-14 2
 0.32277995E 04 0.62544561E 01 0.35984234E 01-0.15289018E-02 0.34408627E-05 3
 -0.17432245E-08 0.12144973E-12 0.31164095E 04 0.24951093E 01 4
 CN2 J 6/66C 1N 200 000 0G 300.000 5000.000 1
 0.43209077E 01 0.24790014E-02-0.94644109E-06 0.16548764E-09-0.10890170E-13 2
 0.68695948E 05-0.48840339E 00 0.35077779E 01 0.72023953E-02-0.75574589E-05 3
 0.42979217E-03-0.94257935E-12 0.63994281E 05 0.60274964E 01 4
 CO J 9/65C 1O 100 000 0G 300.000 5000.000 1
 0.29340636E 01 0.14891390E-02-0.57899684E-06 0.10364577E-09-0.69353550E-14 2
 -0.14245224E 05 0.67479156E 01 0.37100928E 01-0.16190964E-02 0.36923504E-05 3

-0.20319674E-08	0.23053344E-12	-0.14356310E	05	0.2355351F	01	4
COCL	J12/EFC	10	1CL	100	06	1
0.54291236E	01	0.16121535E-02	-0.56006280E-06	0.12127114E-09	-0.82858601F-14	2
-0.93305007E	04	0.36271816E	00	0.42863792E	01	3
0.29647993E-09	-0.77093453E-12	-0.90125212E	04	0.6238030AF	01	4
COCL2	J 6/61C	10	1CL	200	06	1
0.77318082E	01	0.24089287E-02	-0.10111133F-05	0.18936214E-09	-0.13139356F-13	2
-0.29136566E	05	-0.11221874F	02	0.31156139E	01	3
0.12868184E-07	-0.27380865E-11	-0.28043884E	05	0.11755299E	02	4
CCF	J12/EFC	10	1F	100	05	1
0.48998214E	01	0.22179703E-02	-0.92550725E-06	0.12720120E-09	-0.11955343E-13	2
-0.22357984E	05	0.97962087E	00	0.32019727E	01	3
-0.23126069E-08	0.13614353E-11	-0.21817043E	05	0.10047575E	02	4
CCF2	J 3/E5C	10	1F	200	06	1
0.65651527E	01	0.36511407E-02	-0.15332311E-05	0.23720949E-09	-0.19930265E-13	2
-0.78818912E	05	-0.31745228E	01	0.17992182E	01	3
0.19894624E-08	0.11147281E-11	-0.77502762E	05	0.16468950E	02	4
CCS	J 3/E1C	10	1S	100	05	1
0.52392000E	01	0.24100584E-02	-0.96064522E-06	0.17778347E-09	-0.12235704E-13	2
-0.18450455E	05	-0.30910517E	01	0.24625321E	01	3
0.80707736E-08	-0.18327653E-11	-0.17803987E	05	0.19792556E	02	4
CO2	J 2/E5C	10	200	000	06	1
0.44604041E	01	0.30981719F-02	-0.12392571E-05	0.22741325E-09	-0.15525954E-13	2
-0.43961442E	05	-0.98635982E	00	0.24007797E	01	3
0.20021861E-08	0.63274039E-15	-0.48377527E	05	0.96951457E	01	4
CO2-	J12/E6C	10	2E	100	05	1
0.45454640E	01	0.26054316E-02	-0.10928732E-05	0.20454421E-09	-0.14184542E-13	2
-0.54761968E	05	0.18317369E	01	0.34743737E	01	3
-0.99554255E-08	0.36846719E-11	-0.54249049E	05	0.83834329E	01	4
CP	J 6/E2C	1P	100	000	06	1
0.37436112E	01	0.93811496E-03	-0.34116216E-06	0.63775863E-10	-0.44094630E-14	2
0.54969175E	05	0.42305583E	01	0.32335857E	01	3
-0.48985936E-08	0.18766551E-11	0.55196565E	05	0.72701279E	01	4
CS	J12/E2C	1S	100	000	06	1
0.36942533E	01	0.89082274E-03	-0.36800044E-06	0.63778176E-10	-0.47810000E-14	2
0.26452213E	05	0.39176032E	01	0.33093030E	01	3
-0.55253895E-08	0.20392463E-11	0.26658986E	05	0.62942707E	01	4
CS2	J 6/E1C	1S	20	00	06	1
0.59867719E	01	0.16354436E-02	-0.68384845E-06	0.12936890E-09	-0.89167448E-14	2
0.12043850E	05	-0.63998223E	01	0.32144238E	01	3
0.52967662E-08	-0.83022695E-12	0.12745374E	05	0.76195765E	01	4
C2	J 9/61C	200	000	000	06	1
0.41718859E	01	-0.58280144E-04	0.26982465E-06	-0.70416507E-10	0.54949130E-14	2
0.99055653E	05	0.57669265E	00	0.74313577E	01	3
0.13955573E-08	-0.26415452E-11	0.98305909E	05	-0.15764619E	02	4
C2-	J 6/E6C	2E	100	000	06	1
0.36714582F	01	0.80537803E-03	-0.30000042E-06	0.52416166E-10	-0.34375224F-14	2
0.62231672E	05	0.31137872E	01	0.47910076E	01	3
0.24415444E-03	-0.16350431E-11	0.61963602E	05	-0.25794733E	01	4
C2F2	J12/67C	2F	20	00	06	1
0.75164581E	01	0.31686462E-02	-0.13311385E-05	0.24960049E-09	-0.17342072E-13	2
-0.16107655E	03	-0.15081225E	02	0.35345837E	01	3
0.36042985E-08	0.19118951E-12	0.92133562E	03	0.54063023E	01	4
C2H	J 3/E7C	2H	100	000	06	1
0.44297550E	01	0.22119303E-02	-0.59294945E-06	0.94195775E-10	-0.68577594E-14	2
0.55835444E	05	-0.11582893E	01	0.26499400E	01	3
0.65373629E-08	-0.17356273F-11	0.56275751E	05	0.76998609F	01	4
C2HF	J12/67C	2H	1F	10	06	1
0.60949501E	01	0.39432429E-02	-0.14711438F-05	0.25294641E-09	-0.16446663E-13	2
0.12976907E	05	-0.43285075E	01	0.26901770E	01	3
0.14920568E-07	-0.37381925E-11	0.13683223E	05	0.31338073E	01	4
C2H2	J 3/E1C	2H	200	000	06	1
0.45751083E	01	0.51238353F-02	-0.17452354E-05	0.29673065E-09	-0.17951426F-13	2
0.25607428E	05	-0.35737940E	01	0.14192768E	01	3
0.16390872E-07	-0.41345447E-11	0.26188202E	05	0.11393827E	02	4
C2H4	J 9/E5C	2H	400	000	06	1

0.34557152F	01	0.11491803E-01-0.43651750E-05	0.76195095E-09-0.50123200F-13	2
0.44773119E	04	0.26987959E 01 0.14256821E 01	0.11383140E-01 0.79890006E-05	3
-0.16293679E-07	0.67491256E-11	0.53370755E 04	0.14621812F 02	4
C2N	J 3/E7C	2N 100 000 05	300.000 5000.000	1
0.61931308E	01	0.14327539E-07-0.61255161F-06	0.11578707E-09-0.80401339E-14	2
0.64318372E	05-0.84132293E 01	0.32670394E 01	0.99211307E-02-0.83284733E-05	3
0.17650559E-08	0.59632763F-12	0.65589057E 05	0.65692304E 01	4
C2N2	J 3/E1C	2N 200 000 06	300.000 5000.000	1
0.65964935E	01	0.39694131F-02-0.15516161F-05	0.23141546E-09-0.19069442F-13	2
0.34383726E	05-0.10001801E 02	0.39141787E 01	0.14011009E-01-0.17404350E-04	3
0.12012779E-07-0.33565772E-11	0.35514550E 05	0.32384353E 01		4
C20	J 9/E6C	20 100 000 05	300.000 5000.000	1
0.48990313E	01	0.28430384E-02-0.10209669E-05	0.16112165E-09-0.95542914E-14	2
0.32800545E	05-0.91382230E 00	0.35364315F 01	0.69543972E-02-0.53071374E-05	3
0.17030470E-08-0.14108072E-13	0.33151572E 05	0.60172370E 01		4
C3	J12/E0C	300 000 000 06	300.000 5000.000	1
0.47644293E	01	0.27986049E-02-0.11477808E-05	0.21170654E-09-0.14535373E-13	2
0.93736510E	05-0.28157600F 01	0.28254880E 01	0.80526503E-02-0.62007661E-05	3
0.20458584E-08-0.11040561E-12	0.94293793E 05	0.72657659E 01		4
C302	J 6/E8C	30 20 00 06	300.000 5000.000	1
0.81435964E	01	0.54395013E-02-0.22192869E-05	0.40778627E-09-0.27915974F-13	2
-0.14230013E	05-0.15456769E 02	0.37161005F 01	0.19972164E-01-0.20935751E-04	3
0.11750112E-07-0.26529416E-11-0.13089402E	05	0.69298412E 01		4
CL	J 3/E1CL	100 000 000 06	300.000 5000.000	1
0.29595315E	01-0.41899860E-03	0.15980973E-06-0.29102717E-10	0.14673826E-14	2
0.13659143E	05	0.30350159E 01	0.20888310E 01	3
0.22408564E-08-0.33258769E-12	0.13936331E 05	0.72655033E 01		4
CL+	J 6/E5CL	1E -100 000 06	300.000 5000.000	1
0.31290605E	01-0.64678626E-03	0.25414315E-06-0.38607442E-10	0.20947135E-14	2
0.16543356E	06	0.24486633E 01	0.19783295E 01	3
0.63250309E-08-0.16313361E-11	0.16562590E 05	0.77975420E 01		4
CL-	J 6/E5CL	1E 100 000 06	300.000 5000.000	1
0.25000000E	01	0.	0.	2
-0.28874558E	05	0.41872263E 01	0.25000000E 01	3
0.	0.	-0.23874558E 05	0.41372971E 01	4
CLCN	J 6/E6CL	1C 1N 100 06	300.000 5000.000	1
0.54920021E	01	0.20987243E-02-0.77415914E-06	0.13823882E-09-0.92334864E-14	2
0.14749161E	05-0.37436191E 01	0.33390854E 01	0.10397438E-01-0.13704650E-04	3
0.95061962E-08-0.25925260E-11	0.15237539E 05	0.68178759E 01		4
CLF	J 9/E5CL	1F 100 000 06	300.000 5000.000	1
0.41550345E	01	0.43195995E-03-0.16153995E-06	0.30453169E-10-0.21170113E-14	2
-0.74382128E	04	0.22303899E 01	0.23480871E 01	3
0.23634468E-08-0.24187423F-12-0.71277968E	04	0.37639116E 01		4
CLF3	J 9/E5CL	1F 300 000 06	300.000 5000.000	1
0.89535967E	01	0.11722163F-02-0.50895188E-06	0.97567489E-10-0.69858731E-14	2
-0.22075968E	05-0.18094713E 02	0.24949119E 01	0.24718550E-01-0.35139323E-04	3
0.2259591E-07-0.53261979E-11-0.20798640E	05	0.11388534E 02		4
CLO	J 6/E1CL	1C 100 000 06	300.000 5000.000	1
0.40912619E	01	0.50003126E-03-0.13778206F-06	0.35097671E-10-0.24205038E-14	2
0.10853223E	05	0.36057382E 01	0.28179364E 01	3
0.15920942E-08-0.14486242E-13	0.11171397E 05	0.10944828E 02		4
CLC2	J 3/E1CL	10 200 000 06	300.000 5000.000	1
0.57249758E	01	0.14645230F-02-0.59984351E-06	0.11398750E-09-0.79794776E-14	2
0.10606264E	05-0.25921838E 01	0.28878166E 01	0.92876003E-02-0.70824040E-05	3
0.63453376E-09	0.96201805E-12	0.11367377E 05	0.12006873E 02	4
CL2	J 9/E5CL	200 000 000 05	300.000 5000.000	1
0.43077814E	01	0.31182816E-03-0.15310807E-06	0.44511913E-10-0.43057753E-14	2
-0.13458251E	04	0.20666664F 01	0.31316886E 01	3
0.44785641E-08-0.10621859F-11-0.10979696F	04	0.77813424E 01		4
CL20	J12/E5CL	20 100 000 06	300.000 5000.000	1
0.64340062F	01	0.62723309F-03-0.26933252F-06	0.51976394E-10-0.35691545F-14	2
0.84850530E	04-0.49492767E 01	0.32545232E 01	0.12799449E-01-0.17882460E-04	3
0.11264333E-07-0.25984257E-11	0.21657423E 04	0.10558059E 02		4
CS(S)	J 6/E8CS	10 00 00 05	300.000 301.550	1
0.	0.	0.	0.	2
0.	0.	0.31827762F 01-0.49703905E-02	0.13569579E-04	3

0.89561402E-07-0.24031942E-09-0.96298877E 03-0.75956980F 01 4
 CS(L) J 6/68CS 10 00 00 0L 301.550 1500.000 1
 0.33147045E 01 0.52267349E-03-0.45641926E-04-0.95936037E-11 0.55471632E-13 2
 -0.70109826E 03-0.78759204E 01 0.47696835E 01-0.49137505E-02 0.84861109E-05 3
 -0.64184384E-08 0.18034315E-11-0.10158892E 04-0.14960727E 02 4
 CS J 6/68CS 10 00 00 0G 300.000 5000.000 1
 0.18710101E 01 0.14068071E-02-0.10636222E-05 0.30523738E-09-0.19977219E-13 2
 0.86814554E 04 0.10235611E 02 0.24999466E 01 0.10332792E-05-0.35771191E-09 3
 0.49283910E-11-0.19810542E-14 0.84737829E 04 0.63627707E 01 4
 CS+ J 6/68CS 1E -10 00 0G 300.000 5000.000 1
 0.25000000E 01 0. 0. 0. 0. 2
 0.53653730E 05 0.61694923E 01 0.25000000E 01 0. 0. 3
 0. 0. 0.53653730E 05 0.61694925E 01 4
 CSCL(S) J 6/68CS 1CL 10 00 0S 300.000 743.000 1
 0. 0. 0. 0. 0. 2
 0. 0. 0.55453400E 01 0.23305934E-02 0.93570330E-05 3
 -0.99571640E-09 0.38054803E-12-0.55026535E 05-0.20164260E 02 4
 CSCL(S) J 6/68CS 1CL 10 00 0S 743.000 918.000 1
 0. 0. 0. 0. 0. 2
 0. 0. 0.81610737E 01-0.17623568E-02-0.22508516E-06 3
 0.39307317E-08-0.23452341E-11-0.55490431E 05-0.33941396E 02 4
 CSCL(L) J 6/68CS 1CL 10 00 0L 918.000 5000.000 1
 0.33097452E 01 0. 0. 0. 0. 2
 -0.55031161E 05-0.40910133E 02 0.93097452E 01 0. 0. 3
 0. 0. -0.55031161E 05-0.40810133E 02 4
 CSCL J 6/68CS 1CL 10 00 0G 300.000 5000.000 1
 0.44798455E 01 0.10949164E-03-0.39989914E-08 0.20541995E-12 0.22184640E-16 2
 -0.30235809E 05 0.52041565E 01 0.41823030E 01 0.13759553E-02-0.20586233E-05 3
 0.14336474E-08-0.39764546E-12-0.30177927E 05 0.66253273E 01 4
 CSF(S) J 6/68CS 1F 10 00 0S 300.000 976.000 1
 0. 0. 0. 0. 0. 2
 0. 0. 0.56489993E 01 0.19711398E-02 0.66242382E-06 3
 -0.63084871E-09 0.18692339E-12-0.64485102E 05-0.22149959E 02 4
 CSF(L) J 6/68CS 1F 10 00 0L 976.000 5000.000 1
 0.89071617E 01 0. 0. 0. 0. 2
 -0.68066817E 05-0.39912774E 02 0.89071617E 01 0. 0. 3
 0. 0. -0.68066817E 05-0.39912774E 02 4
 CSF J 6/68CS 1F 10 00 0G 300.000 5000.000 1
 0.44373309E 01 0.12715000E-03-0.20547650E-07 0.29813357E-11-0.14774245E-15 2
 -0.44227995E 05 0.32603925E 01 0.37449870E 01 0.30100516E-02-0.45883816E-05 3
 0.32179694E-08-0.83782017E-12-0.44090696E 05 0.71317098E 01 4
 CS2 J 6/68CS 20 00 00 0G 300.000 5000.000 1
 0.46411470E 01 0.10244908E-03 0.10701307E-08 0.55978765E-10-0.77877416E-14 2
 0.11367604E 05 0.76209601E 01 0.45116580E 01 0.17392705E-03 0.36388656E-06 3
 -0.41459947E-09 0.16395515E-12 0.11426704E 05 0.83824693E 01 4
 CS2CL2 J 6/68CS 2CL 20 00 0G 300.000 5000.000 1
 0.99424375E 01 0.62659303E-04-0.26331097E-07 0.43912142E-11-0.33554152E-15 2
 -0.82345855E 05-0.10611221E 02 0.92952112E 01 0.28505600E-02-0.45576019E-05 3
 0.32557731E-08-0.86067362E-12-0.82222862E 05-0.75315139E 01 4
 CS2F2 J 6/68CS 2F 20 00 0G 300.000 5000.000 1
 0.94793725E 01 0.12674229E-03-0.50905253E-07 0.89711762E-11-0.58090960E-15 2
 -0.11005057E 05-0.14067985E 02 0.84425561E 01 0.64921001E-02-0.10832757E-04 3
 0.81791054E-08-0.23173978E-11-0.10978165E 06-0.72614081E 01 4
 E L02/67E 10 00 00 0G 300.000 5000.000 1
 0.25000000E 01 0. 0. 0. 0. 2
 -0.74537496E 03-0.11734026E 02 0.25000000E 01 0. 0. 3
 0. 0. -0.74537500E 03-0.11734026E 02 4
 F J 6/65F 100 000 000 0G 300.000 5000.000 1
 0.27004353E 01-0.22293182E-03 0.97941385E-07-0.19123038E-10 0.13768154E-14 2
 0.87167617E 04 0.38067182E 01 0.28128740E 01-0.33023089E-05-0.12897310E-05 3
 0.16837365E-08-0.64587833E-12 0.86604019E 04 0.30984108E 01 4
 F- J 6/65F 1E 100 000 0G 300.000 5000.000 1
 0.25000000E 01 0. 0. 0. 0. 2
 -0.32044752E 05 0.314845E 01 0.25000000E 01 0. 0. 3
 0. 0. -0.32044752E 05 0.32514846E 01 4
 FCN J 6/61F 1C 1N 100 0G 300.000 5000.000 1

0.50921100E 01	0.24183203E-02-0.97912239E-06	0.17890124E-09-0.12194228E-13	2
-0.32576687E 04	-0.2966F061F 01	0.32675754E 01	3
0.48438881E-08	-0.10902993E-11-0.27875650E 04	0.63527737E 01	4
F0	J12/6EF 10	100 000 00	1
0.39192774E 01	0.70442345E-03-0.26643204E-06	0.49617599E-10-0.33628571E-14	2
0.11793193E 05	0.33155951E 01	0.29680024E 01	3
-0.19066225E-08	0.10614263F-11	0.12087644E 05	4
F02	J 9/FEF 10	200 000 00	1
0.57040935E 01	0.13662889E-02-0.58355374E-06	0.10937214E-09-0.75869181E-14	2
-0.39679673E 03	-0.20810205E 01	0.37505073E 01	3
0.17562504E-08	0.67757430E-13	0.12769462E 03	4
F2	J12/E0F 20	00 00 00	1
0.40397806E 01	0.60869035E-03-0.21494672E-06	0.40596803E-10-0.28294433E-14	2
-0.13123536E 04	0.99528039E 00	0.28445997E 01	3
0.47418780E-09	0.35556237E-12-0.59911761E 03	0.71131622E 01	4
FE(S)	J 3/65FE 100	000 000 05	1
0.40283341E 02	-0.25054763E-01-0.24866004E-04	0.11749263E-07	2
-0.20310190E 05	-0.23775925E 03	0.32514004E 01	3
-0.49585132E-07	0.26137444E-10-0.83324322E 03	-0.14209130E 02	4
FE(S)	J 3/65FE 100	000 000 05	1
0.32005394E 01	0.75484421E-03	0.	2
-0.17210443E 03	-0.14-10926E 02	0.	3
0.	0.	0.	4
FE(S)	J 3/65FE 100	000 000 05	1
0.34018312E 01	0.90581305E-03	0.	2
-0.59567541E 03	-0.16078804E 02	0.	3
0.	0.	0.	4
FE(L)	J 3/65FE 100	000 000 01	1
0.49215842E 01	0.20129179E-03	0.	2
-0.35541952E 03	-0.25191420E 02	0.	3
0.	0.	0.	4
FE	J 3/65FE 100	000 000 00	1
0.34436538E 01	-0.14011625E-02	0.81291351E-06-0.16290473E-09	2
0.49122684E 05	0.25061140E 01	0.26358458E 01	3
0.90994257E-08	-0.28812664E-11	0.49187400E 05	4
FECL	J 6/65FE 100	000 000 00	1
0.46940669E 01	0.11604073E-03-0.20840175E-07	-0.17626556E-11	2
0.28790344E 05	0.41803970E 01	0.37885326E 01	3
0.41797454E-08	-0.94686773E-12	0.29920697E 05	4
FECL2(S)	J 6/65FE 100	000 000 05	1
0.	0.	0.	2
0.	0.	0.71307661E 01	3
0.13155868E-07	-0.40011518E-11-0.43600855E 05	-0.29072053E 02	4
FECL2(L)	J 6/65FE 100	000 000 01	1
0.1228276E 02	0.	0.	2
-0.41107855E 05	-0.53190515E 02	0.1228276E 02	3
0.	0.	-0.41107855E 05	4
FECL2	J 6/65FE 100	000 000 00	1
0.79569177E 01	-0.10430791E-03	0.43393993E-07-0.16106576E-10	2
-0.20226258E 05	-0.18752118E 02	0.38434440E 01	3
0.31321714E-07	-0.89050091E-11-0.19671549E 05	0.77677010E 01	4
FECL3(S)	J 6/65FE 100	000 000 05	1
0.	0.	0.	2
0.	0.	0.11306993E 02	3
0.57778464E-06	-0.19460654E-09-0.51090473E 05	-0.51237249E 02	4
FECL3(L)	J 6/65FE 100	000 000 01	1
0.16102574E 02	0.	0.	2
-0.43435533E 05	-0.67614581E 02	0.16102574E 02	3
0.	0.	-0.43435533E 05	4
FECL3	J 6/65FE 100	000 000 00	1
0.97771106E 01	0.24421362E-03-0.10313944E-06	0.19297426E-10-0.13179299E-14	2
-0.33439578E 05	-0.14562301F 02	0.75614373E 01	3
0.11126368E-07	-0.30022998E-11-0.33013624E 05	-0.39929867E 01	4
FECL(S)	J 6/65FE 100	000 000 05	1
0.58316449E 01	0.14275156E-02-0.93208143E-07	-0.65997763E-11-0.22512147E-13	2
-0.34556902E 05	-0.26446990E 02	0.53195475E 01	3
		0.22096591E-02	4

-0.27929729E-08	0.13320733E-11	-0.34407165E	05	-0.23696034E	02		4
FE0(L)	J 6/65FE	10	100	000	0L	1650.000 5000.000	1
0.82022482E	01	0.		0.		0.	2
-0.33343615E	05	-0.40079129E	02	0.		0.	3
0.	0.	0.		0.		0.	4
FE0	J 9/66FE	10	100	000	0G	300.000 5000.000	1
0.42049317E	01	0.26834452E	-03	-0.89426736E	-07	0.3185911E-10-0.33022543E-14	2
0.28829170E	05	0.48172666E	01	0.28245256E	01	0.43049207E-02-0.41984781E-05	3
0.13201139E	-03	0.71316217E	-13	0.29194035E	05	0.11979013E	4
FE02H2	J12/66FE	10	2H	200	0G	300.000 5000.000	1
0.87968421E	01	0.45844405E	-02	-0.14408771E	-05	0.34177402E-09-0.23047931E-13	2
-0.42754562E	05	-0.17856573E	02	0.14918172E	01	0.38499255E-01-0.61500984E-04	3
0.46635112E	-07	-0.1330872E	-10	-0.41450948E	05	0.16384301E	4
FE02H2(S)	J 6/66FE	10	2H	200	0S	300.000 1500.000	1
0.74031808E	01	0.11921742E	-01	-0.14957611E	-05	0.50526359E-03 0.20037111E-11	2
-0.71592266E	05	-0.34673267E	02	0.10091218E	02	0.44523141E-02 0.40666855E-05	3
-0.40094525E	-03	0.23947164E	-12	-0.2277655E	05	0.44400034E	4
FE03H3(S)	J 6/66FE	10	3H	300	0S	300.000 1500.000	1
0.80223926E	01	0.16420135E	-01	-0.12369378E	-06	0.68192839E-08 0.23276907E-11	2
-0.10321336E	06	-0.37934020E	02	0.44116836E	01	0.32682467E-01-0.22393815E-04	3
0.28646792E	-08	0.22622321E	-11	-0.10271834E	06	0.21331014E	4
H	J 9/65H	100	000	000	0G	300.000 5000.000	1
0.25000000E	01	0.		0.		0.	2
0.25471627E	05	-0.46011763E	00	0.25000000E	01	0.	3
0.	0.	0.25471627E	05	-0.46011762E	00		4
H+	J 6/66H	1E	-100	000	0G	300.000 5000.000	1
0.25000000E	01	0.		0.		0.	2
0.18403344E	06	-0.11538620E	01	0.25000000E	01	0.	3
0.	0.	0.18403344E	06	-0.11538621E	01		4
H-	J 9/65H	1E	100	000	0S	300.000 5000.000	1
0.25000000E	01	0.		0.		0.	2
0.15961045E	05	-0.11524488E	01	0.25000000E	01	0.	3
0.	0.	0.15961045E	05	-0.11524486E	01		4
HALO	J 3/64H	1AL	10	100	0G	300.000 5000.000	1
0.43556053E	01	0.29599933E	-02	-0.12152921E	-05	0.22986419E-09-0.16047592E-13	2
0.21454053E	04	-0.32954973E	01	0.13980220E	01	0.77763784E-02 0.15224672E-05	3
-0.86539734E	-08	0.41709380E	-11	0.31156301E	04	0.12763795E	4
HBO	J12/64H	18	1C	100	0S	300.000 5000.000	1
0.39902745E	01	0.35116761E	-02	-0.14167746E	-05	0.25804765E-09-0.17539792E-13	2
-0.11539403E	05	0.41315742E	00	0.27000640E	01	0.67921406E-02-0.43161135E-05	3
0.21375092E	-08	0.43790703E	-12	-0.11132099E	05	0.72359559E	4
HBO+	J 6/68H	18	1C	1E	-1G	300.000 5000.000	1
0.44547347E	01	0.31423614E	-02	-0.12961293E	-05	0.23975605E-09-0.16390748E-13	2
0.15694872E	06	-0.50143149E	00	0.29798548E	01	0.61956382E-02-0.29948031E-05	3
0.13452306E	-09	0.20881907E	-12	0.16744444E	06	0.73616124E	4
HBO2	J12/64H	18	1C	200	0G	300.000 5000.000	1
0.47383519E	01	0.47718771E	-02	-0.18063494E	-05	0.31492889E-09-0.20738312E-13	2
-0.69243339E	05	-0.33347135E	-02	0.29707966E	01	0.73962644E-02-0.40736842E-06	3
-0.47059022E	-08	0.23548893E	-11	-0.68624111E	05	0.10167820E	4
HBN	J 3/61H	1C	1N	100	0G	300.000 5000.000	1
0.37415749E	01	0.32984095E	-02	-0.12107871E	-05	0.29523624E-09-0.13190218E-13	2
0.14395272E	05	0.18847219E	01	0.24471319E	01	0.87763873E-02-0.10219808E-04	3
0.68098182E	-08	0.17913449E	-11	0.14653425E	05	0.30959213E	4
HCO	J 3/61H	1C	1C	100	0G	300.000 5000.000	1
0.37366720E	01	0.33912031E	-02	-0.12957623E	-05	0.22679230E-09-0.14952372E-13	2
-0.26430557E	04	0.69479829E	01	0.37929190E	01	0.47361919E-04 0.57306920E-05	3
-0.54606603E	-08	0.1619628E	-11	-0.26288218E	04	0.52070412E	4
HCO+	J 6/66H	1C	1C	1F	-1G	300.000 5000.000	1
0.37043178E	01	0.31689422E	-02	-0.11162077E	-05	0.13295523E-09-0.11423033E-13	2
0.19159997E	06	0.22646685E	01	0.24008375E	01	0.94708997E-02-0.12325029E-04	3
0.37365750E	-03	-0.24046919E	-11	0.10131650E	06	0.33016940E	4
HCL	J 9/64H	1CL	100	000	0G	300.000 5000.000	1
0.27665454E	01	0.14281833E	-02	-0.46993000E	-06	0.73499408E-10-0.43731106E-14	2
-0.11917468E	05	0.64983409E	01	0.35248171E	01	0.29924862E-04-0.86221891E-06	3
0.20979721E	-08	-0.0858191E	-12	-0.12150509E	05	0.23957713E	4
HF	J12/62H	1F	100	000	0S	300.000 5000.000	1

0.30075250E 01 0.68441682E-03-0.49447506E-07-0.16420127E-10 0.23547944E-14 2
 -0.33454373E 05 0.37266479E 01 0.34614364E 01 0.36544235E-03-0.10911244E-05 3
 0.12951449E-08-0.40567802E-12-0.33648707E 05 0.10945702E 01 4
 H02 J 3/E4H 10 200 000 0G 300.000 5000.000 1
 0.37866280E 01 0.27585404E-02-0.10165709E-05 0.17193946E-09-0.11021552E-13 2
 0.11888500E 04 0.48147611E 01 0.35094850E 01 0.11499670E-02 0.58784259E-05 3
 -0.77735519E-08 0.29607883E-11 0.13803331E 04 0.68276325E 01 4
 H2 J 3/E1H 20 00 00 0G 300.000 5000.000 1
 0.31001901E 01 0.51119464E-03 0.52644210E-07-0.34969973E-10 0.36945345E-14 2
 -0.87738042E 03-0.19629421E 01 0.30574451E 01 0.26765200E-02-0.59099162E-05 3
 0.55210391E-08-0.18122739E-11-0.98890474E 03-0.22997056E 01 4
 H20(S) L11/65H 20 100 000 0S 200.000 273.150 1
 0. 0. 0. 0. 0. 2
 0. 0. -0.39269330E-01 0.16920420E-01 0. 3
 0. 0. -0.35949581E 05 0.55933784E 00 4
 H20(L) L11/65H 20 100 000 0L 273.150 373.150 1
 0. 0. 0. 0. 0. 2
 0. 0. 0.12712752E 02-0.17662790E-01-0.22556661E-04 3
 0.20820908E-06-0.24078614E-09-0.37483200E 05-0.59115345E 02 4
 H20 J 3/61H 20 100 000 0G 300.000 5000.000 1
 0.27167633E 01 0.29451374E-02-0.80224374E-06 0.10226682E-09-0.48472145E-14 2
 -0.29905826E 05 0.66305671E 01 0.40701275E 01-0.11084439E-02 0.41521180E-05 3
 -0.29637404E-08 0.80702103E-12-0.30279722E 05-0.32270046E 00 4
 H2S J12/65H 2S 100 000 0G 300.000 5000.000 1
 0.28479103E 01 0.38415990E-02-0.14099367E-05 0.24278754E-09-0.15783283E-13 2
 -0.34469739E 04 0.74791412E 01 0.35311293E 01-0.13211956E-03 0.36517726E-05 3
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 H38306 J12/64H 38 30 600 0G 300.000 5000.000 1
 0.20153579E 02 0.13016286E-01-0.50669619E-05 0.90308253E-09-0.60532410E-13 2
 -0.28104092E 06-0.79689531E 02-0.22705116E 01 0.87024834E-01-0.91587714E-04 3
 0.39445392E-07-0.36666035E-11-0.27569523E 02 0.32516454E 02 4
 HE L 5/66HE 100 000 000 0G 300.000 5000.000 1
 0.25000000E 01 0. 0. 0. 0. 2
 -0.74537493E 03 0.91534888E 00 0.25000000E 01 0. 0. 3
 0. 0. -0.74537498E 03 0.91534884E 00 4
 HE+ L12/66HE 1E -100 000 0G 300.000 5000.000 1
 0.25000000E 01 0. 0. 0. 0. 2
 0.24534266E 06 0.16084045E 01 0.25000000E 01 0. 0. 3
 0. 0. 0.24534266E 06 0.16034046E 01 4
 K(S) J12/61K 10 00 00 0S 300.000 336.350 1
 0. 0. 0. 0. 0. 2
 0. 0. 0.17263229E 01-0.98042772E-04 0.13852978E-04 3
 0.57915802E-07-0.11734935E-09-0.69166994E 03-0.23234372E 01 4
 K(L) J12/61K 10 00 00 0L 336.350 2000.000 1
 0.32625048E 01-0.13113792E-03 0.50811991E-06 0.62810507E-10-0.51130459E-13 2
 -0.52525237E 03-0.96002325E 01 0.44202110E 01-0.19475966E-02 0.61695016E-06 3
 0.89316043E-09-0.33655604E-12-0.96275784E 03-0.16042437E 02 4
 K J 6/62K 100 000 000 0G 300.000 5000.000 1
 0.25673650E 01-0.14933596E-03 0.12342444E-06-0.53394240E-10 0.11945426E-13 2
 0.99550531E 04 0.46642081E 01 0.24930967E 01 0.50164177E-04-0.12751224E-06 3
 0.13540491E-09-0.51145936E-13 0.99786380E 04 0.50560478E 01 4
 K+ J 3/65K 1E -100 000 0G 300.000 5000.000 1
 0.25000000E 01 0. 0. 0. 0. 2
 0.61096558E 05 0.43339455E 01 0.25000000E 01 0. 0. 3
 0. 0. 0.61096558E 05 0.43339455E 01 4
 KCL(S) J 3/66K 1CL 100 000 0S 300.000 1044.000 1
 0.89157169E 01-0.20927271E-02 0.47310192E-05 0.70152537E-09-0.55146099E-11 2
 -0.52747066E 05-0.10144200E 02 0.53934311E 01 0.26535242E-02 0.96075655E-06 3
 -0.50251843E-08 0.40721228E-11-0.54748383E 05-0.21536814E 02 4
 KCL(L) J 3/66K 1CL 100 000 0L 1044.000 5000.000 1
 0.88518064E 01 0. 0. 0. 0. 2
 -0.53369478E 05-0.40010059E 02 0. 0. 0. 3
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 KCL J 3/66K 1CL 100 000 0G 300.000 5000.000 1
 0.44635733E 01 0.12229207E-03-0.91719210E-09 0.92645247E-12-0.10407017E-16 2
 -0.27173133E 05 0.32349330E 01 0.39908569E 01 0.21099169E-02-0.31836530E-05 3

0.22525308E-08-0.59094179E-12-0.27080184E 05 0.5498A475E 01 4
 K0 J12/E2K 10 100 000 05 300.000 5000.000 1
 0.43731489E 01 0.19960449E-03-0.56826345E-07 0.10410356E-10-0.7029136A7-15 2
 0.37491801E 04 0.32551045E 01 0.33905136E 01 0.41932012E-02-0.6123994E-05 3
 0.40675370E-08-0.99172754E-12 0.39512947E 04 0.80473015E 01 4
 K2 J12/E1K 200 000 000 06 300.000 5000.000 1
 0.45039995E 01 0.22596406E-03 0.14957172E-07-0.39911532E-11 0.34052376E-15 2
 0.13926067E 05 0.42568563E 01 0.44424903E 01 0.4615A726E-03-0.30025595E-06 3
 0.17502910E-09-0.32470554E-13 0.13941670E 05 0.45868357E 01 4
 K20(S) J 6/E3K 20 100 000 05 300.000 5000.000 1
 0.86890737E 01 0.51097493E-02-0.2036650AE-06 0.53747271E-10-0.10899A23E-14 2
 -0.46449235E 05-0.39589233E 02 0.34449691E 01 0.40567031E-01-0.92051685E-04 3
 0.790060A6E-07-0.27313775E-10-0.4592545AE 05-0.17395210E 02 4
 LI(S) J 6/E2LI 10 00 00 05 300.000 453.690 1
 0. 0. 0. 0. 0. 2
 0. 0. 0.91818617E 01-0.35999310E-01 0.24881854E-05 3
 0.26456527E-06-0.34331039E-09-0.15199533E 04-0.30945954E 02 4
 LI(L) J 6/E2LI 11 00 00 0L 453.690 4000.000 1
 0.36114162E 01-0.18325283E-03 0.40743757E-07 0.26515630E-11-0.11572503E-14 2
 -0.74925732E 03-0.16352732E 02 0.39988094E 01 0.61335444E-03-0.48307646E-05 3
 0.61290368E-08-0.23400340E-11-0.37493992E 03-0.18156235E 02 4
 LI J 6/E2LI 100 000 000 06 300.000 5000.000 1
 0.24737695E 01 0.87439341E-04-0.93773573E-07 0.31327924E-10-0.1757990AE-14 2
 0.18568036E 05 0.25630288E 01 0.2510373AE 01-0.74235730E-04 0.18612567E-06 3
 -0.19540947E-09 0.73145266E-13 0.13551670E 05 0.23902453E 01 4
 LI+ J 3/E5LI 1E -100 000 06 300.000 5000.000 1
 0.25000000E 01 0. 0. 0. 0. 2
 0.81899068E 05 0.17406170E 01 0.25000000E 01 0. 0. 3
 0. 0. 0.8189906AE 05 0.17406170E 01 4
 LI(L) J 6/E2LI 10L 100 000 05 300.000 493.000 1
 0. 0. 0. 0. 0. 2
 0. 0. 0.41095245E 01 0.81891003E-02-0.11541874E-04 3
 0.10595395E-07-0.36457022E-11-0.50608266E 05-0.13298894E 02 4
 LI(L) J 6/E2LI 10L 100 000 0L 493.000 2000.000 1
 0.82149477E 01 0.56391361E-03-0.17350331E-05 0.76595009E-09-0.12379477E-12 2
 -0.50007322E 05-0.39808961E 02 0.10363028E 02-0.47179699E-02-0.16138317E-05 3
 0.80807174E-08-0.44459493E-11-0.50539120E 03-0.49921960E 02 4
 LI(L) J 6/E2LI 10L 100 000 05 300.000 5000.000 1
 0.42712143E 01 0.31400791E-03-0.1012317E-06 0.18451853E-10-0.1239A731E-14 2
 -0.24834442E 05 0.10285692E 01 0.29306905E 01 0.53338642E-02-0.65671979E-05 3
 0.38050160E-08-0.76117455E-12-0.246031A2E 05 0.73150321E 01 4
 LIF(S) J12/E3LI 1F 100 000 05 300.000 1121.300 1
 0.57937896E 01-0.49996725E-03 0.16297053E-05 0.12939534E-03-0.10559079E-11 2
 -0.75512641E 05-0.28854332E 02 0.17624503E 01 0.17550874E-01-0.2914354AE-04 3
 0.22333192E-07-0.69974890E-11-0.74816904E 05-0.99175903E 01 4
 LIF(L) J12/E3LI 1F 100 000 0L 1121.300 5000.000 1
 0.77191711E 01 0. 0. 0. 0. 2
 -0.73822749E 05-0.38813129E 02 0. 0. 0. 3
 0. 0. 0. 0. 4
 LIF J12/E3LI 1F 100 000 06 300.000 5000.000 1
 0.40476615E 01 0.56142555E-03-0.20377763E-06 0.39160917E-10-0.27107364E-14 2
 -0.41317801E 05 0.05825957E 00 0.28623386E 01 0.38923430E-02-0.29052641E-05 3
 0.24730751E-09 0.43954489E-12-0.41005091E 05 0.67357165E 01 4
 LIFO J 6/E5LI 1F 10 100 03 300.000 5000.000 1
 0.59926109E 01 0.11139200E-02-0.47888493E-06 0.91088332E-10-0.63849123E-14 2
 -0.131009A9E 05-0.53497665E 01 0.25001790E 01 0.12661717E-01-0.14157599E-04 3
 0.64506374E-08-0.74261431E-12-0.12265534E 05 0.12130855E 02 4
 LIH(S) J 9/E7LI 1H 100 000 05 300.000 951.800 1
 0. 0. 0. 0. 0. 2
 0. 0. 0.511812E 00 0.12127057E-01-0.86000336E-05 3
 0.56311555E-08-0.12693483E-11-0.11486991E 05-0.39894575E 01 4
 LIH(L) J 9/E7LI 1H 100 000 0L 951.800 5000.000 1
 0.749A1191E 01 0. 0. 0. 0. 2
 -0.1159132E 05-0.40047273E 02 0.74991191E 01 0. 0. 3
 0. 0. -0.11581826E 05-0.4004727AE 02 4
 LIH J 9/E7LI 1H 100 000 06 300.000 5000.000 1

0.35884297E	01	0.10727671E-02	-0.40194588E-06	0.77828557E-10	-0.49269644E-14	2
0.15717625E	05	-0.38820950E	00	0.34209486E	01	-0.69067366E-03
-0.62150348E	-03	0.21531755E	-11	0.15834945E	05	0.10525714E
LIN		J12/6ELI	1N	100	000	06
0.42253077E	01	0.39667187E	-03	-0.12493993E	-06	0.23174759E-10
0.33916952E	95	0.63768563E	00	0.24894300E	01	0.52212534E-02
0.37288997E	-08	-0.72355143E	-12	0.30216323E	05	0.72757056E
LIO		J 3/E4LI	10	100	000	06
0.41876205E	01	0.41186574E	-03	-0.14520296E	-06	0.27253070E-10
0.87795259E	04	0.12182630E	01	0.28383007E	01	0.51538626E-02
0.34114395E	-03	-0.61631343E	-12	0.90594314E	04	0.73999549E
LIG		J12/67LI	10	1E	10	06
0.41810217E	01	0.41785000E	-03	-0.15024843E	-06	0.29397732E-10
-0.93549702E	04	-0.15559110E	00	0.28515866E	01	0.50169880E-02
0.30399451E	-08	-0.47872969E	-12	-0.90778076E	04	0.64462719E
LICH(S)		J 3/66LI	10	1H	100	05
0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.63640356E	-01	0.30407600E-01
0.30692106E	-07	-0.66429719E	-11	-0.59331340E	05	-0.25794094E
LION(L)		J 3/66LI	10	1H	100	0L
0.10436979E	02	0.	0.	0.	0.	0.
-0.60109250E	05	-0.53641166E	02	0.10436979E	02	0.
0.	0.	0.	0.	-0.60109250E	05	-0.53641166E
LION		J 3/66LI	10	1H	100	06
0.40456064E	01	0.23824852E	-02	-0.82302724E	-06	0.13279161E-09
-0.31003210E	05	0.22590447E	01	0.32569330E	01	0.30440910E-02
-0.55750639E	-03	0.24765340E	-11	-0.30730637E	05	0.66566487E
LICN		J 9/66LI	10	1N	100	06
0.54123496E	01	0.12870625E	-02	-0.54667710E	-06	0.10314997E-09
0.19692302E	05	-0.43578702E	01	0.36701164E	01	0.72562177E-02
0.11628312E	-08	0.42704122E	-12	0.20271703E	05	0.66633305E
LI2		J 6/62LI	200	000	000	05
0.44338756E	01	0.22842941E	-03	-0.24519024E	-07	0.39448820E-11
0.24009747E	05	-0.17116905E	01	0.37418914E	01	0.31246294E-02
0.32618304E	-08	-0.85308216E	-12	0.24142156E	05	0.16940721E
LI2CL2		J 6/62LI	2CL	200	000	06
0.95245614E	01	0.52458834E	-03	-0.22337949E	-06	0.41951114E-10
-0.74990263E	05	-0.20044824E	02	0.52801351E	01	0.13344100E-01
0.20313359E	-07	-0.53433247E	-11	-0.74160003E	05	0.26612705E
LI2F2		J12/63LI	2F	200	000	05
0.92241415E	01	0.87023522E	-03	-0.37828706E	-06	0.72506822E-10
-0.11450290E	06	-0.21319163E	02	0.35813313E	01	0.27905498E-01
0.24668598E	-07	-0.62706615E	-11	-0.11336586E	05	0.53542154E
LI20(S)		J 3/64LI	20	100	000	05
0.42774776E	01	0.73921672E	-02	-0.52225090E	-06	0.17364426E-08
-0.73396278E	05	-0.21765497E	02	0.31727239E	00	0.36149356E-01
0.41796437E	-07	-0.11804048E	-10	-0.73106196E	05	0.22888330E
LI20(L)		J 3/64LI	20	100	000	0L
0.12076931E	02	0.	0.	0.	0.	0.
-0.71337921E	05	-0.65174974E	02	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.
LI20		J 3/64LI	20	100	000	06
0.65193748E	01	0.96879443E	-03	-0.41490506E	-06	0.73637337E-10
-0.22255325E	05	-0.10834722E	02	0.39721709E	01	0.97460921E-02
0.36391605E	-08	-0.75658880E	-13	-0.21596988E	05	0.25391411E
LI202		J 3/64LI	20	200	000	06
0.95275260E	01	0.53021013E	-03	-0.23005862E	-06	0.44030231E-10
-0.32132434E	05	-0.21872275E	02	0.55375232E	01	0.17344223E-01
0.19395629E	-07	-0.51207957E	-11	-0.31402044E	05	0.27114759E
LI202H		J 3/66LI	20	2H	200	06
0.89428600E	01	0.60583335E	-02	-0.22032892E	-05	0.37293081E-09
-0.94593042E	05	-0.21057433E	02	0.28083765E	01	0.24969700E-01
0.63288723E	-08	-0.64221372E	-12	-0.93070570E	05	0.99492004E
LI3CL3		J 6/62LI	3CL	300	000	06
0.14319440E	02	0.18854007E	-02	-0.81978330E	-06	0.15735494E-09
-0.12553351E	06	-0.42724175E	02	0.45745959E	01	0.39749239E-01

0.36294145E-07-0.85784700E-11-0.12353351E 06	0.46674442E 01	4
LI3F3 J12/63LI 3F 300 000 0G	300.000 5000.000	1
0.13091417E 02 0.32374694E-02-0.14000897E-05	0.2676663E-09-0.18855216E-13	2
-0.18679660E 06-0.41168173E 02 0.14982352E 01	0.43683009E-01-0.53290482E-04	3
0.23109960E-07-0.49220103E-11-0.13412906E 06	0.16334742E 02	4
MG(S) J 9/62MG 10 00 00 0S	300.000 922.000	1
0. 0. 0. 0. 0.	0.	2
0. 0. 0.20184771E 01	0.52825745E-02-0.89160059E-05	3
0.81194529E-08-0.23538706E-11-0.77246715E 03	0.88131212E 01	4
MG(L) J 9/62MG 10 00 00 0L	922.000 5000.000	1
0.26570516E 01 0.13083966E-02 0.	0. 0.	2
0.22868300E 03-0.10433817E 02 0.26570516E 01	0.13083966E-02 0.	3
0. 0. 0.22568300E 03	0.10433817E 02	4
MG J 9/62MG 100 000 000 0G	300.000 5000.000	1
0.24188605E 01 0.16145771E-03-0.99399205E-07	0.18989312E-10 0.91656165E-16	2
0.17039992E 05 0.40641123E 01 0.24988751E 01	0.87608205E-05-0.23614632E-07	3
0.26287528E-10-0.10308811E-13 0.17008321E 05	0.36263633E 01	4
MG+ J12/67MG 1E -10 00 0S	300.000 5000.000	1
0.25084828E 01-0.17499680E-04 0.12102317E-07	0.34320303E-11 0.34653473E-15	2
0.10571437E 06 0.42685235E 01 0.24961675E 01	0.27410788E-04-0.68663780E-07	3
0.72015616E-10-0.26930064E-13 0.10571774E 06	0.43307379E 01	4
MGCL J 3/66MG 1CL 100 000 0G	300.000 5000.000	1
0.43775833E 01 0.18934173E-03-0.54433592E-07	0.99491031E-11-0.66949611E-15	2
-0.65830826E 04 0.29762332E 01 0.33800534E 01	0.42813389E-02-0.64457333E-05	3
0.44472291E-08-0.11421727E-11-0.63826560E 04	0.77758327E 01	4
MGCL+ J 6/69MG 1CL 1E -10 0S	300.000 5000.000	1
0.63512344E 01-0.37967190E-02 0.24712945E-05	0.50823653E-09 0.33672625E-13	2
0.76480879E 05-0.83035040E 01 0.36012230E 01	0.34791859E-02-0.51353143E-05	3
0.34446337E-08-0.83848206E-12 0.77314688E 05	0.61207176E 01	4
MGCLF J 3/66MG 1CL 1F 100 0G	300.000 5000.000	1
0.55536109E 01 0.49503794E-03-0.21265567E-06	0.40342907E-10-0.29198241E-14	2
-0.70522498E 05-0.61610398E 01 0.39675363E 01	0.10495156E-01-0.14846158E-04	3
0.94797313E-08-0.22227485E-11-0.69974510E 05	0.64280836E 01	4
MSCL2(S) J12/65MG 1CL 200 000 0S	300.000 987.000	1
0. 0. 0. 0. 0.	0.	2
0. 0. 0.54491296E 01	0.16745224E-01-0.25956907E-04	3
0.19111573E-07-0.51059014E-11-0.79343894E 05	0.24261034E 02	4
MGCL2(L) J12/65MG 1CL 200 000 0L	987.000 5000.000	1
0.11071043E 02 0. 0. 0. 0.	0.	2
-0.76294618E 05-0.48972588E 02 0.11071043E 02	0. 0.	3
0. 0. -0.76294618E 05	0.48972588E 02	4
MGCL2 J12/65MG 1CL 200 000 0G	300.000 5000.000	1
0.66909609E 01 0.34055850E-03-0.14507415E-06	0.27277270E-10-0.18889997E-14	2
-0.50324903E 05-0.57783697E 01 0.44799697E 01	0.92693674E-02-0.13850184E-04	3
0.93638025E-08-0.23516224E-11-0.49874382E 05	0.48946211E 01	4
MGF J 3/67MG 1F 100 000 0G	300.000 5000.000	1
0.42110735E 01 0.36113259E-03-0.13239533E-06	0.24644432E-10-0.16919094E-14	2
-0.28059832E 05 0.23145832E 01 0.28664199E 01	0.51625813E-02-0.65086664E-05	3
0.36302039E-08-0.69177563E-12-0.27754352E 05	0.39564751E 01	4
MGF2(S) J 3/66MG 1F 200 000 0S	300.000 1536.000	1
0.66953750E 01 0.43922188E-02-0.11003584E-05	0.53362104E-09 0.31219775E-12	2
-0.13736474E 06-0.32490950E 02 0.21304880E 01	0.28542721E-01-0.45495513E-04	3
0.33548644E-07-0.9548251F-11-0.13678478E 06	0.12050724E 02	4
MGF2(L) J 3/66MG 1F 200 000 0L	1536.000 5000.000	1
0.11357889E 02 0. 0. 0. 0.	0.	2
-0.13400296E 06-0.57018423E 02 0. 0. 0.	0.	3
0. 0. 0. 0. 0.	0.	4
MGF2 J 3/66MG 1F 200 000 0G	300.000 5000.000	1
0.64284668E 01 0.63969935E-03-0.27809763E-06	0.53420244E-10-0.37812854E-14	2
-0.89226616E 05-0.60320744E 01 0.37706721E 01	0.10406351E-01-0.13695278E-04	3
0.80146506E-08-0.16568854E-11-0.88639643E 05	0.70214053E 01	4
MGR J12/66MG 1H 100 000 0G	300.000 5000.000	1
0.34638591E 01 0.12404055E-02-0.50278210E-06	0.93118834E-10-0.66183068E-14	2
0.13176310E 05 0.28845865E 01 0.35102397E 01	0.12368352E-02 0.64246998E-05	3
-0.65054346E-08 0.22803625E-11 0.19293893E 05	0.33604884E 01	4
PGN J 3/64MG 1N 100 000 0G	300.000 5000.000	1

0.42214417E	01	0.36489240E-03	0.12995730E-06	0.24419940E-10	0.16917759E-14	2		
0.33397931E	05	0.27188874E	01	0.28894549E	01	0.51757175E-02	0.65819016E-05	3
0.37218933E-08	0.72385964E-12	0.37681058E	05	0.92844249E	01	4		
MG0(S)	J12/E5HG	10	100	000	05	300.000	3098.000	1
0.51120198E	01	0.17231664E-02	0.90268818E-06	0.26460605E-09	0.28339967E-13	2		
-0.74094363E	05	0.26784367E	02	0.47740339E	00	0.21441338E-01	0.33453071E-04	3
0.24347437E-07	0.66578961E-11	0.77154228E	05	0.45934874E	01	4		
MG0(L)	J12/E5HG	10	100	000	0L	3098.000	5000.000	1
0.72964786E	01	0.	0.	0.	0.	2		
-0.67744028E	05	0.38362761E	02	0.	0.	3		
0.	0.	0.	0.	0.	0.	4		
MG0	J12/E5HG	10	100	000	03	300.000	5000.000	1
0.40654306E	01	0.54784296E-03	0.19704758E-06	0.36606637E-10	0.25102520E-14	2		
-0.81403801E	03	0.31030930E	01	0.28442075E	01	0.41055545E-02	0.35061249E-05	3
0.72885498E-09	0.27783024E-12	0.49777511E	03	0.93349957E	01	4		
MG0H	J E/E7HG	10	1H	100	0G	300.000	5000.000	1
0.44329606E	01	0.25811369E-02	0.91997733E-06	0.15151434E-09	0.93759909E-14	2		
-0.27755885E	05	0.25918925E	00	0.16842602E	01	0.10914848E-01	0.87026993E-05	3
0.13336126E-08	0.94723733E-12	0.27081380E	05	0.14150863E	02	4		
MSCH+	J E/E7HG	10	1H	1F	-13	300.000	5000.000	1
0.47424330E	01	0.22877007E-02	0.80398933E-06	0.13175298E-09	0.82324460E-14	2		
0.70323806E	05	0.18812567E	01	0.17246932E	01	0.13231006E-01	0.14929146E-04	3
0.73413788E-08	0.10182671E-11	0.70977879E	05	0.12933122E	02	4		
MG0H2	J E/E7HG	10	2H	200	0G	300.000	5000.000	1
0.73269210E	01	0.49370374E-02	0.18021108E-05	0.30460208E-09	0.19535992E-13	2		
-0.71137802E	05	0.10591697E	02	0.42789288E	01	0.15680923E-01	0.15568577E-04	3
0.74423876E-08	0.10867487E-11	0.70438934E	05	0.44899763E	01	4		
N	J 3/E1N	100	000	000	0G	300.000	5000.000	1
0.24502682E	01	0.10661458E-03	0.74653373E-07	0.18796524E-10	0.10259839E-14	2		
0.56116040E	05	0.44487581E	01	0.25030714E	01	0.21300191E-04	0.54205297E-07	3
-0.56475602E-10	0.20999044E-13	0.56098904E	05	0.41675764E	01	4		
NF	J E/65N	1F	100	000	0G	300.000	5000.000	1
0.38624046E	01	0.74409961E-03	0.29304178E-06	0.55130022E-10	0.38317928E-14	2		
0.28669390E	05	0.34570237E	01	0.30480680E	01	0.1956867E-02	0.94322448E-06	3
-0.29336643E-08	0.13504454E-11	0.23941633E	05	0.79992363E	01	4		
NF2	J 3/E4N	1F	200	000	0G	300.000	5000.000	1
0.57186890E	01	0.14102822E-02	0.80493363E-06	0.11421911E-09	0.80536431E-14	2		
0.30992965E	04	0.34489259E	01	0.25009872E	01	0.10721062E-01	0.92064150E-05	3
0.19027666E-08	0.71249647E-12	0.39376954E	04	0.12994042E	02	4		
NF3	J 3/E4N	1F	300	000	0G	300.000	5000.000	1
0.79754975E	01	0.22473715E-02	0.97077542E-06	0.18551042E-09	0.13066945E-13	2		
-0.18151986E	05	0.15632481E	02	0.12579876E	01	0.24357895E-01	0.27038511E-04	3
0.12176078E-07	0.13589121E-11	0.16539966E	05	0.13018394E	02	4		
NH	J12/E5N	1H	100	000	0G	300.000	5000.000	1
0.27741580E	01	0.13179393E-02	0.38379707E-06	0.54142146E-10	0.28838332E-14	2		
0.39959049E	05	0.57923234E	01	0.34889532E	01	0.24026519E-03	0.13456768E-05	3
0.22935931E-08	0.95757540E-12	0.39714793E	05	0.18654962E	01	4		
NH2	J12/E5N	1H	200	000	0G	300.000	5000.000	1
0.25769524E	01	0.35896090E-02	0.12276328E-05	0.19549576E-09	0.11873401E-13	2		
0.19335912E	05	0.79074890E	01	0.40385791E	01	0.10098163E-02	0.40120903E-05	3
-0.23095312E-08	0.39022837E-12	0.13973010E	05	0.52444285E	00	4		
NH3	J E/65N	1H	300	000	0G	300.000	5000.000	1
0.24155177E	01	0.61871211E-02	0.21785136E-05	0.37590090E-09	0.24448856E-13	2		
-0.64747177E	04	0.77043482E	01	0.35912768E	01	0.49328668E-03	0.83449322E-05	3
-0.83833385E-08	0.27299092E-11	0.66717143E	04	0.22520966E	01	4		
NO	J E/E3N	10	100	000	0G	300.000	5000.000	1
0.31390000E	01	0.13382281E-02	0.52899318E-06	0.95919332E-10	0.64847932E-14	2		
0.98283290E	04	0.67458125E	01	0.40459521E	01	0.3411743E-02	0.79819190E-05	3
-0.51139316E-08	0.15919076E-11	0.97453934E	04	0.29974988E	01	4		
NO+	J E/66N	10	1E	-100	0G	300.000	5000.000	1
0.28885488E	01	0.15217119E-02	0.57531241E-06	0.10051031E-09	0.65044294E-14	2		
0.11819245E	05	0.70027197E	01	0.36635056E	01	0.11544520E-02	0.21756088E-05	3
-0.48227472E-08	0.27847906E-12	0.11803369E	06	0.31779374E	01	4		
NOCL	J12/E5N	10	100	000	03	300.000	5000.000	1
0.54195728E	01	0.18136944E-02	0.66876691E-06	0.17297226E-09	0.84070915E-14	2		
0.44171534E	04	0.19183665E	00	0.40280304E	01	0.59426529E-02	0.55620366E-05	3

0.29353736E-08-0.66517496E-12	0.4A0344A0E	04	0.69647732E	01	4
N0F	J 6/E1N	10	1F	100	06
0.51906666E	01	0.13924266E-02-0.79642361E-06	0.14626364E-09-0.10097419E-13		2
-0.9675A164E	04-0.62298477E	00	0.32902070E	01	3
0.26529282E-08-0.29528815E-12-0.91566645E	04	0.91451185E	01		4
N02	J 9/E4N	10	200	000	03
0.46240771E	01	0.25260332E-02-0.10609499E-05	0.19879239E-09-0.137993A4E-13		2
0.22599900E	04	0.13324133E	01	0.34589236E	01
-0.95556725E-08	0.36195A81E-11	0.25152265E	04	0.43116983E	01
N02-	J12/E5N	10	2E	100	06
0.50794422E	01	0.20960322E-02-0.99523762E-06	0.16901079E-09-0.11743414E-13		2
-0.45039907E	05-0.16367650E	01	0.29474526E	01	3
-0.75758344E-08	0.34577493E-11-0.44317583E	05	0.10052399E	02	4
N02CL	J12/E5N	10	2CL	100	05
0.72062138E	01	0.29649809E-02-0.12641260E-05	0.23758750E-09-0.16524848E-13		2
-0.11366123E	04-0.99256667E	01	0.30702225E	01	3
0.25890139E-08	0.64589481E-12	0.76657034E	01	0.11618599E	02
N02F	J12/E5N	10	2F	100	06
0.69639166E	01	0.33554437E-02-0.14158297E-07	0.25622227E-09-0.19531606E-13		2
-0.15621287E	05-0.95806218E	01	0.22424380E	01	3
0.32719525E-08	0.59144703E-12-0.14364205E	05	0.14218996E	02	4
N2	J 9/E5N	20	00	00	06
0.28963194E	01	0.15154866E-02-0.57235277E-06	0.93807393E-10-0.65223555E-14		2
-0.90536184E	03	0.61615143E	01	0.36743261E	01-0.12031500E-02
-0.63217559E-09-0.22577253E-12-0.10611588E	04	0.23580424E	01		4
N2C	J 6/E6N	2C	100	000	06
0.59145719E	01	0.17176878E-02-0.73057492E-06	0.13912907E-09-0.96540216E-14		2
0.49688947E	05-0.73960996E	01	0.28823173E	01	3
0.38588460E-08-0.17324120E-12	0.50474679E	05	0.30410039E	01	4
N2H	J12/E5N	2H	400	000	06
0.50347770E	01	0.93256138E-02-0.33626986E-05	0.56308304E-09-0.35859661E-13		2
0.92996644E	04-0.35950952E	01	0.79503836E	00	3
-0.12698753E-09	0.25865213E-11	0.10379887E	05	0.19248696E	02
N20	J12/E4N	20	100	000	06
0.47306679E	01	0.28258267E-02-0.11558115E-05	0.21263683E-09-0.14564087E-13		2
0.81617682E	04-0.17151073E	01	0.26139195E	01	3
0.22275377E-05-0.90650330E-13	0.97590123E	04	0.92266952E	01	4
N204	J 9/E4N	20	400	000	06
0.10506637E	02	0.58723267E-02-0.24766296E-05	0.46556024E-09-0.32402082E-13		2
-0.29609096E	04-0.26252230E	02	0.36662865E	01	3
0.11845939E-08	0.20001618E-11-0.90631797E	03	0.93973337E	01	4
NA(S)	J 6/E2NA	10	00	00	05
0.	0.	0.	0.	0.	
0.	0.	0.24118570E	01	0.89751859E-03	0.10583331E-04
-0.71915700E-05-0.59226613E-11-0.93573157E	03-0.82157280E	01			4
NA(L)	J 6/E2NA	10	00	00	01
0.40097373E	01-0.12933184E-02	0.42443918E-06	0.52391272E-09-0.19396802E-12		2
-0.78115472E	03-0.15366128E	02	0.45673226E	01-0.25257108E-02	0.14840018E-05
0.3A590020E-10-0.92500845E-13-0.97421906E	03-0.18377804E	02			4
NA	J 6/E2NA	100	000	000	06
0.25625078E	01-0.13963284E-03	0.11292708E-06-0.42307732E-10	0.67057055E-14		2
0.12193782E	05	0.38957727E	01	0.24881226E	01
0.22671537E-09-0.95125266E-13	0.12215904E	05	0.42804839E	01	4
NA+	J 3/E5NA	1E	-100	000	06
0.25000000E	01	0.	0.	0.	
0.72599320E	05	0.35374014E	01	0.25000000E	01
0.	0.	0.72599330E	05	0.35374014E	01
NACL	J12/E4NA	1CL	100	000	05
0.44287931E	01	0.15677241E-03-0.23103383E-07	0.47153571E-11-0.28832557E-15		2
-0.23170300E	05	0.22878194E	01	0.37032286E	01
0.34639218E-08-0.91357521E-12-0.23028276E	05	0.57603243E	01		4
NAF	J 6/E4NA	1F	100	000	06
0.43344945E	01	0.25755040E-03-0.79672062E-07	0.14022311E-10-0.95933344E-15		2
-0.36623273E	05	0.12782543E	01	0.31808578E	01
0.46184859E-08-0.11271357E-11-0.36384975E	05	0.68634707E	01		4
NAH	J 3/E3NA	1H	100	000	05

0.38139579E 01	0.85643800E-03	0.31226816E-06	0.58502471E-10	0.40513924E-14	2
0.13633062E 05	0.47100265E 00	0.32203350E 01	0.13996217E-02	0.27141234E-05	3
-0.39950795E-08	0.16722173E-11	0.13940045E 05	0.47913959E 01		4
NAO	J12/E7NA 10	10 00 00	300.000	5000.000	1
0.43924158E 01	0.21320574E-03	0.46220543E-07	0.79751921E-11	0.51735989E-15	2
0.87118995E 04	0.23749263E 01	0.34421007E 01	0.41517241E-02	0.63118368E-05	3
0.44479194E-08	0.11720486E-11	0.83011477E 04	0.69371625E 01		4
NAO-	J12/E7NA 10	1E 10 05	300.000	5000.000	1
0.43368009E 01	0.22344672E-03	0.48212477E-07	0.85720862E-11	0.56004334E-15	2
-0.15946258E 05	0.10004509E 01	0.34186855E 01	0.42117382E-02	0.63104646E-05	3
0.43873515E-08	0.11372639E-11	0.15752234E 05	0.56553725E 01		4
NAOH(S)	J 3/EENA 10	1H 100 05	300.000	592.250	1
0.	0.	0.	0.	0.	2
0.	0.	0.69758356E 01	0.13845649E-01	0.11496912E-03	3
0.30593796E-06	0.22897632E-09	0.53448255E 05	0.37190109E 02		4
NAOH(L)	J 3/EENA 10	1H 100 01	592.250	5000.000	1
0.10774143E 02	0.70452126E-03	0.	0.	0.	2
-0.53503303E 05	0.52256959E 02	0.10774143E 02	0.70452126E-03	0.	3
0.	0.	-0.53503303E 05	0.52256959E 02		4
NACH	J 3/EENA 10	1H 100 06	300.000	5000.000	1
0.44705193E 01	0.19253365E-02	0.62522237E-06	0.95321167E-10	0.55722350E-14	2
-0.26809187E 05	0.23116081E 01	0.37588137E 01	0.41793587E-02	0.26998011E-05	3
0.22226965E-09	0.39074039E-12	0.25645967E 05	0.58652624E 01		4
NA2	J 6/E2NA 200	000 000 06	300.000	5000.000	1
0.44923659E 01	0.19571553E-03	0.22858417E-08	0.10132554E-11	0.10965752E-15	2
0.15136031E 05	0.20044163E 01	0.43197514E 01	0.91397957E-03	0.11333878E-05	3
0.79239225E-09	0.20379253E-12	0.15220419E 05	0.28326974E 01		4
NA2CL2	J12/E4NA 2CL	200 000 06	300.000	5000.000	1
0.98262001E 01	0.19184783E-03	0.81638743E-07	0.15298181E-10	0.10558994E-14	2
-0.71077149E 05	0.17049256E 02	0.79583953E 01	0.83962368E-02	0.13817116E-04	3
0.10277666E-07	0.28544994E-11	0.72725934E 05	0.31334799E 01		4
NA2F2	J 6/E4NA 2F	200 000 06	300.000	5000.000	1
0.97228777E 01	0.30413632E-03	0.12867473E-06	0.24005001E-10	0.16499168E-14	2
-0.10157399E 05	0.19427219E 02	0.69101947E 01	0.12457812E-01	0.20263984E-04	3
0.14892684E-07	0.40960013E-11	0.10134300E 06	0.60424822E 01		4
NE	L 5/E6NE 100	000 000 06	300.000	5000.000	1
0.25000000E 01	0.	0.	0.	0.	2
-0.74537500E 03	0.33420435E 01	0.25000000E 01	0.	0.	3
0.	0.	-0.74537494E 03	0.33420435E 01		4
NE+	L12/E6NE 1E	-100 000 06	300.000	5000.000	1
0.29285147E 01	0.41229320E-03	0.16341709E-06	0.29554891E-10	0.20056917E-14	2
0.25015219E 06	0.24159397E 01	0.21006406E 01	0.32416425E-02	0.56265881E-05	3
0.38693679E-08	0.93291304E-12	0.25029535E 06	0.67098678E 01		4
0	J 6/E7O 100	000 000 06	300.000	5000.000	1
0.25420542E 01	0.27550619E-04	0.31028033E-08	0.45510674E-11	0.43620515E-15	2
0.29230803E 05	0.49203080E 01	0.29464267E 01	0.16321665E-02	0.24210316E-05	3
-0.16029432E-08	0.39909664E-12	0.29147641E 05	0.29579949E 01		4
0+	L12/E6O 1E	-100 001 06	300.000	5000.000	1
0.25060488E 01	0.14464249E-04	0.12446040E-07	0.46958472E-11	0.65549873E-15	2
0.18794705E 06	0.43479741E 01	0.24984794E 01	0.11410972E-04	0.29761395E-07	3
0.32246539E-10	0.12375517E-13	0.18794705E 01	0.43224355E 01		4
C-	J 6/E6O 1E	100 000 06	300.000	5000.000	1
0.25437173E 01	0.53252700E-04	0.25119617E-07	0.71351465E-11	0.39011542E-15	2
0.11480516E 05	0.45202538E 01	0.23115795E 01	0.11975697E-02	0.10710553E-05	3
-0.13479179E-08	0.36682754E-12	0.11428431E 05	0.32402455E 01		4
OH	J 3/E6O 1H	100 000 06	300.000	5000.000	1
0.29106427E 01	0.95921650E-03	0.19441702E-06	0.13786546E-10	0.14224542E-15	2
0.39353815E 04	0.54423445E 01	0.39379943E 01	0.10778875E-02	0.26430378E-06	3
0.18713972E-02	0.22571094E-12	0.35412827E 04	0.49370909E 01		4
OH+	J 3/E6O 1H	1E -100 05	300.000	5000.000	1
0.27544309E 01	0.15025381E-02	0.49411191E-05	0.79367805E-10	0.49153427E-14	2
0.15759366E 05	0.60078407E 01	0.35447365E 01	0.19370343E-03	0.54786182E-06	3
0.18997588E-08	0.94577482E-12	0.15736596E 06	0.14173392E 01		4
OH-	J 3/E6O 1H	1E 100 06	300.000	5000.000	1
0.28772415E 01	0.99323674E-03	0.21102064E-06	0.17074239E-10	0.10219622E-15	2
-0.13124287E 05	0.22625863E 01	0.34554504E 01	0.45712454E-03	0.14904214E-05	3

0.19713513E-08-0.70807531F-12-0.14351348E 05 0.37134167E 00 4
 C2 J 9/E50 20 00 00 05 300.000 5000.000 1
 0.36219535E 01 0.73618264E-03-0.1965222AE-06 0.3620155AE-10-0.29945627E-14 2
 -0.12019825E 04 0.36150960E 01 0.36255985E 01-0.18782184E-02 0.70554544E-05 3
 -0.67635137E-08 0.21555993E-11-0.10475226E 04 0.43052778E 01 4
 G2- J12/E60 2E 100 000 06 300.000 5000.000 1
 0.31147234E 01 0.77444546E-03-0.30677649E-06 0.56619113E-10-0.38229492E-14 2
 -0.69913087E 04 0.29527995E 01 0.31440525E 01 0.12127972E-02 0.23812161E-05 3
 -0.40914092E-08 0.16825304E-11-0.67369752E 04 0.67648687E 01 4
 P J 6/E2P 100 000 00 03 300.000 5000.000 1
 0.2630262AE 01-0.17633559E-03 0.12025113E-07 0.33742455E-10-0.56423035E-14 2
 0.39352993E 05 0.46295137E 01 0.25016145E 01-0.71502000E-05 0.17900937E-07 3
 -0.19050206E-10 0.73374466E-14 0.30107793E 05 0.5365558AE 01 4
 P(S) J 6/E1P 10 00 06 05 300.000 900.000 1
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 0. 0. 0.11869142E 01 0.75957720E-02-0.13635426E-04 3
 0.13366476E-07-0.47391960E-11-0.59485421E 03-0.57859428E 01 4
 P+ J12/E6P 1E -100 000 06 300.000 5000.000 1
 0.29021547E 01-0.58878899E-03 0.31298119E-06-0.59727539E-10 0.39304925E-14 2
 0.16204407E 06 0.39205693E 01 0.43790417E 01-0.64666723E-02 0.99340962E-05 3
 -0.54858021E-08 0.12092857E-11 0.16174775E 06-0.33068769E 01 4
 PCL3 J 9/E2P 1CL 300 000 06 300.000 5000.000 1
 0.94865575E 01 0.56885645E-03-0.24353840E-06 0.46003911E-10-0.32010959E-14 2
 -0.33707085E 05-0.17113973E 02 0.53688177E 01 0.17652493E-01-0.27280124E-04 3
 0.19090652E-07-0.49399143E-11-0.32999165E 05 0.26507301E 01 4
 PF3 J12/E3P 1F 300 000 06 300.000 5000.000 1
 0.84299114E 01 0.17487864E-02-0.75710927E-06 0.14431909E-09-0.10220929E-13 2
 -0.10959235E 06-0.16492072E 02 0.23719035E 01 0.22753583E-01-0.27497236E-04 3
 0.14330466E-07-0.24023335E-11-0.19818123E 06 0.13590601E 02 4
 PH J 6/E7P 1H 100 000 06 300.000 5000.000 1
 0.30745442E 01 0.11698947E-02-0.30381654E-06 0.44436314E-10-0.27000975E-14 2
 0.29525775E 05 0.57548835E 01 0.36803433E 01-0.12756018E-02 0.25932442E-05 3
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 P13 J 6/E2P 1H 300 000 06 300.000 5000.000 1
 0.33448794E 01 0.65770941E-02-0.26336755E-05 0.47744600E-09-0.32354390E-13 2
 0.17937666E 04 0.39416278E 01 0.31581935E 01 0.24941492E-02 0.90255253E-05 3
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 PN J 9/E2P 1N 100 000 06 300.000 5000.000 1
 0.36419226E 01 0.64460672E-03-0.38923480E-06 0.73215826E-10-0.59961632E-14 2
 0.11333688E 05 0.41772775E 01 0.33755239E 01-0.41009386E-03 0.51265151E-05 3
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 0.38389008E 01 0.73137263E-03-0.29549285E-06 0.55095807E-10-0.33604882E-14 2
 -0.19713892E 04 0.45600736E 01 0.39692758E 01-0.27016040E-02 0.77324127E-05 3
 -0.78250095E-08 0.26509901E-11-0.14721788E 04 0.45414990E 01 4
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 0.43563526E 01 0.20240865E-03-0.78680674E-07 0.15193435E-10-0.81648517E-15 2
 0.93838309E 04 0.32161159E 01 0.37492024E 01 0.24320574E-02-0.31177915E-05 3
 0.17650760E-09-0.34202790E-12 0.95171437E 04 0.6197590AE 01 4
 P2 J 6/E1P 200 000 06 05 300.000 5000.000 1
 0.41611733E 01 0.39520800E-03-0.15580330E-06 0.29093474E-10-0.20042454E-14 2
 0.20148755E 05 0.22279293E 01 0.23391107E 01 0.48266193E-02-0.54947488E-05 3
 0.25400507E-08-0.32232453E-12 0.20459594E 05 0.33232470E 01 4
 P4 J 6/E1P 400 000 06 05 300.000 5000.000 1
 0.92252739E 01 0.36854123E-03-0.3775833AE-06 0.72379666E-10-0.51066109E-14 2
 0.12490323E 05-0.19254868E 02 0.35353300E 01 0.24125292E-01-0.36462759E-04 3
 0.24916906E-07-0.63294563E-11 0.13635707E 05 0.77427326E 01 4
 S(S) J12/E5S 10 00 00 05 300.000 388.360 1
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 0. 0. -0.50637425E 01 0.28319353E-02-0.21330205E-04 3
 0.84747862E-05-0.17344967E-08 0.71482679E 03 0.28714074E 02 4
 S(L) J12/E5S 10 00 00 01 388.360 2000.000 1
 0.36536672E 01 0.99033405E-03-0.10114410E-05 0.46536327E-00-0.56679135E-13 2
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 0.13078137E-06-0.35276150E-12 0.12346069E 04 0.54210169E 02 4
 S J12/E5S 100 000 00 00 300.000 5000.000 1

0.29119165F 01-0.56000F35F-03 0.23155555F-06-0.50994412E-10 0.31945420F-14 2
 0.32726267F 05 0.37725044E 01 0.29293157F 01 0.19994083E-03-0.23314920F-05 3
 0.28521102E-08-0.10656090F-11 0.32F86945E 05 0.35000372E 01 4
 S+ L12/6ES 1E -100 000 03 300.000 5000.000 1
 0.24118653E 01 0.22103303E-03-0.18939564E-06 0.61326675E-10-0.53887720E-14 2
 0.15375732E 06 0.58881130F 01 0.25038214E 01-0.62479521E-04 0.15513305E-06 3
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 SF4 J 9/6ES 1F 400 000 06 300.000 5000.000 1
 0.10753578E 02 0.25135146E-02-0.10920195E-05 0.209F2472E-09-0.14A20130F-13 2
 -0.91407009E 05-0.28295056E 02 0.65243888E 00 0.39223804E-01-0.50882830E-04 3
 0.29292955E-07-0.59164774E-11-0.89149574E 05 0.21447238E 02 4
 SF6 J 9/6ES 1F 600 000 06 300.000 5000.000 1
 0.15286816F 02 0.41541264E-02-0.18053249E-05 0.34670283F-09-0.24523633E-13 2
 -0.15234672E 06-0.55069672F 02-0.11646703E 01 0.64060912E-01-0.83337512F-04 3
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 SH J 6/67S 1H 100 000 06 300.000 5000.000 1
 0.30371352E 01 0.12752466E-02-0.42314345E-06 0.67719688E-10-0.40934312F-14 2
 0.16545437E 05 0.60722981E 01 0.44098953E 01-0.220E3747E-02 0.13171081E-05 3
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 0.38493376E 01 0.72756788E-03-0.29370203E-06 0.55013628E-10-0.38123551E-14 2
 0.30459962E 05 0.44179139E 01 0.39422971F 01-0.20035515E-02 0.73534644F-05 3
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 SO J12/65S 10 100 000 06 300.000 5000.000 1
 0.38280162E 01 0.75593144E-03-0.30791631E-06 0.57820156E-10-0.40204449E-14 2
 -0.43632695E 03 0.44528198E 01 0.31224222F 01 0.13727342E-02 0.20611937E-05 3
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 SCF2 J 9/65S 10 1F 200 06 300.000 5000.000 1
 0.81678120E 01 0.20156607E-02-0.86557421F-06 0.16471939E-09-0.11568374E-13 2
 -0.70763942E 05-0.14145544E 02 0.26905686E 01 0.29314017E-01-0.23187553E-04 3
 0.11328486E-07-0.16744583E-11-0.69453573F 05 0.13247024E 02 4
 S02 J 6/61S 10 200 000 06 300.000 5000.000 1
 0.52451364E 01 0.19704204E-02-0.20375769E-06 0.15149969E-09-0.10558004E-13 2
 -0.37558227E 05-0.10873524E 01 0.32665338E 01 0.53237902E-02 0.68437552E-06 3
 -0.52310047E-03 0.25590454E-11-0.35905143E 05 0.96513476E 01 4
 SC2F2 J 3/63S 10 2F 200 06 300.000 5000.000 1
 0.97589416E 01 0.35349972E-02-0.15103050E-05 0.28648297E-09-0.20072393E-13 2
 -0.10668096E 06-0.23029853E 02 0.26823217E 01 0.25219822E-01-0.24789168F-04 3
 0.93820305E-08-0.44501989E-12-0.10487605E 06 0.12842633E 02 4
 S03 J 9/6ES 10 300 000 06 300.000 5000.000 1
 0.70757376E 01 0.31763387E-02-0.13535760E-05 0.25630912E-09-0.17936044E-13 2
 -0.50211376E 05-0.11200793E 02 0.25780385E 01 0.14556335E-01-0.91764173E-05 3
 -0.79203022E-09 0.19709473E-11-0.48931753F 05 0.12251863E 02 4
 S2 J12/65S 200 000 000 06 300.000 5000.000 1
 0.42051134E 01 0.35309150E-03-0.13543069E-06 0.25245375E-10-0.17357439E-14 2
 0.14182904E 05 0.32094717E 01 0.28724248E 01 0.59434461E-02-0.62055277E-05 3
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 SI(S) J 3/67SI 100 000 000 06 300.000 1635.000 1
 0.24753989E 01 0.38112187E-03-0.20939481E-06 0.42757187E-11 0.15006567F-13 2
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 SI(L) J 3/67SI 100 000 000 01 1635.000 5000.000 1
 0.32799915E 01 0. 0. 0. 0. 2
 0.48546547E 04-0.13289281E 02 0. 0. 0. 3
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 0.26506014E 01-0.35763852E-03 0.29592203E-06-0.72804829E-10 0.57963320E-14 2
 0.53437054E 05 0.52204057E 01 0.31792137F 01-0.27646992E-02 0.44784038E-05 3
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 SI+ L12/6ES 1E -100 000 06 300.000 5000.000 1
 0.26645138E 01-0.19509635F-03 0.29017066F-07-0.17351091E-10 0.13133560E-14 2
 0.14791314E 06 0.46289974E 01 0.39497015E 01-0.53831822E-02 0.70533565E-05 3
 -0.52417458E-08 0.12637267F-11 0.14765904F 06-0.15671487E 01 4
 SIC J 3/67SI 10 100 000 03 300.000 5000.000 1
 0.55799933F 01-0.13409344F-02 0.75483047F-06-0.16543778F-09 0.12663345F-13 2
 0.55946120E 05-0.56623593E 01-0.21924695E 01 0.41342700E-01-0.79274113F-04 3

0.60694120E-07-0.16729207E-10	0.85953143E 05	0.28756080E 02	4
SIC2	J 3/67SI 1C 200 000 0G	300.000 5000.000	1
0.57011523E 01	0.21220690F-02-0.11457769E-05	0.3103976AE-09-0.27763897E-13	2
0.72023391E 05	0.49868951F 01	0.38816333E 01	3
0.10573232E-08	0.25513142E-12	0.72558249F 05	4
SICL	J 9/67SI 1CL 100 000 0G	300.000 5000.000	1
0.44179424E 01	0.13137089E-03-0.30782013E-07	0.47502942E-11-0.24135145E-15	2
0.21650362E 05	0.33226345E 01	0.33247525E 01	3
0.25169051E-08	0.65148061E-12	0.21774076E 05	4
SICL2	J12/60SI 1CL 200 000 0G	300.000 5000.000	1
0.66401140E 01	0.40061524E-03-0.17252517E-06	0.32791504E-10-0.22955397F-14	2
-0.21042974E 05	0.44453305E 01	0.40946591E 01	3
0.10778153E-07	0.2680463E-11-0.20524636E 05	0.73395793E 01	4
SICL4	J 9/67SI 1CL 400 000 0G	300.000 5000.000	1
0.12043655E 02	0.10190735E-02-0.44167865E-06	0.84421573E-10-0.59491580F-14	2
-0.52936052E 05	0.29940095E 02	0.61040010E 01	3
0.24448748E-07	0.60370155E-11-0.81705075E 05	0.98955249E 00	4
SIF	J12/63SI 1F 100 000 0G	300.000 5000.000	1
0.41464751E 01	0.42486929E-03-0.1505473AE-06	0.29852749E-10-0.20491743E-14	2
-0.18225468E 04	0.32442007E 01	0.33165872E 01	3
-0.84034933E-09	0.67357144E-12-0.15393631E 04	0.75729103E 01	4
SIF2	J 6/68SI 1F 20 00 0G	300.000 5000.000	1
0.60363216E 01	0.11224411F-02-0.51297359E-06	0.10224952E-09-0.68931139E-14	2
-0.75992284E 05	0.42683330E 01	0.29399908E 01	3
0.57841411E-08	0.65849149E-12-0.75256749E 05	0.11210391E 02	4
SIF4	J 9/63SI 1F 400 000 0G	300.000 5000.000	1
0.1054503AE 02	0.27200200E-02-0.11741279E-05	0.22433362E-09-0.15803156E-13	2
-0.19792290E 06	0.27951944E 02	0.31059749E 01	3
0.12974579E-07	0.13517263E-11-0.19611327E 06	0.9414191AE 01	4
SIN	J12/60SI 1H 100 000 0G	300.000 5000.000	1
0.30623551E 01	0.14953654E-02-0.56220832F-06	0.10102854E-09-0.67870459E-14	2
0.56371778E 05	0.59817282E 01	0.37346289E 01	3
-0.35400381E-08	0.75850849E-12	0.56301206E 05	4
SIN4	J12/60SI 1H 400 000 0G	300.000 5000.000	1
0.44433856E 01	0.86334212E-02-0.35060000E-05	0.64194983E-09-0.43824526E-13	2
0.13468294E 04	0.40777748E 01	0.17519579E 01	3
-0.75058684E-08	0.31897221E-11	0.28880916E 04	4
SIN	J 3/67SI 1N 100 000 0G	300.000 5000.000	1
0.39858621E 01	0.87927056E-05	0.54269539F-06-0.17951017E-09	2
0.43524809E 05	0.31615156E 01	0.31051955E 01	3
-0.3773483E-08	0.16835331E-11	0.43785709E 05	4
SIO	J 9/67SI 10 100 000 0G	300.000 5000.000	1
0.37473335E 01	0.81991943E-03-0.32525396F-06	0.57324962E-10-0.35108944E-14	2
-0.13317430E 05	0.36478404E 01	0.32528277E 01	3
-0.51024483E-08	0.19471317E-11-0.13090340E 05	0.66485803E 01	4
SI02(S)	J 6/67SI 10 200 000 0G	300.000 847.000	1
0.	0.	0.	2
0.	0.	0.37282163E 00	3
-0.87303379E-08	0.12526015E-10-0.11048161E 06	0.21552223E-01-0.14573894E-04	4
SI02(S)	J 6/67SI 1C 200 000 0G	347.000 1079.000	1
0.70854710E 01	0.12077507E-02	0.	2
-0.11178740E 06	0.36198180F 02	0.70854710E 01	3
0.	0.	-0.11178740E 06	4
SIC2(S)	J 6/67SI 10 200 000 0G	1079.000 1996.000	1
0.66032335E 01	0.25955509E-02-0.69075293F-06	0.17550104E-09	2
-0.11150871E 06	0.33656253E 02	0.	3
0.	0.	0.	4
SIC2(S)	J 6/67SI 10 200 000 0G	1996.000 5000.000	1
0.10315204E 02	0.	0.	2
-0.11460598E 06	0.57629533F 02	0.	3
0.	0.	0.	4
SIC2	J 9/67SI 1C 200 000 0G	300.000 5000.000	1
0.53620395E 01	0.17719734F-02-0.75194104E-06	0.14180584E-09-0.08856417F-14	2
-0.38767316E 05	0.69603501F 01	0.37628058F 01	3
0.12995573E-10	0.97544976E-12-0.38035971E 05	0.66549123E 01	4
SIS	J12/60SI 1S 100 000 0G	300.000 5000.000	1

0.41729993E 01	0.39498404E-03	0.1600402E-06	0.39841978E-10	0.21886645E-14	2
0.71535070E 04	0.29342404E 01	0.29507945E 01	0.49935917E-02	0.59703409E-05	3
0.30600935E-08	0.48754490E-12	0.74929303E 04	0.93959024E 01		4
SI2	J 3/67SI	200 000 000 00	300.000 5000.000		1
0.50474139E 01	0.53990034E-03	0.43078376E-06	0.11355206E-09	0.96262871E-14	2
0.69133185E 05	0.19234578E 01	0.38155393E 01	0.19096542E-03	0.59233416E-05	3
-0.57649603E-08	0.14775004E-11	0.69784655E 05	0.57275556E 01		4
SI2C	J 3/67SI	20 100 000 00	300.000 5000.000		1
0.62510388E 01	0.13224176E-02	0.72005214E-06	0.23269424E-09	0.23285148E-13	2
0.62300999E 05	0.72966415E 01	0.40433933E 01	0.73456957E-02	0.66412549E-05	3
0.24885047E-08	0.18196555E-12	0.62935417E 05	0.41712491E 01		4
SI2N	J 3/67SI	2N 100 000 00	300.000 5000.000		1
0.66709912E 01	0.91917882E-03	0.39517130E-06	0.74397145E-10	0.50284691E-14	2
0.45620154E 05	0.78114415E 01	0.36686735E 01	0.11301840E-01	0.13637119E-04	3
0.71633050E-08	0.12373310E-11	0.46313033E 05	0.71095453E 01		4
SI3	J 3/67SI	300 000 000 00	300.000 5000.000		1
0.74213760E 01	0.11703943E-03	0.89820775E-07	0.71935964E-11	0.25670837E-14	2
0.74146699E 05	0.10365274E 02	0.45979129E 01	0.10715274E-01	0.16100422E-04	3
0.10969207E-07	0.27832875E-11	0.74766324E 05	0.34421671E 01		4
END	LAST CARD				