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ADDITION TO THE LEWIS CHEMICAL EQUILIBRIUM PROGRAM TO ALLOW COMPUTATION FROM COAL COMPOSITION DATA

DECEMBER, 1980

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COMPUTER SCIENCES CORPORATION

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DECEMBER, 1980

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1.0 INTRODUCTION

This document reports changes made to the Lewis Chemical Equilibrium Program in order to adapt it for use by the Coal Gasification Project. The program was developed by the Lewis Research Center for analysis of the chemical equilibrium combustion in rocket engines. It can be applied directly to the entrained flow coal gasification process. The particular problem addressed is the reduction of the coal data into a form suitable to the program, since the manual process is involved and error prone. A similar problem in relating the normal output of the program to parameters meaningful to the coal gasification process was also addressed.

The revisions included in this writeup act as buffers on both sides of the Lewis Chemical Equilibrium Program to allow direct processing of raw coal gasification data and the production of data meaningful in coal gasification terms.

This document includes a Program Task Description of the capabilities created by the revisions of the original program. A list is given for the program elements which have been altered. Also included are two sample problems and a printout of the original program with and without the modifications for processing of coal gasification data.

The work was performed for the Engineering Systems Branch (AH33) of the Computer Services Office under contract NAS8-31640. The sponsoring organization was the Coal Gasification Task Team (PF15).

1.1 References

This program is self-contained and requires no other documents for its use and execution. Included for clarification are a memo by David Seymour, "Application of Lewis Chemical Equilibrium Computer Program to Coal Gasification" in Appendix A (Reference 2). If further revisions of this program become necessary, consult the "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shock, and Chapman - Jouget Detonation" by Gordon and McBride, NASA SP-273 (Appendix B, Reference 1).

2.0 PROGRAM TASK DESCRIPTION

The Lewis Chemical Equilibrium Program was revised to include the following capabilities:

1. Accept data in the form of coal and other fuel element compositions and create reactant data compatible with the original program.

2. Store and edit the coal composition data.

3. Increase the number of elements within a compound from four to five.

4. Increase the number of reactants in the system from 15 to 25.

5. Provide a means of removing certain species from consideration during coal calculations.

6. Provide for coal data only, that input temperatures be in ^{o}F and that printout of pressure, temperature, enthalpy and entropy be in English units.

7. Provide, for coal data only, an additional section of output listing.

8. Allow the use of a new pseudo element, inert carbon.

9. Provide a store and edit feature for namelist list.

10. Provide that types of input data, as represented by various menu items, be enterable in any order.

11. Simplify loading the program onto the terminal.

12. Provide a simple means of creating a copy of the system tape with the data from the previous run.

The program which provided the base for the revisions was "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shock, and Chapman-Jouget Detonation" by Gordon and McBride, NASA SP-273. This program had been previously revised to provide interactive input and output via the Marshall Interactive Planning System (MIPS).

A complete listing of the source code is appended so that the changes indicated in the Revisions section may be followed.

3.0 REVISIONS OF LEWIS CHEMICAL EQUILIBRIUM PROGRAM

The current revision is discussed in relation to the changes required in various subroutines and how they relate to the new capabilities. Also discussed are the new inputs and outputs required or generated by the revision. Finally, a complete sample case, for coal data, is presented.

3.1 Storage Element A (Map overlay source code)

A new segment COALCV was added to handle the conversion of coal data to reactant data. Note that this segment is the longest and may at some future time have to be split into more segments.

3.2 Storage Element BLOCK1 (Miscellaneous data - Block data form)

The entry for atomic weight and valence of Deuterium was replaced with the atomic weight and valence of the pseudo element, inert carbon. The element symbol is IC and the weight and valence are those of regular carbon. The inert carbon element is used in the simulation of coal gasifier systems which have an unreacted carbon recycle stream.

3.3 Storage Element BOOT (Bootstrap control section)

The control statements serve to assign, copy and catalog the five files necessary to run the program. The catalog is included to insure that additional runs made on the same day do not have to reload the tape.

Note that BOOT is part of the first file on the system tape for the program. The following control statements are necessary to load the complete system.

```
@ASG,T PUR,U9S,XXXXX
@COPY,G PUR.TPF$.
@ADD TPF$.BOOT
```

The first part of Sample 1 shows the complete loading process.

File LEWIS contains all the subroutines and map elements. File 4 contains the thermodynamic data. Files 8, 10, and 12 contain dummy reactant data, namelist data and coal data, respectively.

3.4 Storage Element CHECK (Subroutine CHECK)

No changes.

3.5 Storage Element COALCV (Subroutine COALCV)

The subroutine COALCV is a new subroutine designed to do the major processing of converting coal composition data to reactant data.

The appended memo "Application of the Lewis Chemical Equilibrium Computer Program to Coal Gasification" by David C. Seymour (A-1) discusses the detailed calculations to be made based on the input data.

The subroutine assumes the existence of a previous set of coal data, stored in file 12. A set of coal reactant data immediately follows the coal data on file 12. This data is in the same form as the reactant data written by subroutine RREAD for data which is entered in the normal fashion. A dummy set of coal data is provided as part of the system tape. The user is queried as to whether he wants a printout of the previous data set. A response of YES produces a listing of the original coal data in the form shown in Sample 2. Regardless of whether a printout of the past data is requested, the past data is always read except for the conditions of first pass and no request for past data.

Table 1 explains the variables used by COALCV to store the coal data and the record groupings of the data. Table 2 explains the various possible measured or empirical values of higher heating value.

After printing the existing data, the user is prompted as to whether he wishes to modify the data, add to the data or continue with the same data. For the continue option, the subroutine exits. For the modify flag, a further prompt is given requesting the data group numbers of the data to be changed. See the last line of Sample 1. Each data group has associated with it a flag which indicates whether that type of data is to be processed. For the modify option, the flags of only those groups requested are turned on. For the add option, all flags are turned on.

Each data group flag is queried. If the flag is on, appropriate prompts are issued and the resulting information as entered by the user is stored in the appropriate variable. Two of the data groups, ash and other fuels, have additional special processing. For those data groups, two paths are possible. If the modify option was chosen, then it is possible to modify, delete or add individual lines to the existing material, via a series of prompts and responses. If the modify option was not chosen, the prompts and responses insert a completely new set of data.

Note that for ash composition, four of the common compounds are prompted for individually. If the weight of any of these is returned as 0 (or blank), that compound is eliminated. Note also that for other fuels, a search is made to determine which fuel number corresponds to water so that the proper water to coal ratio may be computed.

When all the required data groups have been entered, then the calculations outlined in the included paper are done, except for the section "Use and Interpretation of CEC Results". That section is done in another subroutine.

The coal data is saved on file 12 followed by the computed reactant data. The coal data is in the form shown in Table 1. The reactant data is in the same format as for the original program, except that the first record contains the coal to fuel ratio (CF) in addition to the number of reactants (NREAC). The subroutine then returns to the calling routine.

TABLE 1

COALCV VARIABLES

Record 1	
NREAC	Number of reactants
CF	Coal to fuel ratio
HHVV	Higher heating value of coal Btu/lb
WCR	Water to coal ratio
PER	Fraction carbon conversion
Record 2	
CTEMP	Coal temperature (^{o}F)
OTEMP	Oxidizer Temperature (^{o}F)
Record 3	
PROX(3)	Proximate Analysis volatiles, fixed carbon, ash
COAL(5,2)	Coal composition in form element and number in order C, H, N, O, S.
PER	As above in record 2
IE	Pointer to higher heating value table
HH(8)	Measured and empirical higher heating value table. See table 2 for possible values.
Record 4	
NCOAL	Number of other coal elements, other than C, H, N, O, S.
NASH	Number of ash compounds
NFUEL	Number of fuel compounds other than coal.
NOXID	Number of oxidizer compounds.
Record 5*	
CCOMP(12,5)	Other coal components in the form, weight, percent, state, and compound.
ACOMP(11,8)	Ash components in the form, weight percent and compound.
OFUEL(13,8)	Other fuel components in the form, weight, percent, temperature, state and compound.
OXID(11,5)	Oxidizer components in the form, weight percent and compound.

*Compound in this section indicates that a chemical compound is broken down into its component atoms and number of atoms. That is: $CaCO_3$ = Ca 1.0 C 1.0 0 3.0

TABLE 2

Possible Higher Heating Values

1	Measured Data
2	Dulong 1 $145.44(\%C) + 620.28(\%H - 1/8(\%O)) + 40.5(\%S)$
3	Dulong 2 $146.0(\%C) + 620.0(\%H-1/8(\%O)) + 40.5(\%S)$
4	CPP2 $144.9(\%C) + 610.0(\%H-1/8(\%O)) + 55.5(\%S)$
5	Grummel and Davis $\left[\frac{654.3(\%H)}{100. - \%Ash)} + 424.62\right] \left[\frac{\%C}{3} + \%H - \frac{\%O}{8} + \frac{\%S}{8}\right]$
6	Coal Conversion System Technical Data Base (CCSTDB) $146.58(\%C) + 568.78(\%H) + 29.4(\%S)$ $- 6.58(\%Ash) - 51.53(\%O + \%N)$
7	Maximum of 2 through 6
8	Minimum of 2 through 6

3.6 Storage Element CPHS (Subroutine CPHS)

Changes were made in the COMMON area MISC to accommodate 25 instead of 15 reactants. The variables changed were LLMT, BO, BOP, DATA, NAME (first dimension), ANUM (first dimension) PECWT, ENTH, FAZ, RTEMP, DENS, and RMW. In addition, the dimension of NAME (second dimension) and ANUM (second dimension) were changed to accommodate 5 elements within a compound rather than 4. Note that the last column of the array is used to store a flag indicating whether or not the enthalpy of the reactant is to be calculated.

3.7 Storage Element DETON (Subroutine DETON)

Same changes as for CPHS.

3.8 Storage Element EQLBRM (Subroutine EQLBRM)

Same changes as for CPHS.

Also increased temporary storage PROW to 25 from 15.

Added a temperature condition to the error message which states that "100 iterations did not satisfy the convergence requirement".

3.9 Storage Element FROZEN (Subroutine FROZEN)

Same changes as for CPHS.

3.10 Storage Element GAMEFF (Subroutine GAMEFF)

No changes.

3.11 Storage Element GAUSS (Subroutine GAUSS)

No changes.

3.12 Storage Element HCALC (Subroutine HCALC)

Same changes as for CPHS.

In addition the temporary storage area NUM was redimensioned 25 x 6. All references to NAM (N,5) or NAME (N,5) were changed to(N,6). All array processing of ANUM was increased by 1.

3.13 Storage Element LTCPHS (Subroutine LTCPHS)

No changes.

3.14 Storage Element MAIN (Subroutine MAIN - system driver)

Same changes as for CPHS in the data area. Also the addition of COMMON area CFUEL and the addition of a data area (NOMTS) which represent those species which can be eliminated from considera[illegible] when working with coal data. See Table 3 for a summary of the species. The upper limit of 150 possible species is often exceeded when using coal data. The optional omission species can be used to remove some of the least likely possibilities.

In the body of the subroutine the value of CF is initialized to -1.0. If CF remains as -1.0, then the coal data section was never entered since that section will produce a positive value of CF. The CF flag is used in other subroutines to initiate action required by the presence of coal data.

All the entries in namelist, INPT2, are initialized.

The menu of possible choices was expanded by addition of Item 7, 'start program calculation' and Item 8, 'insert or edit coal data.' The wording of Items 1 to 6 were reworked to make them consistent.

A request for Item 8 produces a call to subroutine COALCV and processing returns to the menu list. For menu Item 3, the call is made to subroutine RREAD rather than to subroutine REACT. This is to make the data entry independent of order. The decision on logical flag CALCH was moved to menu Item 7. In the move, references to NAME (N,5) were replaced with (N,6).

Menu Items 4 and 5 were corrected to properly store the species name being placed in the omit and insert lists.

Menu Item 6, concerning namelist, had an edit feature added. A dummy namelist is stored by the system on File 10. The user is queried as to whether he wishes to see the previous namelist. A response of YES prints the previous list and then the user is asked whether he wishes to change the namelist. The program either stops for new namelist data or returns to the menu list. A response of NO in the print namelist question, totally initializes the namelist and then stops to input new items. Return is to the menu list.

TABLE 3

Optional Omission Species

AL(S)	SI(S)
AL(L)	SI(L)
AL CL2	SICL
ALN(S)	SICL2
ALN	SICL3
C	SICL4
C3	SIH
C4	SIH4
C5	SIN
H20(S)	SI2
03	SI20
SI	SI2N
SIC	SI3
SIC2	

Menu Item 7 was added to separate Item 6 from the actual start of the program so that Menu Items 1-6 and 8 can be input in any order. The new section moves the printout of the final namelist from Menu Item 6, the determination of logical CALCH from Menu Item 3 and the initialization of RHOP, VOL and NT from the original initialization area. In addition, this section requests the omission of the special coal data omit candidates.

Some special processing of Menu Item 7 is required by the exclusion of coal data. If the fraction of carbon conversion (PER) is less than 1, the special inert carbon element must be placed in the insert list. If the logical flag ERATIO is false and flag CF is positive then all MIX values must be multiplied by CF. MIX supposedly represents oxidizer to fuel ratio. For coal data, it is more convenient to input oxidizer to fuel ratio. The internally calculated coal to fuel ratio (CF) is then used to adjust to the proper O/F ratio. Also all namelist temperatures read in ^{o}F when coal data is being used, are adjusted to ^{o}K.

3.15 Storage Element MATRIX (Subroutine MATRIX)

Same changes as for CPHS.

3.16 Storage Element OUT1 (Subroutine OUT1 entries OUT2, OUT3, OUT4)

Same changes as for CPHS.

In addition, for coal data only, an additional line is printed at the end of the OUT1 printout. The line identifies oxidizer/coal ratio, water/coal ratio and fraction carbon conversion.

In the OUT2 section, for coal data only, pressures are printed in lbs per square inches, temperatures in °F, enthalpy in Btu/lb, entropy in Btu/(lb °F), and density in lb./cu.ft. The program pauses at the end of OUT2 to produce hardcopy of the output.

In the OUT3 section, for coal data only, an extra header line is printed. It is exactly the same as the line printed by OUT1.

The OUT4 section is new and corresponds exactly to the section "Use and Interpolation of CEC Results."

Sample 3 shows the printout created by each section of OUT1.

3.17 Storage Element PROK (PDP Element PROK)

No changes.

3.18 Storage Element REACT (Subroutine REACT)

Same changes as for CPHS.

Addition of common area CFUEL. Dimension changes of temporary variables ANAME, V, LLMTS, SBOP changes to array processing to handle 25 instead of 15 reactants. Change array processing ANUM and NAME to handle extra element within reactant.

The call to subroutine RREAD was removed and placed in MAIN. REACT now creates the final reactant data arrays by adding reactants placed on the reactant file (4) by the normal reactant input and those coal data reactants which are stored on the coal data file (12). The subroutine uses a two pass system. The first pass reads the first record from the coal data file if CF is -1. This places necessary header data into the system. If any normal reactants exist, they are read into the appropriate data areas. When all the reactants are read, the coal data reactants are read and added to the appropriate data areas.

3.19 Storage Element RKTOUT (Subroutine RKTOUT)

Addition of COMMON area CFUEL.

A call to OUT4 if coal data is present.

3.20 Storage Element ROCKET (Subroutine ROCKET)

Same changes as in CPHS.

Added a prompt for namelist RKTINP.

3.21 Storage Element RREAD (Subroutine RREAD)

Temporary arrays NAME, ANUM, PECWT, MOLE, ENTH, FAZ, RTEMP, FOX, DENS were adjusted to handle 25 instead of 15 reactants. NAME and ANUM were also adjusted to handle an additional element within the reactant. Array processing of these arrays was adjusted accordingly. The COMMON area CFUEL was added.

The first record of the reactant file was amended to include the value of CF. The individual reactant lines were adjusted to isolate the code which indicates that the enthalpy should be calculated. Previously, it had been recorded as part of the NAME array.

In addition, the edit section was made two pass. In the first pass, the data which is added or edited, is placed on the reactant file. Data to be edited also comes from this file. On the second pass, if one is requested, it is taken from the coal reactant data portion of the coal data file. Updates and/or additions are made to this data and the changed data is returned to the coal data file behind the original coal data. Note that the reactant data from the two sources is not added together until subroutine REACT, which is part of the startup routine. The setting of flag FIRST was removed from subroutine RREAD.

3.22 Storage Element SAVE (Subroutine SAVE)

Same changes as for CPHS. Addition of COMMON area CFUEL.

Creation of an additional header line, for coal data only. The line contains oxidizer/coal ratio, water/coal ratio and fraction carbon conversion. This header occurs just before the summation of atoms in the system.. See Sample 2, labeled SAVE.

3.23 Storage Element SEARCH (Subroutine SEARCH)

Same changes as for CPHS. Added a specific number for number of species in system. Also added a pause at the end of the species printout to obtain a hardcopy.

3.24 Storage Element SHCK (Subroutine SHCK)

Same changes as for CPHS.

3.25 Storage Element TAPESAVE (Tape Save Control Section)

The control statements serve to assign a tape, called LEWISTAPE, and copy the five system files into the tape. The following statement is necessary to call the tapesave system:

```
@ADD LEWIS.TAPESAVE
```

3.26 Storage Element THERMP (Subroutine THERMP)

Same changes as for CPHS. Added COMMON area CFUEL.

Addition of a pause to create a hardcopy of the material prior to the output of THERMP.

For coal data only, a call to entry OUT4 of subroutine OUT1.

Also, a pause at the end of THERMP to create a hardcopy before the next data set is processed.

3.27 Storage Element VARFMT (Subroutine VARFMT)

No changes.

3.28 Thermodynamic Data (File 4)

Thermodynamic data for the pseudo element inert carbon was added to the data. The data was that for C(S) with the exception of the compound name and atom name.

4.0 SAMPLE PROBLEM 1

The following pages indicate the procedure to load the Lewis Chemical Equilibrium Program and input new coal data into the system.

The data set which is being illustrated is the same as in the attached memo (A-1).

```
PORT  E8/49   SIGNON   -  HOST1(EX0) UP  HOST2(EX0) UP
PTY#04
ENTER USERID/PASSWORD
>PAYLOADS ESD



$DESTROY USERID/PASSWORD ENTRY
$ENTRY 1100 OPERATING SYSTEM  LEV  AX3GR2BHOST1(RSI)$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
>@RUN LEVIST 1MPD0130,0000.SEVIGNBIM208.30.200
DATE  081880      TIME  094204
>@ASG,T PUP U9S.02130
READY
>@COPY,G PUP  TPF8
FURPUP 28R1H1 E36 S74T11 08/18/80 09.42.46
SEVIGNBIM208$LEVIS(1) COPIED ON 08/04/80 AT 14.23.18
   105 BLOCKS COPIED
EOF ENCOUNTERED ON INPUT TAPE
>@ADD  TPF8 BOOT
READY
READY
READY
READY
READY
READY
READY
READY
READY
READY
READY
FURPUP 28R1H1 E36 S74T11 08/18/80 09 44.26
   105 BLOCKS COPIED
SEVIGNBIM208$4(1) COPIED ON 08/04/80 AT 14.24.49
    17 BLOCKS COPIED
EOF ENCOUNTERED ON INPUT TAPE
SEVIGNBIM208$8(1) COPIED ON 08/04/80 AT 14.25.17
     1 BLOCK  COPIED
EOF ENCOUNTERED ON INPUT TAPE
SEVIGNBIM208$10(1) COPIED ON 08/04/80 AT 14.25.30
     1 BLOCK  COPIED
EOF ENCOUNTERED ON INPUT TAPE
SEVIGNBIM208$12(1) COPIED ON 08/04/80 AT 14.25.49
     1 BLOCK  COPIED
EOF ENCOUNTERED ON INPUT TAPE
READY
>
```

```
@MIPS L
READY
FACILITY WARNING  10000000000
FILE HAS BEEN PREVIOUSLY ASSIGNED (OR FREED)
READY
F.APPLIB 28R1M1 E36 574711 08/21/80 08 11 07
 1 ABS
    12 BLOCKS COPIED
    12 BLOCKS COPIED
    64 BLOCKS COPIED
```

```
  MIPS INITIALIZATION IS IN PROGRESS
 OFF-LINE MAINTENANCE PROCESSOR LAST RUN AT 08/18/80  09:17:37
  TOTAL SUP TIME =   2 17 MIN
SELECT NEW PRINT FILE OPTION:
1   - WRITE PRINT FILE ON PAPER
2   - WRITE PRINT FILE ON FICHE
MIPS:1
     A PRINT FILE HAS BEEN ESTABLISHED NAMED    MPS105551%PSFS.
 INSERT COMMANDS : (INSERT    HELP    FOR TUTORING)
MIPS:&XQT LEWIS B
MIPS:SV ONE
 SAVE COMPLETED
MIPS:RN ONE
MIPS:GO
```

TYPE YES FOR PRINT TO PRINT FILE
MIPS:

LE IS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

- INSERT THERMODYNAMICS DATA
- INSERT LOW TEMP EXTENSION THERMO DATA
- INSERT OR EDIT REACTANTS
- OMIT SPECIES FROM THERMO DATA
- INSERT CONDENSED SPECIES
- INSERT OR EDIT NAMELIST
- START PROGRAM CALCULATION
- INSERT OR EDIT COAL DATA

RETURN - TERMINATE PROGRAM

AIPS78

TYPE YES TO READ IN PREVIOUS COMPOSITION
NIPS>NO

```
                                                                    MIPS)
 TYPE (OPTIONAL) LBS VOLATILES/100 LBS DRY COAL
MIPS)? 54
 TYPE LBS ASH/100 LBS DRY COAL
MIPS)15 93
 TYPE COAL TEMPERATURE IN DEG F
MIPS)??
 TYPE LBS/100 LBS DRY COAL FOR ELEMENTS
 C
MIPS)? 31
 H
MIPS)4 "5"
 N
MIPS), 529
 O
MIPS)+ 343
 S
MIPS)4 1
 TYPE (OPTIONAL) OTHER COAL COMPONENTS
 TYPE LBS/100 LBS DRY COAL STATE AND AND COMPONENT
 COAL TEMPERATURE IS ASSUMED
     EXAMPLE 0 13  1HG  2HCL  2
MIPS)? 13 1HG 2HCL 2
MIPS)
 TYPE LBS 100 LBS DRY ASH FOR COMPONENTS
 STATE ASSUMED SOLID  COAL TEMPERATURE ASSUMED
 SIO2
MIPS)? 69
 FE203
MIPS)2E. 02
 AL203
MIPS)20 23
 FES2
MIPS)?
 CONTINUE WITH ASH COMPONENTS
 LBS/100 LBS DRY ASH AND COMPONENT
     EXAMPLE  0 25  2HTI  1   1HO  2
MIPS)
 TYPE CARBON CONVERSION FRACTION  FOR EXAMPLE. 0 89
MIPS)? 945
 HHV CALCULATION
 0 - ENTER DATA
 1 - DULONG 1          12414 484
 2 - DULONG 2          12451 067
 3 - CPP2              12398 885
 4 - GRUMMEL-DAVIS     12423 143
 5 - CCSTDB            12182 720
 6 - MAX OF ABOVE      12451 067
 7 - MIN OF ABOVE      12182 720
MIPS)0
 ENTER HHV AS BTU/LB COAL
MIPS)12141
 TYPE OTHER FUEL COMPONENTS
 TYPE LBS/LB COAL  TEMPERATURE (DEG F) AND STATE AND COMPONENT
     EXAMPLE  0 31  100   1HG  1HH  2   1HO  1
MIPS)0 1 212  1HG 1HH 2  1HO 1
MIPS)
 TYPE IN OXIDIZER TEMPERATURE  DEG F
MIPS)??
 TYPE OXIDIZER COMPONENTS
 TYPE LBS/100 LBS OXIDIZER AND COMPONENT
    EXAMPLE  95 0  1HO  2
MIPS)95  1HO 2
MIPS)5  2HAR 1
```

INDEX	REACTANT(*)										REL WT/ NO MOLES	MOLE	ENTHALPY/ INT ENERGY	PHASE	TEMP.K	FUEL/ OXID	DENSITY
1	C	49 7311	H	44 3187	N	1 0251	O	3 7243	S	1 2008	730336		-222076 7500	S	298 150	F	00000
2	IC	1 0000		0000		0000		0000		0000	033655		0000*	S	298 150	F	00000
3	CL	2 0000		0000		0000		0000		0000	001182		0000*	G	298 150	F	00000
4	SI	1 0000	O	2 0000		0000		0000		0000	077258		0000*	S	298 150	F	00000
5	FE	2 0000	O	3 0000		0000		0000		0000	037535		0000*	S	298 150	F	00000
6	AL	2 0000	O	3 0000		0000		0000		0000	029116		0000*	S	298 150	F	00000
7	H	2 0000	O	1 0000		0000		0000		0000	090909		0000*	G	373 150	F	00000
8	O	2 0000		0000		0000		0000		0000	950000		0000*	G	298 150	O	00000
9	AR	1 0000		0000		0000		0000		0000	050000		0000*	G	298 150	O	00000

TYPE 1 2 OR 3 TO MODIFY, DELETE, OR ADD A REACTANT (RETURN TO CONTINUE) * INDICATES ENTHALPY TO BE CALCULATED
MIPS>
TYPE YES FOR SPECIAL OMITS FOR COAL DATA
MIPS>YES

LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

1 - INSERT THERMODYNAMICS DATA
2 - INSERT LOW TEMP EXTENSION THERMO DATA
3 - INSERT OR EDIT REACTANTS
4 - OMIT SPECIES FROM THERMO DATA
5 - INSERT CONDENSED SPECIES
6 - INSERT OR EDIT NAMELIST
7 - START PROGRAM CALCULATION
8 - INSERT OR EDIT COAL DATA
RETURN - TERMINATE PROGRAM

MIPS>6

```
TYPE YES FOR PRINT !NPT2 NAMELIST
PIPS>^C
  BEGIN NAMELIST !NPT2 !NPUT
> &INPT2 MIX= 9! P=15  $END
```

```
$INPT2
DETN    =  F
ERATIO  =  F
FA      =  F
FPCT    =  F
HP      =  T
IDEBUG  =          +0
IONS    =  F
MIX     =     91000000E+00,  00000000E+00,  00000000E+00,  00000000E+00
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00
MMHG    =  F
MSQM    =  F
OF      =  T
P       =     15000000E+02,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000030E+00,  00000000E+00,  00000000E+00,
              00002000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+20,  00000000E+00
PSIA    =  T
RKT     =  F
S0      =     00000000E+00
SHOCK   =  F
SO      =     00000000E+00
SP      =  F
SU      =  F
T       =     00000000E+20,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+06,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00
TP      =  F
TU      =  F
UU      =  F
U       =     00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00,  00000000E+00,  00000000E+00,  00000000E+00,
              00000000E+00
$END


READ/COPY - THIS INPUT WILL NOT BE INTERPRETED
MIPS)
```

LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

1 - INSERT THERMODYNAMICS DATA
2 - INSERT LOW TEMP EXTENSION THERMO DATA
3 - INSERT OR EDIT REACTANTS
4 - OMIT SPECIES FROM THERMO DATA
5 - INSERT CONDENSED SPECIES
6 - INSERT OR EDIT NAMELIST
7 - START PROGRAM CALCULATION
8 - INSERT OR EDIT COAL DATA
RETURN - TERMINATE PROGRAM

MIPS??

SPECIES BEING CONSIDERED IN THIS SYSTEM

J12/65	AL	J 6/70	ALCL	J 6/70	ALCL3(S)	J 6/70	ALCL3(L)	J 6/70	ALCL3
J 6/63	ALH	J 6/70	ALO	J 9/64	ALOCL	J12/67	ALOH	J12/68	AL02
J12/68	AL02H	J 6/70	AL2CL6	J 6/72	AL20	J 9/65	AL202	J 6/72	AL203(S)
J 6/72	AL203(L)	L 5/66	AR	J 3/61	C(S)	J12/69	CCL	J12/68	CCL2
J 6/70	CCL3	J12/68	CCL4	J12/67	CH	J12/72	CH2	J 3/61	CH20
J 6/69	CH3	J 3/61	CH4	J 6/69	CN	J 6/66	CNN	J12/70	CN2
J 9/65	CO	J12/65	COCL	J 6/61	COCL2	J 3/61	COS	J 9/65	CO2
J12/62	CS	J 6/61	CS2	J12/69	C2	J12/68	C2CL2	J 3/67	C2H
J 3/61	C2H2	J 9/65	C2H4	L 5/72	C2H6	J 3/67	C2N	J 3/61	C2N2
J 9/66	C2O	J 6/68	C3O2	J 6/72	CL	J 6/66	CLCN	J 6/61	CLO
J 3/61	CLO2	J 9/65	CL2	J12/65	CL2O	J 3/65	FE(S)	J 3/65	FE(S)
J 3/65	FE(S)	J 3/65	FE(L)	J 3/65	FE	J 6/65	FECL	J12/70	FECL2(S)
J12/70	FECL2(L)	J12/70	FECL2	J 6/65	FECL3(S)	J 6/65	FECL3(L)	J 6/65	FECL3
J 6/65	FEO(S)	J 6/65	FEO(L)	J 9/66	FEO	J 6/66	FEO2H2(S)	J12/66	FEO2H2
J 6/66	FEO3H3(S)	J12/70	FE2CL4	J 6/65	FE2O3(S)	J 6/65	FE3O4(S)	J 9/65	H
J 3/64	HALO	J 9/64	HCL	L12/69	HCN	J12/70	HCO	J12/70	HNCO
J 3/63	HNO	J 6/63	HNO2	J 6/63	HNO3	J 3/64	HO2	J 3/61	H2
L11/65	H2O(L)	J 3/61	H2O	L 2/69	H2O2	J12/65	H2S	J 3/61	IC(S)
J 3/61	N	J12/70	NCO	J12/71	NH	J12/65	NH2	J 9/65	NH3
J 6/63	NO	J12/72	NOCL	J 9/64	NO2	J12/65	NO2CL	J12/64	NO3
J 9/65	N2	J12/65	N2H4	J12/64	N2O	J 9/64	N2O4	J12/64	N2O5
J12/70	N3	J 6/62	O	J12/70	OH	J 9/65	O2	J12/65	S(S)
J12/65	S(L)	J 6/71	S	J 6/67	SH	J 8/61	SH	J 6/71	SO
J 6/61	SO2	J 6/71	SO2CL2	J 9/65	SO3	J12/65	S2	J 9/67	SIO
J 6/67	SIO2(S)	J 6/67	SIO2(S)	J 6/67	SIO2(S)	J 6/67	SIO2(L)	J 9/67	SIO2
J12/71	SIS	J 3/67	SI2C						

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MIPS)

OF • 827273

OXIDIZER/COAL• 9100 WATER/COAL• 1000 CARBON CONVERSION• 9450

LOW TEMPERATURE THERMO EXTENSION IN CPHS AT TT • 298 150002 DEGREES KELVIN

	FUEL	OXIDANT	MIXTURE
H CAL/G	- 94422578+03	00000000	- 51674047+03
KG-ATOMS/KG			
C	48142209-01	00000000	26346483-01
H	52995222-01	00000000	29002360-01
N	99234640-03	00000000	54307624-03
O	12785041-01	59377227-01	33879015-01
S	11624349-02	00000000	63615839-03
IC	28020050-02	00000000	15334356-02
CL	33402215-04	00000000	18245889-04
SI	12858276-02	00000000	70368676-03
FE	47009607-03	00000000	25726651-03
AL	57112435-03	00000000	31255561-03
AR	00000000	12516271-02	56665704-03

PT	C	H	N	O	S	IC	CL	SI	FE	AL	AR	
	ADD AL2O3(S)											
1	-10 968	-10 377	-15 904	-24 093	-14 967	-2 659	-29 958	-15 915	-3 639	-14 322	-25 445	17 000
	ADD SIO2(S)											
1	-11 395	-10 436	-15 971	-23 518	-15 114	-2 744	-29 254	-16 363	-4 714	-25 443	-25 528	6 000
	PHASE CHANGE. REPLACE SIO2(S) WITH SIO2(L)											
1	-12 046	-10 542	-16 100	-22 601	-15 427	-2 914	-28 917	-19 308	-6 741	-23 458	-25 686	5 000
	ADD FE(L)											
1	-12 035	-10 540	-16 098	-22 615	-15 421	-2 912	-28 921	-19 367	-6 714	-23 478	-25 684	2 000
1	-12 151	-10 558	-16 116	-22 465	-15 483	-2 937	-28 866	-19 183	-8 080	-23 248	-25 705	4 000

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MIPS)

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

PRESSURES

	CHEMICAL FORMULA										WT FRACTION	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CM3
FUEL	C	49 7311	H	44 3187	N	1 0251	O	3 7243	S	1 2008	73034	-222076 750	S	298 15	0000
FUEL	IC	1 0000									03366	000	S	298 15	0000
FUEL	CL	2 0000									00118	000	G	298 15	0000
FUEL	SI	1 0000	O	2 0000							07726	-217699 047	S	298 15	0000
FUEL	FE	2 0000	O	3 0000							03754	-197250 043	S	298 15	0000
FUEL	AL	2 0000	O	3 0000							02912	-400493 262	S	298 15	0000
FUEL	H	2 0000	O	1 0000							09091	-57189 437	G	373 15	0000
OXIDNT	O	2 0000									95000	000	G	298 15	0000
OXIDNT	AR	1 0000									05000	000	G	298 15	0000

O/F= 8273 PERCENT FUEL= 54 7264 EQUIVALENCE RATIO= 2 1776 DENSITY= 0000

OXIDIZER/COAL= 9100 WATER/COAL= 100 CARBON CONVERSION= 9450

THERMODYNAMIC PROPERTIES

PRESS PSIA	15 000
TEMP DEG F	3447 10
ENTH BTU/LB	-930 13
S BTU/(LB-R)	2 6403
DENSITY L/FT**3	8 492-03
M MOL WEIGHT	23 7175
(DLV/DLP) T	-1 0065
(DLV/DLT) P	1 1430
CP CAL/(G)(K)	7031
GAMMA (S)	1 1753
SON VEL M/SEC	1191 73

READ/COPY - THIS INPUT WILL NOT BE INTERPRETED
MIPS)

OXIDIZER/COAL= 9100 WATER/COAL= 1000 CARBON CONVERSION= 9450

MOLE FRACTIONS

AL2M	7 679-07
AL2O3(S)	3 501-03
AR	1 270-02
CO	5 495-01
COS	4 342-04
CO2	4 032-02
C2	2 344-05
C3	1 022-06
C4	2 785-06
FE(L)	3 811-03
FE	1 876-03
FECL2	9 580-07
FEO	2 159-05
FEO2H2	5 450-05
H	2 188-03
HCL	4 036-04
H2	2 311-01
H2O	8 658-02
H2S	4 854-03
K2O(S)	3 436-02
KCL	8 163-07
N2	6 083-03
O	7 293-07
OH	1 079-04
S	4 359-04
SH	1 895-03
SO	8 704-04
SO2	5 018-04
SO3	2 552-03
SIO	1 995-03
SIO2(L)	1 364-02
SIO2	3 464-06
SIS	1 323-04

HHV COAL B/LB	12141 00
MIXTURE MW	22 406
MF OF CDG	83976
V SAT SCF/LB	29 01858
HHV SAT B/SCF	294 69
EFFICIENCY	70435
V DRY SCF/LB	28 58918
HHV DRY B/SCF	299 12
LHV SAT B/SCF	281 06
LHV DRY B/SCF	285 28
# PER MMBTU	2 84

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MIPS)

5.0 SAMPLE PROBLEM 2

The following pages which could be a continuation of Sample 1, indicate the procedures to be used to edit existing coal data and/or existing namelist data.

The data set, after editing will still be the same as in the attached memo, but additional namelist options are illustrated.

```
TYPE  YES  FOR PRINT TO PRINT FILE
MIPS> NO
```

LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

1 - INSERT THERMODYNAMICS DATA
2 - INSERT LOW TEMP EXTENSION THERMO DATA
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6 - INSERT OR EDIT NAMELIST
7 - START PROGRAM CALCULATION
8 - INSERT OR EDIT COAL DATA
RETURN - TERMINATE PROGRAM

MIPS)8

TYPE YES TO READ IN PREVIOUS COMPOSITION
MIPS>YES

```
 TYPE YES TO READ IN PREVIOUS COMPOSITION
RIPS) ES
 1 - VOLATILE (OPTIONAL) AND ASH AS LBS/100 LBS DRY COAL
      VOLATILE    37 5400
      ASH         19 8300

 2 - COAL TEMPERATURE IN DEG F      77 00

 3 - DRY COAL COMPOSITION AS LBS/100 LBS DRY COAL
      C           67 3100
      H            4 7570
      N            1 5290
      O            6 3430
      S            4 1000

 4 - OTHER COAL COMPONENTS AS LBS/100 LBS DRY COAL, STATE AND COMPOSITION
       1300          G     CL    2 0000          0000          0000          0000          0000

 5 - ASH COMPOSITION AS LBS/100 LBS ASH AND COMPONENT
    53 6800          SI    1 0000  O     2 0000          0000          0000          0000
    26 0800          FE    2 0000  O     3 0000          0000          0000          0000
    20 2300          AL    2 0000  O     3 0000          0000          0000          0000

 6 - FRACTION CARBON CONVERSION       9450

 7 - HEATING VALUE OF COAL BTU/LB     12141 000

 8 - OTHER FUEL COMPONENTS AS LBS/LB COAL, TEMPERATURE IN DEG F, STATE AND COMPOSITION
       1000    212 000 G     H     2 0000  O     1 0000          0000          0000          0000

 9 - OXIDIZER TEMPERATURE IN DEG F      77 00

 10 - OXIDIZER COMPONENTS AS LBS/100 LBS OXIDIZER AND COMPONENT
    95 0000          O     2 0000          0000          0000          0000          0000
     5 0000          AR    1 0000          0000          0000          0000          0000

 TYPE 1 OR 2 TO MODIFY OR REPLACE
     RETURN TO CONTINUE
RIPS)1
 TYPE GROUP NUMBERS OF DATA TO BE CHANGED IN ASCENDING ORDER    FOR EXAMPLE 1 3 7 9
RIPS)2 5 6
```

```
 TYPE COAL TEMPERATURE IN DEG F
MIPS>77
 GROUP NUMBER     5
    1    53 6800                    SI     1 0000  0      2 0000          0000          0000          0000
    2    26 0800                    FE     2 0000  0      3 0000          0000          0000          0000
    3    20 2300                    AL     2 0000  0      3 0000          0000          0000          0000
 TYPE 1-ALTER, 2-DELETE  3-ADD, RETURN TO CONTINUE
MIPS>1
 TYPE LINE NUMBER
MIPS>1
 LBS/100 LBS DRY ASH AND COMPONENT
MIPS>53 68 2HSI 1   1HO 2
    1    53 6800                    SI     1 0000  0      2 0000          0000          0000          0000
    2    26 0800                    FE     2 0000  0      3 0000          0000          0000          0000
    3    20 2300                    AL     2 0000  0      3 0000          0000          0000          0000
 TYPE 1-ALTER  2-DELETE  3-ADD, RETURN TO CONTINUE
MIPS>
 TYPE CARBON CONVERSION FRACTION, FOR EXAMPLE, 0 89
MIPS>2 945
```

INDEX	REACTANT(#)												REL WT/ NO MOLES	MOLE	ENTHALPY/ INT ENERGY		PHASE	TEMP.K	FUEL/ OXID	DENSITY
1	C	49	7311	H	44	3187	N	1	0251	O	3	7243	S	1	2008		730336		-222076	6875	S	298 150	F	00000
2	IC	1	0000			0000			0000			0000			0000		033655			0000#	S	298 150	F	00000
3	CL	2	0000			0000			0000			0000			0000		001182			0000#	G	298 150	F	00000
4	SI	1	0020	O	2	0000			0000			0000			0000		077258			0000#	S	298 150	F	00000
5	FE	2	0000	O	3	0000			0000			0000			0000		037535			0000#	S	298 150	F	00000
6	AL	2	0000	O	3	0000			0000			0000			0000		029116			0000#	S	298 150	F	00000
7	H	2	0000	O	1	0000			0000			0000			0000		000909			0000#	G	373 150	F	00000
8	O	2	0000			0000			0000			0000			0000		050000			0000#	G	298 150	O	00000
9	AR	1	0000			0000			0000			0000			0000		050000			0000#	G	298 150	O	00000

# INDICATES ENTHALPY TO BE CALCULATED

TYPE 1, 2 OR 3 TO MODIFY, DELETE, OR ADD A REACTANT (RETURN TO CONTINUE)
MIPS)
TYPE YES FOR SPECIAL OMITS FOR COAL DATA
MIPS)YES

LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

1 - INSERT THERMODYNAMICS DATA
2 - INSERT LOW TEMP EXTENSION THERMO DATA
3 - INSERT OR EDIT REACTANTS
4 - OMIT SPECIES FROM THERMO DATA
5 - INSERT CONDENSED SPECIES
6 - INSERT OR EDIT NAMELIST
7 - START PROGRAM CALCULATION
8 - INSERT OR EDIT COAL DATA
RETURN - TERMINATE PROGRAM

MIPS>6

```
TYPE YES FOR PRINT INPT2 NAMELIST
MIPS\YES
 $INPT2
 DETN     =  F
 ERATIO   =  F
 FA       =  F
 FPCT     =  F
 HP       =  T
 IDEBUG   =                +0
 IONS     =  F
 MIX      =       91000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00     00000000E+00
 MMHG     =  F
 NSOM     =  F
 OF       =  T
 P        =       15000000E+02,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00
 PSIA     =  T
 RKT      =  F
 S0       =       00000000E+00
 SHOCK    =  F
 SO       =       00000000E+00
 SP       =  F
 SU       =  F
 T        =       00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00
 TP       =  F
 TU       =  F
 UU       =  F
 U        =       00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00,    00000000E+00,    00000000E+00,    00000000E+00,
                  00000000E+00

 $END
 BEGIN NAMELIST INPT2 INPUT
> $INPT2 HP= F , T=2500 , TP= T  $END
```

```
$INPT2
DETN     =  F
ERATIO   =  F
FA       =  F
FPCT     =  F
HP       =  F
IDEBUG   =                +0
IONS     =  F
MIX      =     91000000E+00     00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00     00000000E+00
MMHG     =  F
NSQM     =  F
OF       =  T
P        =     15000000E+02.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00     00000000E+00
PSIA     =  T
RKT      =  F
S0       =     00000000E+00
SHOCK    =  F
SO       =     00000000E+00
SP       =  F
SU       =  F
T        =     25000000E+04.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00     00000000E+00
TP       =  T
TV       =  F
UV       =  F
U        =     00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00.    00000000E+00.    00000000E+00.    00000000E+00.
               00000000E+00

$END


 READ/COPY - THIS INPUT WILL NOT BE INTERPRETED
MIPS>
```

```
LEWIS CHEMICAL EQUILIBRIUM PROGRAM

            MAIN MENU

  1 - INSERT THERMODYNAMICS DATA
  2 - INSERT LOW TEMP EXTENSION THERMO DATA
  3 - INSERT OR EDIT REACTANTS
  4 - OMIT SPECIES FROM THERMO DATA
  5 - INSERT CONDENSED SPECIES
  6 - INSERT OR EDIT NAMELIST
  7 - START PROGRAM CALCULATION
  8 - INSERT OR EDIT COAL DATA
 RETURN - TERMINATE PROGRAM
MIPS>?
```

SPECIES BEING CONSIDERED IN THIS SYSTEM

J12/65	AL	J 6/70	ALCL	J 6/70	ALCL3(S)	J 6/70	ALCL3(L)	J 6/70	ALCL3
J 6/63	ALH	J 6/70	ALO	J 9/64	ALOCL	J12/67	ALOH	J12/68	ALO2
J12/68	ALO2H	J 6/70	AL2CL6	J 6/72	AL2O	J 9/65	AL2O2	J 6/72	AL2O3(S)
J 6/72	AL2O3(L)	L 5/66	AR	J 3/61	C(S)	J12/69	CCL	J12/68	CCL2
J 6/70	CCL3	J12/68	CCL4	J12/67	CH	J12/72	CH2	J 3/61	CH2O
J 6/69	CH3	J 3/61	CH4	J 6/69	CN	J 6/66	CNN	J12/70	CN2
J 9 65	CO	J12/65	COCL	J 6/61	COCL2	J 3/61	COS	J 9/65	CO2
J12/62	CS	J 6/61	CS2	J12/69	C2	J12/68	C2CL2	J 3/67	C2H
J 3/61	C2H2	J 9/65	C2H4	L 5/72	C2H6	J 3/67	C2N	J 3/61	C2N2
J 9/66	C2O	J 6/68	C3O2	J 6/72	CL	J 6/66	CLCN	J 6/61	CLO
J 3/61	CLO2	J 9/65	CL2	J12/65	CL2O	J 3/65	FE(S)	J 3/65	FE(S)
J 3/65	FE(S)	J 3/65	FE(L)	J 3/65	FE	J 6/65	FECL	J12/70	FECL2(S)
J12/70	FECL2(L)	J12/70	FECL2	J 6/65	FECL3(S)	J 6/65	FECL3(L)	J 6/65	FECL3
J 6/65	FEO(S)	J 6/65	FEO(L)	J 9/66	FEO	J 6/66	FEO2H2(S)	J12/66	FEO2H2
J 6/66	FEO3H3(S)	J12/70	FE2CL4	J 6/65	FE2O3(S)	J 6/65	FE3O4(S)	J 9/65	H
J 3/64	HALO	J 9/64	HCL	L12/69	HCN	J12/70	HCO	J12/70	HNCO
J 3/63	HNO	J 6/63	HNO2	J 6/63	HNO3	J 3/64	HO2	J 3/61	H2
L11/65	H2O(L)	J 3/61	H2O	L 2/69	H2O2	J12/65	H2S	J 3/61	IC(S)
J 3/61	N	J12/70	NCO	J12/71	NH	J12/65	NH2	J 9/65	NH3
J 6/63	NO	J12/72	NOCL	J 9/64	NO2	J12/65	NO2CL	J12/64	NO3
J 9/65	N2	J12/65	N2H4	J12/64	N2O	J 9/64	N2O4	J12/64	N2O5
J12/70	N3	J 6/62	O	J12/70	OH	J 9/65	O2	J12/65	S(S)
J12/65	S(L)	J 6/71	S	J 6/67	SH	J 6/61	SH	J 6/71	SO
J 6/61	SO2	J 6/71	SO2CL2	J 9/65	SO3	J12/65	S2	J 9/67	SIO
J 6/67	SIO2(S)	J 6/67	SIO2(S)	J 6/67	SIO2(S)	J 6/67	SIO2(L)	J 9/67	SIO2
J12/71	SIS	J 3/67	SI2C						

READ/COPY - THIS INPUT WILL NOT BE INTERPRETED
MIPS)

OF • 827273

OXIDIZER/COAL• 9100 WATER/COAL• 1000 CARBON CONVERSION• 9450

	FUEL	OXIDANT	MIXTURE
H CAL/G	- 94422572+03	00000000	- 51674044+03
KG-ATOMS/KG			
C	48142289-01	00000000	26346483-01
H	52995222-01	00000000	29002360-01
N	99234840-03	00000000	54307624-03
O	12785041-01	59377227-01	33879015-01
S	11624379-02	00000000	63615839-03
IC	28020050-02	00000000	15334356-02
CL	33340215-04	00000000	18245889-04
SI	12858276-02	00000000	70368676-03
FE	47009607-03	00000000	25726651-03
AL	57112435-03	00000000	31255561-03
AR	00000000	12516271-02	56665704-03

PT	C	H	N	O	S	IC	CL	SI	FE	AL	AR	
	ADD AL2O3(S)											
1	-9 188	-10 135	-15 662	-26 504	-14 718	-2 362	-31 193	-14 064	13(	-13 333	-25 133	17 000
	ADD FE3O4(S)											
1	-9 171	-10 127	-15 660	-26 516	-14 728	-2 362	-30 929	-14 048	13/	-30 310	-25 130	5 000
	ADD SIO2(S)											
1	-9 151	-10 119	-15 659	-26 532	-14 739	-2 362	-30 060	-14 031	-4 764	-30 286	-25 127	5 000
	ADD FE(S)											
1	-8 950	-10 094	-15 650	-26 702	-14 574	-2 362	-30 074	-24 839	-4 538	-30 032	-25 111	5 000
1	-10 979	-10 439	-15 651	-24 994	-14 115	-2 362	-29 706	-28 254	-6 814	-32 593	-25 112	5 000
1	-9 032	-10 102	-15 650	-26 627	-14 561	-2 362	-30 038	-24 989	-6 814	-30 144	-25 111	5 000

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SAVE

EQLBRM

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

TEMPERATURE AND PRESSURE

	CHEMICAL FORMULA										WT FRACTION	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CM3
FUEL	C	49 7311	H	44 3187	N	1 0251	O	3 7243	S	1 2008	73034	-222076 687	S	298 15	0000
FUEL	IC	1 0000									03366	000	S	298 15	0000
FUEL	CL	2 0000									00118	000	G	298 15	0000
FUEL	SI	1 0000	O	2 0000							07726	-217699 047	S	298 15	0000
FUEL	FE	2 0000	O	3 0000							03754	-197250 043	S	298 15	0000
FUEL	AL	2 0000	O	3 0000							02912	-400453 262	S	298 15	0000
FUEL	H	2 0000	O	1 0000							09091	-57189 437	G	373 15	0000
OXIDNT	O	2 0000									95000	000	G	298 15	0000
OXIDNT	AR	1 0000									05000	000	G	298 15	0000

O/F= 8273 PERCENT FUEL= 54 7264 EQUIVALENCE RATIO= 2 1776 DENSITY= 0000

OXIDIZER/COAL= 9100 WATER/COAL= 1000 CARBON CONVERSION= 9450

THERMODYNAMIC PROPERTIES

PRESS PSIA	15 000
TEMP DEG F	2500 00
ENTH BTU/LB	-1394 67
S BTU/(LB-R)	2 5055
DENSITY L/F**3	1 133-02
M MOL WEIGHT	23 9647
(DLV/DLP) T	-1 0006
(DLV/DLT) P	1 0092
CP CAL/(G)(K)	4231
GAMMA (S)	1 2485
SON VEL M/SEC	1040 62

OUT1

OUT2

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MIPS)

OXIDIZER/COAL= 9100 WATER/COAL= 1000 CARBON CONVERSION= 9450

MOLE FRACTIONS

AL2O3(S)	3 521-03
AR	1 277-02
CO	5 397-01
COS	9 251-04
CO2	5 301-02
CS	8 364-06
CS2	3 615-06
FE(S)	5 792-03
FE	2 150-06
FECL2	6 799-07
FEO2H2	2 680-06
H	4 014-05
HCL	4 097-04
H2	2 400-01
H2O	7 442-02
H2S	1 197-02
IC(S)	3 455-02
N2	6 118-03
OH	5 401-07
S	4 332-06
SH	2 246-04
SO	1 140-05
SO2	1 319-05
S2	5 828-04
SIO2(S)	1 586-02

HHV COAL B/LB	12141 60
MIXTURE MW	22 533
MF OF CDG	85165
V SAT SCF/LB	28 26287
HHV SAT B/SCF	290 28
EFFICIENCY	69964
V DRY SCF/LB	28 82986
HHV DRY B/SCF	294 64
LHV SAT B/SCF	276 32
LHV DRY B/SCF	280 47
B PER MMBTU	2 86

OUT3

OUT4

READ/COPY - THIS INPUT WILL NOT BE INTERPRETED
MIPS>

```
LEWIS CHEMICAL EQUILIBRIUM PROGRAM

            MAIN MENU

  1 - INSERT THERMODYNAMICS DATA
  2 - INSERT LOW TEMP EXTENSION THERMO DATA
  3 - INSERT OR EDIT REACTANTS
  4 - OMIT SPECIES FROM THERMO DATA
  5 - INSERT CONDENSED SPECIES
  6 - INSERT OR EDIT NAMELIST
  7 - START PROGRAM CALCULATION
  8 - INSERT OR EDIT COAL DATA
 RETURN - TERMINATE PROGRAM
MIPS>
  . . . . . MIPS MODULE TERMINATED.   SUP'S USED .     26 SECONDS . . . . . .

NORMAL EXIT    CPU TIME        12388      TOTAL SUPS         27808    (MILLISECONDS)
-@@COMPLETE
```

```
 TOTAL SUP TIME =    2.80 MIN
 IS THE CURRENT PRINT FILE TO BE TRANSMITTED?
MIPS>NO
 INSERT COMMANDS   (INSERT    HELP    FOR TUTORING)
MIPS>SP
  MIPS IS EXITING
 PRINT FILES WILL BE DELETED IF NOT TRANSMITTED
 IS THE CURRENT PRINT FILE TO BE TRANSMITTED?
MIPS>NO
NORMAL EXIT    CPU TIME          20      TOTAL SUPS          7084    (MILLISECON
DS)STOP  MIPS
>@FIN



  PUNID  LEWIST   ACCT  1HPD013K0000   PROJECT  SEVIGNBIN208
       LOAD BLANK TP6 N25LEWIS -1 LEWIST
      ***   SAVE  ***   24609 TP6   N25LEWIS
   SEVIGNBIN208*N25LEWIS      24609       082180
      STOP  MIPS
      LEWIST FIN
  TIME      TOTAL  00 02 52 840      CBSUPS   047260104
            CPU    00 00 10 552      I/O   00 01 24 660
            CC/ER  00 01 17 627      WAIT  00 27 40 234
  IMAGES  READ     116        PAGES   13
  START     10 39 03 AUG 18,1980    FIN   11 12 02 AUG 18,1980

**********************************************************************
* THERE WILL BE A USERS MEETING ON 9/10/80 AT 09:00 A.M.  IN THE HOSC *
* CONFERENCE ROOM AT BLDG. 4663.  ALL USERS ARE URGED TO ATTEND.      *
**********************************************************************
----------------------------------------------------------------------
DEMAND USERS   PLEASE KEYIN  @USER*RESPONSE.POLL   PRIOR TO @FIN  ( THANK YOU)
----------------------------------------------------------------------
*TERMINAL INACTIVE*
>
```

APPENDIX A

APPLICATION OF LEWIS CHEMICAL EQUILIBRIUM COMPUTER PROGRAM TO COAL GASIFICATION

BY

DAVID SEYMOUR

This copy of a NASA memo describes the calculations of input and output used in the sample problems for conversion to coal gasification data.

National Aeronautics and
Space Administration

George C. Marshall Space Flight Center
Marshall Space Flight Center, Alabama
35812

NASA

Reply to Attn of PF15 E(80-118)

August 28, 1980

TO: PF15/John P. McCarty

FROM: PF15/David C. Seymour

SUBJECT: Application of the Lewis Chemical Equilibrium Computer Program to Coal Gasification

REF: (a) "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations" NASA SP-273, Gordon and McBride

(b) "Fortran IV Computer Program for Calculation of Thermodynamic and Transport Properties of Complex Chemical Systems", NASA TN-D-7056, Svehla, McBride

In the early 1960's Lewis Research Center developed a chemical equilibrium combustion (CEC) computer program for rocket engine performance analysis (Ref. (a)). Because of the thorough documentation, flexibility, and comprehensive specie library, the program has become an aerospace industry standard.

The CEC program can be applied to entrained flow coal gasification without modification. The complete thermodynamic state can be described for either adiabatic combustion or specified temperature and pressure. The procedures used to apply the program to coal gasification are described here, together with a sample case. Because these procedures are somewhat tedious and error prone, a subroutine has been added to the CEC program which contains these procedures.

The CEC program requires the chemical formula, relative amount and enthalpy of each reactant in the system. For a typical entrained flow gasifier, the reactants include steam, oxygen (with nitrogen and argon impurities) and coal. Due to the complex composition of coal, the chemical formulae for the coal components are generally not supplied and must be determined from an elemental analysis.

Consider the ultimate analysis of the dry Kentucky #9 used by TVA for design criteria.

Coal Composition		Ash Composition	
Element	% Wt.	Compound	% Wt.
C	67.31	S_iO_2	45.94
H	4.757	Al_2O_3	17.31
N	1.529	$F_{e2}O_3$	22.29
O	6.343	C_aO	5.486
S (Pyritic)	2.517	M_gO	1.164
S (Non Pyritic)	1.583	SO_3	3.264
Cl	.131	$N_{a2}O$	.557
Ash	15.83	K_2O	2.336
	100.00	T_iO_2	.742
		Other	.911
			100.00

The term ash used here refers to the residue obtained from complete oxidation of the coal with excess air during a proximate analysis of the coal.

The compounds existing in the coal are unknown. In particular, the composition of the ash is not the same as the composition of the minerals in the coal and thus the ash mass fraction in the coal indicated above is not the true mineral content of the coal. The sodium and potassium, for example, probably exist in the coal as chlorine salts or as part of the other inorganic compounds. Most of the iron in the coal exists as iron pyrite, F_eS_2.

The details of the compounds in the coal and ash are not required for an equilibrium combustion calculation. Only the relative amounts of the elements present must be known. The ash composition shown above is actually an elemental composition with ficticious oxide compounds assumed and is not a real ash composition. The actual ash composition is dependant on the amount of oxygen available during combustion, the combustion temperature, and the rate of cooling of the combustion products.

The ultimate analysis of coal shown above consists of direct measurement of the amount of elemental C, H, N, S, and Cl. The ash weight is then added and the oxygen content is taken to be the difference between 100 and this sum. Thus, if the only remaining element in the coal is oxygen, the oxygen content which is obtained plus the oxygen in the ficticious ash compounds represents the true total elemental oxygen in the coal. The ficticious ash compounds can be used directly to describe the relative amounts of the elements and corrections to the ash content or further assumptions about the coal composition are not required The only exception is that the sulfur in the ash should not be included, since it is already accounted for in the elemental sulfur in the coal. However this correction is smaller than the accuracy of the data and is not included here.

Determination of CEC Reactant Data From Coal Composition

The elemental mass composition of the coal must be converted into a atom/(mole reactant) form for input to the CEC. Since the program is limited to five elements per reactant, a reacting coal is arbitrarily defined to be composed of C, H, N, O and S. Other elements and compounds known to exist in the coal are treated as individual reactants.

Since some of the carbon in the coal may not actually be oxidized, a carbon conversion factor, f, is defined as the mass fraction of carbon which participates in the reaction. The remaining carbon is removed from the reacting coal and treated as in inert solid with carbon thermodynamic properties.

As an example of the procedure, the composition of the reacting coal for the previously described Kentucky #9 is, with f = .945

Coal Element	lb Element / 100 lb coal	lb Element / 100 lb coal	lb Element / 100 lb reacting coal
C	67.31	63.61	79.18
H	4.757	4.757	5.921
N	1.529	1.529	1.903
O	6.343	6.343	7.896
S	4.10	4.10	5.103
Cl	.131	80.337	100.00
Ash	15.83		
	100.00		

Converting to lb-atoms/(lb-mole reacting coal) gives

Element	lb Element / lb-atom	lb-atoms / 100 lb reacting coal	lb-atoms / 100 lb-mole reacting coal
C	12.01	6.593	49.74
H	1.008	5.874	44.31
N	14.007	.136	1.03
O	16.00	.494	3.73
S	32.064	.159	1.20
		13.256	100.00

Then the chemical formula for the reacting coal is

$C_{49.74}\ H_{44.31}\ N_{1.03}\ O_{3.73}\ S_{1.20}$

and it's molecular weight per 100 lb-mole is

$$\left(\frac{100}{13.256}\right) 100 = 754.4 \text{ lb/(100 lb-mole)}$$

$$= 754.4 \text{ g/(100 g-mole reacting coal)}$$

Relative Reactant Weights

In coal gasification it is convenient to use as independent variables the mass ratios water/coal (or steam/coal) and oxygen/coal. The CEC program, however, allows only one independent variable, oxidizer/fuel (O/F). The components of the system identified as oxidyzers as opposed to fuels is completely arbitrary. The distinction between oxidyzer and fuel is only important when running multiple O/F values within a single execution of the program.

The convention selected here is fuel = coal + H_2O + (other fuel compounds),

where coal = reacting coal + minerals + inert C + (other coal compounds).

Oxidyzer = O_2 + (impurities in O_2 feed),

where the other fuel and coal compounds and the O_2 impurities must be included in the CEC thermodynamic data library.

Then

$$\frac{\text{coal}}{\text{fuel}} = \frac{1}{1 + \frac{H_2O}{\text{coal}} + \left(\frac{\text{other fuel compounds}}{\text{coal}}\right)}$$

and the relative weight of reacting coal in the fuel, required for input to the CEC is

$$\frac{\text{reacting coal}}{\text{fuel}} = \frac{\text{coal}}{\text{fuel}} \left(\frac{\text{reacting coal}}{\text{coal}}\right)$$

similarly, for the other components of the fuel,

$$\frac{\text{minerals}}{\text{fuel}} = \frac{\text{coal}}{\text{fuel}} \left(\frac{\text{minerals}}{\text{coal}}\right)$$

$$\frac{\text{inert C}}{\text{fuel}} = \frac{\text{coal}}{\text{fuel}} (1-f) \left(\frac{\text{carbon}}{\text{coal}}\right)$$

$$\frac{H_2O}{\text{fuel}} = \frac{\text{coal}}{\text{fuel}} \left(\frac{H_2O}{\text{coal}}\right)$$

and for the oxidyzer

$$\text{CEC O/F} = \frac{\text{coal}}{\text{fuel}} \left(\frac{O_2}{\text{coal}}\right)$$

where O_2/coal includes the impurities.

As an example, suppose an equilibrium calculation were to be run for Kentucky # 9 with f = .945, H_2O/coal = .10, and O_2/coal = .91, where the O_2 feed is 95% pure O_2 and 5% Ar by volume. Then the relative weights are

$$\frac{\text{coal}}{\text{fuel}} = \frac{1}{1 + .10} = .9091$$

$$\frac{\text{reacting coal}}{\text{fuel}} = .9091\ (.8034) = .7304$$

$$\frac{\text{minerals}}{\text{fuel}} = .9091\ (.1583) = .1439$$

$$\frac{\text{inert C}}{\text{fuel}} = .9091\ (1 - .945)\ (.6731) = .0337$$

$$\frac{H_2O}{\text{fuel}} = .9091\ (.10) = .0909$$

$$\frac{Cl_2}{\text{fuel}} = .9091\ (.00131) = .0012$$

$$1.000$$

$$\frac{O_2}{\text{Oxidyzer}} = .975$$

$$\frac{\text{Ar}}{\text{oxidyzer}} = .025$$

CEC O/F = .9091 (.91) = .8273

The relative weights of the ash components are, considering only the largest three,

$$\frac{SiO_2}{\text{fuel}} = .1439\ \frac{(.4594)}{.8554} = .0773$$

$$\frac{Al_2O_3}{\text{fuel}} = .1439\ \frac{(.1731)}{.8554} = .0291$$

$$\frac{Fe_2O_3}{\text{fuel}} = .1439\ \frac{(.2229)}{.8554} = .0375$$

$$.1439$$

where the remaining ash components have been arbitrarily spread equally between these three.

Determination of Coal Enthalpy from HHV

The CEC program requires an enthalpy for each reactant when calculating adiabatic flame conditions. Enthalpies are not required for calculating equilibrium conditions at specified temperature and pressure. The enthalpy of the reacting coal is the heat of formation at 25°C plus the enthalpy changes from 25°C to the coal temperature. HHV is the heat of combustion at 25°C. where the products of combustion are CO_2, H_2O (l), and SO_2. The HHV of coal is either measured in a calorimeter bomb test or obtained from an empirical formula based on the coal ultimate analysis.

The known HHV_{coal} can be broken down into the reacting components selected for CEC input as

$$HHV_{coal} = HHV_{r.c.} \left(\frac{\text{reacting coal}}{\text{coal}}\right) + HHV_{c} \left(\frac{\text{inert C}}{\text{coal}}\right)$$

The oxides in the ash all have an HHV of zero and do not have to be included here.

The HHV for carbon can be calculated from the heats of formation and the definition of HHV. For carbon,

$$C + O_2 \xrightarrow{25^{\circ}C} CO_2$$

$$HHV_c = (\Delta h_f C + \Delta h_f^{\circ} O_2) - (\Delta h_f CO_2)$$

Where $\Delta h_f C$ = heat of formation of carbon, taken here to be amorphous carbon. $\Delta h_f C = 4680$ BTU/lb-mole

$\Delta h_{CO_2} = -169293$ BTU/lb-mole

$$HHV_c = (4680 + 169293) \frac{1}{12.01} = 14486 \text{ BTU/lb carbon}$$

Then the reacting coal HHV is

$$HHV_{rc} = \frac{HHV_{coal} - 14486 \left(\frac{\text{inert C}}{\text{coal}}\right)}{\frac{\text{reacting coal}}{\text{coal}}}$$

if, in the previous example, HHV_{coal} is given as 12141 BTU/lb coal then

$$HHV_{rc} = \frac{12141 - 14486\ (.037)}{.8034}$$

$$= \frac{12141 - 536}{.8034}$$

$$= 14445 \text{ BTU/lb reacting coal}$$

The heat of formation of the reacting coal can be obtained from the definition of HHV. The reaction is

$$\text{reacting coal} + \text{excess } O_2 \longrightarrow X_c CO_2 + \frac{X_h}{2} H_2O\,(l) + X_s SO_2$$

where X_c, H_h, X_s are the C, H, and S g-atoms per 100 g-moles of reacting coal.

The N and O in the coal are not included since their heat of formation is zero.

Then $$HHV_{rc} = \Delta h_{f_{rc}} - \left(X_c \Delta h_{f_{CO_2}} + \frac{X_h}{2} \Delta h_{f_{H_2O}} + X_s \Delta h_{f_{SO_2}}\right)$$

where $\Delta h_{f_{CO_2}} = -94051.8$ cal/g-mole CO_2

$\Delta h_{f_{H_2O}}\,(l) = -68317.4$ cal/g-mole $H_2O\,(l)$

$\Delta h_{f_{SO_2}} = -70960$ cal/g-mole SO_2

$$\Delta h_{f_{rc}} = HHV_{rc} - X_c\,(94051.8) - X_h\,(68317.4) - X_s\,(70960)$$

where the units of $\Delta h_{f_{rc}}$ required by the CEC are cal/(100 g-mole reacting coal).

In the previous example,

$$HHV_{rc} = (14445 \frac{\text{BTU}}{\text{lb reacting coal}})(\frac{\text{cal/g}}{1.8\ \text{BTU/lb}})(754.4 \frac{\text{g}}{100\ \text{g-mole}})$$

$$= 6.0540 \times 10^6 \text{ cal/(100 g-mole)}$$

and

$$\Delta h_{f_{rc}} = 6.0540 \times 10^6 - (49.74)(94051.8) - \frac{(44.31)}{2}(68317.4) - (1.20)(70960)$$

$$= 6.0540 \times 10^6 - 6.2769 \times 10^6$$

$$= -222890 \text{ cal/(100 g-mole reacting coal)}$$

If the coal temperature were 25°C (77°F), then the coal enthalpy required by the CEC would be $\Delta h_{f_{rc}}$. For temperatures up to about 200°F, the reacting coal enthalpy can be estimated from the emperical equation.

$$h_{rc} - \Delta h_{f_{rc}} = .175\,(T - 77) + .0029 W_v\,(T - 77) + .00025\,(T - 60)^2 - .072$$

where T is the coal temperature in °F and W_v is the percent of volitiles in the dry, ash free coal given by proximate analysis.

If in the previous example, the proximate analysis were

Volitiles	37.54	37.54	44.60
Fixed Carbon	46.63	46.63	55.40
Ash	15.83	84.17	100.00
	100.00		

then $W_v = 44.60$ and if the coal temperature were 100^oF

$$h_{rc} - \Delta h f_{rc} = .175\,(23) + .0029\,(44.6)\,(23) = .00025\,(40)^2 - .072$$

$$= 7.33 \frac{\text{BTU}}{\text{lb reacting coal}}$$

$$= (7.33)\,\frac{754.4}{1.8} = 3072 \text{ cal/(100 g-mole reacting coal}$$

and the enthalpy used in the CEC, h_{rc}, would be

$$h_{rc} = -222890 + 3072 = -219820 \text{ cal/(100 g-mole)}$$

The enthalpy of the remaining reactants will automatically be determined by the CEC program from a specified reactant temperature.

Use and Interpretation of CEC Results

The CEC output consists of the thermodynamic state variables and the specie mole fractions. For coal gasification several other parameters are of interest.

First, the molecular weight output by the program is an effective value meant for use in the ideal gas equation of state. This effective value is the mass of the system per mole of gas in the system and excludes the moles of solids and liquids. To convert to a true ratio of mass/mole for the system,

$$M_w = (\text{CEC } M_w)\,(1 - \sum_{\substack{\text{solid} \\ + \\ \text{liquids}}} X_i)$$

where X_i = CEC mole fraction.

Historically, fuel gas properties are usually quoted on a standard cubic foot basis, with various conventions taken for standard conditions. The standard used here is a saturated gas at 60^oF and 30 in. of mercury. With this standard 385.2 SCF will contain 1 lb-mole of dry fuel gas. If the standard were dry gas at 60^oF and 30 in. of mercury, 379.5 SCF would contain 1 lb-mole of dry fuel gas.

The moles of dry product gas per total moles of reactants is taken to be

$$X_{DP} = X_{CO} + X_{H2} + X_{CH4} + X_{CO2} + X_{N2} + X_{Ar}$$

The volume of clean, dry gas produced per lb of coal is then

$$Y_{DP} = \frac{385.2\, X_{DP}}{M_w} \frac{\text{Reactants}}{\text{coal}}, \text{ SCF/(lb coal)}$$

where the mass fraction $\frac{\text{Reactants}}{\text{coal}}$ can be obtained as $\frac{\text{fuel}}{\text{coal}} + \frac{O_2}{\text{coal}}$.

The higher heating value of the gas, in BTU/SCF, is obtained from the HHV of the constituents as

$$HHV = \frac{319.24\, X_{H2} + 316.06\, X_{CO} + 994.4\, X_{CH4}}{X_{DP}}$$

The lower heating value, which takes water vapor rather than liquid water as the reference state, is given by

$$LHV = \frac{269.71\, X_{H2} + 316.06\, X_{CO} + 895.3\, X_{CH4}}{X_{DP}}$$

Cold gas efficiency, which is the fraction of the coal chemical energy converted to a gas chemical energy, is

$$E = \frac{HHV\ Y_{DP}}{HHV\ coal}$$

where HHV_{coal} is the higher heating value of dry coal and does not include any of the previously discussed corrections for carbon conversion.

The equilibrium thermochemical data provided by the program represent an idealized state and must be applied to actual gasifier operation with caution. The major non-equilibrium effect, unreacted carbon, had been accounted for in this application of the CEC program. However, as the gas/particle mixture is cooled within the gasifier, the chemical reaction rates will decrease and chemical equilibrium will no longer be maintained. A freeze point emperature can be defined as that temperature at which the equilibrium composition approximates the final non-equilibrium temperature. This freeze point temperature must be determined by a finite rate analysis or experimental data. When the freeze point temperature is known, the CEC program can be applied with a specified temperature and pressure to describe the final gas composition.

If transport property data is required, the CEC program described in Ref (B) can be used in lieu of Ref. (A).

David C. Seymour

Distribution:
PF15/Messrs. Rutland/Klan/Irby/Costes/Deaton/Garrett/Hyde/Johnston/
Kramer/Larsen/Lynn/Middleton/Stonemetz
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PD33/Mr. Stafford
PD31/Messrs. Cole/Goss/Steincamp/Wheeler/Belcher
PP03/Mr. Hamaker
EF43/Messrs. Piner/Spear

APPENDIX B

SOURCE LISTING OF PROGRAM ELEMENTS WITH MODIFICATIONS

This is a printout of the Lewis Chemical Equilibrium Program with the modifications necessary for coal gasification data.

B-1

• • • • • • UNIVAC 1100 TIME/SHARING EXEC ACCOUNT NUMBER • 1HPA01R50021 VER. EM 33R3HOST2 SITE • HOST 2 • • • • • • •

RUNID • LEWIST USER ID • PART NUMBER • 00 INPUT DEVICE • CR1 OUTPUT DEVICE • PR2

FILE NAME • PR@000LEWIST CREATED AT: 12:51:12 OCT 15,1980 PRINTED AT: 13:27:53 OCT 15,1980

```
@RUN LEWIST,1,F101R50021,SEVIGNBIN208,30,200

@MSG,N                    REMOVE AT CARD READER      10-15-80          CLOCK NO 2709

@ASG,T PUR,U9S,15753

@COPY,6 PUR.,TPF$.
FURPUR 28R1H1 E33 S74T11 10/15/80 13:09:46
SEVIGNBIN2C0*LEWIS(1) COPIED ON 09/18/80 AT 13:23:53
    105 BLOCKS COPIED.
EOF ENCOUNTERED ON INPUT TAPE

@XQT,A SYS$0MSFC$.LISTIT

@HDG,P       A

@PRT,S     A
FURPUR 28R1H1 E33 S74T11 10/15/80 13:05:53
```

```
SEVIGNBIN208*TPFS(0).A
      1       LIB LEWIS.,MIPS*ILIB.,SYS$*MSFC$.
      2       $EG DRIVER'
      3       IN LEWIS.BLOCK1
      4       IN LEWIS.MAIN
      5       SEG 00*(DRIVER)
      6       IN LEWIS.COALCV
      7       SEG 1*(DRIVER)
      8       IN LEWIS.SEARCH
      9       SEG 2@(DRIVER)
     10       IN LEWIS.REACT
     11       SEG 3@(DRIVER)
     12       IN LEWIS.THERMP
     13       SEG 4*(DRIVER)
     14       IN LEWIS.DETON
     15       SEG 5@(DRIVER)
     16       IN LEWIS.SHCK
     17       SEG 6@(DRIVER)
     18       IN LEWIS.ROCKET

@HOG,P       BLOCK1
```

```
@FOR,S    BLOCK1,BLOCK1
HSA  E3 -10,15/8-13:05:54 (11.)

   BLOCK DATA

   STORAGE USED: CODE(1) 000000; DATA(0) 000000; BLANK COM.ON(2) 000000

    COMMON BLOCKS:

       3   CONSTS 000006
       4   HOLCON 000010
       5   MISC   001701
       6   OUPT   000073


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0005    000640 AM        0005    000705 AM1       0005    001135 ANUM      0005 R 000004 ATAM      0005 R 000235 ATEM
    0003 R  000000 ATMN      0005    000004 AT04      0005    000516 BO        0005    000545 BOP      0005    000706 CPR1
    0005    000634 CPSUM     0005    000654 DATA      0005    00156B DENS      0004 R  000000 END      0005    0017B0 ENLSAV
    0005    000000 ENN       0005    001676 ENNL      0005    001677 ENSAVE    0005    001414 ENTH     0005    000636 EQRAT
    0006 R  000002 FA        0006 R  000003 FAP       0005    001445 FAZ       0006 R  000005 FB       0006 R  000006 FC
    0006 R  000007 FCP       0006 R  000012 FCST      0006 R  000014 FCV       0006 R  000015 FG       0006 R  000017 FGE
    0006 R  000020 FGV       0006 R  000021 FH        0006 R  000023 FI        0006 R  000025 FIV      0006 R  000027 FM
    0004 R  000031 FMT       0006 R  000050 FN        0006 R  000052 FOUR      0005    001527 FOX      0006 R  000053 FP
    0006 R  000054 FS        0006 R  000056 FSV       0006 R  000057 FT        0006 R  000061 FTK      0006 R  000063 FV
    0006 R  000067 FVEL      0006 R  000001 F13       0006 R  000000 F9X       0004 R  000001 GAS      0003 R  000001 GMET
    0005    000642 HPP       0005    000637 HSUB0     0004 I  000002 IE        0004 I  000003 IZER0    0004 I  000004 LANK
    0005    000461 LLMT      0004 I  000005 MOL       0005    000707 NAME      0005    000635 OF       0006 R  000067 ONE
    0004 R  000006 OX        0005    001644 OXF       0003 R  000002 PATM      0005    001363 PECWT    0005    000633 PP
    0003 R  000003 RBAR      0003 R  000004 RBR       0005    000644 RH        0005    001611 RHOP     0005    001612 RMW
    0005    001476 RTEMP     0003 R  000005 RVR       0005    000001 SUMN      0005    000003 SO       0005    000632 THIGH
    0006 R  000070 THREE     0005    001643 TLN       0005    000630 TLOW      0005    000627 TM       0005    000631 TMID
    0005    000002 TT        0006 R  000071 TWO       0005    000646 VMIN      0005    000650 VPLS     0005    000652 WP
    0004 R  000007 ZERO      0006 R  000072 ZEROF
```



```
00101      1*          BLOCK DATA                                                    ATM00001    000000
00101      2*    C                                                                               000000
00102      3*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                   /CONSTS/    000000
00103      4*          COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO             /HOLCON/    000000
00104      5*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                 000000
00104      6*         1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,           000000
00104      7*         2              HSUB0,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),  /MISC/   000000
00104      8*         3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),        000000
00104      9*         4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,         000000
00104     10*         5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                    000000
00105     11*          COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),  /OUPT/   000000
00105     12*         1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/ 000000
00105     13*         2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,   /OUPT/ 000000
00105     14*         3              TWO,ZEROF                                            /OUPT/ 000000
00105     15*   C                                                                               000000
00106     16*          DIMENSION ATAM(3,51),ATEM(3,50)                                          000000
00107     17*          EQUIVALENCE (ATOM(1,1),ATAM),(ATOM(1,52),ATEM)                           000000
```

```
00107   18*     C
00107   19*     C  ATOMIC SYMBOLS, WEIGHTS, AND VALENCES
00110   20*           DATA ATAM/2HH ,1.00797,1.0,2HHE,4.0026,0.0,2HLI,6.939,1.0,2HBE,
00110   21*          1 9.0122,2.0,2HB ,10.811,3.0,2HC ,12.01115,4.0,2HN ,14.0067,0.0,
00110   22*          2 2HO ,15.9994,-2.0,2HF ,18.9984,-1.0,2HNE,20.183,0.0,2HNA,22.9898
00110   23*          3 1H ,2HMG,24.312,2.0,2HAL,26.9815,3.0,2HSI,28.086,4.0,2HP ,30.9738
00110   24*          4,5.0,2HS ,32.064,4.0,2HCL,35.453,-1.0,2HAR,39.948,0.0,2HK ,39.102,
00110   25*          5 1.0,2HCA,40.080,2.0,2HSC,44.956,3.0,2HTI,47.90,4.0,2HV ,50.942,
00110   26*          6 5.0,2HCR,51.996,3.0,2HMN,54.9380,2.0,2HFE,55.847,3.0,2HCO,58.933,
00110   27*          7,2.0,2HNI,58.710,2.0,2HCU,63.540,2.0,2HZN,65.370,2.0,2HGA,69.720,
00110   28*          8 3.0,2HGE,72.590,4.0,2HAS,74.9216,3.0,2HSE,78.960,4.0,2HBR,79.909,
00110   29*          9 -1.0,2HKR,83.80,0.0,2HRB,85.47,1.0,2HSR,87.620,2.0,2HY ,88.905,
00110   30*          A 3.0,2HZR,91.220,4.0,2HNB,92.906,5.0,2HMO,95.94,6.0,2HTC,99.0,7.0,
00110   31*          B 2HRU,101.07,3.0,2HRH,102.905,3.0,2HPD,106.40,2.0,2HAG,107.870,
00110   32*          C 1.0,2HCD,112.40,2.0,2HIN,114.820,3.0,2HSN,118.690,4.0,2HSB,
00110   33*          D 121.750,3.0/
00112   34*           DATA ATEM/2HTE,127.60,4.0,2HI ,126.9044,-1.0,2HXE,131.30,0.0,2HCS,
00112   35*          1 132.905,1.0,2HBA,137.340,2.0,2HLA,138.910,3.0,2HCE,140.120,3.0,
00112   36*          2 2HPR,140.907,3.0,2HND,144.240,3.0,2HPM,145.0,3.0,2HSM,150.350,3.0
00112   37*          3,2HEU,151.960,3.0,2HGD,157.250,3.0,2HTB,158.924,3.0,2HDY,162.50,
00112   38*          4 3.0,2HHO,164.930,3.0,2HER,167.260,3.0,2HTM,168.934,3.0,2HYB,
00112   39*          5 173.040,3.0,2HLU,174.997,3.0,2HHF,178.490,4.0,2HTA,180.948,5.0,
00112   40*          6 2HW ,183.850,6.0,2HRE,186.20,7.0,2HOS,190.20,4.0,2HIR,192.20,4.0,
00112   41*          7 2HPT,195.090,4.0,2HAU,196.967,3.0,2HHG,200.590,2.0,2HTL,204.370,
00112   42*          8 1.0,2HPB,207.190,2.0,2HBI,208.980,3.0,2HPO,210.0,2.0,2HAT,210.0,
00112   43*          9 0.0,2HRN,222.0,0.0,2HFR,223.0,1.0,2HRA,226.0,2.0,2HAC,227.0,3.0,
00112   44*          A 2HTH,232.038,4.0,2HPA,231.0,5.0,2HU ,238.030,6.0,2HNP,237.0,5.0,
00112   45*          B 2HPU,242.0,4.0,2HAM,243.0,3.0,2HCM,247.0,3.0,2HBK,249.0,3.0,2HCF,
00112   46*          C 251.0,3.0,2HES,254.0,0.0,2HFM,253.0,0.0,2HIC,12.01115,4.0/
00112   47*     C      INFORMATION USED IN VARIABLE OUTPUT FORMAT
00114   48*           DATA F9X/3H9X,/,F13/2H13/,FA/6HAE/AT /,FB/6H      /,FC/6HCF    /,  /OUPT/
00114   49*          1      FCV/6HCF VAC/,FG/12HGAMMA (S)   /,FI/12HISP SECONDS /,       /OUPT/
00114   50*          2      FIV/12HIVAC SECONDS/,FM/12HM MOL WEIGHT/,FMT/6H(1H ,2,       /OUPT/
00114   51*          3      6HA6,A2,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,    /OUPT/
00114   52*          4      5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1),/,           /OUPT/
00114   53*          5      FN/12HMACH NUMBER /,FOUR/5HF9.4,/,FP/6HPC/P /,               /OUPT/
00114   54*          6      FT/12H(DLV/DLP) T /,FV/12H(DLV/DLT) P /,ONE/5HF9.1,/,        /OUPT/
00114   55*          7      THREE/5HF9.3,/,TWO/5HF9.2,/,ZERO/5HF9.0,/,FAP/12HPRESS N/M**
00114   56*          82/,FCP/12HCP CAL/(G)(K,2H) /,FCST/12HCSTAR M/SEC /,FGE/6H(EFF) /,
00114   57*          9 FGV/6HGAS VE/,FH/12HENTH CAL/G  /,FS/12HS CAL/(G)(K)/,FSV/6HS ON V
00114   58*          AE/,FTK/12HTEMP DEG. K /,FVEL/6HL M/SE,2HC /
00153   59*           DATA END/3HEND/,GAS/1HG/,IE/1HE/,IZERO/2H00/,LANK/2H  /,MOL/1HM/
00153   60*          1 ,OX/1HO/,ZERO/1HO/,ATMN/101325.0/,RVR/82.0554497/
00153   61*          3 ,GMET/9.806650/,PATM/14.6960060/,RBAR/1.9871650/,RBR/8314.298360/
00172   62*           END                                                  ATM00060  000000

        END OF COMPILATION:        NO  DIAGNOSTICS.

@HDG,P      BOOT

@PRT,S    BOOT
FURPUR 28R1H1 E33 S74T11 10/15/80 13:05:56
```

```
SEVIGNBIN208*TPF%(0).BOOT
      1       @CAT,P LEWIS,F/64/TRK/128
      2       @CAT,P 9,F/64/TRK/1.
      3       @CAT,P 8,F/10/TRK/32
      4       @CAT,P 10,F/10/TRK/32
      5       @CAT,P 12,F/10/TRK/64
      6       @ASG,A LEWIS.
      7       @ASG,A 9.
      8       @ASG,A 8.
      9       @ASG,A 10.
     10       @ASG,A 12.
     11       @COPY TPF$..LEWIS.
     12       @COPY,G PUR.,9.
     13       @COPY,G PUR.,8.
     14       @COPY,G PUR.,10.
     15       @COPY,G PUR.,12.
     16       @FREE PUR.

@HDG,P        CHECK
```

```
@FOR,S    CHECK,CHECK
HSA  E3 -10,15/B0-13:05:57 (2,)

   SUBROUTINE CHECK      ENTRY POINT 000056

   STORAGE USED: CODE(1) 000065; DATA(0) 000013; BLANK COMMON(2) 000000

   EXTERNAL REFERENCES (BLOCK, NAME)

    0003   NERR3S

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000 I 000000 IBLNK2     0000 I 000005 ICHAR1     0000 I 000006 ICHAR2     0000 I 000001 IHIGH     0000 I 000002 ILOW
    0000   000007 INJPS      0000 I 000003 JHIGH      0000 I 000004 JLOW

00101     1*                 SUBROUTINE CHECK(NAME)                                    000000
00101     2*       C                                                                   000000
00101     3*       C         BLANK FILL SPECIES SYMBOLS                                000000
00103     4*                 DATA IBLNK2/2H  /,IHIGH/1HZ/,ILOW/1HA/                    000000
00107     5*                 DATA JHIGH/0/,JLOW/0/ ,ICHAR1/0/,ICHAR2/0/                000000
00114     6*                 FLD(30,6,ICHAR1)=FLD(0,6,NAME)                            000000
00115     7*                 FLD(30,6,ICHAR2)=FLD(6,6,NAME)                            000001
00116     8*                 FLD(30,6,JHIGH)=FLD(0,6,IHIGH)                            000003
00117     9*                 FLD(30,6,JLOW)=FLD(0,6,ILOW)                              000005
00120    10*                 IF(ICHAR1.LT.JLOW .OR. ICHAR1.GT.JHIGH) NAME=IBLNK2       000007
00122    11*                 IF(ICHAR2.LT.JLOW .OR. ICHAR1.GT.JHIGH) FLD(6,6,NAME)=    000027
00122    12*             *   FLD(6,6,IBLNK2)                                           000027
00124    13*                 RETURN                                                    000047
00125    14*                 END                                                       000064

        END OF COMPILATION:        NO  DIAGNOSTICS.

@HDG,P      COALCV
```

```
@FOR,S    COALCV,COALCV
HSA  E3 -10,15,8 0-1 3:05:5 9 (2A,)

 SUBROUTINE COALCV    ENTRY POINT 003674

 STORA  USED: CODE(1) 003713; DATA(0) 003744; BLANK COMMON(2) 000000

  COMMON BLOCKS:

  0003   CFUEL   00000 8
  0004   SPECES  0171 06
  0005   INDX    000021
  0006   CCC     000003

 EXTERNAL REFERENCES (BLOCK, NAME)

  0007   RDYES
  0010   PAGIT
  0011   CHRSIZ
  0012   GOUT
  0013   NNCOD$
  0014   RDATAI
  0015   RDATAF
  0016   NREW$
  0017   NRBU$
  0020   NIO2$
  0021   NIO3$
  0022   NIO1$
  0023   NERR2$
  0024   NWBU$
  0025   NWEF$
  0026   NERR3$

 STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

  0001   000030 10L     0000   002175 100F    0001   001444 1011G   0001   001477 1025G   0001   000460 104L
  0001   001535 1040G   0000   002205 106F    0001   001743 1073G   0000   002233 108F    0001   001764 1107G
  0001   000537 112L    0001   002063 1137G   0001   000554 114L    0001   002075 1147G   0001   000607 120L
  0001   002213 1204G   0001   002213 1207G   0001   002246 1225G   0001   002316 1245G   0001   000617 126L
  0001   002360 1270G   0001   002370 1273G   0001   000635 130L    0001   002454 1322G   0001   002531 1347G
  0001   002541 1354G   0001   002553 1362G   0001   002565 1370G   0001   002576 1375G   0001   002607 1405G
  0001   002683 1426G   0001   002733 1452G   0001   002734 1455G   0001   003021 1504G   0001   003034 1511G
  0001   003035 1514G   0001   003213 1550G   0001   003214 1553G   0001   003253 1574G   0001   003263 1577G
  0001   003322 1615G   0001   003407 1642G   0001   003422 1647G   0001   003423 1652G   0001   003564 1727G
  0001   003564 1731G   0001   003571 1736G   0001   003571 1740G   0001   003576 1745G   0001   003576 1747G
  0001   003603 1758G   0001   003603 1756G   0001   003620 1770G   0001   003624 1774G   0001   000011 205G
  0001   000016 212G    0000   002404 235DF   0001   001102 2352L   0000   002410 2354F   0001   001137 2357L
  0001   001143 2358L   0001   001177 2360L   0001   001250 2364L   0001   001254 2366L   0001   001257 2370L
  0001   001263 2372L   0001   001315 2380L   0001   001352 2386L   0001   002053 2420L   0001   002116 2422L
  0000   002547 2424F   0001   002112 2427L   0001   002152 2428L   0001   002216 2431L   0001   002222 2432L
  0001   002225 2434L   0001   002231 2436L   0001   000126 256G    0001   000126 260G    0001   000133 265G
  0001   000133 267G    0001   000140 274G    0001   000140 276G    0001   000637 300L    0001   000145 303G
```

0001		000145	305G	0001		000693	310L	0001		000660	312L	0001		000675	314L
0001		000710	320L	0001		000716	322L	0001		000727	324L	0001		000740	326L
0001		000762	330L	0001		000773	340L	0001		001013	342L	0001		000240	343G
0001		001060	348L	0001		001063	350L	0001		001386	351L	0001		001366	352L
0001		001410	356L	0001		001421	358L	0001		000273	362G	0001		001502	364L
0001		001524	367L	0001		000302	370G	0001		001562	372L	0001		001565	380L
0001		001600	390L	0000		002533	394F	0001		001773	400L	0001		002020	402L
0001		000343	413G	0001		002031	420L	0001		002267	421L	0001		002301	422L
0001		002347	428L	0001		002352	430L	0001		002405	434L	0001		002410	440L
0001		000434	445G	0001		002423	450L	0001		002437	452L	0001		002443	453L
0001		002501	460L	0001		002504	470L	0001		000160	501L	0001		000515	500G
0001		000523	505G	0001		002767	520L	0001		000611	533G	0001		003078	540L
0001		003276	552L	0001		003301	554L	0000		002020	56F	0001		003361	560L
0001		003455	590L	0000		002032	60F	0000		002055	62F	0001		001030	620G
0001		001122	662G	0001		003662	680L	0000		002100	70F	0001		001245	717G
0001		001300	740G	0001		001323	751G	0001		001334	754G	0001		000316	80L
0001		000357	90L	0000		002131	92F	0000		002143	96F	0004		011052	A
0000	R	000576	ANUM	0000	R	003961	ASH	0000	R	001776	ASHF	0000	R	001640	CC
0003	R	000000	CF	0000	R	002732	COAL	0004		000000	COEF	0005		000001	CONVG
0000	R	001760	CTEMP	0004		010624	DELN	0006		000002	DEMAND	0000	R	001562	DENS
0004		010150	ENLN	0000	R	001447	ENTH	0000	R	002676	FAZ	0000	R	001766	FES2
0000	R	001531	FOX	0006		000000	GRAPH	0000	R	002001	HF1	0000	R	002003	HF2
0000	R	001664	HHT	0000	R	001777	HHV	0003	R	000001	HHVV	0005		000003	HP
0000	R	001657	H2O	0000	I	001637	I	0000	I	003331	IACOMP	0000	I	003961	IASH
0000	I	001645	ICC	0000	I	002744	ICCOMP	0000	I	002732	ICOAL	0000	I	001625	ID
0000	I	001752	IE	0000	I	002676	IFAZ	0000	I	001652	IH2O	0005		000015	IMAT
0000	I	003040	IOFUEL	0000	I	001746	IOPT	0000	I	001760	IOUT	0000	I	003242	IOXID
0005		000016	IQ1	0005		000005	ISV	0004		016266	IUSE	0000	I	001757	J
0000	I	001613	JOPT	0006		000001	JOUT	0005		000014	KMAT	0000	I	001763	KOUT
0000	I	000000	LINE1	0000	I	001767	LL	0000	I	001764	LN	0000	I	001765	L1
0005		000006	MOLES	0000	I	001772	N	0000	I	000007	NAME	0000	I	001754	NASH
0000	I	001747	NDUMMY	0000	I	001755	NFUEL	0000	I	001762	NI	0005		000017	NOF
0000	I	001756	NOXID	0005		000007	NP	0005		000011	NPT	0000	I	001745	NREAC
0005		000010	NT	0000	R	003040	OFUEL	0004	I	010150	OMIT	0000	R	001751	OTEMP
0000	R	001365	PECWT	0003	R	000003	PER	0000	R	002727	PROX	0000	R	002002	PX
0000	R	001632	RMOL	0000	R	001500	RTEMP	0004		004064	S	0000	R	001770	SINRT
0005		000004	SP	0004		015364	SUB	0000	R	001771	SUM	0000	R	001773	SUM1
0000	R	002004	SUM3	0004		016514	TEMP	0005		000002	TP	0003	R	000002	WCR

0001		000677	316L	0001		000145	305G	0001		000693	310L	0001		000660	312L
0001		000751	328L	0001		000710	320L	0001		000716	322L	0001		000727	324L
0001		001017	343L	0001		000762	330L	0001		000773	340L	0001		001013	342L
0001		001377	354L	0001		001060	348L	0001		001063	350L	0001		001386	351L
0001		001520	366L	0001		001410	356L	0001		001421	358L	0001		000273	362G
0001		001567	382L	0001		001524	367L	0001		000302	370G	0001		001562	372L
0001		000335	406G	0001		001600	390L	0000		002533	394F	0001		001773	400L
0001		002305	423L	0001		000343	413G	0001		002031	420L	0001		002267	421L
0001		002412	442L	0001		002347	428L	0001		002352	430L	0001		002405	434L
0001		000444	454G	0001		000434	445G	0001		002423	450L	0001		002437	452L
0001		002706	504L	0001		002501	460L	0001		002504	470L	0001		000160	501L
0001		000626	543G	0001		000523	505G	0001		002767	520L	0001		000611	533G
0000		002024	58F	0001		003276	552L	0001		003301	554L	0000		002020	56F
0001		001112	654G	0001		003455	590L	0000		002032	60F	0000		002055	62F
0001		001245	722G	0001		001122	662G	0001		003662	680L	0000		002100	70F
0000		002122	84F	0001		001300	740G	0001		001323	751G	0001		001334	754G
0000	R	003331	ACOMP	0004		011052	A	0001		000316	80L	0000		002143	96F
0000	R	002744	CCOMP	0000	R	001640	CC	0000	R	001776	ASHF	0000	R	003961	ASH
0000	R	001774	CSUM	0005		000001	CONVG	0004		000000	COEF	0000	R	002732	COAL
0004		004312	EN	0000	R	001562	DENS	0006		000002	DEMAND	0004		010624	DELN
0000	R	002000	FES2C	0000	R	001766	FES2	0000	R	002676	FAZ	0000	R	001447	ENTH
0000	R	001734	HH	0000	R	002003	HF2	0000	R	002001	HF1	0006		000000	GRAPH
0004		010376	HO	0005		000003	HP	0000	R	000001	HHVV	0000	R	001777	HHV
0000	I	001744	IC	0000	I	003961	IASH	0000	I	003331	IACOMP	0000	I	001637	I
0005		000000	IDEBUG	0000	I	001625	ID	0000	I	002732	ICOAL	0000	I	002744	ICCOMP
0000		003713	INJPS	0005		000015	IMAT	0000	I	001652	IH2O	0000	I	002676	IFAZ
0000	I	002727	IPROX	0000	I	003242	IOXID	0000	I	001760	IOUT	0000	I	001746	IOPT
0000	I	001761	JJ	0000	I	001757	J	0004		016266	IUSE	0005		000005	ISV
0005		000012	L	0000	I	001763	KOUT	0005		000014	KMAT	0006		000001	JOUT
0000	I	001416	MOLE	0000	I	001765	L1	0000	I	001764	LN	0000	I	001767	LL
0000	I	001753	NCOAL	0000	I	001754	NASH	0000	I	000007	NAME	0000	I	001772	N
0005		000020	NOMIT	0005		000017	NOF	0000	I	001762	NI	0000	I	001755	NFUEL
0005	I	000013	NS	0000	I	001745	NREAC	0005		000011	NPT	0005		000007	NP
0000	R	003242	OXID	0000	R	001751	OTEMP	0000	R	002002	PX	0000	R	003040	OFUEL
0007	L	000000	RDYES	0000	R	001770	SINRT	0004		016660	SLN	0004		004064	S
0000	R	001775	SUM2	0000	R	001773	SUM1	0003	R	000002	WCR	0000	R	001771	SUM

```
00101     1*          SUBROUTINE COALCV(FIRST)                                                    000000
00101     2*    C        USE MIPS INPUT ROUTINES TO READ COAL CONVERSION                          000000
00101     3*    C             AND CREATE SIMULATED REACTANT CARDS                                 000000
00103     4*          COMMON /CFUEL/CF,HHVV,WCR,PER                                               000000
00104     5*          COMMON /SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)            000000
00104     6*         X   ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(150,2),SLN(150)          000000
00105     7*          COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,                000000
00105     8*         X   KMAT,IMAT,IQ1,NOF,NOMIT                                                 000000
00106     9*          COMMON /CCC/GRAPH,JOUT,DEMAND                                               000000
00107    10*          INTEGER OMIT                                                                000000
00110    11*          DIMENSION OMIT(3,50)                                                        000000
00111    12*          EQUIVALENCE (OMIT(1,1),ENLN(1))                                             000000
00112    13*          LOGICAL FIRST,RDYES                                                         000000
00113    14*          DIMENSION LINE1(7)                                                          000000
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00114   15*          DATA LINE1/42H TYPE YES TO READ IN PREVIOUS COMPOSITION /                    000000
00114   16*    C     DATA ARRAYS FOR REACTANT CARDS                                               000000
00116   17*          DIMENSION NAM (15,25), ANUM(15,25),PECWT(25),MOLE(25),ENTH(25),              000000
00116   18*         X   FAZ(25),PTEMP(25),FOX(25),DENS(25)                                        000000
00117   19*          DIMENSION IFAZ(15)                                                           000000
00120   20*          EQUIVALENCE (FAZ(1),IFAZ(1))                                                 000000
00120   21*    C     ARRAYS FOR COAL DATA                                                         000000
00121   22*          DIMENSION IPROX(3)                                                           000000
00122   23*          DIMENSION PROX(3),COAL(5,2),ICOAL(5,2),CCOMP(12,5),ICCOMP(12,5),             000000
00122   24*         X   OFUEL(13,10),IOFUEL(13,10),OXID(11,5),IOXID(11,5),                        000000
00122   25*         X   ACOMP(11,8),IACOMP(11,8)                                                 000000
00123   26*          EQUIVALENCE (PROX(1),IPROX(1))                                               000000
00124   27*          EQUIVALENCE (COAL(1,1),ICOAL(1,1))                                           000000
00125   28*          EQUIVALENCE (CCOMP(1,1),ICCOMP(1,1))                                         000000
00126   29*          EQUIVALENCE (OFUEL(1,1),IOFUEL(1,1))                                         000000
00127   30*          EQUIVALENCE (OXID(1,1),IOXID(1,1))                                           000000
00130   31*          EQUIVALENCE (ACOMP(1,1),IACOMP(1,1))                                         000000
00131   32*          DIMENSION JOPT(10)                                                           000000
00132   33*          DIMENSION ID(5),RMOL(5)                                                      000000
00133   34*          DATA (ID(I),I=1,5)/'C','H','N','O','S'/                                      000000
00135   35*          DATA (RMOL(I),I=1,5)/12.01115,1.00797,14.0067,15.994,32.064/                 000000
00137   36*          DIMENSION ASH(10,5),IASH(10,5)                                               000000
00140   37*          EQUIVALENCE (ASH(1,1),IASH(1,1))                                             000000
00141   38*          DATA (IASH(I,1),I=1,10,2)/'SI','O',3*' '/                                    000000
00143   39*          DATA (IASH(I,2),I=1,10,2)/'FE','O',3*' '/                                    000000
00145   40*          DATA (IASH(I,3),I=1,10,2)/'AL','O',3*' '/                                    000000
00147   41*          DATA (IASH(I,4),I=1,10,2)/'FE','S',3*' '/                                    000000
00151   42*          DATA (ASH(I,1),I=2,10,2)/1.,2.,3*0./                                         000000
00153   43*          DATA (ASH(I,2),I=2,10,2)/2.,3.,3*0./                                         000000
00155   44*          DATA (ASH(I,3),I=2,10,2)/2.,3.,3*0./                                         000000
00157   45*          DATA (ASH(I,4),I=2,10,2)/1.,2.,3*0./                                         000000
00161   46*          DIMENSION CC(5),ICC(5)                                                       000000
00162   47*          DATA (ICC(I),I=1,5)/'C   ',4*' '/                                            000000
00164   48*          DATA (CC(I),I=1,5)/1.,4*0./                                                  000000
00166   49*          DIMENSION IH2O(5),H2O(5)                                                     000000
00167   50*          DATA (IH2O(I),I=1,5)/'H','O',3*' '/                                          000000
00171   51*          DATA (H2O(I),I=1,5)/2.,1.,3*0./                                              000000
00173   52*          DIMENSION HHT(40),HH(8)                                                      000000
00174   53*          DATA (HHT(I),I=1,40)/                                                        000000
00174   54*         X' 0 - E','NTER D','ATA   ',2*'       ',                                      000000
00174   55*         X' 1 - D','ULONG ','1     ',2*'       ',                                      000000
00174   56*         X' 2 - D','ULONG ','2     ',2*'       ',                                      000000
00174   57*         X' 3 - C','PP2   ',3*'      ',                                             000000
00174   58*         X' 4 - G','RUMMEL','-DAVIS',2*'       ',                                     000000
00174   59*         X' 5 - C','CSTOB ',3*'      ',                                             000000
00174   60*         X' 6 - M','AX OF ','ABOVE ',2*'       ',                                     000000
00174   61*         X' 7 - M','IN OF ','ABOVE ',2*'       '                                      000000
00174   62*         X   /                                                                        000000
00176   63*          DATA IC/12/                                                                  000000
00200   64*          CALL PAGIT                                                                   000000
00201   65*          CALL CHRSIZ(4)                                                               000001
00202   66*          NREAC=0                                                                      000004
00203   67*          IOPT=0                                                                       000005
00204   68*          DO 2 I=1,10                                                                  000011
00207   69*        2 JOPT(I)=1                                                                    000011
00211   70*          DO 12 I=1,5                                                                  000016
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00214    71*        12 ICOAL(I,1)=ID(I)                                          000016
00214    72*     C     FOR FIRST PASS DO NOT CHECK SAVED DATA                    000016
00216    73*           IF (.NOT.FIRST) GO TO 10                                  000020
00220    74*           IF ( NOT.RDYES(LINE1,42)) GO TO 300                       000022
00222    75*        10 CONTINUE                                                  000030
00222    76*     C     READ IN PREVIOUS COAL DATA                                000030
00223    77*           REWIND IC                                                 000030
00224    78*           READ (IC) NDUMMY,CF,HHVV,WCR,PER                          000032
00233    79*           READ (IC) CTEMP,OTEMP                                     000043
00237    80*           READ (IC) PROX,COAL,PER,IE,HH                             000051
00246    81*           READ (IC) NCOAL,NASH,NFUEL,NOXID                          000071
00259    82*           READ (IC) ((ICCOMP(I,J),I=1,12),J=1,NCOAL),               000112
00254    83*          X    ((ACOMP(I,J),I=1,11),J=1,NASH),                      000112
00254    84*          X    ((OFUEL(I,J),I=1,13),J=1,NFUEL),                     000112
00254    85*          X    ((OXID(I,J),I=1,11),J=1,NOXID)                       000112
00254    86*     C     DISPLAY PRESENT COAL DATA                                 000112
00312    87*           IF (FIRST) GO TO 50                                       000150
00314    88*           IF (.NOT.RDYES(LINE1,42)) GO TO 300                       000152
00316    89*        50 CONTINUE                                                  000160
00317    90*           CALL GOUT(' 1 - VOLATILE (OPTIONAL) AND ASH AS LBS/100 LBS DRY COA  000160
00317    91*          XL',56)                                                   000160
00320    92*           ENCODE (56,IOUT) PROX(1)                                  000163
00323    93*        56 FORMAT (6X,'VOLATILE',F10.4)                              000171
00324    94*           CALL GOUT(IOUT,24)                                        000171
00325    95*           ENCODE (58,IOUT) PROX(3)                                  000175
00330    96*        58 FORMAT (6X,'ASH',5X,F10.4)                                000203
00331    97*           CALL GOUT(IOUT,24)                                        000203
00332    98*           CALL GOUT(' ',1)                                          000207
00333    99*           ENCODE (60,IOUT) CTEMP                                    000213
00336   100*        60 FORMAT (' 2 - COAL TEMPERATURE IN DEG F',F10.2)           000221
00337   101*           CALL GOUT(IOUT,40)                                        000221
00340   102*           CALL GOUT(' ',1)                                          000225
00341   103*           CALL GOUT(' 3 - DRY COAL COMPOSITION AS LBS/100 LBS DRY COAL',49)  000231
00342   104*           DO 66 I=1,5                                               000240
00345   105*           ENCODE (62,IOUT) ICOAL(I,1),COAL(I,2)                     000240
00351   106*        62 FORMAT (5X,A4,5X,F10.4)                                   000246
00352   107*           CALL GOUT(IOUT,24)                                        000246
00353   108*        66 CONTINUE                                                  000253
00355   109*           CALL GOUT(' ',1)                                          000253
00356   110*           CALL GOUT(' 4 - OTHER COAL COMPONENTS AS LBS/100 LBS DRY COAL, STA  000257
00356   111*          XTE AND COMPOSITION',73)                                  000257
00357   112*           IF (NCOAL.EQ.0) GO TO 80                                  000263
00361   113*           DO 72 I=1,NCOAL                                           000265
00364   114*           ENCODE (70,IOUT) CCOMP(1,I),ICCOMP(2,I),                  000273
00364   115*          X    (ICCOMP(J*2+1,I),CCOMP(J*2+2,I),J=1,5)                000273
00375   116*        70 FORMAT (F10.4,10X,A4,5(2X,A2,2X,F8.4))                    000306
00376   117*           CALL GOUT(IOUT,94)                                        000306
00377   118*        72 CONTINUE                                                  000316
00401   119*        80 CALL GOUT(' ',1)                                          000316
00402   120*           CALL GOUT(' 5 - ASH COMPOSITION AS LBS/100 LBS ASH AND COMPONENT',  000321
00402   121*          X    53)                                                   000321
00403   122*           IF (NASH.EQ.0) GO TO 90                                   000325
00405   123*           DO 88 I=1,NASH                                            000327
00410   124*           ENCODE (84,IOUT) ACOMP(1,I),(IACOMP(J*2,I),ACOMP(J*2+1,I),J=1,5)  000335
00420   125*        84 FORMAT (F10.4,19X,5(2X,A2,2X,F8.4))                       000347
00421   126*           CALL GOUT(IOUT,94)                                        000347
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00422  127*      88 CONTINUE                                                    000357
00424  128*      90 CALL GOUT(' ',1)                                            000357
00425  129*         ENCODE (92,IOUT) PER                                        000362
00430  130*      92 FORMAT (' 6 - FRACTION CARBON CONVERSION',F10.4)            000370
00431  131*         CALL GOUT(IOUT,41)                                          000370
00432  132*         CALL GOUT(' ',1)                                            000374
00433  133*         ENCODE (96,IOUT) HH(IE+1)                                   000400
00436  134*      96 FORMAT (' 7 - HEATING VALUE OF COAL BTU/LB',F13.3)          000410
00437  135*         CALL GOUT(IOUT,46)                                          000410
00440  136*         CALL GOUT(' ',1)                                            000414
00441  137*         CALL GOUT(' 8 - OTHER FUEL COMPONENTS AS LBS/LB COAL, TEMPERATURE  000420
00441  138*        XIN DEG F, STATE AND COMPOSITION',86)                        000420
00442  139*         IF (NFUEL.EQ.0) GO TO 104                                   000424
00444  140*         DO 102 I=1,NFUEL                                            000426
00447  141*         ENCODE (100,IOUT) OFUEL(1,I),OFUEL(2,I),IOFUEL(3,I),        000434
00447  142*        X    (IOFUEL(J*2+2,I),OFUEL(J*2+3,I),J=1,5)                  000434
00461  143*      100 FORMAT (F10.4,F10.3,1X,A3,5(2X,A2,2X,F8.4))                000450
00462  144*         CALL GOUT(IOUT,94)                                          000450
00463  145*      102 CONTINUE                                                   000460
00465  146*      104 CALL GOUT(' ',1)                                           000460
00466  147*         ENCODE (106,IOUT) OTEMP                                     000463
00471  148*      106 FORMAT (' 9 - OXIDIZER TEMPERATURE IN DEG F',F10.2)        000471
00472  149*         CALL GOUT(IOUT,44)                                          000471
00473  150*         CALL GOUT(' ',1)                                            000475
00474  151*         CALL GOUT(' 10 - OXIDIZER COMPONENTS AS LBS/100 LBS OXIDIZER AND C  000501
00474  152*        XOMPONENT',63)                                               000501
00475  153*         IF (NOXID.EQ.0) GO TO 112                                   000505
00477  154*         DO 110 I=1,NOXID                                            000507
00502  155*         ENCODE (108,IOUT) OXID(1,I),(IOXID(J*2,I),OXID(J*2+1,I),J=1,5)  000515
00512  156*      108 FORMAT (F10.4,14X,5(2X,A2,2X,F8.4))                        000527
00513  157*         CALL GOUT(IOUT,94)                                          000527
00514  158*      110 CONTINUE                                                   000537
00516  159*      112 CALL GOUT(' ',1)                                           000537
00517  160*         CALL GOUT(' TYPE 1 OR 2 TO MODIFY OR REPLACE',33)           000542
00520  161*         CALL GOUT('      RETURN TO CONTINUE',23)                    000546
00521  162*         IOPT=0                                                      000552
00522  163*      114 CONTINUE                                                   000554
00523  164*         CALL RDATAI(1,IOPT,$114)                                    000554
00524  165*         IF (IOPT.LT.0.OR.IOPT.GT.2) GO TO 114                       000560
00526  166*         IF (IOPT.EQ.0) GO TO 680                                    000575
00530  167*         GO TO (120,300),IOPT                                        000577
00530  168*  C      SELECT GROUPS TO BE CHANGED                                 000577
00531  169*      120 CONTINUE                                                   000611
00532  170*         DO 124 I=1,10                                               000611
00535  171*      124 JOPT(I)=0                                                  000611
00537  172*         CALL GOUT (' TYPE GROUP NUMBERS OF DATA TO BE CHANGED IN ASCENDING  000612
00537  173*        X ORDER.   FOR EXAMPLE 1 3 7 9',83)                          000612
00540  174*      126 CONTINUE                                                   000617
00541  175*         CALL RDATAI(10,JOPT,$126)                                   000617
00542  176*         DO 130 I=10,1,-1                                            000626
00545  177*         JJ=JOPT(I)                                                  000626
00546  178*         IF (JJ.EQ.0) GO TO 130                                      000627
00550  179*         JOPT(I)=0                                                   000631
00551  180*         JOPT(JJ)=JJ                                                 000633
00552  181*      130 CONTINUE                                                   000637
00552  182*  C      ADD OR UPDATE COAL DATA                                     000637
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00554   183*        300 CONTINUE                                                    000637
00555   184*            CALL PAGIT                                                  000637
00556   185*            IF (JOPT(1).EQ.0) GO TO 314                                 000640
00556   186*      C     READ IN PROXIMATE ANALYSIS DATA                             000640
00560   187*        310 CALL GOUT(' TYPE (OPTIONAL) LBS VOLATILES/100 LBS DRY COAL',47) 000643
00561   188*            CALL RDATAF(1,PROX(1),$310)                                 000646
00562   189*            IF (IPROX(1).EQ.'      ') PROX(1)=0.                        000653
00564   190*        312 CALL GOUT(' TYPE LBS ASH/100 LBS DRY COAL',30)              000660
00565   191*            CALL RDATAF(1,PROX(3),$312)                                 000663
00566   192*            PROX(2)=100.-PROX(1)-PROX(3)                                000670
00567   193*        314 IF (JOPT(2).EQ.0) GO TO 320                                 000675
00567   194*      C     READ IN COAL TEMPERATURE                                    000675
00571   195*        316 CALL GOUT(' TYPE COAL TEMPERATURE IN DEG F',31)             000677
00572   196*            CALL RDATAF(1,CTEMP,$316)                                   000702
00573   197*        320 IF (JOPT(3).EQ.0) GO TO 340                                 000710
00573   198*      C     READ IN REACTING COAL COMPOSITION                           000710
00575   199*            CALL GOUT(' TYPE LBS/100 LBS DRY COAL FOR ELEMENTS',39)     000711
00576   200*        322 CALL GOUT(' C',2)                                           000716
00577   201*            CALL RDATAF(1,COAL(1,2),$322)                               000721
00600   202*        324 CALL GOUT(' H',2)                                           000727
00601   203*            CALL RDATAF(1,COAL(2,2),$324)                               000732
00602   204*        326 CALL GOUT(' N',2)                                           000740
00603   205*            CALL RDATAF(1,COAL(3,2),$326)                               000743
00604   206*        328 CALL GOUT(' O',2)                                           000751
00605   207*            CALL RDATAF(1,COAL(4,2),$328)                               000754
00606   208*        330 CALL GOUT(' S',2)                                           000762
00607   209*            CALL RDATAF(1,COAL(5,2),$330)                               000765
00610   210*        340 IF (JOPT(4).EQ.0) GO TO 350                                 000773
00610   211*      C     READ IN OTHER COAL COMPONENTS                               000773
00612   212*            CALL GOUT(' TYPE (OPTIONAL) OTHER COAL COMPONENTS',38)      000774
00613   213*            CALL GOUT(' TYPE LBS/100 LBS DRY COAL,STATE AND AND COMPONENT',50) 001000
00614   214*            CALL GOUT(' COAL TEMPERATURE IS ASSUMED',28)                001004
00615   215*            NI=1                                                        001010
00616   216*        342 CALL GOUT('     EXAMPLE 0.13  1HG  2HCL  2.',32)            001013
00617   217*        343 DO 344 J=1,5                                                001017
00622   218*            ICCOMP(J*2+1,NI)=2H                                         001030
00623   219*        344 CCOMP(J*2+2,NI)=0.                                          001031
00625   220*            CCOMP(1,NI)=0.                                              001033
00626   221*            ICCOMP(2,NI)='      '                                       001035
00627   222*        346 CALL RDATAF(12,CCOMP(1,NI),$342)                            001037
00630   223*            IF (CCOMP(1,NI)) ,348,                                      001046
00633   224*            IF (ICCOMP(1,NI).EQ.'      ') GO TO 348                     001050
00635   225*            NI=NI+1                                                     001053
00636   226*            GO TO 343                                                   001056
00637   227*        348 NCOAL=NI-1                                                  001060
00640   228*        350 IF (JOPT(5).EQ.0) GO TO 380                                 001063
00642   229*            IF (IOPT.NE.1) GO TO 351                                    001064
00644   230*            ENCODE (2350,IOUT) JOPT(5)                                  001067
00647   231*      2350  FORMAT (' GROUP NUMBER',I5)                                 001075
00650   232*            CALL GOUT(IOUT,18)                                          001075
00651   233*      2352  IF (NASH.EQ.0) GO TO 2357                                  001102
00653   234*            DO 2356 I=1,NASH                                            001103
00656   235*            ENCODE (2354,IOUT) I,ACOMP(1,I),                            001112
00656   236*           X   (IACOMP(J*2,I),IACOMP(J*2+1,I),J=1,5)                    001112
00667   237*      2354  FORMAT (I4,F10.4,14X,5(2X,A2,2X,F8.4))                     001126
00670   238*            CALL GOUT(IOUT,98)                                          001126
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00671  239*      2356 CONTINUE                                                  001137
00673  240*      2357 CALL GOUT(' TYPE 1-ALTER, 2-DELETE, 3-ADD, RETURN TO CONTINUE',50)  001137
00674  241*      2358 KOUT=0                                                    001143
00675  242*           CALL RDATAI(1,KOUT,$2358)                                 001143
00676  243*           IF (KOUT.LT.0.OR.KOUT.GT.3) GO TO 2358                    001150
00700  244*           IF (KOUT.EQ.0) GO TO 2380                                 001165
00702  245*           IF (KOUT.EQ.3) GO TO 2370                                 001167
00704  246*           CALL GOUT(' TYPE LINE NUMBER.',17)                        001172
00705  247*      2360 LN=0                                                      001177
00706  248*           CALL RDATAI(1,LN,$2360)                                   001177
00707  249*           IF (LN.LE.0.OR.LN.GT.NASH) GO TO 2360                     001204
00711  250*           IF (KOUT.EQ.1) GO TO 2366                                 001221
00711  251*     C     DELETE                                                    001221
00713  252*           L1=LN+1                                                   001224
00714  253*           IF (LN.EQ.NASH) GO TO 2364                                001227
00716  254*           DO 2362 I=L1,NASH                                         001234
00721  255*           DO 2362 J=1,11                                            001245
00724  256*           ACOMP(J,I-1)=ACOMP(J,I)                                   001245
00725  257*      2362 CONTINUE                                                  001250
00730  258*      2364 NASH=NASH-1                                               001250
00731  259*           GO TO 2352                                                001252
00731  260*     C     ALTER                                                     001252
00732  261*      2366 NI=LN                                                     001254
00733  262*           GO TO 2372                                                001255
00733  263*     C     ADD                                                       001255
00734  264*      2370 NASH=NASH+1                                               001257
00735  265*           NI=NASH                                                   001261
00735  266*     C     READ IN NEW DATA                                          001261
00736  267*      2372 CALL GOUT(' LBS/100 LBS DRY ASH AND COMPONENT',34)        001263
00737  268*           DO 2374 J=1,5                                             001266
00742  269*           IACOMP(J*2,NI)=2H                                         001300
00743  270*      2374 ACOMP(J*2+1,NI)=0.                                        001301
00745  271*           CALL RDATAF(11,ACOMP(1,NI),$2372)                         001303
00746  272*           GO TO 2352                                                001313
00746  273*     C     CHECK FOR FES2                                            001313
00747  274*      2380 FES2=0.                                                   001315
00750  275*           DO 2386 I=1,NASH                                          001315
00753  276*           DO 2384 J=1,5                                             001334
00756  277*           IF (IACOMP(J*2,I).NE.IASH(J*2-1,4)) GO TO 2386            001334
00760  278*           IF (ACOMP(J*2+1,I).NE.ASH(J*2,4)) GO TO 2386              001337
00762  279*      2384 CONTINUE                                                  001346
00764  280*           FES2=ACOMP(1,I)                                           001346
00765  281*           GO TO 380                                                 001350
00766  282*      2386 CONTINUE                                                  001354
00770  283*           GO TO 380                                                 001354
00771  284*       351 CONTINUE                                                  001356
00771  285*     C     READ IN ASH COMPONENTS                                    001356
00772  286*           CALL GOUT(' TYPE LBS/100 LBS DRY ASH FOR COMPONENTS',40)  001356
00773  287*           CALL GOUT(' STATE ASSUMED SOLID. COAL TEMPERATURE ASSUMED.',47)  001361
00774  288*       352 CALL GOUT(' SIO2',5)                                      001366
00775  289*           CALL RDATAF(1,ACOMP(1,1),$352)                            001371
00776  290*       354 CALL GOUT(' FE2O3',6)                                     001377
00777  291*           CALL RDATAF(1,ACOMP(1,2),$354)                            001402
01000  292*       356 CALL GOUT(' AL2O3',6)                                     001410
01001  293*           CALL RDATAF(1,ACOMP(1,3),$356)                            001417
01002  294*       358 CALL GOUT(' FES2',5)                                      001421
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01003   295*          CALL RDATAF(1,ACOMP(1,9),$358)                                  001424
01004   296*          FES2=ACOMP(1,9)                                                 001431
01005   297*          IF (IACOMP(1,9).EQ.'      ') FES2=0.                            001433
01007   298*          J=0                                                             001437
01007   299*    C     REMOVE ANY ZERO COMPONENTS                                      001437
01010   300*          DO 369 I=1,9                                                    001440
01013   301*          IF (ACOMP(1,I)) ,369,                                           001450
01016   302*          IF (IACOMP(1,I).EQ.'      ') GO TO 369                          001452
01020   303*          J=J+1                                                           001455
01021   304*          ACOMP(1,J)=ACOMP(1,I)                                           001461
01022   305*          IF (I.NE.J) ACOMP(1,I)=0.                                       001462
01024   306*          DO 362 LL=1,10                                                  001466
01027   307*    362   ACOMP(LL+1,J)=ASH(LL,I)                                        001477
01031   308*    369   CONTINUE                                                       001504
01033   309*          NI=J+1                                                          001504
01033   310*    C     ADD OTHER ASH COMPONENTS                                        001504
01034   311*          CALL GOUT(' CONTINUE WITH ASH COMPONENTS',,29)                  001507
01035   312*          CALL GOUT(' LBS/100 LBS DRY ASH AND COMPONENT',,38)             001613
01036   313*    366   CALL GOUT('      EXAMPLE  0.25  2HTI  1.  1HO  2.',,38)         001520
01037   314*    367   DO 368 J=1,5                                                   001524
01042   315*          IACOMP(J+2,NI)=2H                                               001535
01043   316*    368   ACOMP(J+2+1,NI)=0.                                           001536
01045   317*    370   CALL RDATAF(11,ACOMP(1,NI),$366)                             001540
01046   318*          IF (ACOMP(1,NI)) ,372,                                          001550
01051   319*          IF (IACOMP(1,NI).EQ.'      ') GO TO 372                         001552
01053   320*          NI=NI+1                                                         001555
01054   321*          GO TO 367                                                       001560
01055   322*    372   NASH=NI-1                                                     001562
01056   323*    380   IF (JOPT(4).EQ.0) GO TO 390                                  001565
01056   324*    C     READ COAL CONVERSION FRACTION                                   001565
01060   325*    382   CALL GOUT(' TYPE CARBON CONVERSION FRACTION, FOR EXAMPLE, 0.89',  001567
01060   326*         X   51)                                                          001567
01061   327*          CALL RDATAF(1,PER,$382)                                         001572
01061   328*    C     COMPUTE VALUES FOR HHV BY DIFFERENT FORMULAS                    001572
01062   329*    390   CONTINUE                                                       001600
01063   330*          HH(2)=145.44*COAL(1,2)+620.28*(COAL(2,2)-0.125*COAL(4,2))       001600
01063   331*         X  +40.50*COAL(5,2)                                              001600
01064   332*          HH(3)=146.0*COAL(1,2)+620.0*(COAL(2,2)-0.125*COAL(4,2))         001614
01064   333*         X  +40.50*COAL(5,2)                                              001614
01065   334*          HH(4)=144.9*COAL(1,2)+610.0*(COAL(2,2)-0.125*COAL(4,2))         001623
01065   335*         X   +55.56*COAL(5,2)                                             001623
01066   336*          HH(5)=(654.3*COAL(2,2)/(100.-PROX(3))+429.62)*                  001634
01066   337*         X   (COAL(1,2)/3.+COAL(2,2)-0.125*(COAL(4,2)-COAL(5,2)))        001634
01067   338*          HH(6)=146.58*COAL(1,2)+568.78*COAL(2,2)+29.8*COAL(5,2)          001653
01067   339*         X   -6.58*PROX(3)-51.53*(COAL(3,2),COAL(4,2))                    001653
01070   340*          HH(7)=AMAX1(HH(2),HH(3),HH(4),HH(5),HH(6))                      001673
01071   341*          HH(8)=AMIN1(HH(2),HH(3),HH(4),HH(5),HH(6))                      001715
01072   342*          DO 392 I=2,8                                                    001743
01075   343*          ENCODE (394,HHT(I*5-1)) HH(I)                                   001743
01100   344*    392   CONTINUE                                                       001753
01102   345*    394   FORMAT (F12.3)                                               001753
01103   346*          IF (JOPT(7).EQ.0) GO TO 420                                     001753
01105   347*          CALL GOUT(' HHV CALCULATION',16)                                001755
01106   348*          DO 398 I=1,8                                                    001764
01111   349*          CALL GOUT(HHT(I*5-4),30)                                        001764
01112   350*    398   CONTINUE                                                       001773
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01114  351*      400 CALL RDATAI(1,IE,$400)                                    001773
01115  352*          IF (IE.LT.0.OR.IE.GT.8) GO TO 400                         001777
01117  353*          IF (IE.GT.0) GO TO 420                                    002014
01121  354*      402 CALL GOUT(' ENTER HHV AS BTU/LB COAL',25)                 002020
01122  355*          CALL RDATAF(1,HH(1),$402)                                 002023
01123  356*      420 HHVV=HH(IE*1)                                             002031
01124  357*          IF (JOPT(8).EQ.0) GO TO 440                               002033
01126  358*          IF (IOPT.NE.1) GO TO 421                                  002035
01130  359*          ENCODE (2350,IOUT, JOPT(8)                                002040
01133  360*          CALL GOUT(IOUT,18)                                        002046
01134  361*     2420 IF (NFUEL.EQ.0) GO TO 2427                                002053
01136  362*          DO 2426 I=1,NFUEL                                         002064
01141  363*          ENCODE (2424,IOUT) I,OFUEL(1,I),OFUEL(2,I),OFUEL(3,I),    002063
01141  364*         X    (IOFUEL(J*2+2,I),OFUEL(J*2+3,I),J=1,5)                 002063
01154  365*     2424 FORMAT (I4,F10.4,F10.3,1X,A3,5(2X,A2,2X,F8.4))            002101
01155  366*          CALL GOUT(IOUT,98)                                        002101
01156  367*     2426 CONTINUE                                                  002112
01160  368*     2427 CALL GOUT(' TYPE 1-ALTER, 2-DELETE, 3-ADD, RETURN TO CONTINUE',50)  002112
01161  369*     2422 KOUT=0                                                    002116
01162  370*          CALL RDATAI(1,KOUT,$2422)                                 002116
01163  371*          IF (KOUT.LT.0.OR.KOUT.GT.3) GO TO 2422                    002123
01165  372*          IF (KOUT.EQ.0) GO TO 430                                  002140
01167  373*          IF (KOUT.EQ.3) GO TO 2434                                 002142
01171  374*          CALL GOUT(' TYPE LINE NUMBER',17)                         002145
01172  375*     2428 LN=0                                                      002152
01173  376*          CALL RDATAI(1,LN,$2428)                                   002152
01174  377*          IF (LN.LE.0.OR.LN.GT.NFUEL) GO TO 2428                    002157
01176  378*          IF (KOUT.EQ.1) GO TO 2432                                 002174
01176  379*     C    DELETE                                                    002174
01200  380*          L1=LN+1                                                   002177
01201  381*          IF (LN.EQ.NFUEL) GO TO 2431                               002202
01203  382*          DO 2430 I=1,NFUEL                                         002205
01206  383*          DO 2430 J=1,13                                            002213
01211  384*          OFUEL(J,I-1)=OFUEL(J,I)                                   002213
01212  385*     2430 CONTINUE                                                  002216
01215  386*     2431 NFUEL=NFUEL-1                                             002216
01216  387*          GO TO 2420                                                002220
01216  388*     C    ALTER                                                     002220
01217  389*     2432 NI=LN                                                     002222
01220  390*          GO TO 2436                                                002223
01220  391*     C    ADD                                                       002223
01221  392*     2434 NFUEL=NFUEL+1                                             002225
01222  393*          NI=NFUEL                                                  002227
01222  394*     C    READ IN NEW DATA                                          002227
01223  395*     2436 CALL GOUT(' TYPE LBS/LB COAL, TEMPERATURE (DEG F) AND STATE AND CO  002231
01223  396*         XMPONENT',63)                                              002231
01224  397*          DO 2438 I=1,5                                             002234
01227  398*          IOFUEL(J*2+2,NI)=2H                                       002246
01230  399*     2438 OFUEL(J*2+3,NI)=0.                                        002247
01232  400*          OFUEL(1,NI)=0.                                            002251
01233  401*          OFUEL(2,NI)=0.                                            002253
01234  402*          IOFUEL(3,NI)='  '                                         002254
01235  403*          CALL RDATAF(13,OFUEL(1,NI),$2436)                         002256
01236  404*          GO TO 2420                                                002265
01237  405*      421 CONTINUE                                                  002267
01237  406*     C    READ IN OTHER FUEL COMPONENTS                             002267
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01240     407*          CALL GOUT(* TYPE OTHER FUEL COMPONENTS*,27)                                    002267
01241     408*          CALL GOUT(* TYPE LBS/LB COAL, TEMPERATURE (DEG F) AND STATE AND CO             002272
01241     409*         XMPONENT*,63)                                                                   002272
01242     410*          NI=1                                                                           002276
01243     411*      422 CALL GOUT(*     EXAMPLE  0.31  100.  1HG  1HH  2.  1HO  1.*,47)               002301
01249     412*      423 DO 429 J=1,5                                                                   002305
01247     413*          IOFUEL(J*2-2,NI)=2H                                                            002316
01250     414*      429 OFUEL(J*2-1,NI)=0.                                                             002317
01252     415*          OFUEL(1,NI)=0.                                                                 002321
01253     416*          OFUEL(2,NI)=0.                                                                 002323
01254     417*          IOFUEL(3,NI)='  '                                                              002329
01255     418*      426 CALL RDATAF(11,OFUEL(1,NI),$4221)                                              002326
01256     419*          IF (OFUEL(1,NI)) ,428,                                                         002335
01261     420*          IF (IOFUEL(1,NI).EQ.'  ') GO TO 428                                            002337
01263     421*          NI=NI+1                                                                        002342
01264     422*          GO TO 423                                                                      002345
01265     423*      428 NFUEL=NI-1                                                                     002347
01266     424*      430 WCR=0.                                                                         002352
01267     425*          DO 434 I=1,NFUEL                                                               002352
01272     426*          DO 432 J=1,5                                                                   002370
01275     427*          IF (IOFUEL(J*2-2,I).NE.IH20(J)) GO TO 434                                      002370
01277     428*          IF (OFUEL(J*2-1,I).NE.H20(J)) GO TO 434                                        002373
01301     429*      432 CONTINUE                                                                       002401
01303     430*          WCR=OFUEL(1,I)                                                                 002401
01304     431*          GO TO 440                                                                      002403
01305     432*      434 CONTINUE                                                                       002410
01307     433*      440 IF (JOPT(9).EQ.0) GO TO 450                                                    002410
01307     434*    C     READ IN OXIDIZER TEMPERATURE                                                   002410
01311     435*      442 CALL GOUT(* TYPE IN OXIDIZER TEMPERATURE, DEG F*,36)                           002412
01312     436*          CALL RDATAF(1,OTEMP,$442)                                                      002415
01313     437*      450 IF (JOPT(10).EQ.0) GO TO 470                                                   002423
01313     438*    C     READ IN OXIDIZER COMPONENTS                                                    002423
01315     439*          CALL GOUT(* TYPE OXIDIZER COMPONENTS*,25)                                      002426
01316     440*          CALL GOUT(* TYPE LBS/100 LBS OXIDIZER AND COMPONENT*,40)                       002430
01317     441*          NI=1                                                                           002434
01320     442*      452 CALL GOUT(*     EXAMPLE  95.0  AHO  2.*,27)                                    002437
01321     443*      453 DO 454 J=1,5                                                                   002443
01324     444*          IOXID(J*2-1,NI)=2H                                                             002450
01325     445*      454 OXID(J*2-1,NI)=0.                                                              002455
01327     446*      456 CALL RDATAF(11,OXID(1,NI),$452)                                                002457
01330     447*          IF (OXID(1,NI)) ,460,                                                          002467
01333     448*          IF (IOXID(1,NI).EQ.'  ') GO TO 460                                             002471
01335     449*          NI=NI+1                                                                        002474
01336     450*          GO TO 453                                                                      002477
01337     451*      460 NOXID=NI-1                                                                     002501
01340     452*      470 CONTINUE                                                                       002504
01340     453*    C     COMPUTATION FOR COAL CARD                                                      002504
01341     454*          SINRT=COAL(1,2)*(1.-PER)                                                       002504
01342     455*          COAL(1,2)=COAL(1,2)*PER                                                        002507
01343     456*          SUM=0.                                                                         002512
01344     457*          N=NREAC+1                                                                      002513
01345     458*          NS=N                                                                           002516
01346     459*          DO 482 I=1,5                                                                   002531
01351     460*      482 SUM=SUM+COAL(I,2)                                                              002531
01353     461*          DO 484 I=1,5                                                                   002541
01356     462*      484 ANUM(N,I)=(COAL(I,2)/SUM)*100.                                                 002541
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01360  486*          SUM1=0.                                                  002545
01361  487*          DO 488 I=1,5                                             002553
01364  488*          ANUM(N,I)=ANUM(N,I)/PMOL(I)                              002553
01365  489*      488 SUM1=SUM1+ANUM(N,I)                                      002555
01367  490*          DO 488 I=1,5                                             002565
01372  491*      488 ANUM(N,I)=(ANUM(N,I)/SUM1)*100.                          002565
01372  492*      C   CREATE COAL CARD                                         002565
01375  493*          DO 499 I=1,5                                             002576
01377  494*      499 NAME(N,I)=ICOAL(I,1)                                     002576
01401  495*          NAME(N,6)=1H                                             002600
01402  496*          ANUM(N,6)=0.                                             002602
01402  497*      C   COMPUTE COAL/FUEL RATIO                                  002607
01403  498*          CSUM=0.                                                  002603
01404  499*          DO 498 I=1,NFUEL                                         002607
01407  500*      498 CSUM=CSUM+OFUEL(1,I)                                     002607
01411  501*          CF=1.0/(1.0+CSUM)                                        002617
01412  502*          PECWT(N)=CF*SUM/100.                                     002616
01413  503*          MOLE(N)=1H                                               002621
01414  504*          FAZ(N)=1HS                                               002623
01415  505*          RTEMP(N)=(CTEMP-32.)/1.8+273.15                          002625
01416  506*          FOX(N)=1HF                                               002632
01417  507*          DENS(N)=0.                                               002634
01420  508*          NREAC=NREAC+1                                            002635
01420  509*      C   CREATE INERT CARBON CARD                                 002635
01421  510*          IF (PER-1.) ,504,                                        002640
01424  511*          N=NREAC+1                                                002643
01425  512*          DO 500 I=1,6                                             002645
01430  513*          NAME(N,I)=4H                                             002653
01431  514*      500 ANUM(N,2)=0.                                             002654
01433  515*          NAME(N,1)='IC  '                                         002656
01434  516*          ANUM(N,1)=1.                                             002660
01435  517*          PECWT(N)=CF*SINRT/100.                                   002662
01436  518*          MOLE(N)=1H                                               002666
01437  519*          ENTH(N)=0.                                               002667
01440  520*          NAME(N,6)=2H00                                           002670
01441  521*          FAZ(N)=1HS                                               002672
01442  522*          RTEMP(N)=RTEMP(NS)                                       002674
01443  523*          FOX(N)=1HF                                               002677
01444  524*          DENS(N)=0.                                               002701
01445  525*          NREAC=NREAC+1                                            002702
01445  526*      C   CREATE OTHER COAL COMPONENTS CARDS                       002702
01446  527*      504 IF (NCOAL.EQ.0) GO TO 520                                002706
01450  528*          N=NREAC                                                  002707
01451  529*          DO 508 I=1,NCOAL                                         002715
01456  530*          DO 506 J=1,5                                             002734
01457  531*          NAME(N+I,J)=ICCOMP(J*2+1,I)                              002734
01460  532*      506 ANUM(N+I,J)=CCOMP(J*2+2,I)                               002735
01462  533*          PECWT(N+I)=CCOMP(1,I)*CF/100.                            002740
01463  534*          MOLE(N+I)=1H                                             002744
01466  535*          IFAZ(N+I)=ICCOMP(2,I)                                    002746
01465  536*          ENTH(N+I)=0.                                             002750
01466  537*          NAME(N+I,6)=2H00                                         002753
01467  538*          ANUM(N+I,6)=0.                                           002753
01470  539*          RTEMP(N+I)=(CTEMP-32.)/1.8+273.15                        002754
01471  540*          FOX(N+I)=1HF                                             002756
01472  541*          DENS(N+I)=0.                                             002760
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01473  519*      508 CONTINUE                                                  002767
01475  520*      520 NREAC=NREAC+NCOAL                                         002767
01475  521*    C     CREATE CARDS FOR ASH COMPONENTS                         002767
01476  522*          N=NREAC                                                   002771
01477  523*          SUM2=0.                                                   002772
01500  524*          IF (ASH.EQ.0) GO TO 540                                   002773
01502  525*          ASHF=CF*PROX(3)/100.                                      002775
01503  526*          DO 522 I=1,NASH                                           003010
01506  527*      522 SUM2=SUM2+ACOMP(1,I)                                      003021
01510  528*          DO 528 I=1,NASH                                           003035
01513  529*          DO 526 J=1,5                                              003035
01516  530*          NAME(N+I,J)=IACOMP(J*2,I)                                 003036
01517  531*      526 NUM(N+I,J)=ACOMP(J*2+1,I)                                 003036
01521  532*          PECWT(N+I)=(ACOMP(1,I)*ASHF)/SUM2                         003041
01522  533*          MOLE(N+I)=1H                                              003045
01523  534*          FAZ(N+I)=1HS                                              003047
01524  535*          ENTH(N+I)=0.                                              003051
01525  536*          NAME(N+I,6)=2H00                                          003052
01526  537*          ANUM(N+I,6)=0.                                            003054
01527  538*          RTEMP(N+I)=(CTEMP-32.)/1.8+273.15                         003055
01530  539*          FOX(N+I)=1HF                                              003057
01531  540*          DENS(N+I)=0.                                              003061
01532  541*      528 CONTINUE                                                  003070
01534  542*      540 NREAC=NREAC+NASH                                          003070
01534  543*    C     COMPUTE ENTHALPY FOR COAL                               003070
01535  544*          FES2=FES2*ASHF/(SUM2*CF)                                  003072
01536  545*          HHV=((HHVV-14485.7*SINRT/100.)/1.8)*(100./SUM)*(100./SUM1)*100.  003100
01537  546*          FES2C=(100./(1.8*119.85))*(100./SUM)*(100./SUM1)*FES2     003117
01540  547*          HF1=-ANUM(NS,1)*94051.8-0.5*ANUM(NS,2)*68317.4            003124
01540  548*         X   -ANUM(NS,5)*70960.-FES2C*197650.                       003124
01541  549*          PX=100.*PROX(1)/(PROX(1)+PROX(2))                         003141
01542  550*          HF2=(.175*(CTEMP-77)+.002*PX*(CTEMP-77)+                  003147
01542  551*         X   0.00025*(CTEMP-60)**2-0.07225)*(100./SUM1)*(100./1.8)  003147
01543  552*          ENTH(NS)=HHV+HF1+HF2                                      003167
01543  553*    C     CREATE CARDS FOR OTHER FUEL COMPONENTS                    003167
01544  554*          N=NREAC                                                   003172
01545  555*          IF (NFUEL.EQ.0) GO TO 560                                 003173
01547  556*          DO 548 I=1,NFUEL                                          003200
01552  557*          DO 546 J=1,5                                              003214
01555  558*          NAME(N+I,J)=IOFUEL(J*2+2,I)                               003214
01556  559*      546 ANUM(N+I,J)=OFUEL(J*2+3,I)                                003215
01560  560*          PECWT(N+I)=OFUEL(1,I)*CF                                  003220
01561  561*          MOLE(N+I)=1H                                              003223
01562  562*          IFAZ(N+I)=IOFUEL(3,I)                                     003225
01563  563*          ENTH(N+I)=0.                                              003227
01564  564*          NAME(N+I,6)=2H00                                          003230
01565  565*          ANUM(N+I,6)=0.                                            003232
01566  566*          RTEMP(N+I)=(OFUEL(2,I)-32.)/1.8+273.15                    003233
01567  567*          FOX(N+I)=1HF                                              003240
01570  568*          DENS(N+I)=0.                                              003242
01571  569*      548 CONTINUE                                                  003253
01571  570*    C     LOOK UP CARBON                                          003253
01573  571*          DO 552 I=1,NFUEL                                          003253
01576  572*          DO 550 J=1,5                                              003263
01601  573*          IF (NAME(N+I,J).NE.ICC(J)) GO TO 552                      003263
01603  574*          IF (ANUM(N+I,J)-CC(J)) 552,,552                           003266
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01606  575*        550 CONTINUE                                                  003274
01610  576*            GO TO 55                                                  003274
01611  577*        552 CONTINUE                                                  003277
01613  578*            GO TO 560                                                 003277
01613  579*      C     CREATE INERT CARBON CARD FOR RECYCLE CARBON               003277
01616  580*        554 DO 556 J=1,6                                              003301
01617  581*            NAME(N+NFUEL+1,J)=NAME(N+I,J)                             003322
01620  582*        556 ANUM(N+NFUEL+1,J)=ANUM(N+I,J)                             003323
01622  583*            NAME(N+NFUEL,1)=1HC                                       003326
01623  584*            PECWT(N+NFUEL+1)=(1.-PER)*PECWT(N+I)                      003331
01624  585*            PECWT(N+I)=PER*PECWT(N+I)                                 003336
01625  586*            MOLE(N+NFUEL+1)=MOLE(N+I)                                 003341
01626  587*            FAZ(N+NFUEL+1)=FAZ(N+I)                                   003343
01627  588*            ENTH(N+NFUEL+1)=ENTH(N+I)                                 003345
01630  589*            RTEMP(N+NFUEL,1)=RTEMP(N+I)                               003347
01631  590*            FOX(N+NFUEL+1)=FOX(N+I)                                   003351
01632  591*            DENS(N+NFUEL+1)=DENS(N+I)                                 003353
01633  592*            NREAC=NREAC+1                                             003355
01634  593*        560 NREAC=NREAC+NFUEL                                         003361
01634  594*      C     CREATE CARDS FOR OXIDIZER COMPONENTS                      003361
01635  595*            N=NREAC                                                   003363
01636  596*            IF (NOXID.EQ.0) GO TO 590                                 003364
01640  597*            SUM3=0.                                                   003366
01641  598*            DO 572 I=1,NOXID                                          003376
01644  599*        572 SUM3=SUM3+OXID(1,I)                                       003407
01646  600*            DO 578 I=1,NOXID                                          003423
01651  601*            DO 576 J=1,5                                              003423
01654  602*            NAME(N+I,J)=IOXID(J*2,I)                                  003423
01655  603*        576 ANUM(N+I,J)=OXID(J*2+1,I)                                 003424
01657  604*            PECWT(N+I)=OXID(1,I)/SUM3                                 003427
01660  605*            MOLE(N+I)=1H                                              003432
01661  606*            FAZ(N+I)=1HG                                              003434
01662  607*            ENTH(N+I)=0.                                              003436
01663  608*            NAME(N+I,6)=2H00                                          003437
01664  609*            ANUM(N+I,6)=0.                                            003441
01665  610*            RTEMP(N+I)=(OTEMP-32.)/1.8+273.15                         003442
01666  611*            FOX(N+I)=1HO                                              003444
01667  612*            DENS(N+I)=0.                                              003446
01670  613*        578 CONTINUE                                                  003455
01672  614*        590 NREAC=NREAC+NOXID                                         003455
01672  615*      C     SAVE COAL DATA                                            003455
01673  616*            COAL(1,2)=COAL(1,2)/PER                                   003457
01674  617*            REWIND IC                                                 003462
01675  618*            WRITE (IC) NREAC,CF,HHVY,WCR,PER                          003465
01704  619*            WRITE (IC) CTEMP,OTEMP                                    003476
01710  620*            WRITE (IC) PROX,COAL,PER,IE,HH                            003504
01717  621*            WRITE (IC) NCOAL,NASH,NFUEL,NOXID                         003524
01725  622*            WRITE (IC) ((CCOMP(I,J),I=1,12),J=1,NCOAL),               003552
01725  623*           X    ((ACOMP(I,J),I=1,11),J=1,NASH),                       003552
01725  624*           X    ((OFUEL(I,J),I=1,13),J=1,NFUEL),                      003552
01725  625*           X    ((OXID(I,J),I=1,11),J=1,NOXID)                        003552
01725  626*      C     WRITE OUT REACTANT FILE                                   003552
01763  627*            WRITE (IC) NREAC,CF                                       003606
01767  628*            DO 610 I=1,NREAC                                          003620
01772  629*            WRITE (IC) (NAME(I,J),ANUM(I,J),J=1,5),PECWT(I),MOLE(I),  003620
01772  630*           X   ENTH(I),NAME(I,6),ANUM(I,6),FAZ(I),RTEMP(I),FOX(I),DENS(I)  003620
```

```
02012     631*        610 CONTINUE                                    003696
02014     632*            ENDFILE IC                                  003696
02015     633*        680 CONTINUE                                    003652
02016     634*            RETURN                                      003652
02017     635*            END                                         003712
```

END OF COMPILATION: NO DIAGNOSTICS.

```
@HDG,P      CPHS
```

```
@FOR,S    CPHS,CPHS
HSA  E3 -10/15/80-13:06:13 (11,)

    SUBROUTINE CPHS      ENTRY POINT 000567

    STORAGE USED: CODE(1) 000603; DATA(D) 000160; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003   SPECES  017106
     0004   MISC    001701
     0005   INDX    000041
     0006   LOWTH   001201
     0007   CCC     000003

    EXTERNAL REFERENCES (BLOCK, NAME)

     0010   NWDUS
     0011   NIO2S
     0012   ALOG
     0013   NIO1S
     0014   NERR3S

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001    000031 10L      0001    000207 171G     0001    000217 174G     0001    000093 20L      0001    000351 221G
     0001    000462 254G     0001    000065 30L      0001    000067 31L      0001    000157 32L      0000    000041 3333F
     0001    000164 40L      0001    000176 60L      0001    000230 70L      0001    000233 80L      0001    000412 87L
     0000    000060 88F      0001    000472 89L      0001    000531 90L      0000    000103 904F     0003    011052 A
     0004    000640 AM       0004    000705 AM1      0004    001135 ANUM     0004    000004 ATOM     0004    000519 BO
     0004    000545 BOP      0005    000036 CALCH    0003 R  000000 COEF     0005    000001 CONVG    0006 R  000361 CPL
     0004    000706 CPR1     0004 R  000634 CPSUM    0000 R  000040 CPUSED   0000 R  000035 CPX      0000 R  000007 CPXX
     0004    000654 DATA     0003    010624 DELN     0007    000002 DEMAND   0004    001560 DENS     0003 R  004312 EN
     0003    010150 ENLN     0004    001700 ENLSAV   0004    000000 ENN      0004    001676 ENNL     0004    001677 ENSAVE
     0004    001814 ENTH     0004    000636 EQRAT    0004    001945 FAZ      0004    001527 FOX      0007    000000 GRAPH
     0006 R  000551 HL       0005    000003 HP       0004    000642 HPP      0004    000637 HSUBO    0000 R  000034 HX
     0000 R  000013 HXX      0003 R  010376 HO       0000 I  000037 I        0005    000030 IC       0005    000000 IDEBUG
     0000 I  000001 IER      0000 I  000023 IEXTND   0006 I  001131 ILSP     0005    000015 IMAT     0000 I  000002 IMSG
     0005    000132 INJPS    0005    000023 IONS     0005    000021 IP       0005    000037 IOSAVE   0005    000016 IQ1
     0005    000005 ISV      0005    000034 IT       0003 I  016266 IUSE     0000 I  000026 IX       0005 I  000031 J
     0005    000026 JLIQ     0007 I  000001 JOUT     0005    000025 JSOL     0000 I  000024 K        0000 I  000025 KK
     0005    000014 KMAT     0000 I  000027 KX       0004    000463 LLMT     0005    000040 LSAVE    0000 I  000036 M
     0005    000006 MOLES    0004    000707 NAME     0005    000024 NC       0005    000022 NEWR     0005    000035 NFZ
     0005    000012 NLM      0006 I  000000 NLTSP    0005    000017 NOF      0005    000020 NOMIT    0005    000007 NP
     0005 I  000011 NPT      0005    000027 NREAC    0005 I  000013 NS       0000 I  000000 NSPP1    0005    000010 NT
     0000 I  000030 NTUP     0004    000635 OF       0004    001644 OXF      0004    001363 PECWT    0004    000633 PP
     0004    000644 RH       0004    001611 RHOP     0004    001612 RMW      0004    001476 RTEMP    0003 R  004064 S
     0005    000033 SHOCK    0006 R  000741 SL       0003    016660 SLN      0005    000004 SP       0003 I  015364 SUB
     0006 I  000001 SUBLT    0004    000001 SUMN     0000 R  000033 SX       0000 R  000017 SXX      0004    000003 SO
     0003    016514 TEMP     0004    000632 THIGH    0006 R  000171 TL       0004 R  001643 TLN      0000 R  000032 TLNS
     0004 R  000670 TLOW     0004    000627 TM       0004 R  000631 TMID     0005    000002 TP       0004 R  000002 TT
     0000 R  000031 TTS      0000 R  000003 TXX      0004    000646 VMIN     0005    000032 VOL      0004    000650 VPLS
```

000[9] 000652 wP

```
00101     1*          SUBROUTINE CPHS                                                    000002
00101     2*    C                                                                        000002
00101     3*    C     CALCULATES THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES         000002
00101     4*    C                                                                        000002
00101     5*    C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)    000002
00101     6*    C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)     000002
00101     7*          INCLUDE SPECPK                                                     000002
00107     8*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),          000002
00107     9*         1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,     000002
00107    10*         2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),     /MISC/ 000002
00107    11*         3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),  000002
00107    12*         4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,   000002
00107    13*         5              RMM(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV              000002
00110    14*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,    /INDX/ 000002
00110    15*         1              KMAT,IMAT,IQ,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/ 000002
00110    16*         2              NREAC,IC,J,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE      /INDX/ 000002
00111    17*          COMMON /LOWTH/ NLTSP,SUBLT(90,3),TL(90,3),CPL(90,3),HL(90,3),      /LOWTH/ 000002
00111    18*         1               SL(90,3),ILSP(90)                                  /LOWTH/ 000002
00111    19*    C                                                                        000002
00112    20*             COMMON /CCC/ GRAPH,JOUT,DEMAND                                  000002
00112    21*    C                                                                        000002
00113    22*          DATA IER/0/,IMSG/-1/                                               000002
00116    23*          DIMENSION TXX(4),CPXX(4),HXX(4),SXX(4)                  CPHS  20   000002
00117    24*          INTEGER SUB,SUBLT                                                  000002
00117    25*    C                                                                        000002
00120    26*          IEXTND = 0                                              CPHS 190   000002
00121    27*          IF(TT.LT.TLOW) IEXTND = 1                               CPHS 200   000003
00123    28*          IF(IEXTND.NE.0) IMSG = IMSG + 1                         R FEB-3    000011
00125    29*          IF(IMSG.NE.0) GO TO 10                                  R FEB-3    000016
00127    30*          IF(IEXTND.NE.0) WRITE(JOUT,3333) TT                                000020
00133    31*    3333  FORMAT (//25X,48HLOW TEMPERATURE THERMO EXTENSION IN CPHS AT TT =,  000031
00133    32*         1        F12.6,15H DEGREES KELVIN//)                               000031
00134    33*      10  K = 1                                                             000031
00135    34*          IF (TT.LE.TMID) K=2                                     CPHS 240   000032
00137    35*          KK=0                                                    CPHS 250   000040
00140    36*          CPSUM=0.                                                CPHS 260   000041
00141    37*    20    IF (COEF(K,1,J).NE.0.) GO TO 30                         CPHS 270   000043
00143    38*          IF (IUSE(J).LT.0) GO TO 40                              CPHS 280   000047
00145    39*          KK=K                                                    CPHS 290   000053
00146    40*          K=1                                                     CPHS 300   000055
00147    41*          IF (KK.EQ.1) K=2                                        CPHS 310   000057
00151    42*       30 IF (IEXTND .NE. 0)  GO TO 60                                       000065
00153    43*       31 S(J) = ((((COEF(K,5,J)/4.0)*TT + COEF(K,4,J)/3.0)*TT + COEF(K,3,J)  000067
00153    44*         1       /2.0)*TT + COEF(K,2,J))*TT + COEF(K,1,J)*TLN + COEF(K,7,J)  000067
00154    45*          HO(J)=(((((COEF(K,5,J)/5.)*TT+COEF(K,4,J)/4.)*TT+COEF(K,3,J)/3.)*TTCPHS 370   000114
00154    46*         1+COEF(K,2,J)/2.)*TT+COEF(K,1,J)+COEF(K,6,J)/TT                     CPHS 380   000114
00155    47*          CPSUM=CPSUM+((((COEF(K,5,J)*TT+COEF(K,4,J))*TT+COEF(K,3,J))*TT+COECPHS 390   000140
00155    48*         1F(K,2,J))*TT+COEF(K,1,J))*EN(J,NPT)                               CPHS 400   000140
00156    49*       32 IF (KK .EQ. 0)  GO TO 40                                           000157
00160    50*          K=KK                                                    CPHS 430   000160
00161    51*          KK=0                                                    CPHS 440   000162
```

```
00162    52*      40  IF (J .EQ. NS)  RETURN                                                  000164
00164    53*          J=J+1                                                    CPHS 460       000171
00165    54*          GO TO 20                                                 CPHS 470       000174
00166    55*      60  IF (NLTSP .EQ. 0)  GO TO 31                                            000176
00170    56*          DO 70 IX = 1,NLTSP                                       CPHS 500       000177
00173    57*          DO 65 KK = 1,3                                                          000217
00176    58*      65  IF (SUB(J,KK) .NE. SUBL(IX,KK))  GO TO 70                             000217
00201    59*          GO TO 80                                                 CPHS 540       000226
00202    60*      70  CONTINUE                                                 CPHS 550       000231
00204    61*          GO TO 3                                                  CPHS 560       000231
00205    62*      80  NTUP = ILSP(IX)                                                        000233
00206    63*          IF(TT.LT.TL(IX,1)) GO TO 90                              CPHS 590       000238
00210    64*          TTS = TT                                                 CPHS 600       000241
00211    65*          TLNS= TLN                                                CPHS 610       000243
00212    66*          TT = TLOW                                                CPHS 620       000245
00213    67*          TLN= ALOG(TT)                                            CPHS 630       000247
00214    68*          KK = 2                                                   CPHS 640       000253
00215    69*          SX =(((((COEF(KK,6,J)/6.)*TT+COEF(KK,5,J)/5.)*TT+COEF(KK,4,J)/4.)*TT+COEF(KK,3,J)/3.)*TT+COEF(KK,2,J)/2.)  CPHS 650  000255
00215    70*       1     *TT+COEF(KK,2,J))*TT+COEF(KK,1,J)*TLN+COEF(KK,7,J)         CPHS 660       000255
00216    71*          HX =(((((COEF(KK,5,J)/5.)*TT+COEF(KK,4,J)/4.)*TT+COEF(KK,3,J)/3.)  CPHS 670  000301
00216    72*       1     *TT+COEF(KK,2,J)/2.)*TT+COEF(KK,1,J)+COEF(KK,6,J)/TT       CPHS 680       000301
00217    73*          CPX=(((COEF(KK,5,J)*TT+COEF(KK,4,J))*TT+COEF(KK,3,J))*TT    CPHS 690       000325
00217    74*       1     +COEF(KK,2,J))*TT+COEF(KK,1,J)                          CPHS 700       000325
00220    75*          DO 86 KK = 1,NTUP                                                       000351
00223    76*          TXX(KK) = TL(IX,KK)                                                     000351
00224    77*          CPXX(KK) = CPL(IX,KK)                                                   000352
00225    78*          HXX(KK) = HL(IX,KK)                                                     000354
00226    79*      86  SXX(KK) = SL(IX,KK)                                                     000356
00230    80*          TXX(NTUP+1) = TT                                         CPHS 770       000361
00231    81*          CPXX(NTUP+1) = CPX                                       CPHS 780       000363
00232    82*          HXX(NTUP+1) = HX                                         CPHS 790       000365
00233    83*          SXX(NTUP+1) = SX                                         CPHS 800       000367
00234    84*          TT = TTS                                                 CPHS 820       000371
00235    85*          TLN = TLNS                                               CPHS 830       000373
00236    86*          M = 1                                                                   000375
00237    87*          I = 1                                                                   000377
00240    88*          IF (TT .LT. TXX(M))  I = -1                                             000400
00242    89*      87  IF (TT .GE. TXX(M) .AND. TT .LE. TXX(M+1))  GO TO 89                    000412
00244    90*          M = M + I                                                               000430
00245    91*          IF (M .LT. NTUP + 1 .AND. M .GT. 0)  GO TO 87                           000433
00247    92*          WRITE (JOUT,88) TT,M,NTUP,(I,TXX(I), I = 1,4)                          000450
00261    93*      88  FORMAT (//50X,29H*CPHS* VARIABLE OUTSIDE TABLE//45X,4HTT =,1PE15.8    000470
00261    94*       1,5H  M =,I2,8H  NTUP =,I2//(50X,4HTXX(,I1,3H) =,E15.8))               000470
00262    95*          GO TO 31                                                            000470
00263    96*      89  S(J) = SXX(M) + (SXX(M+1)-SXX(M))*(TT-TXX(M))/(TXX(M+1)-TXX(M))       000472
00264    97*          HO(J) = HXX(M) + (HXX(M+1)-HXX(M))*(TT-TXX(M))/(TXX(M+1)-TXX(M))       000506
00265    98*          CPUSED = CPXX(M)+(CPXX(M+1)-CPXX(M))*(TT-TXX(M))/(TXX(M+1)-TXX(M))     000514
00266    99*          CPSUM = CPSUM + CPUSED * EN(J,NPT)                       CPHS 940       000522
00267   100*          GO TO 32                                                 CPHS 950       000527
00270   101*      90  IF (IER .LT. 1)  WRITE (JOUT,904) TT                                   000531
00274   102*     904  FORMAT (//25X,60HERROR DURING LOW TEMPERATURE THERMO EVALUATION IN     000542
00274   103*       1 CPHS, TT =,F12.6,15H DEGREES KELVIN//)                                  000542
00275   104*          IER = 1                                                                 000542
00276   105*          GO TO 31                                                                000544
00277   106*          END                                                                     000602
```

END OF COMPILATION: NO DIAGNOSTICS.

@HDG,P DETON

```
2F0R,S    DETON,DETON
HSA  E3 -10/15/80-13:06:18 (12,)
```

SUBROUTINE DETON ENTRY POINT 001331

STORAGE USED: CODE(1) 001347; DATA(0) 000201; BLANK COMMON(2) 000000

COMMON BLOCKS:

```
0003   CONSTS 000006
0004   HOLCON 000010
0005   POINTS 000335
0006   MISC   001701
0007   INDX   000091
0010   PERF   000166
0011   OUPT   000073
0012   CCC    000003
```

EXTERNAL REFERENCES (BLOCK, NAME)

```
0013   NEWOF
0014   HCALC
0015   OUT1
0016   EQLBRM
0017   OUT2
0020   OUT3
0021   SAVE
0022   NWDUS
0023   NIO2S
0024   XPRR
0025   EXP
0026   SQRT
0027   NIO1S
0030   NIO3S
0031   NERR3S
```

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

```
0001   001305 1000L    0000   000035 11F     0001   000005 1306    0001   000040 1466    0001   000566 1506
0001   000053 1546    0000   000044 190F     0000   000053 203F    0001   000255 2056    0001   000176 2146
0000   000055 30F     0001   000651 3416    0001   000672 3526    0001   000711 3626    0001   000717 3676
0001   000563 406L    0001   000750 4016    0001   000767 4116    0001   001004 4226    0001   001024 4336
0001   001055 4516    0000   000114 46F     0001   001100 4646    0001   001115 4756    0000   000102 5F
0001   001123 5026    0001   001142 5146    0001   001157 5256    0001   001176 5356    0001   001216 5466
0000   000120 58F     0000   000123 68F     0001   000016 7L      0001   000615 860L    0000   000130 868F
0001   001251 870L    0001   001270 902L    0000 R 000032 ALAM    0000 R 000017 ALFA    0006   000640 AM
0006 R 000705 AM1     0006   001135 ANUM    0010   000133 APP     0003   000000 ATMN    0006   000004 ATOM
0000 R 000022 A11     0000 R 000023 A12     0000 R 000024 A21     0000 R 000025 A22     0006   000514 B0
0006   000545 B0P     0000 R 000026 B1      0000 R 000027 B2      0007   000036 CALCH   0007   000001 CONVG
0006 R 000654 CP      0005 R 000032 CPR     0006 R 000706 CPR1    0006   000634 CPSUM   0012   000002 DEMAND
0006   001560 DENS    0005 R 000064 DLVPT   0005 R 000047 DLVTP   0004   000000 END     0006   001700 ENLSAV
0006   000000 ENN     0006   001676 ENNL    0006   001677 ENSAVE  0006   001414 ENTH    0010 L 000165 EOL
```

```
0006  000636 EQRAT     0011    000002 FA        0011    000003 FAP       0006  001445 FAZ       0011  R 000005 FB
0011    000006 FC      0011  R 000007 FCP       0011    000012 FCST      0011  000014 FCV       0011    000015 FG
0011    000017 FGE     0011    000020 FGV       0000  R 000040 FG1       0011  R 000021 FH      0011    000023 FI
0011    000025 FIV     0011  R 000027 FM        0000  R 000001 FMM       0011  R 000031 FMT     0011    000050 FN
0011  R 000052 FOUR    0006    001527 FOX       0011    000053 FP        0000  R 000003 FPP     0000  R 000002 FP1
0000  R 000004 FRA     0000  R 000005 FRB       0011    000054 FS        0011  R 000056 FSV     0011  R 000067 FT
0011    000061 FTK     0000  R 000006 FTT       0000  R 000007 FUD       0011    000063 FV        0011  R 000065 FVEL
0011  R 000001 F13     0011    000000 F9X       0000  R 000014 GAM       0005  R 000101 GAMMAS  0004    000001 GAS
0003    000001 GMET    0010  R 000150 GM1       0012    000000 GRAPH     0007  L 000003 HP      0006    000642 HPP
0006  R 000637 HSUBO   0005  R 000000 HSUM      0010  R 000064 H1        0007    000030 IC        0007  I 000000 IDEBUG
0004    000002 IE      0000  I 000011 II        0007    000015 IMAT      0000    000143 INJPS     0000  I 000010 IOF
0007    000023 IONS    0007  I 000021 IP        0007    000037 IQSAVE    0007    000016 IQ1       0007  I 000034 IT
0000  I 000012 ITR     0004  I 000003 IZEPO     0000  I 000034 J         0007    000026 JLIQ      0012  I 000001 JOUT
0007    000025 JSOL    0007    000031 JS1       0007  I 000005 K         0007    000014 KMAT      0004    000004 LANK
0006    000463 LLMT    0007    000040 LSAVE     0004    000005 MOL       0007    000006 MOLES     0006  I 000707 NAME
0007    000024 NC      0007    000022 NEWR      0007    000035 NFZ       0007    000012 NLM       0007  I 000017 NOF
0007    000020 NOMIT   0007  I 000007 NP        0007  I 000011 NPT       0007  I 000027 NREAC   0007    000013 NS
0007  I 000010 NT      0006  R 000635 OF        0011  R 000067 ONE       0004    000006 OX        0006  R 001644 OXF
0005  R 000116 P       0003    000002 PATM      0010  R 000000 PCP       0006    001363 PECWT     0006  R 000633 PP
0005  R 000217 PPP     0000  R 000013 PP1       0010  R 000101 PUB       0003  R 000003 RBAR    0003  R 000004 RBR
0006    000644 RH      0006    001611 RHOP      0000  R 000020 RK        0006    001612 RMW       0010  R 000047 RRHO
0000  R 000021 RR1     0006  R 001476 RTEMP     0003    000005 RVR       0007    000033 SHOCK     0005  R 000251 SONVEL
0007    000004 SP      0005    000015 SSUM      0006    000001 SUMN      0006    000003 SO        0005  R 000150 T
0000  R 000016 TEM     0006    000632 THIGH     0011  R 000070 THREE     0006    001643 TLN       0006    000630 TLOW
0006    000627 TM      0006    000631 TMID      0005    000320 TOTN      0007  L 000002 TP      0006  R 000002 TT
0005  R 000266 TTT     0000  R 000015 TT1       0010  R 000116 TUB       0011  R 000071 TWO     0000  R 000033 UD
0005  R 000202 V       0005    000303 VLM       0006    000646 VMIN      0010  R 000032 VMOC    0007    000032 VOL
0006    000650 VPLS    0005  R 000234 WM        0006    000652 WP        0000  R 000030 X1      0000  R 000031 X2
0004    000007 ZERO    0011    000072 ZEROF
```

```
00101     1*          SUBROUTINE DETON                                                    000000
00101     2*    C                                                          00343900       000000
00101     3*    C     CHAPMAN-JOUGUET DETONATIONS                          00344000       000000
00101     4*    C                                                                         000000
00103     5*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR          /CONSTS/       000000
00104     6*          COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO    /HOLCON/       000000
00105     7*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)         000000
00105     8*         1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)    000000
00105     9*         2 ,VLM(13),TOTN(13)                                                 000000
00106    10*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),           000000
00106    11*         1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,     000000
00106    12*         2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),     /MISC/ 000000
00106    13*         3              CP(25)  ,AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),  000000
00106    14*         4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,   000000
00106    15*         5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV              000000
00107    16*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,K,MOLES,NP,NT,NPT,NLM,NS,       /INDX/ 000000
00107    17*         1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/ 000000
00107    18*         2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE    /INDX/ 000000
00110    19*          COMMON /PERF/ PCP(26),VMOC(13),RRHO(13),H1(13),PUB(13),           /PERF/ 000000
00110    20*         1              TUB(13),APP(13),GM1(13),EQL                         /PERF/ 000000
00111    21*          COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),     /OUPT/ 000000
00111    22*         1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/ 000000
00111    23*         2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,  /OUPT/ 000000
```

```
00111  24*        3              TW0,ZERO                                  /OUPT/      000000
00111  25*  C                                                                          000000
00112  26*           COMMON /CCC/ GRAPH,JOUT,DEMAND                                    000000
00112  27*  C                                                                          000000
00113  28*        LOGICAL EQL,HP,TP                                                   000000
00114  29*        DATA FG1/6HGAMMA1/,FMM/6HM/M1  /,FP1/6HP1 AT M/,FPP/6HP/P1  /,      000000
00114  30*       1 FRA/6HRHO/RH/,FRB/6HO1     /,FTT/6HT/T1  /,FUD/6HDET VE/          000000
00114  31*  C                                                                          000000
00125  32*        XX(A,X,B,Y,C,D) = (A*X-B*Y)/(A*C-B*D)                               000000
00125  33*  C                                                                          000000
00126  34*        IOF = 0                                                             000000
00127  35*        DO 9 II = 1,NREAC                                                   000000
00132  36*      9 NAME(II,6)=ZERO                                                     000005
00134  37*        TT = 0.                                                             000007
00135  38*        IF (T(1) .LE. 0.0)  T(1) = RTEMP(1)                                 000010
00137  39*      7 IOF = IOF+1                                                         000016
00140  40*        OF = OXF(IOF)                                                       000021
00141  41*        CALL NEWOF                                                          000023
00142  42*        WRITE(JOUT,11)                                                      000025
00144  43*     11 FORMAT(33H1DETONATION VELOCITY CALCULATIONS)                        000032
00145  44*        DO 902 IT = 1,NT                                                    000032
00150  45*        TT = T(IT)                                                          000040
00151  46*        CALL HCALC                                                          000042
00152  47*        CALL OUT1                                                           000044
00153  48*        DO 902 IP=1,NP                                                      000046
00156  49*        H1(NPT) = RBAR*HSUBO                                                000055
00157  50*        TUB(NPT) = T(IT)                                                    000061
00160  51*        PUB(NPT) = P(IP)                                                    000063
00161  52*        CP(NPT) = RBAR*CPR1                                                 000065
00162  53*        ITR= 0                                                              000070
00163  54*        TT= 3800.                                                           000071
00164  55*        PP1= 15.                                                            000073
00165  56*        PP = PP1*P(IP)                                                      000075
00166  57*        HSUBO = H1(NPT)/RBAR + 0.750*T(IT)*PP1/AM1                          000077
00167  58*        TP = .FALSE.                                                        000105
00170  59*        HP= .TRUE.                                                          000106
00171  60*        CALL EQLBRM                                                         000110
00172  61*        HSUBO = H1(NPT)/RBAR                                                000117
00173  62*        HP= .FALSE.                                                         000122
00174  63*        IF (TT .LE. 0.0)  GO TO 902                                         000123
00176  64*        GAM= GAMMAS(NPT)                                                    000126
00177  65*        TT1 = TT/T(IT)                                                      000137
00200  66*        II= 0                                                               000142
00201  67*        TEM=TT1-.75*PP1/(CPR(NPT)*AM1)                                      000143
00203  68*        WRITE(JOUT,190)TT                                                   000150
00205  69*     190 FORMAT(8HOT EST.=,F8.2/11X,4HP/P1,17X,4HT/T1)                      000160
00206  70*        WRITE(JOUT,203) II,PP1,TT1                                          000160
00213  71*        DO 202 II = 1,3                                                     000176
00216  72*        ALFA = WM(NPT)/AM1/TT1                                              000176
00217  73*        PP1= (1.+GAM)*(1.+(1.-4.*GAM*ALFA/(1.+GAM)**2)**.5)/(2.*GAM*ALFA)   000201
00220  74*        RK=PP1*ALFA                                                         000220
00221  75*        TT1= TEM+.5*PP1*GAM*(RK*RK-1.)/(AM1*CPR(NPT)*RK)                    000222
00222  76*     202  WRITE(JOUT,203) II,PP1,TT1                                       000235
00230  77*      203 FORMAT (I5,2E20.8)                                                000247
00231  78*        TP= .TRUE.                                                          000247
00232  79*        TT = TT1*T(IT)                                                      000251
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```
00233    80*        205 ITR= ITR+1                                                  000255
00234    81*            PP = PP1*P(IP)                                              000257
00235    82*            CALL EQLBRM                                                 000262
00236    83*            IF (NPT.EQ.0) GO TO 1000                                    000264
00240    84*            IF (TT .LE. 0.0)  GO TO 860                                 000266
00242    85*            GAM= GAMMAS(NPT)                                            000272
00243    86*            RR1 = PP1*WM(NPT)/AM1/TT1                                   000274
00244    87*            A11= 1./PP1 + GAM*RR1*DLVPT(NPT)                            000302
00245    88*            A12= GAM*RR1*DLVTP(NPT)                                     000310
00246    89*            A21= .5*GAM*(RR1**2-1.-DLVPT(NPT)*(1.+RR1**2))*DLVTP(NPT)-1.  000314
00247    90*            A22=-.5*GAM*DLVTP(NPT)*(RR1**2+1.)-WM(NPT)*CPR(NPT)         000330
00250    91*            B1= 1./PP1-1.+GAM*(RR1-1.)                                  000343
00251    92*            B2 = WM(NPT)*(HSUM(NPT) - H1(NPT)/RBAR)/TT - 0.5*GAM*(RR1**2 - 1.)  000353
00252    93*            X1 = XX(A22,B1,A12,B2,A11,A21)                              000370
00253    94*            X2 = XX(A11,B2,A21,B1,A22,A12)                              000400
00254    95*            ALAM= 1.                                                    000412
00255    96*            TEM = X1                                                    000414
00256    97*            IF(TEM.LT.0.)  TEM = -TEM                                   000416
00260    98*            IF(X2.GT.TEM)  TEM=X2                                       000423
00262    99*            IF (-X2.GT.TEM) TEM = -X2                                   000431
00264   100*            IF(TEM.GT.0.4) ALAM=.4/TEM                                  000437
00266   101*            PP1= PP1*EXP(X1*ALAM)                                       000446
00267   102*            TT1= TT1*EXP(X2*ALAM)                                       000456
00270   103*            TT = TT1*T(IT)                                              000466
00271   104*            UD = RR1*SQRT(RBR*GAM*TT/WM(NPT))                           000470
00272   105*            WRITE(JOUT,30)ITR,PP1,TT1,RR1,X1,X2                         000503
00302   106*         30 FORMAT 7HOITER =,I2,5X,6HP/P1 =,E15.8,5X,6HT/T1 =,E15.8,5X,10HRHO/  000516
00302   107*           1RHO1 =,E15.8/7X,13HDEL LN P/P1 =,E15.8,5X,13HDEL LN T/T1 =,E15.8)  000516
00302   108*      C      CONVERGENCE TEST                                            000516
00303   109*            IF(ITR.LE.10 .AND. TEM.GT.0.5E-04)  GO TO 205               000516
00305   110*            RRHO(NPT)=RR1                                               000534
00306   111*            IF (CP(NPT) .LE. 0.0)  GO TO 40                             000536
00310   112*            GM1(NPT) = CP(NPT)/(CP(NPT) - RBAR/AM1)                     000541
00311   113*            VMOC(NPT) = UD/SQRT(RBR*GM1(NPT)*T(IT)/AM1)                 000547
00312   114*            GO TO 150                                                   000561
00313   115*         40 GM1(NPT) = 0.                                               000563
00314   116*            VMOC(NPT) = 0.                                              000569
00315   117*        150 K = 0                                                       000566
00316   118*            IF (IP .EQ. NP .AND. IT .EQ. NT .OR. TT .LE. 0.0)  GO TO 860  000566
00320   119*            K = NPT                                                     000610
00321   120*            IF(NPT.NE.13)  GO TO 870                                    000612
00321   121*      C  OUTPUT                                                         000612
00323   122*        860 WRITE(JOUT,5)                                               000615
00325   123*          5 FORMAT(1H1,42X,46HDETONATION PROPERTIES OF AN IDEAL REACTING GAS )  000621
00326   124*            CALL OUT1                                                   000621
00327   125*            WRITE(JOUT,46)                                              000623
00331   126*         46 FORMAT(13H UNBURNED GAS//)                                  000633
00332   127*            FMT(3) = F13                                                000633
00333   128*            FMT(4) = FOUR                                               000635
00334   129*            WRITE(JOUT,FMT) FP1,FB,FB,(PUB(J), J = 1,NPT)               000637
00345   130*            FMT(4) = TWO                                                000650
00346   131*            WRITE(JOUT,FMT) FT,FB,(TUB(J), J = 1,NPT)                   000656
00356   132*            WRITE(JOUT,FMT) FH,FB,(H1(J), J = 1,NPT)                    000675
00366   133*            DO 56 J = 1,NPT                                             000717
00371   134*            V(J) = AM1                                                  000717
00372   135*         56 SONVEL(J) = SQRT(RBR*GM1(J)*TUB(J)/AM1)                     000720
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00374   134*          FMT(4) = THREE                                          000732
00375   137*          WRITE(JOUT,FMT) FM,FB,(V(J), J = 1,NPT)                 000734
00405   138*          FMT(4) = FOUR                                           000753
00406   139*          WRITE(JOUT,FMT) FCP,(CP(J), J = 1,NPT)                  000755
00415   140*          WRITE(JOUT,FMT) FG1,FB,FB,(GM1(J), J = 1,NPT)           000772
00426   141*          FMT(4) = ONE                                            001007
00427   142*          WRITE(JOUT,FMT) FSV,FVEL,(SONVEL(J), J = 1,NPT)         001011
00437   143*          WRITE(JOUT,58)                                          001027
00441   144*       58 FORMAT(11H0BURNED GAS//)                                001034
00442   145*          FMT(3) = ONE                                            001034
00443   146*          CALL OUT2                                               001036
00444   147*          WRITE(JOUT,68)                                          001040
00446   148*       68 FORMAT(22H0DETONATION PARAMETERS //)                    001050
00447   149*          FMT(4) = THREE                                          001050
00450   150*          DO 70 J = 1,NPT                                         001055
00453   151*          V(J) = PPP(J)/PUB(J)                                    001055
00454   152*          PCP(J) = TTT(J)/TUB(J)                                  001057
00455   153*       70 SONVEL(J) = SONVEL(J)*RRHO(J)                           001062
00457   154*          WRITE(JOUT,FMT) FPP,FB,FB,(V(J), J = 1,NPT)             001066
00470   155*          WRITE(JOUT,FMT) FTT,FB,FB,(PCP(J), J = 1,NPT)           001103
00501   156*          DO 73 J = 1,NPT                                         001123
00504   157*       73 V(J) = WM(J)/AM1                                        001123
00506   158*          FMT(4) = FOUR                                           001126
00507   159*          WRITE(JOUT,FMT) FNM,FB,FB,(V(J), J = 1,NPT)             001130
00520   160*          WRITE(JOUT,FMT) FRA,FRB,FR,(RRHO(J), J = 1,NPT)         001145
00531   161*          WRITE(JOUT,FMT) FM,FB,(VMOC(J), J = 1,NPT)              001162
00541   162*          FMT(4) = ONE                                            001201
00542   163*          WRITE(JOUT,FMT) FUD,FVEL,(SONVEL(J), J = 1,NPT)         001203
00552   164*          EQL=.TRUE.                                              001221
00553   165*          CALL OUT3                                               001223
00554   166*          IF (K .EQ. 0 .AND. IOF .EQ. NOF) GO TO 1000             001225
00556   167*          IDEBUG = IDEBUG-13                                      001237
00557   168*          WRITE(JOUT,868)                                         001242
00561   169*       868 FORMAT(1H1)                                            001247
00562   170*          NPT = 0                                                 001247
00563   171*       870 NPT = NPT + 1                                          001281
00564   172*          IF (K .EQ. 1) K = -1                                    001253
00566   173*          CALL SAVE                                               001260
00567   174*          WRITE(JOUT,868)                                         001262
00571   175*       902 CONTINUE                                               001274
00574   176*          IF(IOF.GE.NOF) GO TO 1000                               001274
00576   177*          IDEBUG = IDEBUG+13                                      001300
00577   178*          GO TO 7                                                 001303
00600   179*      1000 IP = .FALSE.                                           001305
00601   180*          RETURN                                                  001305
00602   181*          END                                                     001306

      END OF COMPILATION:        NO  DIAGNOSTICS.

$HDG,P      EQLBRM
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@FOR,S    EQLBRM,EQLBRM
HSA  E3 -10/15/80-13:06:23 (16,)

   SUBROUTINE EQLBRM    ENTRY POINT 003120

   STORAGE USED: CODE(1) 003136; DATA(0) 000461; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   CONSTS 000006
    0004   HOLCON 000010
    0005   POINTS 000335
    0006   SPECES 017106
    0007   MISC   001701
    0010   DOUBLE 001560
    0011   INDX   000041
    0012   PERF   000166
    0013   CCC    000003

   EXTERNAL REFERENCES (BLOCK, NAME)

    0014   CPYS
    0015   MATRIX
    0016   GAUSS
    0017   ALOG
    0020   NWDUS
    0021   NIO1S
    0022   NIO2S
    0023   EXP
    0024   NERR3S

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001   001202 100L      0001   001211 101L      0001   002172 1027G     0001   002222 1037G     0000   000233 110F
    0001   001452 111L      0001   001575 1115L     0001   001633 1116L     0001   001517 113L      0001   002503 1134G
    0001   001513 114L      0001   002511 1140G     0001   001542 115L      0001   002551 1156G     0001   001660 116L
    0001   002624 1160L     0001   002454 1165L     0001   002716 1171L     0000   000214 1183F     0001   002644 1205G
    0001   002676 1223G     0001   002741 1244G     0001   002046 131L      0001   001747 130L      0000   000321 136F
    0001   002660 143L      0000   000257 144F      0001   002263 147L      0001   002276 148L      0001   000116 151G
    0001   002516 153L      0001   002312 154L      0000   000265 156F      0001   002342 157L      0001   002401 158L
    0001   002437 159L      0001   002152 160L      0000   000277 161F      0001   000151 165G      0001   002630 165L
    0001   002650 166L      0000   000307 168F      0001   002616 169L      0001   002621 170L      0001   002725 171L
    0000   000111 172F      0001   000430 174L      0001   002062 183L      0001   003013 186L      0000   000165 1924F
    0001   003002 199L      0000   000326 201F      0001   001561 2115L     0001   000244 2216      0001   000277 2326
    0000   000072 244F      0001   000325 245G      0001   000332 2516      0001   000374 2706      0001   000406 2776
    0000   000220 306F      0001   000464 315G      0001   000512 3246      0001   000131 33L       0001   000613 3606
    0000   003103 373F      0001   002653 40L       0001   000721 4166      0001   000732 4226      0001   000155 43L
    0001   001003 4456      0001   001141 4776      0001   000125 499L      0001   001172 5066      0001   001252 5316
    0001   001413 6006      0001   000213 62L       0001   000251 63L       0001   001464 6316      0001   000302 67L
    0001   001625 6736      0001   001642 7046      0001   000342 72L       0001   001722 7266      0000   000107 73F
    0000   000140 74F       0001   001760 7466      0000   000324 771F      0000   000075 772F      0001   000412 7731
    0001   000524 774L      0001   000536 775L      0000   000144 776F      0001   000747 80L       0001   000766 83L
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0001  001023 B4L          0001  001036 B5L          0001  000571 B71L         0001  003071 B73L         0000  000117 B74F
0001  001332 B17L         0000  000196 923F         0001  000171 B2nF         0000  000210 925F         0001  000603 9661
0001  000622 968L         0001  000632 969L         0001  001111 97L          0001  000635 970L         0001  000644 973L
0000  000232 973F         0000  000250 974F         0001  000654 997L         0006 R 011052 A            0000 R 000061 AA
0012  000150 AEAT         0007  000640 AM           0000 R 000054 AMBDA        0000 R 000055 AMBDA1       0007  000705 AM1
0007  001135 ANUM         0012 R 000133 APP          0003  000000 ATMN         0007  000004 ATOM           0007 R 000614 B0
0007  000545 BOP          0011  000036 CALCH         0006  000000 COEF         0011 L 000001 CONVG         0005 R 000032 CPR
0007  000706 CPR1         0007 R 000634 CPSUM        0000 R 000040 CRITV        0007  000654 DETA         0000 R 000067 DELF
0006 R 010624 DELN         0013  000002 DEMAND       0007  015600 DENS         0000 R 000053 DLNT         0005 R 000064 DLVPT
0005 R 000047 DLVTP        0006 R 009312 EN           0004  000000 END          0000 R 000037 ENL          0006 R 010150 ENLN
0007  001700 ENLSAV        0007 R 000000 ENN          0007 R 001676 ENNL         0007  001677 ENSAVE       0000 R 000045 ENSOL
0007  001414 ENTH          0012  000165 EQL          0007 R 000636 EORAT        0007  001445 FAZ          0000 R 000057 FNEG1
0000 R 000060 FNEG2        0007  001527 FOX          0010 D 000000 G            0005 R 000101 GAMMAS       0004  000001 GAS
0003  000001 GMET          0013  000000 GRAPH        0011 L 000003 HP           0007  000642 HPP          0007  000637 HSUBO
0005 R 000000 HSUM         0006 R 010376 HO           0000 I 000044 I            0011 L 000030 IC           0011 I 000000 IDEBUG
0004 I 000002 IE           0011 I 000015 IMAT         0000 I 000053 INC          0000  000421 INJPS        0011 L 000023 IONS
0011  000021 IP            0011  000037 IOSAVE       0011 I 000016 IQ1          0000 I 000047 IQ2          0000 L 000034 ISING
0011  000005 ISV           0011  000034 IT           0000 I 000042 ITNUMB       0006 I 016266 IUSE         0004  000003 IZERO
0000 I 000043 J            0000 I 000070 JDELF        0000 I 000051 JJ           0000 I 000065 JKG          0011 I 000026 JLIQ
0013 I 000001 JOUT         0011 I 000025 JSOL         0011 I 000031 JS1          0000 I 000064 KG           0011 I 000014 KMAT
0011 I 000012 L            0004  000004 LANK         0007 I 000463 LLMT         0000 L 000035 LOGV         0011  000040 LSAVE
0004  000006 MOL           0011  000006 MOLES        0007  000707 NAME         0011 I 000024 NC           0000 I 000052 NEN
0011  000022 NEWR          0011  000035 NFZ          0011  000017 NOF          0011  000020 NOMIT        0011  000007 NP
0011 I 000011 NPT          0011  000027 NREAC        0011 I 000013 NS           0000 I 000000 NSPP1        0011  000010 NT
0000 I 000050 NTZERO       0000 I 000046 NUMB         0007  000635 OF          0004  000006 OX           0007  016444 OXF
0005  000116 P             0003  000002 PATM         0012  000000 PCP          0007  002365 PECWT        0007 R 000633 PP
0005 R 000217 PPP          0000 R 000001 PROW         0003  000003 RBAR         0003  000004 RBR          0007  000644 RH
0007  001611 RHOP          0000 L 000036 RITE         0007  001012 RMW          0007  001476 RTEMP        0003 R 000005 RVR
0006 R 004064 S            0011 L 000033 SHOCK        0000 R 000041 SIZEF        0006  016660 SLN          0005  000751 SONVEL
0011 L 000004 SP           0012  000047 SPIM         0000 R 000062 SS           0005 R 000015 SSUM         0006 R 015564 SUB
0012  000101 SUBAR         0000 D 000032 SUM          0007 R 000001 SUMN         0000 R 000056 SUM1         0012  000116 SUPAR
0007 R 000003 SO           0005 R 000150 T            0006 R 016514 TEMP         0007 R 000632 THIGH        0007 R 001643 TLN
0007 R 000630 TLOW         0007 R 000627 TM           0000 R 000066 TMELT        0007  000631 TMID         0000 R 000071 TN
0005 R 000320 TOTN         0011 L 000002 TP           0007 R 000002 TT           0005 R 000266 TTT          0005  000202 V
0012  000064 VACT         0005 D 000303 VLM          0007  000646 VMIN         0012  000032 VMOC         0011 L 000032 VOL
0007  000650 VPLS         0005 R 000234 WM           0007  000652 WP           0010 D 001510 X            0004  000007 ZERO
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00101      1*            SUBROUTINE EQLBRM                                                    EQLN0002   000000
00101      2*      C                                                                                       000000
00101      3*      C  ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES               EQLN0003   000000
00101      4*      C                                                                           EQLN0004   000000
00103      5*            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                           /CONSTS/   000000
00104      6*            COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO                     /HOLCON/   000000
00105      7*            COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                      000000
00105      8*           1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)                 000000
00105      9*           2 ,VLM(13),TOTN(13)                                                               000000
00105     10*      C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)                   000000
00105     11*      C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                    000000
00106     12*            INCLUDE SPECPK                                                                    000000
00112     13*            COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,10),LLMT(25),BO(25),                          000000
00112     14*           1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,                    000000
00112     15*           2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),      /MISC/       000000
00112     16*           3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),                000000
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00112    17*          4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,                    000000
00112    18*          5              RMW(25),TLN,OXF(26),ENNL,ENSAV,ENLSAV                                000000
00113    19*           COMMON /DOUBLE/ G(20,21), X(20)                                  EQLN0013          000000
00114    20*           COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,    /INDX/             000000
00114    21*          1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/         000000
00114    22*          2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCN,IGSAVE,LSAVE    /INDX/         000000
00115    23*           COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),      /PERF/             000000
00115    24*          1              SUPAR(13),APP(13),AFAT(13),EQL                     /PERF/             000000
00115    25*     C                                                                                         000000
00116    26*              COMMON /CCC/ GRAPH,JOUT,DEMAND                                                  000000
00116    27*     C                                                                                         000000
00117    28*           DIMENSION PROD(25)                                                                 000000
00120    29*           DOUBLE PRECISION G,SUM,X                                                           000000
00121    30*           LOGICAL CONVG,HP,ICIONS,ISING,LOGV,RITE,SHOCK,SP,TP,VOL                            000000
00121    31*     C                                                                                         000000
00122    32*           ENL = ENNL                                                                         000000
00123    33*           RITE = .FALSE.                                                                     000001
00124    34*           IF(IDEBUG.GT.0.AND.NPT.GE.IDEBUG) RITE=.TRUE.                                      000002
00126    35*           CRITV = 5.0E-6                                                                     000021
00127    36*           SIZEF = 0.                                                                         000023
00130    37*           ISING = .FALSE.                                                                    000024
00131    38*           LOGV = .FALSE.                                                                     000025
00132    39*           IF (VOL)  PP = RVR*ENN*TT/VLM(NPT)                                                 000026
00134    40*           TLN = ALOG(TT)                                                                     000040
00135    41*           CONVG = .FALSE.                                                                    000044
00136    42*           ITNUMB = 100                                                                       000045
00137    43*           JS1 = 1                                                                            000047
00140    44*           CALL CPHS                                                                          000051
00141    45*           TM = ALOG(PP/ENN)                                                                  000053
00141    46*     C     IF(IC) PREVIOUS POINT HAD SINGULAR MATRIX                                          000053
00142    47*           IF(IC)  GO TO 966                                                                  000062
00144    48*           IF (.NOT.IONS.OR.IE.EQ.LLMT(L)) GO TO 33                                           000064
00146    49*           L = L+1                                                                            000102
00147    50*           IQ1 = IQ1+1                                                                        000105
00150    51*           DO 499 J = 1,NS                                                                    000116
00153    52*           IF (A(L,J) .EQ.0.) GO TO 499                                                       000116
00155    53*           EN(J,NPT) = 1.E-8                                                                  000117
00156    54*           ENLN(J) = -18.420680                                                               000121
00157    55*           IUSE(J) = 0                                                                        000123
00160    56*       499 CONTINUE                                                                           000131
00162    57*        33 IF(NPT.EQ.1.AND..NOT.SHOCK)  WRITE(JOUT,244)(LLMT(I),I=1,L)                        000131
00171    58*       244 FORMAT (4HOPT ,14(5X,A4))                                                          000155
00171    59*     C     BEGIN ITERATION                                                                    000155
00172    60*        43 IF(IC)  GO TO 1171                                                                 000155
00174    61*           IF (.NOT.CONVG)  GO TO 62                                                          000156
00176    62*           SUMN = ENN                                                                         000166
00177    63*           IF(JSOL.EQ.0)  GO TO 62                                                            000170
00201    64*           ENSOL = EN(JSOL,NPT)                                                               000172
00202    65*           EN(JSOL,NPT) = EN(JSOL,NPT)+EN(JLIQ,NPT)                                           000176
00203    66*           IUSE(JLIQ) = -IUSE(JLIQ)                                                           000200
00204    67*           IQ1 = IQ1-1                                                                        000202
00205    68*           DLVTP(NPT) = 0.                                                                    000205
00206    69*           CPR(NPT) = 0.                                                                      000206
00207    70*           GAMMAS(NPT) = 0.                                                                   000207
00210    71*           LOGV = .TRUE.                                                                      000210
00211    72*        62 CALL MATRIX                                                 EQLN0048            000213
```

```
00212    73*          NUMP = ITI - ITNUMB                                          000214
00213    74*          IQ2 = IQ1 + 1                                                000217
00214    75*          IF(.NOT.CONVG)    GO TO 67                                   000222
00216    76*          IF (LOGV.AND.JSOL.EQ.0) GO TO 63                             000224
00220    77*          DO 182 I=1,L                                        EQLN0140 000244
00223    78*      182 PROW(I) = G(IQ1,I)                                           000244
00225    79*          IF (.NOT.LOGV) GO TO 67                                      000246
00225    80*    C     LOGV = .TRUE.-- SET UP MATRIX TO SOLVE FOR DLVPT             000246
00227    81*       63 G(IQ1,IQ2) = ENN                                             000251
00230    82*          J = IQ1 - 1                                                  000260
00231    83*          DO 777 I = 1,J                                               000270
00234    84*      777 G(I,IQ2) = G(I,IQ1)                                          000277
00236    85*       67 IF(.NOT.RITE)  GO TO 72                                      000302
00240    86*          WRITE(JOUT,772) NUM                                          000303
00243    87*      772 FORMAT (11HOITERATION  ,I3,6X,7HMATRIX //)                   000325
00244    88*          DO 911 I=1,IMAT                                     EQLN0051 000325
00247    89*      911 WRITE(JOUT,73) (G(I,J), J = 1,KMAT)                          000325
00256    90*       72 IF(CONVG) IMAT=IMAT-1                                        000342
00260    91*          J = IMAT                                                     000346
00261    92*          CALL GAUSS                                                   000350
00262    93*          IF (J .NE. IMAT) GO TO 774                                   000352
00264    94*          IF(.NOT.RITE)  GO TO 773                                     000355
00266    95*          WRITE(JOUT,373)(LLMT(I),I=1,L)                               000363
00274    96*      373 FORMAT (7HOMOLE ,9(A9,1X))                                   000377
00275    97*          WRITE(JOUT,73)(X(I),I=1,IMAT)                                000377
00303    98*       73 FORMAT (9E14.6)                                  EQLN0062 000412
00304    99*      773 IF(.NOT.CONVG)  GO TO 85                                     000412
00306   100*          IF(.NOT.LOGV)  GO TO 174                                     000413
00310   101*          IF(JSOL.NE.0) ENSOL(JSOL,NPT)=ENSOL                          000421
00312   102*          GO TO 171                                                    000426
00313   103*      174 SUM = 0.                                            EQLN0148 000430
00314   104*          DO 175 J=1,L                                        EQLN0149 000431
00317   105*      175 SUM = SUM + PROW(J)*X(J)                                     000464
00321   106*          DLVTP(NPT) = 1.+G(IQ2,IQ1)/ENN-SUM/ENN  - X(IQ1)    EQLN0151 000470
00322   107*          CPR(NPT) = G(IQ2,IQ2)                               EQLN0152 000502
00323   108*          DO 176 J=1,IQ1                                      EQLN0153 000512
00326   109*      176 CPR(NPT) = CPR(NPT) - G(IQ2,J)*X(J)                          000512
00330   110*          LOGV = .TRUE.                                       EQLN0155 000520
00331   111*          GO TO 62                                                     000522
00331   112*    C  SINGULAR MATRIX                                                 000522
00332   113*      774 IF(.NOT.CONVG)  GO TO 775                                    000524
00332   114*    C     IF(ISING)  SINGULAR ONCE                                     000524
00332   115*    C     IF(IC)     SINGULAR TWICE                                    000524
00334   116*          WRITE(JOUT,172)                                              000525
00336   117*      172 FORMAT(28HODERIVATIVE MATRIX SINGULAR )                      000532
00337   118*          IC = .TRUE.                                                  000532
00340   119*          GO TO 1171                                                   000534
00341   120*      775 IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 871 000536
00343   121*          WRITE(JOUT,874)                                              000562
00345   122*      874 FORMAT(26HOLOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE 000567
00345   123*         1BEEN INCLUDED ON AN INSERT CARD, RESTART )                   000567
00346   124*          GO TO 873                                                    000567
00347   125*      871 WRITE(JOUT,74)                                               000571
00351   126*       74 FORMAT(16HOSINGULAR MATRIX)                                  000575
00352   127*          IF(IC)  GO TO 873                                            000575
00354   128*          IF (ISING) GO TO 997                                         000577
```

```
00356  129*          NTZER0 = 0                                                    000601
00357  130*    966   DO 970 JJ = 1, NS                                           000603
00362  131*          IF(IUSE(JJ)) 970,968,967                                      000613
00365  132*    967   IF (EN(JJ,NPT)) 969,973,969                                 000616
00370  133*    968   IF (EN(JJ,NPT) .GT. 0.0) GO TO 969                         000622
00372  134*          EN(JJ,NPT) = 1.0E-6                                           000626
00373  135*          ENLN(JJ) = -13.815511                                         000626
00374  136*          GO TO 970                                                     000630
00375  137*    969   NTZERO = NTZERO+1                                           000632
00376  138*    970   CONTINUE                                                     000637
00400  139*          IF(.NOT.IC) GO TO 971                                         000637
00402  140*          IC = .FALSE.                                                  000641
00403  141*          GO TO 43                                                      000642
00404  142*    971   ISING = .TRUE.                                               000644
00405  143*          WRITE(IOUT,776)                                               000645
00407  144*    776   FORMAT (8HORESTART)                                         000652
00410  145*          GO TO 43                                                      000652
00411  146*    997   IF(NTZERO.NE.L-1.OR.EQRAT.GT.1.00001.OR.EQRAT.LT..99999) GO TO 873  000664
00413  147*          ENN=0.                                                        000710
00414  148*          NEN = 0                                                       000711
00415  149*          DO 83 I=1,L                                                   000721
00420  150*          JJ = 0                                                        000724
00421  151*          DO 80 J=1,NS                                                  000732
00424  152*          IF (EN(J,NPT) .EQ. 0.0 .OR. A(I,J) .EQ. 0.0) GO TO 80         000732
00426  153*          IF (JJ .NE. 0) GO TO 83                                       000742
00430  154*          JJ = J                                                        000744
00431  155*    80    CONTINUE                                                      000752
00433  156*          NEN = NEN+1                                                   000752
00434  157*          EN(JJ,NPT) = BO(I)/A(I,JJ)                                    000755
00435  158*    83    CONTINUE                                                      000767
00437  159*          IF(NEN.LT.NTZERO) GO TO 873                                   000767
00441  160*          CONVG = .TRUE.                                                000773
00442  161*          IC = .TRUE.                                                   000775
00443  162*          HSUM(NPT) = 0.                                                000776
00444  163*          DO 84 J=1,NS                                                  001003
00447  164*          IF (EN(J,NPT) .LE. 0.0) GO TO 84                              001003
00451  165*          ENN = EN(J,NPT)+ENN                                           001005
00452  166*          ENLN(J) = ALOG(EN(J,NPT))                                     001010
00453  167*          HSUM(NPT) = HSUM(NPT) + EN(J,NPT)*HO(J)                       001016
00456  168*    84    CONTINUE                                                      001025
00456  169*          TM = ALOG(PP/ENN)                                             001025
00457  170*          GO TO 43                                                      001038
00460  171*    85    ITNUMB= ITNUMB-1                                  EQLN0068    001036
00461  172*          IF (ITNUMB .LT. 30) CRITV = CRITV + 2.50E-7                   001040
00461  173*    C     OBTAIN CORRECTIONS TO THE ESTIMATES               EQLN0070    001040
00463  174*          JJ = L + 1                                                    001047
00464  175*          IF(VOL) X(IO2)=X(IO1)                                         001060
00466  176*          IF(TP) X(IO2)=0.                                              001066
00470  177*          DLNT= X(IO2)                                      EQLN0072    001073
00471  178*          SUM = X(IO1)                                                  001076
00472  179*          IF(.NOT.VOL) GO TO 97                                         001101
00474  180*          X(IO1) = 0.                                                   001103
00475  181*          SUM =  -DLNT                                                  001105
00476  182*    97    DO 101 J=1,NS                                                 001111
00501  183*          IF (IUSE(J)) 101,98,100                                       001145
00504  184*    98    DELN(J) = HO(J)*DLNT-HO(J)+S(J)-ENLN(J)-TM+SUM                001151
```

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00505  185*          DO 99 I = 1,L                                                    001172
00510  186*       99 DELN(J) = DELN(J) + A(I,J)*X(I)                                  001172
00512  187*          GO TO 101                                                        001200
00513  188*      100 DELN(J) = X(JJ)                                                  001202
00514  189*          JJ = JJ + 1                                                      001205
00515  190*      101 CONTINUE                                          EQLN0079       001213
00517  191*          AMBDA= 1.                                         EQLN0080       001213
00520  192*          AMBDA1= 1.                                        EQLN0081       001215
00521  193*          SUM = X(IQ1)                                                     001216
00522  194*          IF(SUM.LT.0.)  SUM=-SUM                                          001222
00524  195*          IF(DLNT.GT.SUM)  SUM=DLNT                                        001230
00526  196*          IF(-DLNT.GT.SUM)  SUM=-DLNT                                      001236
00530  197*          DO 917 J=1,NS                                     EQLN0088       001252
00533  198*          IF (IUSE(J).NE.0) GO TO 917                                      001252
00535  199*          IF (EN(J,NPT) .GT. 0.0 .AND. DELN(J) .GT. SUM)  SUM = DELN(J)    001253
00537  200*          IF (EN(J,NPT) .GT. 0.0 .OR. DELN(J) .LE. 0.0)  GO TO 917         001272
00541  201*          SUM1 = (-9.212-ENLN(J)+ ENL)/(DELN(J)-X(IQ1))                    001306
00542  202*          IF(SUM1.LT.0.)  SUM1=-SUM1                                       001316
00544  203*          IF (SUM1.LT.AMBDA1) AMBDA1 = SUM1                                001323
00546  204*      917 CONTINUE                                          EQLN0089       001334
00550  205*          IF(SUM.GT.2.)AMBDA=2./SUM                         EQLN0090       001334
00552  206*          IF (AMBDA1.LT.AMBDA) AMBDA = AMBDA1                              001340
00554  207*          IF(.NOT.RITE)  GO TO 111                                         001352
00556  208*          WRITE(JOUT,923) II,ENN, ENL,PP,TM,AMBDA                          001354
00566  209*      923 FORMAT (3HOT=,E15.8,6H  ENN=,E15.8,7H  ENNL=E15.8,5H  PP=,E15.8,  001367
00566  210*         1 9H  LN P/N=E15.8,8H  AMBDA=E15.8 )                              001367
00567  211*          IF(VOL)  WRITE(JOUT,1924) VLM(NPT)                               001367
00573  212*     1924 FORMAT(8H VOLUME=,E15.8,2HCC)                                    001401
00574  213*          WRITE(JOUT,924)                                                  001401
00576  214*      924 FORMAT(1HO,18X,2HNI,12X,5HLN NI,8X,9HDEL LN NI,10X,4HH/RT,9X,4HSO/ 001413
00576  215*         1R,12X,6H-GO/RT,9X,5H-G/RT  )                                     001413
00577  216*          DO 926 J=1,NS                                                    001413
00602  217*          FNEG1 = S(J)-HO(J)                                               001413
00603  218*          FNEG2 = FNEG1                                                    001415
00604  219*          IF(IUSE(J).EQ.0)  FNEG2=FNEG2-ENLN(J)-TM                         001416
00606  220*      926 WRITE(JOUT,925) SUB(J,1),SUB(J,2),SUB(J,3),EN(J,NPT),ENLN(J),    001424
00606  221*         A                DELN(J),HO(J),S(J),FNEG1,FNEG2                   001424
00623  222*      925 FORMAT (1X,3A4,7E15.6)                                           001444
00624  223*          WRITE(JOUT,110)                                                  001444
00626  224*      110 FORMAT(1HO)                                                      001452
00626  225*        C     APPLY CORRECTIONS TO ESTIMATES                  EQLN0096       001452
00627  226*      111 SUM = 0.                                                         001452
00630  227*          DO 113 J=1,NS                                     EQLN0099       001453
00633  228*          IF (IUSE(J)) 113,112,114                                         001464
00636  229*      112 ENLN(J)=ENLN(J)+AMBDA*DELN(J)                     EQLN0100       001467
00637  230*          EN(J,NPT) = 0.                                    EQLN0101       001473
00640  231*          IF (ENLN(J) + 19.4206810 .LE. ENL)  GO TO 113                    001474
00642  232*          EN(J,NPT) = EXP(ENLN(J))                                         001500
00643  233*          SUM = SUM+EN(J,NPT)                                              001506
00644  234*          GO TO 113                                                        001511
00645  235*      114 EN(J,NPT) = EN(J,NPT) + AMBDA * DELN(J)                          001513
00646  236*      113 CONTINUE                                                         001521
00650  237*          SUMN = SUM                                                       001521
00651  238*          IF (TP) GO TO 115                                 EQLN0104       001523
00653  239*          TLN= TLN+AMBDA*DLNT                               EQLN0105       001525
00654  240*          TP     = EXP(TLN)                                 EQLN0106       001531
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00655  241*          JS1 = 1                                                    001535
00656  242*          CALL CPHS                                                  001537
00657  243*      115 IF(VOL) GO TO 2115                                         001542
00661  244*          ENL = ENL+AMBDA*X(IQ1)                                     001543
00662  245*          ENN = EXP(ENL)                                             001553
00663  246*          GO TO 1115                                                 001557
00664  247*     2115 ENN = SUMN                                                 001561
00665  248*          ENNL = ALOG(ENN)                                           001562
00666  249*          PP = RVR*TT*ENN/VLM(NPT)                                   001566
00667  250*     1115 TM = ALOG(PP/ENN)                                          001575
00670  251*          IF (LLMT(L).NE.IE) GO TO 116                               001603
00670  252*     C    CHECK ON REMOVING IONS                                     001603
00672  253*          DO 1116 J = 1,NS                                           001625
00675  254*          IF (A(L,J).EQ.0.) GO TO 1116                               001625
00677  255*          IF (ENI(J,NPT).GT.0.) GO TO 116                            001627
00701  256*     1116 CONTINUE                                                   001642
00703  257*          DO 1118 J=1,NS                                             001642
00706  258*     1118 IF (A(L,J) .NE. 0.0) IUSE(J) = + 10000                     001642
00711  259*          L = L-1                                                    001650
00712  260*          IQ1 = IQ1-1                                                001653
00713  261*          GO TO 43                                                   001656
00713  262*     C    TEST FOR CONVERGENCE                          EQLN0110     001656
00714  263*      116 IF (ITNUMB.EQ.0) GO TO 13                     EQLN0112     001660
00716  264*          IF (AMBDA.LT.1.) GO TO 43                     EQLN0113     001661
00720  265*          SUM = (ENN-SUMN)/ENN                                       001674
00721  266*          IF (SUM.LT.0.) SUM = -SUM                                  001704
00723  267*          IF (SUM .GT. CRITV)  GO TO 43                              001712
00725  268*          DO 130 J=1,NS                                 EQLN0115     001722
00730  269*          IF (IUSE(J).LT.0) GO TO 130                                001722
00732  270*          AA= DELN(J)/SUMN                                           001725
00733  271*          IF(AA.LT.0.)  AA=-AA                                       001730
00735  272*          IF (IUSE(J).EQ.0) AA = AA*EN(J,NPT)                        001735
00737  273*          IF (AA .GT. CRITV)  GO TO 43                               001742
00741  274*      130 CONTINUE                                                   001751
00741  275*     C    CALCULATE ENTROPY, CHECK ON DELTA S FOR SP PROBLEMS        001751
00743  276*          TOTN(NPT) = 0.                                             001751
00744  277*          SSUM(NPT) = 0.                                             001753
00745  278*          DO 183 J=1,NS                                 EQLN0133     001760
00750  279*          IF(IUSE(J).LT.0)  GO TO 183                                001760
00752  280*          TOTN(NPT) = TOTN(NPT) + EN(J,NPT)                          001762
00753  281*          SS = S(J)                                                  001765
00754  282*          IF(IUSE(J).EQ.0) SS=SS-ENLN(J)-TM                          001767
00756  283*          SSUM(NPT) = SSUM(NPT)+SS*EN(J,NPT)                         001775
00757  284*      183 CONTINUE                                      EQLN0136     002004
00761  285*          IF(.NOT.SP.OR.NPT.EQ.1)  GO TO 13                          002004
00763  286*          SS = SSUM(NPT) -SO                                         002014
00764  287*          IF(SS.LT.(-0.00005).OR.SS.GT.0.00005)  GO TO 43            002020
00766  288*          IF(RITE)  WRITE(JOUT,1183)  SS                             002035
00772  289*     1183 FORMAT(12HODELTA S/R =,E15.8)                              002046
00773  290*       13 CONVG= .TRUE.                                 EQLN0117     002046
00774  291*          IF(TT    .LT.TLOW.OR.TT    .GT.THIGH)WRITE(JOUT,306)TT,NPT  002047
01001  292*      306 FORMAT(17HOTHE TEMPERATURE=E12.4,26H IS OUT OF RANGE FOR POINT,I5)EQLN0119  002074
01002  293*          IF(ITNUMB.NE.0) GO TO 160                                  002074
01004  294*          WRITE(JOUT,973) NPT                                        002076
01007  295*      973 FORMAT (//5X,69H100 ITERATIONS DID NOT SATISFY THE CONVERGENCE REQ  002104
01007  296*         1UIREMENTS FOR POINT,I3/)                                   002104
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01010   297*          WRITE (JOUT,974) TT                                    002104
01013   298*      974 FORMAT (5X,'aaaa TEMPERATURE=',F12.8,' aaaa')          002112
01014   299*          IF (.NOT.MP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.) GO TO 873  002112
01016   300*          WRITE(JOUT,874)                                        002137
01020   301*          TT = T(1)                                              002144
01021   302*          RETURN                                                 002146
01021   303*      C   CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES.  002146
01022   304*      160 IF(NC.EQ.0) GO TO 143                                  002152
01024   305*          SIZEF = 0.                                             002153
01025   306*          INC = 0                                                002154
01026   307*          DO 170 J = 1,NS                                        002172
01031   308*          IF (IUSE(J).EQ.0 .OR. IUSE(J).EQ.-10000) GO TO 170     002172
01033   309*          INC = INC + 1                                          002204
01034   310*          IF(RITE) WRITE(JOUT,144)(SUB(J,I),I=1,3),TEMP(INC,1),TEMP(INC,2),  002207
01034   311*         1IUSE(J),EN(J,NPT)                                      002207
01047   312*      144 FORMAT (1HO,3A8,2F10.3,3X,5HIUSE=,I4,E15.7)            002241
01050   313*          IF (EN(J,NPT)) 146,148,169                             002241
01053   314*      146 IF (J.NE.JSOL .AND. J .NE.JLIQ) GO TO 147              002244
01055   315*          JSOL = 0                                               002260
01056   316*          JLIQ = 0                                               002261
01057   317*      147 IQ1 = IQ1 - 1                                          002263
01060   318*          EN(J,NPT) = 0.                                         002265
01061   319*          GO TO 166                                              002266
01062   320*      148 KG = 1                                                 002270
01063   321*          IF(IUSE(J).EQ.-IUSE(J+1)) GO TO 154                    002271
01065   322*          IF (J .EQ. 1 .OR. IUSE(J) .NE. -IUSE(J-1)) GO TO 153   002274
01067   323*          KG = -1                                                002307
01070   324*      154 JKG = J + KG                                           002312
01071   325*          IF (EN(JKG,NPT).LT.0.) GO TO 170                       002314
01073   326*          TMELT = TEMP(INC,1)                                    002321
01074   327*          IF (TMELT .EQ. TEMP(INC+KG,2)) GO TO 158               002324
01076   328*          TMELT = TEMP(INC,2)                                    002330
01077   329*          IF (TMELT .EQ. TEMP(INC+KG,1)) GO TO 157               002332
01101   330*          WRITE(JOUT,156)                                        002334
01103   331*      156 FORMAT (50H03 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER  )  002342
01103   332*      C  JTH SPECIES A SOLID (EN=0), (J+KG)TH SPECIES A LIQUID (EN IS +)  002342
01104   333*      157 IF (TT .GT. TMELT .OR. (TP .AND. TT .EQ. TMELT)) GO TO 169  002342
01106   334*          IF (TP .OR. TT .LE. TMELT - 150.0) GO TO 1165          002361
01110   335*          JSOL = J                                               002373
01111   336*          JLIQ = JKG                                             002375
01112   337*          GO TO 159                                              002377
01112   338*      C  JTH SPECIES A LIQUID(EN=0), (J+KG)TH SPECIES A SOLID (EN IS +)  002377
01113   339*      158 IF (TT .LT. TMELT .OR. (TP .AND. TT .EQ. TMELT)) GO TO 169  002401
01115   340*          IF (TP .OR. TT .GE. TMELT + 150.0) GO TO 1165          002420
01117   341*          JSOL = JKG                                             002432
01120   342*          JLIQ = J                                               002434
01121   343*      159 TLN = ALOG (TMELT)                                     002437
01122   344*          TT = TMELT                                             002482
01123   345*          EN(JKG,NPT) = .5 * EN(JKG,NPT)                         002444
01124   346*          EN(J,NPT) = EN(JKG,NPT)                                002451
01125   347*          GO TO 165                                              002452
01125   348*      C  WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH FN          002452
01126   349*      1165 EN(J,NPT) = EN (JKG, NPT)                             002454
01127   350*          IUSE(J) = -IUSE(J)                                     002457
01130   351*          IUSE (JKG) = -IUSE(JKG)                                002461
01131   352*          EN(JKG,NPT)= 0.                                        002464
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01132  353*          WRITE(JOUT,161) (SUB(JKG,I), I = 1,3),(SUB(J,I), I = 1,3)                    002471
01144  354*     161  FORMAT (10X,22HPHASE CHANGE, REPLACE ,3A4,6H WITH ,3A4)                       002514
01145  355*          GO TO 90                                                                     002514
01146  356*      153 IF (TT.LT.TEMP(INC,1) .AND.TEMP(INC,1).NE.TLOW) GO TO 169                    002516
01150  357*          IF (TT.GT.TEMP(INC,2)) GO TO 169                                             002533
01152  358*          SUM = 0.                                                                     002902
01153  359*          DO 167 I = 1,L                                                               002551
01156  360*     167  SUM = SUM + A(I,J)*X(I)                                                      002551
01160  361*          DELF = HO(J)-S(J)-SUM                                                        002555
01161  362*          IF(RITE)  WRITE(JOUT,168)DELF,SIZEF                                          002563
01166  363*      168 FORMAT (17H GO-SUM(AIJ*PI) =E15.7,10X,18HPREVIOUS DELTA G =,E15.7)           002574
01167  364*          IF(DELF.GE.SIZEF .OR. DELF.GE.0.1 GO TO 169                                  002578
01171  365*          SIZEF = DELF                                                                 002611
01172  366*          JDELF = J                                                                    002613
01173  367*      169 IF(INC.EQ.NC) GO TO 1160                                                     002616
01175  368*      170 CONTINUE                                                                     002624
01177  369*     1160 IF (SIZEF.EQ.0.) GO TO 143                                                   002624
01201  370*          J = JDELF                                                                    002625
01202  371*      165 IQ1 = IQ1 + 1                                                                002630
01203  372*          WRITE(JOUT,136) (SUB(J,I), I = 1,3)                                          002632
01211  373*     136  FORMAT (10X,9HADD ,3A4)                                                      002650
01212  374*      166 IUSE(J) = - IUSE(J)                                                          002650
01213  375*       40 CONVG = .FALSE.                                                              002653
01214  376*          JS1 = 1                                                                      002653
01215  377*          CALL CPHS                                                                    002655
01216  378*      143 TN = NUMB                                                                    002660
01217  379*          IF (.NOT. SHOCK)  WRITE(JOUT,771) NPT,(X(I), I = 1,L),TN                     002662
01230  380*      771 FORMAT (I3,14F9.3)                                                           002703
01231  381*          JS1 = 1                                                                      002703
01232  382*          IF(TP.AND.CONVG)  CALL CPHS                                                  002705
01234  383*          ITNUMB = 100                                                                 002712
01235  384*          GO TO 43                                                      EQLN0124       002714
01235  385*    C     CALCULATE EQUILIBRIUM PROPERTIES                              EQLN0128       002714
01236  386*     1171 DLVPT(NPT) = -1.                                                             002716
01237  387*          DLVTP(NPT) = 1.                                                              002720
01240  388*          CPR(NPT) = CPSUM                                                             002721
01241  389*          GO TO 199                                                                    002723
01242  390*      171 SUM = 0.                                                                     002725
01243  391*          DO 179 J = 1,L                                                EQLN0167       002726
01246  392*      179  SUM = SUM + PROW(J)*X(J)                                                    002741
01250  393*          DLVPT(NPT) = -2.+SUM/ENN+ X(IQ1)                              EQLN0170       002745
01251  394*          IF (JLIQ .EQ. 0)  GO TO 199                                                  002754
01253  395*          IUSE(JLIQ) = -IUSE(JLIQ)                                                     002756
01254  396*          HSUM(NPT) = HSUM(NPT)+EN(JLIQ,NPT)*(HO(JLIQ)-HO(JSOL))                       002761
01255  397*          IQ1 = IQ1+1                                                                  002772
01256  398*          GAMMAS(NPT) = -1./DLVPT(NPT)                                                 002775
01257  399*          GO TO 186                                                                    003000
01260  400*      199 GAMMAS(NPT) = -1./(DLVPT(NPT)+(DLVTP(NPT)**2)*ENN/CPR(NPI))   EQLN0171       003002
01261  401*      186 TTT(NPT) = TT                                                 EQLN0178       003013
01262  402*          ENNL = ENL                                                                   003015
01263  403*          PPP(NPT) = PP                                                                003017
01264  404*          VLM(NPT) = RVR*ENN*TT/PP                                                     003021
01265  405*          HSUM(NPT) = HSUM(NPT)*TT                                                     003026
01266  406*          WM(NPT) = 1./ENN                                              EQLN0180       003031
01267  407*          IF (.NOT. RITE)  RETURN                                                      003035
01271  408*          WRITE(JOUT,201) NPT,APP(NPT),PP,TT,HSUM(NPT),SSUM(NPT),WM(NPT),              003042
```

```
01271    409*          1 CPR(NPT),OLVPT(NPT),OLVTP(NPT),GAMMAS(NPT),VLM(NPT)                    003092
01307    410*       201 FORMAT (7HOPOINT=I3,3X,4HPCP=E13.6,3X,2HP=E13.6,3X,2HT=E13.6,3X,4H      003065
01307    411*          1H/R=E13.6,3X,4HS/R=E13.6//3X,3HMV=E13.6,3X,5HCP/R=E13.6,3X,6HOLVPT      003065
01307    412*          2=E13.6,3X,6HOLVTP=E13.6,3X,9HGAMMA(S)=E13.6,3X,2HV=,E13.6)              003065
01310    413*           RETURN                                                                  003065
01310    414*     C     ERROR. SET TT=0                                                         003065
01311    415*       873 TT=0.                                                                   003071
01312    416*           NPT = NPT-1                                                             003071
01313    417*           RETURN                                                                  003074
01314    418*           END                                                                     003135
```

END OF COMPILATION: NO DIAGNOSTICS.

@HD6,P FROZEN

```
@FOR,S    FROZEN,FROZEN
HSA  E3 -10/15/80-13:06:33 (10.)

    SUBROUTINE FROZEN    ENTRY POINT 000345

    STORAGE USED: CODE(1) 00036: DATA(0) 000041: BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003   COMSIS 000006
     0004   POINTS 000335
     0005   SPECES 017106
     0006   MISC   001701
     0007   INDX   000041

    EXTERNAL REFERENCES (BLOCK, NAME)

     0010   CPHS
     0011   ALOG
     0012   EXP
     0013   NERR3S

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001   000066 1356   0001   000251 2076   0001   000022 S1L    0001   000050 S5L    0001   000120 60L
     0001   000165 81L    0001   000313 901L   0001   000321 903L   0005   011052 A      0004   000640 AM
     0006   000705 AM1    0006   001135 ANUM   0003   000000 ATMN   0006   000004 ATOM   0006   000514 BD
     0006   000545 BOP    0007   000036 CALCH  0000 R 000005 CC     0005   000000 COEF   0007 L 000001 CONV6
     0004 R 000032 CPR    0006   000706 CPR1   0006 R 000634 CPSUM  0006   000654 DATA   0005   010624 DELN
     0006   001560 DENS   0000 R 000007 DLNT   0004 R 000064 DLVPT  0004 R 000047 DLVTP  0005 R 004312 EN
     0005   010150 ENLN   0006   001700 ENLSAV 0006   000000 ENN    0006   001676 ENNL   0006   001677 ENSAVE
     0006   001414 ENTH   0006   000636 FORAT  0006   001445 FAZ    0006   001527 FOX    0004 R 000101 GAMMAS
     0003   000001 GMET   0007 L 000003 HP     0006   000642 HPP    0006 R 000637 HSUBO   0004 R 000000 HSUM
     0005 R 010376 HO     0007   000030 IC     0007   000000 IDEBUG 0007   000015 IMAT   0000 I 000010 INC
     0000   000015 INJPS  0007   000023 IONS   0007   000021 IP     0007   000037 IOSAVE 0007   000016 IOI
     0007   000005 ISV    0007   000034 IT     0005 I 016266 IUSE   0000 I 000004 J      0007   000026 JLIQ
     0007   000025 JSOL   0007 I 000031 JS1    0007   000014 KMAT   0006   000463 LLMT   0007   000040 LSAVE
     0007   000006 MOLES  0006   000707 NAME   0007 I 000024 NC     0007   000022 NEWR   0007 I 000035 NFZ
     0007   000012 NLM    0007   000017 NOF    0007   000020 NOMIT  0007   000007 NP     0007 I 000011 NPT
     0007   000027 NREAC  0007 I 000013 NS     0000 I 000000 NSPP1  0007   000010 NT     0006   000635 OF
     0006   001644 OXF    0004   000116 P      0003   000002 PATM   0006   001363 PECNT  0006 R 000633 PP
     0004 R 000217 PPP    0003   000003 RBAR   0003   000004 RBR    0006   000644 RH     0006   001611 RHOP
     0006   001612 RMW    0000 R 000001 RNV    0006   001476 RTEMP  0003 R 000005 RVR    0005 R 004064 S
     0007   000033 SHOCK  0005   016660 SLN    0004   000251 SONVEL 0007 L 000004 SP     0000 R 000006 SS
     0004 R 000015 SSUM   0005   015364 SUB    0000 R 000003 SUMH   0006   000001 SUMN   0000 R 000002 SUMS
     0006 R 000003 SO     0004   000150 T      0005 R 016514 TEMP   0006   000632 TNIGH  0006 R 001643 TLN
     0006 R 000630 TLOW   0006   000627 TM     0006   000631 TMID   0004 R 000320 TOTN   0007   000002 TP
     0006 R 000002 TT     0004 R 000266 TTT    0004   000202 V      0004 R 000303 VLM    0006   000646 VMIN
     0007 L 000032 VOL    0006   000650 VPLS   0004 R 000234 WM     0006   000652 WP
```

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00101     1*          SUBROUTINE FROZEN                                          FRO20002   000000
00101     2*    C                                                                FRO20001   000000
00101     3*    C     (FROZEN COMPOSITION EXPANSION ONLY)                        FRO20004   000000
00101     4*    C                                                                FRO20005   000000
00101     5*          COMMON /CONSTS/ AIMN,GMET,PATM,RBAR,RBR,RVR                /CONSTS/   000000
00104     6*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)           000000
00104     7*         1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)     000000
00104     8*         2 ,VLM(13),TOTN(13)                                                   000000
00104     9*    C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)       000000
00104    10*    C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)       000000
00105    11*          INCLUDE SPECPR                                                        000000
00111    12*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),             000000
00111    13*         1              BOP(25,2),TM,TLOW,THIO,THIGH,PP,CPSUM,OF,EQRAT,       000000
00111    14*         2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),NPLS(2),WP(2),  /MISC/ 000000
00111    15*         3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(23,6),PECNT(25),    000000
00111    16*         4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,     000000
00111    17*         5              RM(25),TLN,DXE(26),ENNL,ENSAVE,ENLSAV                 000000
00112    18*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,MP,NT,NPT,NLM,NS,  /INDX/ 000000
00112    19*         1              RMAT,IMAT,IOI,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/ 000000
00112    20*         2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IGSAVE,LSAVE    /INDX/ 000000
00112    21*    C                                                                            000000
00113    22*          LOGICAL CONVG,HP,SP,VOL                                               000000
00113    23*    C                                                                           000000
00114    24*          CONVG = .FALSE.                                                       000000
00115    25*          TLN = ALOG(TT)                                                        000000
00116    26*          IF (VOL)  RNV = RVR/(VLM(NPT)*WM(NFZ))                                000004
00120    27*       51 SUMS=0.                                                             000022
00121    28*          SUMH = 0.                                                           000022
00122    29*          JS1 = 1                                                             000023
00123    30*          J = NPT                                                             000025
00124    31*          NPT = NFZ                                                           000027
00125    32*          CALL CPHS                                                           000031
00126    33*          CC = CPSUM                                                          000033
00127    34*          IF(.NOT.VOL)  GO TO 55                                              000035
00131    35*          CC = CPSUM-1./WM(NFZ)                                               000037
00132    36*          PP = RNV*TT                                                         000044
00133    37*       55 NPT = J                                                             000050
00134    38*          DO 60 J = 1,NS                                                      000051
00137    39*          IF (EN(J,NFZ) .LE. 0.0)  GO TO 60                                   000066
00141    40*          SS = S(J)                                                           000070
00142    41*          IF(IUSE(J).EQ.0)  SS=SS-ALOG(EN(J,NFZ)*PP*WM(NFZ))                  000072
00144    42*          SUMS = SUMS+SS*EN(J,NFZ)                                            000105
00145    43*          IF (CONVG.OR.HP)  SUMH=SUMH+HO(J)*EN(J,NFZ)                         000111
00147    44*       60 CONTINUE                                                  FRO20058   000122
00151    45*          IF (CONVG) GO TO 81                                       FRO20059   000122
00153    46*          IF(SP)  DLNT=(SUMS-SO)/CC                                           000124
00155    47*          IF(HP)  DLNT=(SUMH-HSUBO/TT)/CC                                     000132
00157    48*          TLN=TLN-DLNT                                              FRO20061   000141
00160    49*          IF(DLNT.LT.0.) DLNT=-DLNT                                           000144
00162    50*          IF(DLNT.LT.0.5E-4)  CONVG=.TRUE.                                    000151
00164    51*          TT = EXP(TLN)                                                       000157
00165    52*          GO TO 51                                                  FRO20063   000163
00166    53*       81 TTT(NPT)= TT                                                        000165
00167    54*          SSUM(NPT)= SUMS                                                     000167
00170    55*          HSUM(NPT)= TT*SUMH                                                  000171
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00171   56*         GAMMAS(NPT)= CPSUM/(CPSUM-1./WM(NFZ))                    000173
00172   57*         VLM(NPT) = RVR*TT/(WM(NFZ)*PP)                           000202
00173   58*         WM(NPT) = WM(NFZ)                                        000210
00174   59*         DLVPT(NPT) = -1.                                         000212
00175   60*         DLVTP(NPT) = 1.                                          000214
00176   61*         TOTN(NPT) = TOTP(NFZ)                                    000215
00177   62*         PPP(NPT) = PP                                            000217
00200   63*         CPR(NPT)= CPSUM                                          000221
00201   64*         IF (TT.LT.(TLOW-150.))GO TO 903                          000223
00203   65*         IF (NC .EQ. 0) RETURN                                    000230
00205   66*         INC =0                                                   000244
00206   67*         DO 901 J = 1,NS                                          000251
00211   68*         IF (IUSE(J) .EQ. 0 .OR. IUSE(J) .EQ. - 10000) GO TO 901  000251
00213   69*         INC = INC+1                                              000263
00214   70*         IF (EN(J,NFZ) .LE. 0.0) GO TO 901                        000267
00216   71*         IF (TT.LT.TEMP(INC,1)-50. .OR. TT.GT.TEMP(INC,2)+50.) GO TO 903  000272
00220   72*   901 CONTINUE                                                   000315
00222   73*         RETURN                                                   000315
00223   74*   903 TT=0.                                                      000321
00224   75*         NPT= NPT-1                                               000321
00225   76*         RETURN                                                   000324
00226   77*         END                                    FR020084          000357
```

END OF COMPILATION: NO DIAGNOSTICS.

B-43

&HDG,P GAMEFF

```
$FOR,S    GAMEFF,GAMEFF
HSA  E3 -10/15/80-13:06:42 (2,)

   SUBROUTINE GAMEFF    ENTRY POINT 000176

   STORAGE USED: CODE(1) 000217; DATA(0) 000044; BLANK COMMON(2) 000000

   EXTERNAL REFERENCES (BLOCK, NAME)
    0003   XPRR
    0004   SQRT
    0005   NERR36

   STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)
    0001   000036 10L      0001   000025 1D86     0001   000132 20L      0001   000152 50L      000C R 000002 ANK
    0000 R 000006 CFA      0000 R 000005 CGAM     0000 R 000001 G        0000 R 000004 GM       0000 R 000003 GP
    0000 I 000000 I        0000   000019 INJPS
```

```
00101      1*            SUBROUTINE GAMEFF (V,GAMMAS,A,N,M)                                    000025
00103      2*            DIMENSION A(1,1),GAMMAS(13),M(13),V(13)                               000025
00103      3*      C                                                                           000025
00104      4*            DO 50 I = 2,N                                                         000025
00107      5*            G = GAMMAS(I)                                                         000025
00110      6*            ANK = +1.0                                                            000126
00111      7*            IF (G .GT. 1.0)  GO TO 10                                             000036
00113      8*            G = 1.0010                                                            000033
00114      9*       10   GP = G + 1.0                                                          000036
00115     10*            GM = G - 1.0                                                          000040
00116     11*            CGAM = SQRT(G)*(2.0/GP)**(GP/(2.0*GM))                                000043
00117     12*            CFA = CGAM*SQRT(2.0*G*(1.0 - (1.0/A(I))**(GM/G))/GM)                  000063
00120     13*            IF (ABS(V(I) - CFA) .LE. 5.0E-5)  GO TO 50                            000110
00122     14*            IF (G .LT. 2.0)  GO TO 20                                             000115
00124     15*            IF (ANK .LT. 0.0)  GO TO 50                                           000121
00126     16*            ANK = -1.0                                                            000124
00127     17*            G = GAMMAS(I)                                                         000126
00130     18*            GO TO 10                                                              000130
00131     19*       20   G = G + ANK*(V(I) - CFA)                                             000132
00132     20*            IF (G .GT. 1.0)  GO TO 10                                             000136
00134     21*            IF (ANK .LT. 0.0)  GO TO 50                                           000141
00136     22*            ANK = -1.0                                                            000144
00137     23*            G = GAMMAS(I)                                                         000146
00140     24*            GO TO 10                                                              000150
00141     25*       50   M(I) = G                                                             000152
00143     26*            RETURN                                                                000157
00144     27*             END                                                                  000216

       END OF COMPILATION:       NO  DIAGNOSTICS.
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BMDS,P GAUSS

```
@FOR,S   GAUSS,GAUSS
HSA  E3 -10/15/80-13:06:54 (7,)

    SUBROUTINE GAUSS      ENTRY POINT 000911

    STORAGE USED: CODE(1) 000931; DATA(0) 000126; BLANK COMMON(2) 000000

     COMMON BLOCKS:

    0003   DOUBLE 001560
    0004   INDX   000001

    EXTERNAL REFERENCES (BLOCK, NAME)

    0005   NERR38

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001   000107 10L       0001   000011 106       0001   000043 1206      0001   000062 1276      0001   000130 1526
     0001   000181 1676      0001   000204 1776      0001   000115 8L        0001   000256 210       0001   000257 2136
     0001   000141 22L       0001   000361 23L       0001   000333 2316      0001   000167 31L       0001   000275 45L
     0001   000303 47L       0001   000390 51L       0001   000020 8L        0001   000101 9L        0004   000036 CALCH
     0000 D 000000 COEFX     0004   000001 CONV6     0003 D 000000 G         0004   000003 HP        0000 I 000086 I
     0004   000030 IC        0004   000000 IDEBUG    0000   000071 INJPS     0004   000023 IONS      0004   000021 IP
     0004   000037 IQSAVE    0004   000016 IQ1       0004   000005 ISV       0004   000034 IT        0004 I 000015 IUSE
     0000 I 000054 IUSE1     0000 I 000057 J         0004   000026 JLIQ      0004   000025 JSOL      0004   000031 JS1
     0000 I 000061 K         0004   000014 KMAT      0004   000040 LSAVE     0004   000006 MOLES     0004   000024 NC
     0004   000022 NEWR      0004   000035 NFZ       0004   000012 NLM       0000 I 000055 NN        0004   000017 NOF
     0004   000020 NOMIT     0004   000007 NP        0004   000011 NPT       0004   000027 NREAC     0004   000013 NS
     0004   000010 NT        0004   000033 SHOCK     0004   000004 SP        0000 D 000050 SUM       0000 R 000060 TEMP
     0004   000002 TP        0004   000032 VOL       0003 D 001510 X         0000 D 000052 Z

00101     1*          SUBROUTINE GAUSS                                                          000000
00103     2*          COMMON/DOUBLE/G(20,21),X(20)                                              000000
00104     3*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,    /INDX/  000000
00104     4*         1              KMAT,IUSE,IQ1,NCF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/  000000
00104     5*         2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE    /INDX/  000000
00105     6*          DOUBLE PRECISION COEFX(20),G,SUM,X,Z                                      000000
00105     7*     C    BEGIN ELIMINATION OF NNTH VARIABLE                                00020000 000000
00106     8*          IUSE1=IUSE+1                                                      00020300 000000
00107     9*          DO 45 NN = 1,IUSE                                                         000002
00112    10*          IF (NN .NE. IUSE)  GO TO 8                                                000011
00114    11*          IF (G(NN,NN))  31,23,31                                                   000014
00114    12*     C    SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW                        00020600 000014
00117    13*        8 DO 18 I=NN,IUSE                                                           000020
00122    14*          COEFX(I) = 1.0E38                                                         000047
00123    15*          IF(G(I,NN).EQ.0.)  GO TO 18                                               000051
00125    16*          COEFX(I) = 0.                                                             000054
00126    17*          DO 10 J=NN,IUSE1                                                          000062
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00131    18*          SUM = G(I,J)                                                000062
00132    19*          IF(SUM.LT.0.)  SUM=-SUM                                     000064
00134    20*          IF(J.NE.NN)  GO TO 9                                        000072
00136    21*          Z = SUM                                                     000075
00137    22*          GO TO 10                                                    000077
00140    23*        9 IF(SUM.GT.COEFX(I))  COEFX(I)=SUM                           000101
00142    24*       10 CONTINUE                                                    000111
00144    25*          COEFX(I) = COEFX(I)/Z                                       000111
00145    26*       18 CONTINUE                                                    000121
00147    27*          TEMP = 1.0E38                                               000121
00150    28*          I=0                                            00207200     000123
00151    29*          DO 22 J = NN,IUSE                                           000130
00154    30*          IF (COEFX(J) .GE. TEMP)  GO TO 22                           000130
00156    31*          TEMP = COEFX(J)                                             000134
00157    32*          I=J                                            00207600     000136
00160    33*       22 CONTINUE                                       00207700     000143
00162    34*          IF (I .EQ. 0)  GO TO 23                                     000143
00162    35*    C     INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH 00208200     000143
00162    36*    C     VARIABLE FROM THE REMAINING EQUATIONS              00208300 000143
00162    37*    C       INTERCHANGE EQUATIONS I AND NN                   00208500 000143
00164    38*          IF (NN .EQ. I)  GO TO 31                                    000145
00166    39*          DO 30 J = NN,IUSE1                                          000150
00171    40*          Z=G(I,J)                                         00208900   000161
00172    41*          G(I,J)=G(NN,J)                                   00209000   000162
00173    42*       30 G(NN,J) = Z                                                 000164
00173    43*    C     DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH 00209300    000164
00173    44*    C     VARIABLE FROM THE REMAINING EQUATIONS              00209400 000164
00175    45*       31 K = NN + 1                                         00209600 000167
00176    46*          DO 36 J = K, IUSE1                                 00209700 000171
00201    47*          IF(G(NN,NN).EQ.0.)  GO TO 23                                000204
00203    48*       36 G(NN,J) = G(NN,J)/G(NN,NN)                                  000207
00205    49*          IF (K .EQ. IUSE1)  GO TO 45                                 000214
00207    50*          DO 44 I = K,IUSE                                            000217
00212    51*          DO 44 J = K,IUSE1                                           000257
00215    52*       44 G(I,J) = G(I,J) - G(I,NN)*G(NN,J)                           000257
00220    53*       45 CONTINUE                                       00210500     000300
00220    54*    C     BACKSOLVE FOR THE VARIABLES                    00210700     000300
00222    55*          K = IUSE                                       00211000     000300
00223    56*       47 J = K + 1                                      00211100     000303
00224    57*          X(K) = 0.0D0                                   00203800     000305
00225    58*          SUM = 0.0                                      00211200     000312
00226    59*          IF (IUSE .LT. J)  GO TO 51                                  000313
00230    60*          DO 50 I = J,IUSE                                            000316
00233    61*       50 SUM = SUM + G(K,I)*X(I)                                     000333
00235    62*       51 X(K) = G(K,IUSE1) - SUM                                     000340
00236    63*          K = K - 1                                      00211800     000350
00237    64*          IF (K .NE. 0)  GO TO 47                                     000353
00241    65*          RETURN                                                      000355
00242    66*       23 IUSE = IUSE-1                                               000361
00243    67*          RETURN                                                      000363
00244    68*          END                                                         000430

      END OF COMPILATION:       NO  DIAGNOSTICS.
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@HDG,P      HCALC
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@FOR,S   HCALC,HCALC
HSA  E3 -10/15/80-13:06:58 (11,)

    SUBROUTINE HCALC     ENTRY POINT 000526

    STORAGE USED: CODE(1) 000542; DATA(0) 000066; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003   CONSTS 000006
     0004   HOLCON 000010
     0005   POINTS 000101
     0006   SPECES 017106
     0007   MISC   001701
     0010   INDX   000041
     0011   CCC    000003

    EXTERNAL REFERENCES (BLOCK, NAME)

     0012   CPHS
     0013   ALOG
     0014   NWDUS
     0015   NIO2S
     0016   NERR3S

    STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001   000070 143G     0001   000107 15L      0001   000131 16L      0001   000145 145G     0001   000154 172G
     0001   000162 177G     0001   000204 210G     0001   000275 227G     0001   000170 30L      0001   000026 4L
     0001   000177 50L      0001   000432 500L     0001   000251 55L      0001   000265 56L      0001   000307 70L
     0001   000467 75L      0000   000010 76F      0001   000477 80L      0000   000024 85F      0001   000037 9L
     0001   000312 90L      0006 R 011052 A        0004 I 002001 AG       0007 R 000690 AM       0007 R 000705 AM1
     0000 R 000002 ANN      0007 R 001135 ANUM     0003   000000 ATMN     0007   000004 ATOM     0004 I 000004 BLK
     0007   000514 BO       0007   000545 BOP      0010 L 000036 CALCM    0006   000000 COEF     0010   000001 CONVG
     0005   000032 CPR      0007 R 000706 CPR1     0007 R 000634 CPSUM    0007 R 000654 DATA     0006   010624 DELN
     0011   000002 DEMAND   0007   001560 DENS     0005   000064 DLVPT    0005   000047 DLVTP    0006 R 004312 EN
     0004   000000 END      0000 R 000007 ENJ      0006   010150 ENLN     0007   001700 ENLSAV   0007   000000 ENN
     0007   001676 ENNL     0007   001677 ENSAVE   0007 R 001914 ENTH     0007   000636 EORAT    0007 I 001445 FAZ
     0007 I 001527 FOX      0003   000001 GMET     0011   000000 GRAPH    0010   000003 HP       0007 R 000642 HPP
     0007 R 000637 HSUBO    0005   000000 HSUM     0006 R 010376 HO       0000 I 000005 I        0010   000030 IC
     0010   000000 IDEBUG   0004   000002 IE       0010   000015 IMAT     0000   000044 INJPS    0010   000023 IONS
     0010   000021 IP       0010   000037 IQSAVE   0010   000016 IQ1      0000 I 000006 IS       0010   000005 ISV
     0010   000034 IT       0006 I 016266 IUSE     0004 I 000003 IZERO    0010 I 000031 J        0010   000026 JLIO
     0011 I 000001 JOUT     0010   000025 JSOL     0000 I 000004 K        0010   000014 KMAT     0010 I 000012 L
     0007 I 000463 LLMT     0010   000040 LSAVE    0004   000005 MOL      0010 L 000006 MOLES    0000 I 000003 N
     0007 I 000707 NAME     0010   000024 NC       0010   000022 NEWR     0010   000035 NFZ      0010   000017 NOF
     0010   000020 NOMIT    0010   000007 NP       0010 I 000011 NPT      0010 I 000027 NREAC    0010 I 000013 NS
     0000 I 000000 NSPP1    0010   000010 NT       0007 I 001135 NUM      0007 R 000635 OF       0004 I 000006 OX
     0007   001644 OXF      0003   000002 PATM     0007 R 001363 PECNT    0007 R 000633 PP       0003 R 000003 RBAR
     0003   000004 RBR      0007   000644 RH       0007   001611 RHOP     0007 R 001612 RHW      0007 R 001476 RTEMP
     0003   000005 RVR      0006 R 004064 S        0010 L 000033 SHOCK    0006   016660 SLN      0010   000004 SP
     0005 R 000015 SSUM     0006   015364 SUB      0007   000001 SUMN     0007   000003 SO       0006 R 016514 TEMP
```

```
0007 R 000632 THIGH     0007 R 001643 TLN       0007 R 000630 TLOW      0007 R 000627 TM        0007  000631 TMID
0010   000002 TP        0000 R 000001 TSAVE     0007 R 000002 TT        0007   000646 VMIN      0010 L 000032 VOL
0007   000650 VPLS      0007 R 000652 WP        0004   000007 ZERO
```

```
00101     1*          SUBROUTINE HCALC                                                                    000000
00101     2*    C  CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS                                   000000
00103     3*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                    /CONSTS/             000000
00104     4*          COMMON /HOLCON/ END,AG,IE,IZERO,BLK,MOL,OX,ZERO                /HOLCON/             000000
00105     5*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVIP(13),DLVPI(13)                         000000
00108     6*    C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)                     000000
00105     7*    C   1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                      000000
00106     8*          INCLUDE SPECPK                                                                      000000
00112     9*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                           000000
00112    10*        1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,                      000000
00112    11*        2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),      /MISC/          000000
00112    12*        3              DATA(25),AMI,CPRI,NAME(25,6),ANUM(25,6),PECWT(25),                   000000
00112    13*        4              EMTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,                    000000
00112    14*        5              RHW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                               000000
00113    15*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,      /INDX/           000000
00113    16*        1              KMAT,IMAT,IQ1,MOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,   /INDX/           000000
00113    17*        2              NREAC,IC,J,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE       /INDX/           000000
00113    18*    C                                                                                       000000
00114    19*          COMMON /CCC/ GRAPH,JOUT,DEMAND                                                      000000
00114    20*    C                                                                                       000000
00115    21*          DIMENSION NUM(25,6)                                                                 000000
00116    22*          EQUIVALENCE (ANUM,NUM)                                                              000000
00117    23*          INTEGER AG,BLK,FAZ,FOX,OX                                                           000000
00120    24*          LOGICAL CALCH,MOLES,SHOCK,VOL                                                       000000
00121    25*          TSAVE = TT                                                                          000000
00122    26*          IF (AM(1) .GT. 0.0 .AND. AM(2) .GT. 0.0)  GO TO 4                                   000001
00124    27*          AM1= AM(2)                                                                          000015
00125    28*          IF (AM(2) .LE. 0.0)  AM1 = AM(1)                                                    000017
00127    29*          GO TO 9                                                                             000024
00130    30*        4 AM1=(OF+1.)*AM(1)*AM(2)/(AM(1)+OF*AM(2))                                            000026
00131    31*        9 TM = 0.                                                                             000037
00132    32*          IF(PP.GT.0.) TM = ALOG(PP*AM1)                                                      000037
00134    33*          SSUM(NPT) = 0.                                                                      000051
00135    34*          HPP(1) = 0.                                                                         000053
00136    35*          HPP(2) = 0.                                                                         000054
00137    36*          HSUBO = 0.                                                                          000055
00140    37*          CPR1 = 0.                                                                           000056
00141    38*          ANN = (1.+OF)                                                                       000057
00141    39*    C     LOOP ON REACTANTS. IF OXIDANT, K = 1, IF FUEL, K = 2.                               000057
00142    40*          DO 900 N=1,NREAC                                                                    000070
00145    41*          K=2                                                                                 000070
00146    42*          IF(FOX(N).EQ.OX)K=1                                                                 000072
00150    43*          IF (NAME(N,6).NE.IZERO) GO TO 90                                                    000077
00152    44*          IF(.NOT.CALCH)  GO TO 15                                                            000102
00154    45*          TT = RTEMP(N)                                                                       000104
00154    46*    C  IS TT IN RANGE                                                                         000104
00155    47*       15 IF (SHOCK)  GO TO 16                                                                000107
00157    48*          IF (TT .LT. TLOW - 100.0 .OR. TT .GT. THIGH + 1000.0)  GO TO 75                     000110
00161    49*       16 J=NUM(N,6)                                                                          000134
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```
00162   50*          IF (J.NE.0) GO TO 90                                    000136
00164   51*          DO 10 J=1,L                                             000145
00167   52*       10 DATA(J) = 0.0                                           000145
00171   53*          DO 30 I=1,S                                             000154
00174   54*          IF (ANUM(N,I) .LE. 0.0) GO TO 50                        000154
00176   55*          DO 20 J=1,L                                             000162
00201   56*       20 IF (LLMT(J) .EQ. NAME(N,I)) GO TO 30                    000162
00204   57*       30 DATA(J) = DATA(J) + ANUM(N,I)                           000170
00206   58*       50 IS=0                                                    000177
00207   59*          DO 70 J=1,NS                                            000177
00212   60*          IF(IUSE(J).EQ.0)GO TO 55                                000204
00214   61*          IS = IS+1                                               000206
00215   62*          IF(FAZ(N).EQ.AG)GO TO 70                                000212
00217   63*          IF(TT.GT.TEMP(IS,2).AND.TEMP(IS,2).NE.THIGH) GO TO 70   000215
00221   64*          IF(TT.LT.TEMP(IS,1).AND.TEMP(IS,1).NE.TLOW) GO TO 70    000232
00223   65*          GO TO 56                                                000247
00224   66*       55 IF(FAZ(N).NE.AG.AND.FAZ(N).NE.BLK) GO TO 70             000251
00226   67*       56 DO 60 I=1,L                                             000265
00231   68*       60 IF (A(I,J) .NE. DATA(I)) GO TO 70                       000275
00234   69*          NUM(N,6)=J                                              000303
00235   70*          GO TO 90                                                000305
00236   71*       70 CONTINUE                                                000310
00240   72*          GO TO 80                                                000310
00241   73*       90 IF (MOLES)      ENJ = PECWT(N)/WP(K)                    000312
00243   74*          IF (.NOT.MOLES)      ENJ = PECWT(N)/RMM(N)              000325
00245   75*          ENJ = ENJ/ANN                                           000332
00246   76*          IF(K.EQ.1)  ENJ = ENJ*OF                                000335
00250   77*          IF (NAME(N,6).NE.IZERO) GO TO 500                       000343
00252   78*          I = NS                                                  000346
00253   79*          NS = J                                                  000350
00254   80*          TLN = ALOG(TT)                                          000352
00255   81*          IF(.NOT.CALCH)  EN(J,NPT) = ENJ                         000356
00257   82*          CALL CPHS                                               000363
00260   83*          NS = I                                                  000366
00261   84*          IF (HO(J).GT.-.01 .AND. HO(J).LT..01) HO(J) = 0.        000371
00263   85*          RTEMP(N) = TT                                           000411
00264   86*          IF(VOL) HO(J)=HO(J)-1.                                  000413
00266   87*          ENTH(N) = RBAR*TT*HO(J)                                 000421
00267   88*          CPR1 = CPR1 + CPSUM                                     000426
00270   89*       500 HSUBO = HSUBO + ENTH(N)*ENJ                            000432
00271   90*          HPP(K) = HPP(K)+ENTH(N)*ENJ                             000440
00272   91*       900 SSUM(NPT) = SSUM(NPT) + ENJ*(S(J) - ALOG(ENJ) - TM)    000446
00274   92*          TT = TSAVE                                              000456
00275   93*          HSUBO = HSUBO/RBAR                                      000460
00276   94*          RETURN                                                  000463
00277   95*       75 WRITE(JOUT,76)                                          000467
00301   96*       76 FORMAT (//20X,57HREACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA
00301   97*         1IN HCALC/)                                             000473
00302   98*          RETURN                                                  000473
00303   99*       80 WRITE(JOUT,85) N                                        000477
00306  100*       85 FORMAT (//20X,I2,42HTH REACTANT IS NOT IN THERMO DATA IN HCALC/)  000504
00307  101*          RETURN                                                  000504
00310  102*          END                                                     000541
```

END OF COMPILATION: NO DIAGNOSTICS.

```
@PRT,S LISTIT
FURPUR 28R1 E33 S74T11 10/15/80 13:07:03
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```
SEVIGNBIN208.TPF$(0).LISTIT
      1       @FOR,S LEWIS.BLOCK1,LEWIS.BLOCK1
      2       @FOR,S LEWIS.CPHS,LEWIS.CPHS
      3       @FOR,S LEWIS.DETON,LEWIS.DETON
      4       @FOR,S LEWIS.FOLBRM,LEWIS.FOLBRM
      5       @FOR,S LEWIS.FROZEN,LEWIS.FROZEN
      6       @FOR,S LEWIS.GAMEFF,LEWIS.GAMEFF
      7       @FOR,S LEWIS.GAUSS,LEWIS.GAUSS
      8       @FOR,S LEWIS.HCALC,LEWIS.HCALC
      9       @FOR,S LEWIS.LTCPHS,LEWIS.LTCPHS
     10       @FOR,S LEWIS.MAIN,LEWIS.MAIN
     11       @FOR,S LEWIS.MATRIX,LEWIS.MATRIX
     12       @FOR,S LEWIS.OUT1,LEWIS.OUT1
     13       @FOR,S LEWIS.REACT,LEWIS.REACT
     14       @FOR,S LEWIS.RKTOUT,LEWIS.RKTOUT
     15       @FOR,S LEWIS.ROCKET,LEWIS.ROCKET
     16       @FOR,S LEWIS.RREAD,LEWIS.RREAD
     17       @FOR,S LEWIS.SAVE,LEWIS.SAVE
     18       @FOR,S LEWIS.SEARCH,LEWIS.SEARCH
     19       @FOR,S LEWIS.SHCK,LEWIS.SHCK
     20       @FOR,S LEWIS.THERMP,LEWIS.THERMP
     21       @FOR,S LEWIS.VARFMT,LEWIS.VARFMT
     22       @BRKPT PRINT$

@MDG,P        LTCPHS
```

```
@FOR,S    LTCPHS,LTCPHS
HSA  E3 -10/15/80-13:07:03 (2.)

    SUBROUTINE LTCPHS    ENTRY POINT 000205

    STORAGE USED: CODE(1) 000221; DATA(0) 000130; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003   CONSTS 000006
     0004   LOWTH  001201

    EXTERNAL REFERENCES (BLOCK, NAME)

     0005   PAUSIT
     0006   CHRSIZ
     0007   GOUT
     0010   RDATAI
     0011   RDCHAR
     0012   NDCODS
     0013   RDATAF
     0014   NIO1S
     0015   NIO2S
     0016   NERR3S

    STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001   000006 IOL      0000   000072 100F     0001   000025 1246     0001   000045 1326     0001   000111 1946
     0001   000113 1976     0001   000124 1566     0001   000026 20L      0001   000051 30L      0001   000122 96L
     0003   000000 ATMN     0004 R 000361 CPL      0003   000001 GMET     0004 R 000551 HL       0000 I 000066 I
     0004 I 001131 ILSP     0000 I 000024 IMN      0000   000107 INJPS    0000 I 000000 INLTMN    0000 I 000012 ISNMN
     0000 I 000015 ITMPMN   0000 I 000067 J        0000 I 000071 K        0004 I 000000 NLTSP     0000 I 000070 NT
     0003   000002 PATM     0003 R 000003 RBAR     0003   000004 RBR      0000 R 000062 RDUM      0003   000005 RVR
     0004 R 000741 SL       0004 R 000001 SUBLT    0004 R 000171 TL

00101     1*          SUBROUTINE LTCPHS                                          LTCP  10    000000
00101     2*    C                                                                            000000
00101     3*    C       PROCESS LOW TEMPERATURE  CP,H,S  (VIA MIPS I/O)                      000000
00101     4*    C                                                                            000000
00101     5*    C       DIMENSION MIPS OUTPUT ARRAYS                                         000000
00103     6*            DIMENSION INLTMN(10),ISNMN(3),ITMPMN(7),IMN(5,6),RDUM(4)             000000
00103     7*    C                                                                            000000
00104     8*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                /CONSTS/  000000
00105     9*          COMMON /LOWTH/ NLTSP,SUBLT(40,3),TL(40,3),CPL(40,3),HL(40,3),/LOWTH/  000000
00105    10*         1               SL(40,3),ILSP(40)                           /LOWTH/  000000
00105    11*    C                                                                            000000
00105    12*    C       SET DATA FOR MIPS OUTPUT                                             000000
00106    13*            DATA INLTMN/24HTYPE THE NUMBER OF LOW T,                             000000
00106    14*         1    36HEMPERATURE SPECIES TO BE ENTERED    /                          000000
```

```
00110   15*           DATA ISNMN/18HTYPE SPECIES NAME /                          000000
00112   16*           DATA ITMPMN/42HTYPE NUMBER OF TEMPERATURES,THIS SPECIES<4/  000000
00114   17*           DATA IMN/36HTYPE  TL,CPL,HL,SL  WHERE -          ,          000000
00114   18*         1           36H  TL-TEMPERATURE                    ,          000000
00114   19*         2           36H CPL-CONSTANT PRESSURE SPECIFIC HEAT,          000000
00114   20*         3           36H  HL-ENTHALPY                       ,          000000
00114   21*         4           36H  SL-ENTROPY                        /          000000
00114   22*   C                                                                   000000
00116   23*           NLTSP=0                                                     000000
00117   24*           CALL PAGI                                                   000000
00120   25*           CALL CHRSIZ(3)                                              000002
00121   26*    10     CALL GOUTLINL(MN,56)                                        000006
00122   27*           CALL RDATAI(1,NLTSP,*10)                                    000011
00122   28*   C                                                                   000011
00122   29*   C           LOOP FOR EACH SPECIES                                   000011
00123   30*               DO 60 I=1,NLTSP                                         000016
00126   31*    20         CALL GOUT(ISNMN,17)                                     000026
00127   32*               CALL RDCHAR(RDUM,2,-1,*20)                              000031
00130   33*               DECODE(100,RDUM) (SUBLT(I,J),J=1,3)                     000037
00136   34*    30         CALL GOUT(ITMPMN,42)                                    000051
00137   35*               CALL RDATAI(1,NT,*30)                                   000056
00140   36*               IF(NT.LT.1 .OR. NT.GT.3) GO TO 30                       000064
00142   37*               ILSP(I)=0                                               000102
00142   38*   C                                                                   000102
00142   39*   C               LOOP FOR EACH TEMPERATURE                           000102
00143   40*                   DO 50 K=1,NT                                        000103
00146   41*                   DO 45 J=1,5                                         000113
00151   42*                   CALL GOUT(IMN(J,1),36)                              000113
00152   43*    45             CONTINUE                                            000124
00154   44*    46             CONTINUE                                            000124
00155   45*                   DO 48 J=1,4                                         000124
00160   46*                   RDUM(J)=0.                                          000124
00161   47*    48             CONTINUE                                            000125
00163   48*                   CALL RDATAF(4,RDUM,*46)                             000125
00164   49*                   TL(I,K)=RDUM(1)                                     000132
00165   50*                   CPL(I,K)=RDUM(2)                                    000136
00166   51*                   HL(I,K)=RDUM(3)                                     000136
00167   52*                   SL(I,K)=RDUM(4)                                     000140
00170   53*                   ILSP(I)=ILSP(I)+1                                   000142
00171   54*                   CPL(I,K)=CPL(I,K)/RBAR                              000145
00172   55*                   HL(I,K)=HL(I,K)/(TL(I,K)*RBAR)                      000147
00173   56*                   SL(I,K)=SL(I,K)/RBAR                                000152
00174   57*    50             CONTINUE                                            000163
00174   58*   C                                                                   000163
00174   59*   C           END SPECIES LOOP                                        000163
00176   60*    60         CONTINUE                                                000163
00176   61*   C                                                                   000163
00200   62*               RETURN                                                  000163
00200   63*   C                                                                   000163
00201   64*   100         FORMAT(3A4)                                             000220
00201   65*   C                                                                   000220
00202   66*               END                                                     000220
```

END OF COMPILATION: NO DIAGNOSTICS.

```
aFOR,S    MAIN,MAIN
HSA  E3 -10/15S/0B-13:07:06 (39.)
```

MAIN PROGRAM

STORAGE USED: CODE(1) 001516; DATA(0) 000720; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003	CONSTS	000006
0004	HOLCOM	000010
0005	POINTS	000335
0006	SPECES	017106
0007	MISC	001701
0010	INDX	000041
0011	PERF	000166
0012	CCC	000003
0013	CFUEL	000004
0014	MIN2	000002

EXTERNAL REFERENCES (BLOCK, NAME)

0015	RDYES
0016	MPSINT
0017	PAGIT
0020	CHRSIZ
0021	GOUT
0022	RDATAI
0023	RREAD
0024	COALCV
0025	LYCPHS
0026	RDCHAR
0027	NDCOD$
0030	MOVABS
0031	MOLDIT
0032	REACT
0033	SEARCH
0034	THERMP
0035	DETON
0036	ROCKET
0037	SHCK
0040	MPSTRM
0041	MINTR$
0042	MWDUS
0043	MIO2S
0044	MERR2S
0045	MREWS
0046	MRDUS
0047	MIO3S
0050	MIO1S
0051	MRWLS
0052	MWWLS
0053	MWEFS
0054	ALOG
0055	MSTOP$

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0		000530	10F	0001		000406	108L	0		000233	11L	0001		000601	11211L
0001		0	0379	1212L	0001		000733	1219L	0001		0	1037	1x05L	0001	
0001		000419	181L	0001		000057	2L	0000		000537	20F	0001		000078	203L
0001		000452	206L	0000		000522	207F	0001		000506	208L	0000		000648	21F
0000		00	0615	211F	0001		000762	213L	0001		00	0777	214L	0001	
0001		000403	25L	0001		001506	3L	0001		001446	301L	0001		001450	302L
0001		001122	307L	0001		001104	322L	0001		001153	323L	0001		000367	3276
0001		000437	3526	0001		000471	3676	0001		000243	34L	0000		000377	4006
0001		001363	432L	0000		000526	5F	0001		000706	5176	0001		000714	5226
0001		000756	546G	0001		001014	5716	0001		001050	6106	0001		001104	6256
0001		001267	707G	0001		001124	722L	0000		000637	724F	0001		001331	7246
0001		001404	746G	0001		001254	746L	0001		001381	748L	0001		001416	7516
0001		001452	760L	0001		001462	761L	0001		001476	800L	0001		000246	90L
0006	R	011052	A	0011		000150	AEAT	0007		000640	AM	0007		000705	AM1
0011		000133	APP	0703	R	000000	ATMN	0007		000004	ATOM	0004	I	000004	BLANK
0007	R	000545	BOO	0010	L	000036	CALCM	0013	R	000000	CF	0006		000000	CDCF
0005		000032	CPR	0007		000706	CPR1	0007		000634	CPSUM	0007	I	000654	DATA
012		000002	DEMAND	0007		001560	DEMS	000	L	000200	DETM	0005		000064	DLVPT
0006	R	004312	EN	0004	I	000000	END	0006	R	010150	ENLN	0007		001700	ENLSAV
0007	R	001676	ENML	0007		001677	ENSAVE	0006	I	010624	ENSERT	0007		001434	ENTM
0007	R	000636	EORAT	0000	L	000245	ERATIO	000	L	000246	FA	0007		001445	FAZ
0007		001527	FOX	0000	L	000247	FPCT	0005		000101	GAMMAS	0006		000001	GMET
0012		000000	GRAPH	0013		000001	HHVV	0010	L	000003	HP	0007		000642	HPP
005		000000	HSUM	0006		010376	HO	0008	I	000231	I	0010		000030	IC
0010	I	000000	IDEBUG	0004	I	000002	IE	0010		000015	IMAT	0000	I	000260	INAM
0000	I	000232	INSERT	0010	L	000023	IONS	0010		000021	IP	0010		000037	IOSAVE
0000	I	000264	IST	0010		000005	ISV	0010	I	000034	IT	0006	I	010266	IUSE
0000	I	000263	J	0010		000026	JLIQ	0012	I	000001	JOUT	0010		000028	JSOL
0010		000014	KMAT	0010	I	000012	L	0007	I	000463	LLMT	0010		000040	LSAVE
0007	R	001644	MIX	0000	I	000235	MLOW	0000	L	000250	MMMG	0004		000005	MOL
0007	I	000707	NAME	0010	I	000024	NC	0000	I	000236	NCO	0010	L	000022	NEWR
000	I	000234	NMLT	0010	I	000017	NOF	0010	I	000020	NOMIT	0000	I	000003	NOMTS
0010		000011	NPT	0010	I	000027	NREAC	0010	I	000013	NS	0000	I	000261	NSERT
0000	L	000251	NSQM	0010	I	000010	NT	0010	I	000000	N1	0010	I	000001	N2
0006	I	010150	OMIT	0004		000006	OX	0007	R	001644	OXF	0007	R	000635	OXFL
0003	R	000002	PATM	0011		000000	PCP	0007		001363	PECWT	0013	R	000003	PER
0005		000217	PPP	0000	L	000252	PSIA	0003	R	000003	RBAR	0003		000004	RBR
0015	L	000000	RDYES	0000	I	000001	REAC	0007		000644	RH	0007	R	001611	RHOP
0007		001612	RHW	0007		001476	RTEMP	0003		000005	RVR	0006		004064	S
006		016660	SLN	0007	R	000003	SO	005		000251	SONVEL	0010	L	000004	SP
0005		000015	SSUM	0006	I	015364	SUR	0011		000101	SUBAR	0007	R	000001	SUMN
0000	L	000254	SV	0007	R	000003	SQ	0005	R	000150	T	0006		016514	TEMP
0000	I	000002	TMRM	0007		001643	TLN	0007	R	000630	TLOW	0007		000627	TM
0005		000320	TOTN	0010	L	000002	TP	0007		000002	TT	0005		000266	TTT
0000	L	000256	UV	0005	R	000202	V	0011		000064	VACI	0005		000303	VLM
0011		000032	VMOC	0010	L	000032	VOL	0007	R	000650	VPLS	0013		000002	WCR
0007	R	000652	WP	0004		000007	ZERO								

```
00100      1*      C  MAIN PROGRAM                                          MAIN0002   00000
00100      2*      C                                                                   00000
00101      3*            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,PBR,RVR        /CONSTS/   00000
```

```
00103     4*          COMMON /MOLCON/ END,GAS,IE,IZ,BLANK,MOL,OX,ZERO                    /MOLCON/   000001
00104     5*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVIP(13),DLVPT(13)                   000001
00104     6*         1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),             000001
00104     7*         2 ,VLM(13),TOTN(13)                                                            000001
00104     8*    C     COMMON/SPECES/COEF(2,7,150),S(150),ENI(150,13),ENLN(150),MO(150)             000001
00104     9*    C    1 ,DELN(150),A(15,150),SUB(150,1),IUSE(150),TEMP(50,2),SLN(150)               000001
00105    10*          INCLUDE SPECPR                                                                 000001
00111    11*          COMMON /MISC/ ENN,SUMN,TT,S0,ATOM(3,101),LLMT(25),BD(25),                      000001
00111    12*         1              BDP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EGRAT,                000001
00111    13*         2              HSUB0,AM(2),MPP(2),RM(2),VMIN(2),VPLS(2),WP(2),     /MISC/     000001
00111    14*         3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(13,6),PECNT(25),             000001
00111    15*         4              EMIM(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RMOP,              000001
00111    16*         5              RMW(25),TLN,OXF(26),ENML,ENSAVE,ENLSAV                         000001
00112    17*          COMMON /INOX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,MP,MT,NPT,L,NS,       /INOX/     000001
00112    18*         1              NMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,    /INOX/     000001
00112    19*         2              NREAC,IC,JSJ,VOL,SHOCK,IT,NFZ,CALCM,IOSAVE,LSAVE      /INOX/     000001
00113    20*          COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),          /PERF/     000001
00113    21*         1              SUPAR(13),APP(13),AEAT(13),EOL                         /PERF/     000001
00113    22*    C                                                                                    000001
00114    23*              COMMON /CCC/ GRAPH,JOUT,DEMAND                                           000001
00115    24*          COMMON /CFUEL/CF,NNVV,NCP,PER                                                000001
00116    25*          COMMON /NIN2/N1,N2                                                           000001
00117    26*          INTEGER BLANK,DATA,END,ENSERT,OMIT,REAC,SUB,THRM                             000001
00120    27*          DIMENSION NOMTS(150)                                                         000001
00121    28*          DATA (NOMTS(I),I=1,8)/                                                       000001
00121    29*         X'AL(L*,*)   *,*     *,*AL(L*,*)   *,*     *,                               000001
00121    30*         X'ALCL*,*2   *,*     *,*ALN(*,*S)  *,*     *,                               000001
00121    31*         X'ALN  *,*   *,*     *,*C    *,*   *,*     *,                               000001
00121    32*         X'C3   *,*   *,*     *,*C4   *,*   *,*     *,                               000001
00121    33*         X'C5   *,*   *,*     *,                                                     000001
00121    34*         X'H2O(*,*S)  *,*     *,                                                     000001
00121    35*         X'O3   *,*   *,*     *,*SI   *,*   *,*     *,                               000001
00121    36*         X'SIC  *,*   *,*     *,*SIC2*,*   *,*     *,                               000001
00121    37*         X'SI(S*,*)   *,*     *,*SI(L*,*)   *,*     *,                               000001
00121    38*         X'SICL*,*    *,*     *,*SICL*,*2   *,*     *,                               000001
00121    39*         X'SICL*,*3   *,*     *,*SICL*,*4   *,*     *,                               000001
00121    40*         X'SIH  *,*   *,*     *,*SIH4*,*    *,*     *,                               000001
00121    41*         X'SIN  *,*   *,*     *,*SI2  *,*   *,*     *,                               000001
00121    42*         X'SI2O*,*    *,*     *,*SI2N*,*    *,*     *,                               000001
00121    43*         X'SI3  *,*   *,*     *,                                                     000001
00121    44*         X   /                                                                        000001
00123    45*          DATA INSERT,MII,NMLT,REAC,THRM/9HINSERT,9HOMIT,9HNAME,9HREAC,9HNUMBER/       000001
00131    46*          DATA MLOW/9HLOW /                                                            000001
00133    47*          DIMENSION ENSERT(3,3),NCD(9),OMIT(3,3)                                       000001
00134    48*          DIMENSION RDUM(2)                                                            000001
00135    49*          EQUIVALENCE (DELN,ENSERT),(ENLN,OMIT),(MIX,OXF),(OF,OXFL),(SO,S0)            000001
00136    50*          LOGICAL CALCM,DETN,EOL,ERATIO,FA,FPCT,HP,IONS,MMHG,MOLES,NEWR,               000001
00136    51*         1        NSOK,OF,PSIA,RKT,SHOCK,SP,SV,TP,TV,UV,VOL                           000001
00136    52*    C                                                                                  000001
00137    53*              LOGICAL ROVFS,FIRST                                                      000001
00137    54*    C                                                                                  000001
00140    55*          REAL MIX(26)                                                                 000001
00140    56*    C                                                                                  000001
00141    57*          NAMELIST /INPT2/ DETN,ERATIO,FA,FPCT,HP,IDEBUG,IONS,MIX,MMHG,NSOK,  /INPT2/  000001
00141    58*         1                 OF,P,PSIA,RKT,SO,SHOCK,SO,SP,SV,T,TP,TV,UV,V      /INPT2/  000001
00142    59*          DATA INAM/10/                                                                000001
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00142    60*     C                                                                  000001
00144    61*             FIRST=.TRUE.                                               000001
00145    62*                CALL MPSINT                                             000003
00146    63*             CF=1.0                                                     000005
00147    64*             N1=0                                                       000007
00150    65*             N2=0                                                       000010
00151    66*           1 WRITE(JOUT,400)                                            000011
00153    67*             DO 30 I=1,6                                                000021
00156    68*             MIX(I) = 0.0                                               000021
00157    69*             P(I)= 0.                                    ODE  115       000021
00160    70*             T(I)= 0.                                    ODE  116       000022
00161    71*         300 VI(I) = 0.0                                                000023
00163    72*             TP = .FALSE.                                ODE  123       000025
00164    73*             HP=.TRUE.                                                  000026
00165    74*             TV = .FALSE.                                               000030
00166    75*             UV = .FALSE.                                               000031
00167    76*             SV = .FALSE.                                               000032
00170    77*             RKI=.FALSE.                                                000033
00171    78*             SO=0.0                                                     000034
00172    79*             SP=.FALSE.                                                 000036
00173    80*             SHOCK = .FALSE.                             ODE  129       000036
00174    81*             DETN = .FALSE.                              ODE  130       000037
00175    82*             MMHG   = .FALSE.                            ODE  133       000040
00176    83*             PSIA = .TRUE.                                              000041
00177    84*             NSOM = .FALSE.                                             000043
00200    85*             IONS = .FALSE.                                             000044
00201    86*             IDEBUG = 0                                                 000045
00202    87*             FA = .FALSE.                                               000046
00203    88*             OF = .TRUE.                                                000047
00204    89*             ERATIO = .FALSE.                                           000051
00205    90*             FPCT = .FALSE.                                             000052
00206    91*             EQL = .TRUE.                                ODE  145       000053
00207    92*             NEWR = .FALSE.                              MAIN00^2       000055
00210    93*         400 FORMAT(1H1)                                 MAIN0025       000057
00211    94*           2 CONTINUE                                                   000057
00212    95*             NREAC=0                                                    000057
00213    96*             NSERT=0                                                    000057
00214    97*             NOMIT=0                                                    000060
00215    98*                CALL PAGIT                                              000061
00216    99*                JOUT=6                                                  000063
00217   100*             IF(IRDYES('TYPE  YES  FOR PRINT TO PRINT FILE',35)) JOUT=31 000065
00221   101*       203      CONTINUE                                               000075
00222   102*                CALL PAGIT                                              000075
00223   103*                CALL CHRSIZ(1)                                          000076
00224   104*                CALL GOUT('LEWIS CHEMICAL EQUILIBRIUM PROGRAM',34)      000101
00225   105*                CALL GOUT(' ',1)                                        000105
00226   106*                CALL GOUT('          MAIN MENU',19)                     000111
00227   107*                CALL GOUT(' ',1)                                        000115
00230   108*                CALL GOUT(' 1 - INSERT THERMODYNAMICS DATA',31)         000121
00231   109*                CALL GOUT(' 2 - INSERT LOW TEMP EXTENSION THERMO DATA',42) 000125
00232   110*                CALL GOUT(' 3 - INSERT OR EDIT REACTANTS',29)           000131
00233   111*                CALL GOUT(' 4 - OMIT SPECIES FROM THERMO DATA',34)      000135
00234   112*                CALL GOUT(' 5 - INSERT CONDENSED SPECIES',29)           000141
00235   113*                CALL GOUT(' 6 - INSERT OR EDIT NAMELIST',28)            000145
00236   114*                CALL GOUT(' 7 - START PROGRAM CALCULATION',30)          000151
00237   115*                CALL GOUT(' 8 - INSERT OR EDIT COAL DATA',29)           000155
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00240   116*            CALL GOUT(' RETURN - TERMINATE PROGRAM',27)                    000161
00241   117*             ICARD=0                                                       000165
00242   118*           CALL CHRSIZ(4)                                                  000166
00243   119*              CALL RDATA(1,ICARD,$203)                                     000171
00244   120*              IF(ICARD.EQ.0) GO TO 3                                       000176
00245   121*           IF (ICARD.LT.0.OR.ICARD.GT.8) GO TO 203                         000200
00250   122*           GO TO (90,39,11,205,10,210,215,15),ICARD                        000215
00251   123*     C                                                                     000215
00250   124*     C          CALL SUBROUTINE TO READ REACTANT CARDS                     000215
00251   125*        11 CALL RREAD(FIRST)                                               000233
00252   126*           GO TO 203                                                       000235
00253   127*     C     COAL COMPOSITION INPUT                                        000235
00253   128*        15 CALL COALCV(FIRST)                                            000237
00254   129*           GO TO 203                                                       000241
00255   130*     C                                                                     000241
00254   131*     C     READ LOW TEMPERATURE EXTENSION THERMO DATA                     000241
00255   132*        39 CALL LTCPHS                                                    000243
00256   133*           GO TO 203                                                       000244
00256   134*     C                                                                     000244
00256   135*     C     READ THERMO DATA FROM CARDS AND STORE ON  TAPE 9               000244
00257   136*        90 NEWR = .TRUE.                                                  000246
00260   137*           REWIND 9                                                        000247
00261   138*              CALL GOUT('ADD THERMO DATA HERE',20)                         000252
00262   139*           READ(5,5) TLOW,TMID,THIGH                                       000256
00267   140*         5 FORMAT (3F10.3)                                                 000266
00270   141*           WRITE (9,5) TLOW,TMID,THIGH                                     000266
00275   142*        97 READ (5,10) (DATA(I),I=1,16),NCD(1)                           000277
00301   143*        10 FORMAT(3A9,6X,2A3,9(A2,F3.0),A1,2F10.3,I5)                    000310
00302   144*           IF(DATA(1).EQ.BLANK) DATA(1)=END                              000310
00309   145*           WRITE (9,10) (DATA(I),I=1,16)                                 000315
00307   146*           IF(DATA(1).EQ.END)  GO TO 203                                 000325
00311   147*           READ (5,20) (DATA(I), I = 1,5),NCD(2),(DATA(J), J = 6,10),NCD(3),  000330
00311   148*          1            (DATA(I), I = 11,14),NCD(4)                       000330
00321   149*        20 FORMAT(5E15.8,I5/5E15.8,I5/4E15.8,I20)                        000350
00322   150*           WRITE (9,21) (DATA(I), I = 1,14)                              000350
00325   151*        21 FORMAT(5E15.8/5E15.8/4E15.8)                                  000367
00326   152*           DO 25  I=1,4                                                  000367
00331   153*           IF(NCD(I).EQ.I)  GO TO 25                                     000367
00333   154*           WRITE(JOUT,22) (DATA(J),J=1,3)                                000372
00336   155*        22 FORMAT(28HOERROR IN ORDER OF CARDS FOR ,3A9)                  000404
00337   156*        25 CONTINUE                                                      000404
00341   157*           GO TO 97                                                      000404
00341   158*     C                                                                     000404
00341   159*     C    CHECK INSERT CARDS                                             000404
00342   160*       108      CONTINUE                                                 000406
00343   161*                CALL PAGIT                                               000406
00344   162*                CALL GOUT('TYPE SPECIES TO INSERT(1 PER LINE)',34)       000407
00345   163*       181      CONTINUE                                                 000414
00346   164*                CALL RDCHAR(RDUM,2,-1,$203)                              000414
00347   165*                NSERT=NSERT+1                                            000421
00350   166*                DECODE (207,RDUM) (ENSERT(I,NSERT),I=1,3)                000424
00356   167*                GO TO 181                                                000442
00356   168*     C                                                                     000442
00356   169*     C    CHECK OMIT CARDS                                               000442
00357   170*       205      CONTINUE                                                 000440
00360   171*                CALL PAGIT                                               000440
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00361  172*            CALL GOUT('TYPE SPECIES TO OMIT FROM THERMO DATA',37)                    000445
00362  173*      206   CONTINUE                                                                 000452
00363  174*            CALL RDCHAR(RDUM,2,-1,$208)                                              000452
00364  175*            NOMIT=NOMIT+1                                                            000457
00365  176*            DECODE (2,207,RDUM) (OMIT(I,NOMIT),I=1,3)                                000462
00373  177*      207   FORMAT(3A4)                                                              000503
00374  178*            GO TO 206                                                                000503
00375  179*        208 CONTINUE                                                  MAIN0062       000505
00376  180*            NEWR= .TRUE.                                                             000505
00377  181*            REWIND 4                                                                 000506
00400  182*            GO TO 203                                                 MAIN0063       000511
00400  183*      C                                                                              000511
00400  184*      C     BEGIN NAMELIST INPT2                                      MAIN0065       000511
00401  185*        210 CALL PAGE                                                                000513
00402  186*            IF (.NOT.RDYES('TYPE YES FOR PRINT INPT2 NAMELIST',35)) GO TO 1211       000514
00402  187*      C     ACCESS THE ORIGINAL NAMELIST FROM PREVIOUS RUN                           000514
00403  188*            REWIND INAM                                                              000521
00405  189*            READ (INAM,INPT2)                                                        000524
00410  190*            WRITE (6,INPT2)                                                          000530
00413  191*            GO TO 1212                                                               000534
00413  192*      C     RESET ALL PARTS OF NAMELIST                                              000534
00414  193*       1211 DO 1210 I=1,26                                                           000540
00417  194*            MIX(I)=0                                                                 000540
00420  195*            P(I)=0                                                                   000540
00421  196*            T(I)=0                                                                   000541
00422  197*       1210 V(I)=0                                                                   000542
00424  198*            TP=.FALSE.                                                               000544
00425  199*            HP=.TRUE.                                                                000545
00426  200*            TV=.FALSE.                                                               000547
00427  201*            UV=.FALSE.                                                               000550
00430  202*            SV=.FALSE.                                                               000551
00431  203*            RKT=.FALSE.                                                              000552
00432  204*            SO=0.0                                                                   000553
00433  205*            SP=.FALSE.                                                               000554
00434  206*            SHOCK=.FALSE.                                                            000555
00435  207*            DETN=.FALSE.                                                             000556
00436  208*            MMHG=.FALSE.                                                             000557
00437  209*            PSIA=.TRUE.                                                              000560
00440  210*            NSOM=.FALSE.                                                             000562
00441  211*            IONS=.FALSE.                                                             000563
00442  212*            IDEBUG=0                                                                 000564
00443  213*            FA=.FALSE.                                                               000565
00444  214*            OF=.TRUE.                                                                000566
00445  215*            ERATIO=.FALSE.                                                           000570
00446  216*            FPCT=.FALSE.                                                             000571
00447  217*            GO TO 11211                                                              000572
00450  218*       1212 IF (.NOT.RDYES('TYPE YES TO CHANGE NAMELIST',27))                        000574
00450  219*           X   GO TO 203                                                            000574
00452  220*      11211 WRITE (6,211)                                                           000601
00454  221*      211       FORMAT(' BEGIN NAMELIST INPT2 INPUT')                               000605
00455  222*       2211 CONTINUE                                                                000605
00456  223*            READ(5,INPT2)                                             MAIN0086       000605
00456  224*      C     STORE NAMELIST                                                           000605
00461  225*            REWIND INAM                                                              000611
00462  226*            WRITE (INAM,INPT2)                                                       000614
00465  227*            ENDFILE INAM                                                             000620
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00466   228*          CALL MOVABS(B00,50)                                    000623
00467   229*          CALL HOLDIT                                            000627
00470   230*          GO TO 203                                              000631
00471   231*      215 CONTINUE                                               000633
00472   232*          FIRST=.FALSE.                                          000633
00473   233*          CALL PAGIT                                             000633
00474   234*          CALL GOUT(' ',1)                                       000635
00475   235*          REWIND INAM                                            000641
00476   236*          READ (INAM,INPT2)                                      000644
00501   237*          WRITE (6,INPT2)                                        000650
00504   238*          CALL MOVABS(500,50)                                    000654
00505   239*          CALL HOLDIT                                            000660
00506   240*          CALL PAGIT                                             000662
00507   241*          CALL GOUT(' ',1)                                       000664
00510   242*          CALL REACT                                             000670
00511   243*          IF (CF) 1215,,                                         000672
00514   244*          IF (.NOT.ADYES('TYPE YES FOR SPECIAL OMITS FOR COAL DATA',40))  000675
00515   245*         X   GO TO 1215                                          000675
00516   246*          DO 12 I=1,27                                           000706
00521   247*          DO 12 J=1,3                                            000714
00524   248*       12 OMIT(J,NOMIT+I)=NOMTS(I,3-3+J)                         000721
00527   249*          NOMIT=NOMIT+27                                         000727
00530   250*      1215 CALCH=.FALSE.                                         000733
00531   251*          DO 755 I=1,NREAC                                       000733
00534   252*          IF (NAME(I,6).EQ.IZ) CALCH=.TRUE.                      000740
00536   253*       755 CONTINUE                                              000746
00540   254*          IF (ERATIO) GO TO 213                                  000746
00542   255*          IF (CF) 213,,                                          000750
00545   256*          DO 212 I=1,26                                          000756
00550   257*       212 MIX(I)=MIX(I)*CF                                      000756
00552   258*       213 IF (PER-1.0) ,214,                                    000762
00555   259*          NSERT=NSERT+1                                          000764
00556   260*          ENSERT(1,NSERT)='IC(S'                                 000770
00557   261*          ENSERT(2,NSERT)=')    '                                000772
00560   262*          ENSERT(3,NSERT)='     '                                000774
00561   263*       214 CONTINUE                                              000772
00562   264*          RHOP=0.                                                000777
00563   265*          VOL=.FALSE.                                            000777
00564   266*          NT=1                                                   001000
00565   267*          IF(.NOT.TV.AND..NOT.UV.AND..NOT.SV)  GO TO 309         001002
00567   268*          VOL = .TRUE.                                           001007
00570   269*          DO 1304  I=1,26                                        001014
00573   270*          IF (P(I) .GT. 0.0)  P(I) = 1.0/P(I)                    001014
00575   271*          IF (V(I) .GT. 0.0)  P(I) = V(I)                        001022
00577   272*          IF (P(I) .LE. 0.0)  GO TO 1305                         001027
00601   273*      1304 NP = I                                                001032
00603   274*      1305 TP = TV                                               001037
00604   275*           HP = UV                                               001040
00605   276*           SP = SV                                               001042
00606   277*           GO TO 322                                             001044
00607   278*       309 DO 305  I=1,26                                        001050
00612   279*           IF (P(I) .LE. 0.0)  GO TO 322                         001050
00614   280*           NP = I                                    MAIN0090    001053
00615   281*           IF (MMHG) P(NP) = P(NP)/760.                          001057
00617   282*           IF (PSIA)  P(NP) = P(NP)/PATM                         001065
00621   283*       305 IF (NSOM)  P(NP) = P(NP)/ATMN                         001073
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00624  284*       322 DO 307 IT = 1,26                                                    001106
00627  285*           IF (T(IT) .LE. 0.0)  GO TO 722                                      001106
00631  286*           IF (CF+1.0) ,307,                                                   001111
00634  287*           T(IT)=(T(IT)-32.)/1.8+273.15                                        001114
00635  288*       307 NT = IT                                                             001122
00637  289*       722 DO 625 IST = 1,26                                                   001130
00642  290*           IF (MIX(IST) .GT. 0.0)  GO TO 323                                   001130
00646  291*           IF(IST.NE.1) GO TO 745                                              001133
00650  292*           WRITE(JOUT,724)                                                     001136
00651  293*       724 FORMAT (//45X,40HNO INPT2 VALUE GIVEN FOR FA, FPCT, OR OF//)        001143
00653  294*           IF (WP(2) .GT. 0.0)  OXFL = WP(1)/WP(2)                             001143
00659  295*           GO TO 333                                                           001151
00659  296*       323 OXFL=MIX(IST)                                                       001153
00655  297*           IF(FA) OXFL =1./   MIX(IST)                                         001154
00657  298*           IF(FPCT) OXFL =(100.-   MIX(IST))/   MIX(IST)                      001161
00661  299*           IF(.NOT.ERATIO)  GO TO 333                                          001167
00663  300*           EQRAT = MIX(IST)                                                    001171
00669  301*           IF(EQRAT.EQ.1.)  EQRAT = 1.000005                                   001173
00666  302*           OXFL   = (-EQRAT*VMIN(2)-VPLS(2))/(VPLS(1)+EQRAT*VMIN(1))           001200
00667  303*       333 OXF(IST) = OXFL                                                     001211
00670  304*       625 NOF = IST                                                           001212
00672  305*       745 IF (.NOT. IONS .OR. LLMT(L) .EQ. IE)  GO TO 746                     001217
00676  306*           L = L+1                                                             001227
00675  307*           IF(LLMT(L).NE.IE)  NEWR=.TRUE.                                      001232
00677  308*           REWIND 9                                                            001242
00700  309*           LLMT(L) = IE                                                        001245
00701  310*           BOP(L,1) = 0.                                                       001250
00702  311*           BOP(L,2) = 0.                                                       001251
00703  312*           GO TO 748                                                           001252
00706  313*       746 IF(LLMT(L).NE.IE)  GO TO 748                                        001256
00706  314*           DO 747  J=1,NS                                                      001257
00711  315*       747 IF (A(L,J) .NE. 0.0)  IUSE(J) = - 10000                             001267
00714  316*           L = L-1                                                             001275
00715  317*       748 IF(NEWR)  CALL SEARCH                                               001301
00715  318*     C     INITIAL ESTIMATES                                                   001301
00717  319*           SO = SO/RBAR                                                        001304
00720  320*           ENN = .1                                                            001307
00721  321*           ENNL = -2.3025851                                                   001311
00722  322*           SUMN = ENN                                          MAIN0141        001313
00723  323*           DO 432 J=1,NS                                       MAIN0145        001331
00726  324*           IF(IUSE(J).GT.0)  IUSE(J)=-IUSE(J)                                  001331
00730  325*           IF(IUSE(J).EQ.-10000.AND.IONS)  IUSE(J) = 0                         001335
00732  326*           EN(J,1) = 0.                                                        001346
00733  327*           ENLN(J) = 0.                                                        001347
00734  328*           IF (IUSE(J).NE.0)  GO TO 432                                        001350
00736  329*           EN(J,1) = ENN/(NS - NC)                                             001352
00737  330*           ENLN(J) = ALOG(EN(J,1))                                             001354
00740  331*       432 CONTINUE                                                            001369
00742  332*           IQ1= L+1                                                            001364
00743  333*           IF (NC.EQ.0.OR.NSERT.EQ.0) GO TO 790                                001367
00745  334*           DO 302 I=1,NSERT                                                    001377
00750  335*           DO 301 J=1,NS                                                       001416
00753  336*           IF(IUSE(J).EQ.0) GO TO 301                                          001421
00755  337*           DO 299 IST = 1,3                                                    001430
00760  338*       299 IF (SUB(J,IST) .NE. ENSERT(IST,I))  GO TO 301                       001430
00763  339*           IQ1= IQ1+1                                                          001437
```

```
00764   340*          IUSE(J)= -IUSE(J)                                    001442
00765   341*          GO TO 302                                            001444
00766   342*      301 CONTINUE                                             001452
00770   343*      302 CONTINUE                                             001452
00772   344*      790 IF (.NOT. TP .AND. .NOT. MP .AND. .NOT. SP) GO TO 791 001452
00774   345*          CALL THERMP                                          001456
00775   346*          GO TO 800                                            001460
00776   347*      791 IF (DETN) CALL DETON                                 001462
01000   348*          IF(RKT) CALL ROCKET                                  001465
01002   349*          IF(SHOCK) CALL SHCK                                  001471
01004   350*      800 NSERT = 0                                            001476
01005   351*          CALL MOVABS(600,50)                                  001476
01006   352*          CALL HOLDIT                                          001502
01007   353*          GO TO 2                                              001504
01010   354*        3     CONTINUE                                         001506
01011   355*              CALL MPSTRM                                      001506
01012   356*              STOP                                             001507
01013   357*          END                                        MAIN0153  001513
```

END OF COMPILATION: NO DIAGNOSTICS.

aH06,P MATRIX

```
@F0R,S    MATRIX,MATRIX
HSA  E3 -10/15/80-13:07:13 (11.)
```

SUBROUTINE MATRIX ENTRY POINT 001063

STORAGE USED: CODE(1) 001107; DATA(0) 000116; BLANK COMMON(2) 000000

COMMON BLOCKS:

```
0003   POINTS 000335
0004   SPECES 017106
0005   MISC   001701
0006   DOUBLE 001560
0007   INDX   000041
```

EXTERNAL REFERENCES (BLOCK, NAME)

```
0010   NERR3S
```

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

```
0001   000102 124G      0001   000103 1276      0001   000126 1406      0001   000215 154G      0001   000244 161B
0001   000672 175L      0001   000677 185L      0001   000453 2176      0001   001011 230L      0001   000567 244G
0001   000606 247G      0001   000623 257G      0001   001026 260L      0001   000757 303G      0001   001023 317G
0001   000276 55L       0001   000346 59L       0001   000372 62L       0001   000376 64L       0001   000511 65L
0001   000405 70L       0004 R 011052 A         0005   000490 AM        0005   000708 AM1       0005   001138 ANUM
0005   000004 ATOM      0005 R 000514 BD        0005   000545 BOP       0007   000036 CALCH     0004   000000 COEF
0007 L 000001 CONVG     0003   000032 CPR       0005   000706 CPR1      0005 R 000634 CPSUM     0005   000654 DATA
0004   010624 DELN      0005   001560 DENS      0003   000064 DLVPT     0003   000047 DLVTP     0004 R 004312 EN
0000 P 000013 ENERGY    0004 R 010150 ENLN      0005   001700 ENLSAV    0005 R 000000 ENN       0005   001676 ENNL
0005   001677 ENSAVE    0005   001414 ENTH      0005   000636 EQRAT     0000 R 000010 F         0005   001445 FAZ
0005   001527 FOX       0006 D 000000 G         0003   000101 GAMMAS    0007 L 000003 HP        0005   000642 HPP
0005 R 000617 HSUBO     0003 R 000000 HSUM      0004 R 010376 HO        0000 I 000003 I         0007   000030 IC
0007   000058 IDEBUG    0007 I 000015 IMAT      0000   000023 INJPS     0007   000023 IONS      0007   000021 IP
0007   000017 IQSAVE    0007 I 000016 IQ1       0000 I 000001 IQ2       0000 I 000002 IQ3       0007   000005 ISV
0007   000034 IT        0004 I 016266 IUSE      0000 I 000007 J         0007   000024 JLIQ      0007   000025 JSOL
0007   000031 JS1       0000 I 000004 K         0000 I 000006 KK        0007 I 000014 KMAT      0007 I 000012 L
0005   000463 LLMT      0007   000040 LSAVE     0007   000006 MOLES     0005   000707 NAME      0007   000024 NC
0007   000022 NEWR      0007   000035 NFZ       0007   000017 NOF       0007   000020 NOMIT     0007   000007 NP
0007 I 000011 NPT       0007   000027 NREAC     0007 I 000013 NS        0000 I 000000 NSPP1     0007   000010 NT
0005   000635 OF        0003   001694 OXF       0003   000116 P         0005   001363 PECWT     0005   000633 PP
0003   000217 PPP       0005   000644 RH        0005   001611 RHOP      0005   001612 RMW       0005   001976 RTEMP
0004 R 004064 S         0007   000033 SHOCK     0004   016660 SLN       0003   000251 SONVEL    0007 L 000004 SP
0000 R 000012 SS        0000 R 000005 SSS       0003   000015 SSUM      0004   015364 SUB       0005 R 000001 SUMN
0005 R 000003 SO        0003   000150 T         0004   016514 TEMP      0000 R 000012 TERM1     0005   000632 THIGH
0005   001693 TLN       0005   000630 TLOW      0005 R 000627 TM        0005   000631 TMID      0003   000320 TOTN
0007 L 000002 TP        0005 R 000002 TT        0003   000266 TTT       0003   000202 V         0003   000303 VLM
0005   000646 VMIN      0007 L 000032 VOL       0005   000650 VPLS      0003   000234 WM        0005   000652 WP
0006 D 001510 X
```

```
00101     1*          SUBROUTINE MATRIX                                          MATX0001   000030
00101     2*    C                                                                           000030
00103     3*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)           000030
00103     4*         1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)      000030
00103     5*         2 ,VLM(13),TOTM(13)                                                   000030
00103     6*    C    COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)       000030
00103     7*    C   1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)      000030
00104     8*          INCLUDE SPECPK                                                      000030
00110     9*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),           0000030
00110    10*         1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,LSUM,OF,EQRAT,       000030
00110    11*         2              HSUBO,AM(2),HPP(2),RM(2),WMM(2),WPLS(2),WP(2),  /MISC/ 000030
00110    12*         3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECNT(25),   000030
00110    13*         4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,    000030
00110    14*         5              RHW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV               000030
00111    15*          COMMON /DOUBLE/ G(20,21), X(20)                          MATX0012   000030
00112    16*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,  /INDX/ 000030
00112    17*         1              KMAT,IMAT,IQ1,NOF,NONIT,IP,NEWR,IONS,NC,JSOL,JL10,  /INDX/ 000030
00112    18*         2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE  /INDX/ 000030
00112    19*    C                                                                           000030
00113    20*          DOUBLE PRECISION G,X                                                000030
00114    21*          LOGICAL CONVG,HP,SP,TP,VOL                                          000030
00114    22*    C                                                                           000030
00115    23*          IQ2 = IQ1 + 1                                                       000030
00116    24*          IQ3 = IQ2 + 1                                                       000033
00117    25*          KMAT = IQ3                                               MATX0018   000035
00120    26*          IF(.NOT.CONVG.AND.TP) KMAT = IQ2                         MATX0019   000036
00122    27*          IMAT = KMAT - 1                                          MATX0020   000046
00122    28*    C     CLEAR MATRIX STORAGES TO ZERO                            MATX0022   000046
00123    29*          DO 211 I=1,IMAT                                                     000057
00126    30*          DO 211 K=1,KMAT                                                     000103
00131    31*      211 G(I,K) = 0.000                                                      000103
00134    32*          SSS = 0.                                                            000111
00135    33*          HSUM(NPT) = 0.                                                      000112
00135    34*    C     BEGIN SET UP OF ITERATION MATRIX                         MATX0028   000112
00136    35*          KK = L                                                              000114
00137    36*          DO 65  J=1,NS                                            MATX0031   000127
00142    37*          IF(IUSE(J).LT.0)  GO TO 65                                          000141
00144    38*          IF(IUSE(J).GT.0)  GO TO 70                                          000145
00146    39*          F = (HO(J)-S(J)+ENLN(J)+TM)*EN(J,NPT)                               000150
00147    40*          SS = HO(J)*EN(J,NPT) - F                                            000157
00150    41*          TERM1 = HO(J)*EN(J,NPT)                                             000161
00151    42*          IF (KMAT .EQ. IQ2) TERM1 = F                             MATX0037   000163
00153    43*          DO 55 I = 1, L                                           MATX0038   000174
00153    44*    C     CALCULATE THE ELEMENTS  R(I,K)                           MATX0040   000174
00156    45*          IF (A(I,J) .EQ. 0.) GO TO 55                             MATX0042   000232
00160    46*          DO 15  K=I, L                                            MATX0044   000234
00163    47*       15 G(I,K) = G(I,K) + A(K,J)*A(I,J)*EN(J,NPT)                           000244
00165    48*          G(I,IQ1) = G(I,IQ1) + A(I,J)*EN(J,NPT)                             000251
00166    49*          G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM1                           MATX0048   000255
00167    50*          IF (CONVG .OR.TP) GO TO 55                               MATX0049   000261
00171    51*          G(I,IQ3)= G(I,IQ3)+A(I,J)*F                              MATX0050   000263
00172    52*          IF (SP) G(IQ2,I) = G(IQ2,I) + A(I,J)*SS                  MATX0051   000267
00174    53*       55 CONTINUE                                                 MATX0052   000305
00176    54*          IF (KMAT .EQ. IQ2) GO TO 69                              MATX0053   000305
00200    55*          IF(CONVG.OR.HP) GO TO 59                                 MATX0054   000310
```

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00202   86*          G(IQ2,IQ1) = G(IQ2,IQ1) + SS                                MATX0055   000323
00203   87*          G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*SS                              MATX0056   000326
00204   88*          G(IQ2,IQ3) = G(IQ2,IQ3)+(S(J) - ENLN(J)-TM)*F               MATX0057   000334
00205   89*          GO TO 62                                                    MATX0058   000344
00206   90*       59 G(IQ2,IQ2) = G(IQ2,IQ2) + HO(J)**2*EN(J,NPT)                           000346
00207   91*          IF (CONVG) GO TO 68                                         MATX0060   000362
00211   92*          G(IQ2,IQ3)=G(IQ2,IQ3)+HO(J)*F                               MATX0061   000364
00212   93*       62 G(IQ1,IQ3)=G(IQ1,IQ3)+F                                     MATX0062   000372
00213   94*       68 G(IQ1,IQ2)=G(IQ1,IQ2)+TERM1                                 MATX0063   000376
00214   95*          GO TO 65                                                             000403
00214   96*       C  CONDENSED SPECIES                                                    000403
00215   97*       70 KK = KK + 1                                                          000405
00216   98*          DO 75  I = 1,L                                                       000407
00221   99*          G(I,KK) = A(I,J)                                                     000453
00222  100*       75 G(I,KMAT) = G(I,KMAT) - A(I,J)*EN(J,NPT)                             000459
00224  101*          G(KK,IQ2) = HO(J)                                                    000462
00225  102*          G(KK,KMAT) = HO(J) - S(J)                                            000465
00226  103*          HSUM(NPT) = HSUM(NPT) + HO(J)*EN(J,NPT)                              000471
00227  104*          IF(.NOT.SP) GO TO 65                                                 000477
00231  105*          SSS = SSS + S(J)*EN(J,NPT)                                           000501
00232  106*          G(IQ2,KK) = S(J)                                                     000505
00233  107*       68 CONTINUE                                                 MATX0064   000520
00235  108*          SSS = SSS + G(IQ2,IQ1)                                               000520
00236  109*          HSUM(NPT) = HSUM(NPT) + G(IQ1,IQ2)                                   000527
00237  110*          G(IQ1,IQ1) = SUMN - ENN                                              000537
00237  111*       C  REFLECT SYMMETRIC PORTIONS OF THE MATRIX                 MATX0066   000537
00240  112*          K = IQ1                                                              000543
00241  113*          IF (HP .OR. CONVG)  K = IQ2                                          000545
00243  114*          DO 102 I = 1,K                                                       000562
00246  115*          DO 102 J = I,K                                                       000604
00251  116*       102 G(J,I) = G(I,J)                                                     000606
00251  117*       C  COMPLETE THE RIGHT HAND SIDE                             MATX0074   000606
00254  118*          IF(CONVG)  GO TO 175                                     MATX0076   000612
00256  119*          DO 185 I=1,L                                             MATX0077   000623
00261  120*          X(I)=BO(I)-G(I,IQ1)                                                  000623
00262  121*       185 G(I,KMAT) = G(I,KMAT) + X(I)                                        000625
00264  122*          G(IQ1,KMAT) = G(IQ1,KMAT)+ENN-SUMN                       MATX0080   000630
00264  123*       C  COMPLETE ENERGY ROW AND TEMPERATURE COLUMN               MATX0082   000630
00265  124*          IF (KMAT .EQ. IQ2) GO TO 185                             MATX0084   000636
00267  125*          IF (SP)ENERGY = SO+ENN-SUMN - SSS                                    000641
00271  126*          IF(HP)ENERGY=HSUBO/TT - HSUM(NPT)                                    000656
00273  127*          G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY                                        000665
00274  128*       175 G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM                            MATX0088   000672
00275  129*       185 IF (.NOT. VOL .OR. CONVG)  RETURN                                   000677
00275  130*       C  CONSTANT VOLUME MATRIX                                               000677
00277  131*          K = IQ1 - 1                                                          000704
00300  132*          IF(KMAT.EQ.IQ2) GO TO 230                                            000707
00302  133*          DO 220 I = 1,K                                                       000721
00305  134*          G(IQ1,I) = G(IQ2,I)-G(IQ1,I)                                         000757
00306  135*          G(I,IQ1) = G(I,IQ2)-G(I,IQ1)                                         000761
00307  136*       220 G(I,IQ2) = G(I,IQ3)                                                 000764
00311  137*          G(IQ1,IQ1) = G(IQ2,IQ2)-G(IQ1,IQ2)-G(IQ2,IQ1)                        000767
00312  138*          G(IQ1,IQ2) = G(IQ2,IQ3)-G(IQ1,IQ3)                                   000774
00313  139*          IF (HP)  G(IQ1,IQ2) = G(IQ1,IQ2) + ENN                               001001
00315  140*          GO TO 260                                                            001007
00316  141*       230 DO 240 I = 1,K                                                      001011
```

```
00321   112*      240  G(I,IQ1) = G(I,IQ2)                              001023
00323   113*      260 KMAT = IMAT                                        001026
00324   114*          IMAT = IMAT-1                                      001027
00325   115*          RETURN                                             001031
00326   116*          END                              MATX00?0          001106
```

END OF COMPILATION: NO DIAGNOSTICS.

@MOG.P OUT1

```
@FOR,S    OUT1 OUT1
HP3A  E3 -10/15/80-13:07:18 (15,)


    SUBROUTINE OUT1      ENTRY POINT 002156
               OUT2      ENTRY POINT 002161
               OUT3      ENTRY POINT 002164
               OUT4      ENTRY POINT 002167


    STORAGE USED: CODE(1) 002172; DATA(0) 000655; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   CONSTS 000006
    0004   HOLCON 000010
    0005   POINTS 000335
    0006   SPECES 017106
    0007   MISC   001701
    0010   INDX   000041
    0011   PERF   000166
    0012   OUPT   000073
    0013   CC     000003
    0014   CFUEL  000004


    EXTERNAL REFERENCES (BLOCK, NAME)

    0015   VARFMT
    0016   MOVABS
    0017   HOLDIT
    0020   PAGIT
    0021   NWDUS
    0022   NIO1S
    0023   NIO2S
    0024   NIO3S
    0025   SORT
    0026   MERR3S


    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000   000371 1F      0001   000034 10L     0001   001440 1014G   0001   001443 1020G   0001   001470 1034G
    0001   001477 1042G   0001   001510 1045G   0001   001520 1050G   0001   001564 1066G   0001   001573 1072G
    0001   001621 1107G   0001   001627 1115G   0001   001643 1124G   0001   001673 1135G   0001   001752 1153G
    0001   001760 1161G   0001   002030 1176G   0001   002042 1205G   0001   002054 1214G   0001   002066 1223G
    0001   002100 1232G   0001   002112 1241G   0001   001044 130L    0001   000025 154G    0001   001120 160L
    0001   000043 164G    0001   001144 170L    0001   001152 175L    0001   001221 177L    0001   001257 179L
    0001   001261 180L    0000   000377 2F      0000   000333 20F     0001   000112 200G    0001   001334 200L
    0001   001371 210L    0001   001373 211L    0000   000353 22F     0000   000310 240F    0001   000213 247G
    0001   000235 261G    0001   000276 277G    0000   000406 280F    0000   000422 290F    0001   000036 30L
    0000   000450 300F    0000   000452 310F    0001   000320 310G    0000   000416 320F    0001   000334 321G
    0001   000362 332G    0000   000412 340F    0001   000404 3436    0001   000420 3506    0001   000447 3646
    0001   000471 375G    0001   000501 4036    0001   000522 414G    0001   000544 4256    0001   000560 4326
    0001   000606 445G    0001   000065 45L     0001   000623 455G    0001   000647 471G    0000   000471 490F
    0000   000472 492F    0001   000217 50L     0001   001451 500L    0001   000670 502G    0000   000477 504F
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0001		001533	S08L	0001		001536	S10L	0001		000711	S136	0001		001604	S14L
0000		000509	S20F	0001		000717	S206	0000		000511	S24F	0001		000734	S276
0001		000753	S33F	0000		000525	S42F	0000		000532	S44F	0001		000763	S456
0000		000546	S48F	0000		000554	S50F	0000		000562	S52F	0001		001007	S556
0001		001100	6136	0001		001106	6206	0001		001131	6316	0001		001140	6366
0001		001157	6506	0001		001216	6616	0001		001247	6736	0001		001275	7156
0001		001331	7276	0001		000342	74L	0001		001362	7416	0000		000405	80F
0011		000150	ACAT	0007		000640	AN	0007		000705	AN1	0007	R	001138	ANUM
0003	R	000000	ATMN	0007		000004	ATOM	0007		000514	B0	0007		000545	B0P
0014	R	000000	CF	0000	R	000103	CMW	0006		000000	COEF	0000	R	000047	COF
0005	R	000032	CPR	0007		000706	CPR1	0007		000634	CPSUM	0007		000654	DATA
0013		000002	DEMAND	0007	R	001560	DENS	0005	R	000640	DLVPT	0005	R	000043	DLVTP
0000	R	000167	EE	0006	R	004312	EN	0004		000000	END	0004		010150	ENLN
0007		000000	ENN	0007		001676	ENNL	0007		001677	ENSAVE	0007	R	001414	ENTH
0007	R	000636	EQRAT	0012		000002	FA	0012	R	000003	FAP	0007	R	001445	FAZ
0012		000006	FC	0012	R	000007	FCP	0012		000012	FCST	0012		000014	FCV
0012		000017	FGE	0012		000020	FGV	0012	R	000021	FH	0000	R	000036	FMH
0012		000026	FGV	0012	R	000027	FM	0012	R	000031	FMT	0012		000050	FN
0007	I	001527	FOX	0012		000053	FP	0000	R	000046	FPC	0000	R	000032	FPP
0000	R	000040	FSS	0012	R	000056	FSV	0012	R	000057	FT	0012	R	000061	FTR
0012	R	000063	FV	0012	R	000065	FVEL	0000	R	000001	FVLM	0012	R	000001	F13
0005	R	000101	GAMMAS	0004		000001	GAS	0003		000001	GMET	0013		000000	GRAPN
0000	R	000221	HHVD	0000	R	000152	HHVS	0014	R	000001	HHVV	0010		000003	HP
0007		000637	HSUB0	0005	R	000000	HSUM	0006		010376	HO	0000	I	000002	I
0010		000000	IDEBUG	0000	I	000261	IDG	0004		000002	IE	0000	I	000050	IFLAG
0010		000015	IMAT	0000	I	000253	INDX	0000		000624	INJPS	0010		000023	IONS
0010		000037	IOSAVE	0010		000016	IO1	0006	I	015364	ISUB	0010		000005	ISV
0006	I	016266	IUSE	0004		000003	IZ	0000	I	000045	J	0010		000026	JLIQ
0010		000025	JSOL	0010		000031	JS1	0000	I	000043	K	0010		000014	KMAT
0000	R	000066	LHVD	0000	R	000051	LHVS	0007		000463	LIMT	0010		000008	LSAVE
0000	I	000306	L3	0000	I	000307	L4	0004		000005	MOL	0010	L	000003	MOLES
0007	I	000707	NAME	0010		000024	NC	0000	I	000044	ND	0010		000022	NEWR
0010		000012	NLM	0010		000017	NOF	0010		000020	NOMIT	0010		000007	NP
0010	I	000027	NREAC	0010	I	000013	NS	0000	I	000000	NSPP1	0010		000010	NT
0012	R	000067	ONE	0004	I	000006	OX	0007		001644	OXF	0005		000116	P
0011		000000	PCP	0007	R	001363	PECNT	0014	R	000001	PER	0007		000033	PP
0003	R	000003	RBAR	0003	R	000004	RRR	0007		000644	RW	0007	R	001611	RWOP
0007	R	001476	RTEMP	0003		000005	RVR	0006		004064	S	0010		000033	SHOCK
0005	R	000251	SONVEL	0010		000004	SP	0011		000047	SPIN	0005	R	000018	SSUM
0011		000101	SUBAR	0000	R	000303	SUM	0007		000001	SUMN	0011		000116	SUPAR
0005		000150	T	0006		016514	TEMP	0007		000632	THIGH	0012		000070	THREE
0007		000630	TLOW	0007		000627	TM	0007		000631	TMID	0005	R	000320	TOTN
0007		000002	TT	0005	R	000266	TTT	0012	R	000071	TWO	0005	R	000202	V
0005	R	000303	VLM	0007		000646	VMIN	0011		000032	VMOC	0010	L	000032	VOL
0014	R	000002	WCR	0005	R	000234	WM	0007		000652	WP	0000	R	000120	XDP
0000	R	000135	YDPS	0000	R	000020	YN	0000	R	000025	YX	0006	R	010376	Z
0012		000072	ZEROF												

00101	1•		SUBROUTINE OUT1	OUTP0001	000000
00101	2•	C			000000
00103	3•		COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR	/CONSTS/	000000
00104	4•		COMMON /HOLCON/ END,GAS,IE,IZ,LAMK,MOL,OX,ZERO	/HOLCON/	000000
00105	5•		COMMON/POINTS/MSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)		000000

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00105     6.      1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WW(13),SONVEL(13),TTT(13)                    000000
00105     7.      2 ,VLM(13),TOTN(13)                                                                  000000
00105     8.  C    COMMON/SPECES/COEF(2,7,150),S(150),EN(150,3),ENLN(150),HO(150)                      000000
00105     9.  C   1 ,DELH(150),A(15,150),SUB(150,3),IUSE(150),TEMP(150,2),SLN(150)                     000000
00106    10.      INCLUDE SPECPR                                                                       000000
00112    11.      COMMON /MISC/ ENN,SUMN,TT,XO,ATOM(3,101),ELMT(25),BG(25),                            000000
00112    12.     1              BOP(25,2),TM,TLOW,TMID,TMIGH,PP,CPSUM,OF,EQRAT,                      000000
00112    13.     2              HSUBO,AM(2),HPP(2),RHI(2),VMIN(2),VPLS(2),WP(2),      /MISC/         000000
00112    14.     3              DATA(25),AM1,CP91,NAME(25,6),ANUM(25,6),PECUT(25),                   000000
00112    15.     4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,                    000000
00112    16.     5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                               000000
00113    17.      COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,MP,MT,MPT,NLM,NS,      /INDX/         000000
00113    18.     1              KMAT,IMAT,IO1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,LIQ,    /INDX/         000000
00113    19.     2              NREAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCM,IOSAVE,LSAVE     /INDX/         000000
00114    20.      COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),         /PERF/         000000
00114    21.     1              SUPAR(13),APP(13),AEAT(13),EQL                       /PERF/         000000
00115    22.      COMMON /OUPT/ FGX,F13,FAX,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),    /OUPT/         000000
00115    23.     1              FGE,FGW,FM(21,FI(2),FIM(2),FM(2),MT(15),FN(2),FOUR,  /OUPT/         000000
00115    24.     2              FP,FS(2),FSV,FT(2),FTM(2),FV(2),FVEL(2),ONE,THREE,   /OUPT/         000000
00115    25.     3              TWO,ZEROF                                            /OUPT/         000000
00115    26.  C                                                                                      000000
00116    27.          COMMON /CCC/GRAPH,JOUT,DEMAND                                                  000000
00117    28.      COMMON /CFUEL/CF,HHVV,WCR,PER                                                      000000
00117    29.  C                                                                                      000000
00120    30.      DIMENSION FVLM(2),HEAD(9),MW(2,2),YN(5),YX(5),Z(10,3)                              000000
00121    31.      DIMENSION FPP(2),FTR(2),FMM(2),FSS(2)                                              000000
00122    32.      DATA (FPP(I),I=1,2)/'PRESS ','PSIA  '/                                             000000
00124    33.      DATA (FTR(I),I=1,2)/'TEMP D','EG F  '/                                             000000
00126    34.      DATA (FMM(I),I=1,2)/'ENTH B','TU/LB '/                                             000000
00130    35.      DATA (FSS(I),I=1,2)/'S BTU/','(LB-R)'/                                             000000
00132    36.      EQUIVALENCE (Z,MO)                                                                 000000
00133    37.      INTEGER FOX,OX                                                                     000000
00134    38.      LOGICAL EQL,MOLES,VOL                                                              000000
00134    39.  C                                                                        OUTP0021     000000
00134    40.  C   HEAD = (1XA6,2X5(A2,F8.5,3X), 5X,F7.5,F13.3,4X,A1,F10.2,F9.4)                      000000
00134    41.  C                                                                                      000000
00135    42.      DATA (HEAD/6H(1XA6,,6H2X5(A2,6H,F8.4,,6H3X), 5,6HX,F7.5,6H,F13.3,                  000000
00135    43.     1     6H,4X,A1,6H,F10.2,6H,F9.4)/,YN/6H2X1(A2,6H2X2(A2,6H2X3(A2,                  000000
00135    44.     2     6H2X4(A2,6H2X5(A2/,YX/6H3X),57,6H3X),44,6H3X),31,6H3X),18,                   000000
00135    45.     3 6H3X), 5/,MW/24HMWT FRACTION    MOLES    /,FVLM/12HVOLUME CC/G /                 000000
00138    46.  C                                                                                      000000
00143    47.      K = 1                                                                              000000
00144    48.      IF (MOLES) K = 2                                                                   000001
00146    49.      WRITE(JOUT,240) MW(1,K),MW(2,K)                                                    000005
00152    50.  240 FORMAT (77X,2A6,34H ENTHALPY   STATE   TEMP    DENSITY/10X,                       000025
00152    51.     1        16HCHEMICAL FORMULA,65X,7HCAL/MOL,10X,6HDEG. K,3X,5HG/CM3)                 000025
00153    52.      DO 60 K = 1,NREAC                                                                  000028
00156    53.      IF (FOX(K) .NE. OX)  GO TO 10                                                      000025
00160    54.      ND = 6HOXIDNT                                                                      000030
00161    55.      GO TO 30                                                            OUT1 580       000032
00162    56.   10 ND = 6HFUEL                                                                        000034
00163    57.   30 DO 40 J=1,5                                                         OUT1 610       000036
00166    58.   40 IF(ANUM(K,J) .LE. 0. .OR. NAME(K,J) .EQ. LANK)  GO TO 45                          000043
00171    59.      J=6                                                                                000062
00172    60.   45 J=J-1                                                                             000065
00173    61.      HEAD(2) = YN(J)                                                                    000073
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00174    62*          HEAD(9) = YX(J)                                                    000075
00175    63*       60 WRITE(JOUT,HEAD, ND,(NAME(K,I),ANUM(K,I),I = 1,3),PECNT(K),        000077
00175    64*      1                ENTHN(K),FAZ(K),RTEMP(K),DENS(K)                    000077
00213    65*          FPC = 100./(1.+OF)                                                 000126
00214    66*          WRITE(JOUT,20) OF ,FPC,FORAT,RHOP                                  000133
00222    67*       20 FORMAT (1HO,1SX, 4HO/F=, F8.4,8X,13HPERCENT SUL=,F8.4,8X,          000144
00222    68*      1  19HEQUIVALENCE RATIO= ,F7.4,8X,8HDENSITY=,F8.4)                     000144
00223    69*          IF (CF+1.0) ,60,                                                   000144
00226    70*          COF=OF/CF                                                          000147
00227    71*          WRITE (JOUT,22) COF,WCR,PER                                        000152
00236    72*       22 FORMAT (21X,'OXIDIZER/COAL=',F8.4,5X,'WATER/COAL=',F8.4,          000163
00236    73*      X   5X,'CARBON CONVERSION=',F8.4)                                     000163
00235    74*       60 RETURN                                                          000163
00235    75*     C                                                                    000163
00236    76*          ENTRY OUT2                                                         000165
00236    77*     C    VOLUME                                                          000165
00237    78*          FMT(3) = ONE                                                       000165
00240    79*          IF(.NOT.VOL) GO TO 80                                              000167
00242    80*          CALL VARFMT(VLM,NPT)                                               000171
00243    81*          WRITE(JOUT,FMT) FVLM,FB,(VLM(I), I = 1,NPT)                        000175
00253    82*     C    PRESSURE                                          OUTP0038         000175
00253    83*       80 IFLAG=0                                                          000217
00254    84*          IF (CF+1.0) ,82,                                                   000217
00257    85*          IFLAG=1                                                            000222
00260    86*       82 DO 85 I=1,NPT                                                    000225
00263    87*          IF (IFLAG.EQ.0) V(I)=ATMN*PPP(I)                                   000235
00265    88*          IF (IFLAG.EQ.1) V(I)=PATM*PPP(I)                                   000241
00267    89*       85 CONTINUE                                                         000251
00271    90*          CALL VARFMT(V,NPT)                                                 000251
00272    91*          IF (IFLAG.EQ.0) WRITE (JOUT,FMT) FAP,FB,(V(I),I=1,NPT)             000255
00303    92*          IF (IFLAG.EQ.1) WRITE (JOUT,FMT) FPP,FB,(V(J),J=1,NPT)             000301
00303    93*     C    TEMPERATURE                                       OUTP0047         000301
00314    94*          FMT(3) = F13                                                       000323
00315    95*          FMT(4) = TWO                                                       000325
00316    96*          IF (IFLAG.EQ.1) GO TO 74                                           000327
00320    97*          DO 72 J=1,NPT                                                      000330
00323    98*       72 TTT(J)=(TTT(J)-273.15)*1.8+32.                                   000330
00325    99*       74 IF (IFLAG.EQ.0) WRITE (JOUT,FMT) FTK,FB,(TTT(J),J=1,NPT)        000342
00336   100*          IF (IFLAG.EQ.1) WRITE (JOUT,FMT) FTR,FB,(TTT(J),J=1,NPT)        000365
00336   101*     C    ENTHALPY                                          OUTP0056         000365
00347   102*          DO 75 I=1,NPT                                     OUTP0058         000407
00352   103*          V(I)=RBAR*HSUM(I)                                                  000420
00353   104*          IF (IFLAG.EQ.1) V(I)=V(I)*1.8                                      000422
00355   105*       75 CONTINUE                                                         000431
00357   106*          IF (IFLAG.EQ.0) WRITE (JOUT,FMT) FH,FB,(V(J),J=1,NPT)           000431
00370   107*          IF (IFLAG.EQ.1) WRITE (JOUT,FMT) FHH,FB,(V(J),J=1,NPT)          000452
00370   108*     C    ENTROPY                                           OUTP0064         000452
00401   109*          FMT(4) = FOUR                                                      000470
00402   110*          DO 78 I = 1,NPT                                                    000501
00405   111*       78 V(I) = RBAR*SSUM(I)                                              000501
00407   112*          IF (IFLAG.EQ.0) WRITE (JOUT,FMT) FS,FB,(V(J),J=1,NPT)           000504
00420   113*          IF (IFLAG.EQ.1) WRITE (JOUT,FMT) FSS,FB,(V(J),J=1,NPT)          000525
00420   114*     C    DENSITY                                                         000525
00431   115*          DO 70 I = 1,NPT                                                    000547
00436   116*          IF (VLM(I).GT.0) V(I)=1./VLM(I)                                    000560
00436   117*          IF (IFLAG.EQ.1) V(I)=V(I)*2206./35.31                              000565
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00440  118*       70 CONTINUE                                                    000575
00442  119*          IF (IFLAG.EQ.0) WRITE (JOUT,1) (V(J),J=1,NPT)               000575
00451  120*        1 FORMAT (1X,14HDENSITY G/CC  ,1P13E9.3)                      000611
00452  121*          IF (IFLAG.EQ.1) WRITE (JOUT,2) (V(J),J=1,NPT)               000611
00461  122*        2 FORMAT (1X,'DENSITY L/F**3',1P13E9.3)                       000626
00462  123*          WRITE(JOUT,80)                                              000626
00464  124*       80 FORMAT ( 1H )                                  OUTP0070    000633
00464  125*  C    MOLECULAR WEIGHT                                  OUTP0072    000633
00465  126*          WRITE(JOUT,FMT) FM,FB,(WM(J), J = 1,NPT)                    000633
00465  127*  C    (DLV/DLP)T                                        OUTP0080    000633
00475  128*          IF (EQL)  WRITE(JOUT,FMT) FV,FB,(DLVPT(J), J = 1,NPT)       000652
00475  129*  C    (DLV/DLT)P                                        OUTP0083    000652
00506  130*          IF (EQL)  WRITE(JOUT,FMT) FV,FB,(DLVTP(J), J = 1,NPT)       000673
00506  131*  C    HEAT CAPACITY                                     OUTP0087    000673
00517  132*          DO 85  I=1,NPT                                OUTP0089    000717
00522  133*       85 V(I) = RBAR*CPR(I)                                          000717
00524  134*          WRITE(JOUT,FMT) FCP,(V(J), J = 1,NPT)                       000722
00529  135*  C    GAMMA(S)                                          OUTP0093    000722
00533  136*          WRITE(JOUT,FMT) FG,FB,(GAMMAS(J), J = 1,NPT)                000737
00533  137*  C    SONIC VELOCITY                                    OUTP0097    000737
00543  138*          FMT(4) = TWO                                                000756
00544  139*          DO 95 I = 1,NPT                               OUTP0100    000763
00547  140*       95 SONVEL(I) = SQRT(RBR*GAMMAS(I)*TTT(I)/WM(I))                000763
00551  141*          WRITE(JOUT,FMT) FSV,FVEL,(SONVEL(J), J = 1,NPT)             000777
00561  142*          CALL MOVABS(500,50)                                         001012
00562  143*          CALL HOLDIT                                                 001016
00563  144*          CALL PAGIT                                                  001020
00564  145*          RETURN                                                      001022
00564  146*  C                                                 OUTP0104    001022
00565  147*          ENTRY OUT1                                                  001025
00566  148*          IF (CF+1.0) ,130,                                           001025
00571  149*          COF=OF/CF                                                   001030
00572  150*          WRITE (JOUT,22) COF,WCR,PER                                 001033
00577  151*      130 WRITE (JOUT,80)                                             001044
00601  152*          ND = 0                                                      001050
00601  153*  C       MOLE FRACTIONS EQUILIBRIUM OR FROZEN              OUT12270  001050
00602  154*          WRITE(JOUT,280)                                             001051
00604  155*      280 FORMAT (15HOMOLE FRACTIONS/)                                001056
00605  156*          IF (.NOT. EQL)  GO TO 175                                   001086
00605  157*  C       EQUILBRIUM MOLE FRACTIONS                                   001056
00607  158*          DO 170 K=1,NS                                 OUT12330    001100
00612  159*          DO 140 I=1,NPT                                OUT12340    001100
00615  160*      140 V(I) = EN(K,I)/TOTN(I)                                      001100
00617  161*          DO 150 I=1,NPT                                OUT12370    001106
00622  162*      150 IF (V(I) .GE. 5.0E-7)  GO TO 160                            001106
00625  163*          ND = 1                                                      001114
00626  164*          GO TO 170                                     OUT12400    001116
00627  165*      160 WRITE(JOUT,340) (SUB(K,J), J = 1,3),FB,(V(I), I = 1,NPT)    001120
00642  166*      340 FORMAT (1H ,3A4,A2,1P13E9.3)                                001150
00643  167*      170 CONTINUE                                      OUT12430    001150
00643  168*  C       OUTPUT COMPLETE GO EXIT                       OUT12590    001150
00645  169*          GO TO 211                                     OUT12600    001150
00645  170*  C       FROZEN MOLE FRACTIONS                                       001150
00646  171*      175 J = 0                                                       001152
00647  172*          DO 179 K = 1,NS                               OUT12630    001152
00652  173*          V(J+1) = EN(K,1)/TOTN(1)                                    001164
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00653   174*          IF (V(J+1) .LT. 5.0E-7)  ND = 1                                    001170
00655   175*          IF (V(J+1) .LT. 5.0E-7)  GO TO 177                                 001177
00655   176*    C     OUTPUT VALUE ACCEPTED                                  OUT12660    001177
00657   177*          J = J + 1                                                          001204
00660   178*          DO 176 I = 1,3                                                     001207
00663   179*    176   Z(J,I) = SUB(K,I)                                                  001216
00665   180*    177   IF (J .NE. 4 .AND. K .NE. NS)  GO TO 179                          001221
00667   181*          IF (J .EQ. 0)  GO TO 180                                           001234
00671   182*          WRITE(JOUT,320) (Z(I,1),Z(I,2),Z(I,3),V(I), I = 1,J)              001236
00702   183*    320   FORMAT (1H ,4(3A4,F11.8,5X))                                     001255
00703   184*          J = 0                                                              001255
00704   185*    179   CONTINUE                                               OUT12780    001261
00706   186*    180   IF (ND .EQ. 0)  GO TO 211                                         001261
00710   187*          WRITE(JOUT,290)                                                    001262
00712   188*    290   FORMAT (///1X,116HADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHO 001267
00712   189*         1SE MOLE FRACTIONS WERE LESS THAN 5.0E-7 FOR ALL ASSIGNED CONDITION 001267
00712   190*         2S//)                                                              001267
00713   191*          J = 0                                                              001267
00714   192*          DO 210 K=1,NS                                          OUT12780    001275
00717   193*          DO 190 I=1,NPT                                         OUT12790    001307
00722   194*    190   IF( (EN(K,I)/TOTN(I)) .GE. (5.0E-7) ) GO TO 200       OUT12800    001307
00725   195*          J = J + 1                                                          001327
00726   196*          DO 195 I = 1,3                                                     001322
00731   197*    195   Z(J,I) = SUB(K,I)                                                 001331
00733   198*    200   IF (J .NE. 10 .AND. K .NE. NS)  GO TO 210                        001334
00735   199*          IF (J .EQ. 0)  GO TO 211                                           001347
00737   200*          WRITE(JOUT,300) (Z(I,1),Z(I,2),Z(I,3), I = 1,J)                    001351
00747   201*    300   FORMAT (10(1X,3A4))                                  OUT13100    001367
00750   202*          J = 0                                                              001367
00751   203*    210   CONTINUE                                               OUT12900    001373
00751   204*    C     REMOVE TO IMPROVE PRINTOUT FOR COAL CALCULATIONS                   001373
00751   205*    C        WHICH ARE ALWAYS IN WEIGHT FRACTION                             001373
00753   206*          211 RETURN                                                         001373
00754  *DIAGNOSTIC*  CONTROL CAN NEVER REACH THE NEXT STATEMENT
00754   207*          IF (.NOT.MOLES) WRITE (JOUT,310)                                   001375
00757   208*    310   FORMAT (//1X,77HNOTE, WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND O 001404
00757   209*         IF OXIDANT IN TOTAL OXIDANTS)                                       001404
00760   210*          RETURN                                                             001404
00761   211*          ENTRY OUT4                                                         001407
00762   212*          REAL LHVS,LHVD                                                     001407
00763   213*          DIMENSION CHW(13),XDP(13),YDPS(13),HHVS(13),EE(13),YDP(13),        001407
00763   214*         X   HHVD(13),LHVS(13),LHVD(13),DOL(13)                              001407
00764   215*          DIMENSION ISUB(150,3)                                              001407
00765   216*          EQUIVALENCE (ISUB(1,1),SUB(1,1))                                   001407
00766   217*          DIMENSION INDX(6)                                                  001407
00767   218*          DIMENSION IDG(6,3)                                                 001407
00770   219*          DATA (IDG(1,I),I=1,3)/'CO  ',2*' '/                                001407
00772   220*          DATA (IDG(2,I),I=1,3)/'CO2 ',2*' '/                                001407
00774   221*          DATA (IDG(3,I),I=1,3)/'CH4 ',2*' '/                                001407
00776   222*          DATA (IDG(4,I),I=1,3)/'H2  ',2*' '/                                001407
01000   223*          DATA (IDG(5,I),I=1,3)/'N2  ',2*' '/                                001407
01002   224*          DATA (IDG(6,I),I=1,3)/'AR  ',2*' '/                                001407
01004   225*          WRITE (JOUT,490)                                                   001407
01006   226*    490   FORMAT (1H )                                                       001414
01007   227*          WRITE (JOUT,492) HHVV                                              001414
01012   228*    492   FORMAT (1X,'HHV COAL B/LB',1X,F9.2)                              001440
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01013  229*        DO 502 I=1,NPT                                          001440
01016  230*        SUM=0.                                                  001440
01017  231*        DO 500 J=1,NS                                           001443
01022  232*        IF (IUSE(J).NE.0) GO TO 500                             001443
01024  233*        SUM=SUM+EN(J,I)/TOTN(I)                                 001444
01025  234*  500   CONTINUE                                                001453
01027  235*        CMW(I)=WM(I)*SUM                                        001453
01030  236*  502   CONTINUE                                                001461
01032  237*        WRITE (JOUT,504) (CMW(I),I=1,NPT)                       001461
01040  238*  504   FORMAT (1X,'MIXTURE MW',4X,13F9.3)                      001477
01040  239*  C     LOCATE DRY ELEMENTS                                     001477
01041  240*        DO 510 I=1,6                                            001477
01044  241*        DO 508 J=1,NS                                           001510
01047  242*        DO 506 K=1,3                                            001520
01052  243*        IF (IDG(I,K).NE.ISUB(J,K)) GO TO 508                    001520
01054  244*  506   CONTINUE                                                001527
01056  245*        INDX(I)=J                                               001527
01057  246*        GO TO 510                                               001531
01060  247*  508   CONTINUE                                                001534
01062  248*        INDX(I)=0                                               001534
01063  249*  510   CONTINUE                                                001540
01065  250*        DO 516 I=1,NPT                                          001540
01070  251*        SUM=0.                                                  001567
01071  252*        DO 514 J=1,6                                            001573
01074  253*        IJ=INDX(J)                                              001573
01075  254*        IF (IJ.EQ.0) GO TO 514                                  001574
01077  255*        SUM=SUM+EN(IJ,I)                                        001576
01100  256*  514   CONTINUE                                                001605
01102  257*        XDP(I)=SUM/TOTN(I)                                      001605
01103  258*  516   CONTINUE                                                001612
01105  259*        WRITE (JOUT,520) (XDP(I),I=1,NPT)                       001612
01113  260*  520   FORMAT (1X,'MF OF CDG',5X,13F9.5)                       001627
01114  261*        DO 522 I=1,NPT                                          001627
01117  262*        YDPS(I)=(385.2*XDP(I)/CMW(I))*((1./CF)*(1.+OF))         001627
01120  263*  522   CONTINUE                                                001634
01122  264*        WRITE (JOUT,524) (YDPS(I),I=1,NPT)                      001634
01130  265*  524   FORMAT (1X,'Y SAT SCF/LB',2X,13F9.5)                    001646
01131  266*        L1=INDX(1)                                              001646
01132  267*        L3=INDX(3)                                              001650
01133  268*        L4=INDX(4)                                              001652
01134  269*        DO 530 I=1,NPT                                          001662
01137  270*        SUM=0.                                                  001675
01140  271*        IF (L4.NE.0) SUM=SUM+319.29*EN(L4,I)/TOTN(I)            001677
01142  272*        IF (L1.NE.0) SUM=SUM+316.06*EN(L1,I)/TOTN(I)            001710
01144  273*        IF (L3.NE.0) SUM=SUM+994.4*EN(L3,I)/TOTN(I)             001721
01146  274*        HHVS(I)=SUM/XDP(I)                                      001732
01147  275*  530   CONTINUE                                                001737
01151  276*        WRITE (JOUT,532) (HHVS(I),I=1,NPT)                      001737
01157  277*  532   FORMAT (1X,'HHV SAT B/SCF',1X,13F9.2)                   001760
01160  278*        DO 538 I=1,NPT                                          001760
01163  279*        EE(I)=HHVS(I)*YDPS(I)/HHVV                              001760
01164  280*        YDP(I)=379.5*YDPS(I)/385.2                              001764
01165  281*        HHVD(I)=(385.2/379.5)*HHVS(I)                           001770
01166  282*        IF (L4.NE.0) LHVS(I)=HHVS(I)-(1059.9*18./385.2)*(EN(L4,I)/TOTN(I))  001773
01156  283*       X   /XDP(I)                                              001773
01170  284*        LHVD(I)=LHVS(I)*385.2/379.5                             002004
```

```
01171   285*        DOL(I)=10000.*(1.25*HHVV/10000.+OF/CF)/(HHVS(I)+YDPS(I))          002012
01172   286*    538 CONTINUE                                                          002021
01174   287*        WRITE (JOUT,542) (EE(I),I=1,NPT)                                  002021
01202   288*    542 FORMAT (1X,'EFFICIENCY',4X,13F9.5)                                002033
01203   289*        WRITE (JOUT,544) (YDP(I),I=1,NPT)                                 002033
01211   290*    544 FORMAT (1X,'Y DRY SCF/LB',2X,13F9.5)                              002045
01212   291*        WRITE (JOUT,546) (HHVD(I),I=1,NPT)                                002045
01220   292*    546 FORMAT (1X,'HHV DRY B/SCF',1X,13F9.2)                             002057
01221   293*        WRITE (JOUT,548) (LHVS(I),I=1,NPT)                                002057
01227   294*    548 FORMAT (1X,'LHV SAT B/SCF',1X,13F9.2)                             002071
01230   295*        WRITE (JOUT,550) (LHVD(I),I=1,NPT)                                002071
01236   296*    550 FORMAT (1X,'LHV DRY B/SCF',1X,13F9.2)                             002103
01237   297*        WRITE (JOUT,552) (DOL(I),I=1,NPT)                                 002103
01245   298*    552 FORMAT (1X,'$ PER MMBTU',3X,13F9.2)                               002115
01246   299*    560 CONTINUE                                                          002115
01247   300*        RETURN                                                            002115
01250   301*        END                                              OUTP0137         002171
```

END OF COMPILATION: 1 DIAGNOSTICS.

@HDG,P PROK

```
@PDP,LWF   PROK PROK
PDP12R1 R72-16 10/15/80 13:07:27 (0,0)       RI
PE0001       SPECPK PROC
  0002            COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)
  0003           1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)
  0004            DATA NS/PP1/151/
  0005       END

END PDP  ERRORS : NONE


@MDG,P       @EAC
```

```
AFOR,S   REACT,REACT
HSA  E3 -10/15/80-13:07:28 (31,)

    SUBROUTINE REACT     ENTRY POINT 001077

    STORAGE USED: CODE(1) 001111: DATA(0) 000367; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003   HOLCON 000010
     0004   MISC   001701
     0005   INOX   000041
     0006   CCC    000003
     0007   CFUEL  000004

    EXTERNAL REFERENCES (BLOCK, NAME)

     0010   COUT
     0011   RNCODS
     0012   MOVABS
     0013   HOLDIT
     0014   PAGIT
     0015   NREWS
     0016   NRBUS
     0017   NI02S
     0020   NI01S
     0021   NWDUS
     0022   NERR3S

    STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001   000327 101L     0001   000003 132G     0001   000013 143G     0001   000072 18L      0001   000074 20L
     0001   000463 200L     0001   000521 204L     0001   000106 206G     0001   000557 210L     0000   000318 212F
     0001   000566 214L     0001   000736 218L     0001   000740 220L     0001   001002 222L     0001   001005 224L
     0001   001022 226L     0001   001042 229L     0001   001056 230L     0001   000146 232G     0001   000233 267G
     0001   000243 275G     0000   000301 30F      0001   000256 304G     0001   000300 317G     0001   000377 342G
     0001   000226 37L      0001   000512 400G     0001   000534 414G     0001   000554 430G     0001   000617 447G
     0001   000270 45L      0001   000275 46L      0001   000662 460G     0001   000712 473G     0001   000311 50L
     0001   000766 510G     0001   000771 513G     0001   001012 531G     0001   001033 543G     0001   001046 552G
     0003   000042 6L       0004 R 000640 AM       0004   000705 AM1      0004 R 000707 ANAME    0004 R 001135 ANUM
     0004 R 000004 ATOM     0004   000514 BO       0004 R 000545 BOP      0005   000036 CALCH    0007 R 000000 CF
     0005   000001 CONVG    0004   000706 CPR1     0004   000634 CPSUM    0004 R 000654 DATA     0006   000002 DEMAND
     0004 R 001560 DENS     0003   000000 END      0004   001700 ENLSAV   0004   000000 ENN      0004   001676 ENNL
     0004   001677 ENSAVE   0004 R 001414 ENTH     0004   000636 EQRAT    0004 R 001405 FAZ      0004 I 001527 FOX
     0003   000001 GAS      0006   000000 GRAPH    0007 R 000001 HHVV     0005   000003 HP       0004 R 000642 HPP
     0004   000637 HSUBO    0000 I 000262 I        0005 I 000030 IC       0005   000000 IDEBUG   0003   000002 IE
     0005   000018 IMAT     0000   000344 INJPS    0000 I 000271 IO       0005   000023 IONS     0000 I 000235 IOUT
     0005   000021 IP       0005   000037 IQSAVE   0005   000016 IQ1      0005   000005 ISV      0005   000034 IT
     0003 I 000003 IZERO    0000 I 000266 J        0000 I 000275 JJ       0005   000026 JLIO     0006 I 000001 JOUT
     0005   000025 JSOL     0005   000031 JS1      0000 I 000265 K        0005   000014 KMAT     0005 I 000012 L
     0003 I 000004 LANK     0000 I 000145 LINE1    0000 I 000172 LINE2    0000 I 000215 LINE3    0004 I 000463 LLMT
     0000 I 000032 LLMTS    0005   000040 LSAVE    0003 I 000005 MOL      0000 I 000272 MOLE     0005 L 000006 MOLES
```

0000	I	000270	N	0004	I	000707	NAME	0000	I	000273	NAST	0005		000024	NC
0000	I	000300	NDUMMY	0005	L	000022	NEWR	0000	I	000267	NFUEL	0005		000035	NFZ
0000	I	000277	NN1	0005		000017	NOF	0005	I	000020	NOMIT	0005		000007	NP
0005		000027	NREAC	0005		000013	NS	0005		000010	NT	0000	I	000263	N3
0000	I	000264	N8	0003	I	000006	OX	0004		001644	OXF	0000	R	000276	PCNT
0007	R	000003	PER	0009		000633	PP	0004	R	000044	RH	0004		001611	RHOP
0000	R	000274	RM	0004	R	001612	RMW	0004	R	001476	RTEMP	0000	R	000063	SBOP
0005		000033	SHOCK	0005		000004	SP	0004		000001	SUMN	0009		000003	SO
0004		001643	TLN	0004		000630	TLOW	0009		000627	TM	0004		000631	TMID
0004		000632	THIGH	0005		000002	TP	0004		000002	TT	0000	R	000001	V
0004	R	000646	VMIN	0007	R	000002	WCR	0004	R	000652	WP	0005	I	000007	ZERO
0005		000032	VOL	0004	R	000650	VPLS								

```
00101     1*            SUBROUTINE REACT                                                        000003
00101     2*      C                                                                             000003
00103     3*            COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO          /HOLCON/   000003
00109     4*            COMMON /MISC/ EMN,SUMN,TT,SO,ATOM(3,10),LLMT(25),BOP(25),             000003
00104     5*           1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,        000003
00104     6*           2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),  /MISC/ 000003
00104     7*           3              DATA(25),AM1,CPR1,NAME(25,6),AMOM(25,6),PECWT(25),     000003
00104     8*           4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RMOP,      000003
00104     9*           5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                 000003
00105    10*            COMMON /INDX/ IDEBUG,CONVG,IP,MP,SP,ISV,MOLES,NP,NT,NPI,L,NS,  /INDX/ 000003
00105    11*           1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/ 000003
00105    12*           2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE    /INDX/ 000003
00105    13*     C                                                                             000003
00106    14*           COMMON /CCC/ GRAPH,JOUT,DEMAND                                         000003
00106    15*     C                                                                             000003
00107    16*           COMMON /CFUEL/CF,HHVV,WCR,PER                                          000003
00110    17*           DATA NLS/0/                                                            000003
00112    18*           DIMENSION ANAME(25,6),V(25),LLMTS(25),SBOP(25,2)                       000003
00113    19*           EQUIVALENCE (NAME,ANAME)                                               000003
00114    20*           INTEGER FOX,OX,ZERO                                                    000003
00115    21*           LOGICAL MOLES,NEWR                                                     000003
00116    22*           DIMENSION LINE1(21),LINE2(19),LINE3(16)                                000003
00117    23*           DIMENSION IOUT(21)                                                     000003
00120    24*           DATA (LINE1(I),I=1,21)/' INDEX',4*'      ',                            000003
00120    25*          X   'REACTA','NT(#) ',3*'      ','     R',                             000003
00120    26*          X   'EL WT/','   MOL','E  ENT','HALPY/',                               000003
00120    27*          X   '   PHA','SE  TE','MP,K  ',' FUEL/','  DENS','ITY   '/            000003
00122    28*           DATA (LINE2(I),I=1,19)/10*'      ',                                   000003
00122    29*          X   '     N','O MOLE','S     ','   INT',                              000003
00122    30*          X   ' ENERG','Y     ',2*'      ',' OXID'/                            000003
00124    31*           DATA (LINE3(I),I=1,16)/8*'      ',                                   000003
00124    32*          X   '  #   ','   IND','ICATES',' ENTHA','LPY TO',' BE CA',             000003
00124    33*          X   'LCULAT','ED    '/                                                000003
00124    34*     C                                                                             000003
00126    35*           DATA N3/8/,N8/12/                                                      000003
00131    36*                                                                                  000003
00131    37*     C                                                                  RCTN0022   000003
00131    38*           DO 8 K = 1,2                                                           000003
00134    39*           WP(K)=0.                                                               000003
00135    40*           HPP(K)=0.                                                              000003
00136    41*           RH(K)=0.                                                               000004
00137    42*           VPLS(K)=0.                                                             000005
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```
00140   43.         VMIN(K)=0.                                          000006
00141   44.         AM(K)=0.                                            000007
00142   45.         DO 8 J=1,25                                         000013
00145   46.         LLMT(J)=0                                           000013
00146   47.       8 BOP(J,K) = 0.0                                      000013
00151   48.         NFUEL = 0                                           000017
00152   49.         N=1                                                 000020
00152   50.   C     WRITE REACTANT HEADER                               000020
00153   51.         CALL GOUT(LINE1,126)                                000022
00154   52.         CALL GOUT(LINE2,114)                                000026
00155   53.         L=1                                                 000032
00156   54.         IO=43                                               000034
00156   55.   C     READ REACTANTS                                      000034
00157   56.            REWIND IO                                        000036
00160   57.       6 READ (IO) NREAC,CF                                  000042
00164   58.      10 IF (IO.EQ.NB) GO TO 20                              000047
00166   59.         IF (CF.LT.1.0) GO TO 18                             000052
00171   60.         REWIND IO                                           000056
00172   61.         READ (N8) NREAC,CF,HHVV,HCR,PER                     000060
00201   62.      18 IF (NREAC.EQ.0.0) GO TO 200                         000072
00203   63.      20    CONTINUE                                         000074
00204   64.         READ (IO) (NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),  000074
00204   65.        X    NAME(N,6),ANUM(N,6),FAZ(N),                     000074
00204   66.        X    RTEMP(N),FOX(N),DENS(N)                         000074
00224   67.         NAST=1H                                             000124
00225   68.         IF (NAME(N,6).EQ.2H00) NAST=1H*                     000127
00227   69.         ENCODE (30,IOUT) N,(NAME(N,J),ANUM(N,J),J=1,5),PECWT(N),MOLE,  000135
00227   70.        X    ENTH(N),NAST,FAZ(N),RTEMP(N),FOX(N),DENS(N)     000135
00247   71.         CALL BOUT(IOUT,126)                                 000164
00250   72.      30 FORMAT (1X,I2,2X,5(A2,F8.4,2X),F10.6,2X,A1,F13.4,A1,3X,A1,F12.3,  000170
00250   73.        X    3X,A1,F12.5,1X)                                 000170
00251   74.         IF(L.EQ.0)GO TO 20                                  000170
00253   75.         IF (MOLE .EQ. MOL)  MOLES = .TRUE.                  000172
00253   76.   C     IF OXIDANT, K = 1; IF FUEL, K = 2.                  000172
00255   77.         IF(FOX(N).EQ.ZERO)  FOX(N)=OX                       000177
00257   78.         IF (PECWT(N) .LE. 0.0)  PECWT(N) = 1.0              000205
00261   79.         K = 1                                               000213
00262   80.         IF(FOX(N).EQ.OX)  GO TO 37                          000215
00264   81.         K = 2                                               000221
00265   82.         NFUEL = NFUEL+1                                     000223
00266   83.      37 DO 38 J=1,25                                        000226
00271   84.      38 DATA(J) = 0.0                                       000233
00273   85.         RM=0.                                               000234
00274   86.         DO 100 JJ=1,6                                       000243
00277   87.         IF (ANUM(N,JJ) .LE. 0.0)  GO TO 101                 000243
00301   88.         IF (NAME(N,JJ) .EQ. ZERO)  NAME(N,JJ) = OX          000246
00303   89.         DO 41 J=1,15                                        000256
00306   90.         I = J                                               000256
00307   91.         IF(LLMT(J).EQ.0) GO TO 45                           000260
00311   92.      41 IF (NAME(N,JJ) .EQ. LLMT(J))  GO TO 46              000262
00314   93.      45 L = I                                               000270
00315   94.         LLMT(J)=NAME(N,JJ)                                  000272
00316   95.      46 DO 48 I = 1,101                                     000300
00321   96.      48 IF (ATOM(1,I) .EQ. ANAME(N,JJ))  GO TO 50           000300
00324   97.         L=0                                                 000306
00325   98.         GO TO 20                                            000307
```

```
00326   99*        50  RM = RM * ANUM(N,JJ)*ATOM(2,I)                                  000311
00327  100*            W(J) = ATOM(J,I)                                                 000317
00330  101*       100  DATA(J) = ANUM(N,JJ)                                            000321
00332  102*       101  PCNT=PECNT(N)                                                   000327
00333  103*            IF(MOLES) PCNT=PCNT*RM                                         000332
00335  104*            WP(K)=WP(K) + PCNT                                             000337
00336  105*            IF (NAME(N,6).NE.IZERO) HPP(K)=HPP(K)+ENTH(N)*PCNT/RM          000343
00340  106*            AM(K)=AM(K)+PCNT/RM                                            000365
00341  107*            DO 110  J=1,L                                                  000377
00344  108*       110  BOP(J,K) = DATA(J)*PCNT/RM + BOP(J,K)                        000377
00346  109*            IF (DENS(N) .GT. 0.0)  RH(K) = RH(K) + PCNT/DENS(N)            000404
00350  110*            RM(N1) = RM                                                    000415
00351  111*            N = N+1                                                        000420
00352  112*            IF (N.EQ.26) GO TO 200                                         000423
00354  113*            IF (IO.EQ.N3.AND.N-1.EQ.NREAC) GO TO 200                       000425
00356  114*            IF (IO.EQ.N8.AND.N-1.EQ.NN1+NREAC) GO TO 200                   000442
00360  115*            GO TO 20                                                       000461
00361  116*       200  NN1=N-1                                                        000463
00362  117*            IF (IO.EQ.N8) GO TO 204                                        000465
00364  118*            IO=N8                                                          000470
00365  119*            REWIND IO                                                      000472
00366  120*            READ (IO) NREAC,CF,HHVV,WCR,PER                                000475
00375  121*            IF (NREAC.EQ.0) GO TO 204                                      000506
00377  122*            DO 202 I=1,4                                                   000512
00402  123*            READ (IO) NDUMMY                                               000512
00405  124*       202  CONTINUE                                                       000517
00407  125*            GO TO 6                                                        000517
00410  126*       204  NREAC=NN1                                                     000521
00411  127*            IF(NFUEL.GT.0)  GO TO 210                                      000522
00411  128*  C         100 PERCENT OXIDANT, CALL REACTANTS FUEL                       000522
00413  129*            DO 205  N=1,NREAC                                              000534
00416  130*       205  FOX(N) = BLANK                                                 000534
00420  131*            RH(2) = RH(1)                                                  000536
00421  132*            RH(1) = 0.                                                     000540
00422  133*            WP(2) = WP(1)                                                  000541
00423  134*            WP(1) = 0.                                                     000543
00424  135*            HPP(2) = HPP(1)                                                000544
00425  136*            AM(2) = AM(1)                                                  000546
00426  137*            AM(1) = 0.                                                     000550
00427  138*            DO 208  J=1,L                                                  000554
00432  139*       208  BOP(J,2) = BOP(J,1)                                          000554
00434  140*       210  IF (L.NE.0) GO TO 214                                        000557
00436  141*            WRITE (JOUT,212)                                               000560
00440  142*       212  FORMAT ('0','ERROR IN REACTANT DATA')                        000566
00441  143*       214  CALL GOUT(' ',1)                                             000566
00442  144*            CALL GOUT(LINE3,96)                                            000571
00443  145*            CALL MOVABS(500,50)                                            000575
00444  146*            CALL HOLDIT                                                    000601
00445  147*            CALL PAGIT                                                     000603
00446  148*            DO 220 K=1,2                                                   000605
00451  149*            IF (WP(K) .LE. 0.0)  GO TO 220                                 000637
00453  150*            HPP(K)=HPP(K)/WP(K)                                            000642
00454  151*            AM(K) = WP(K)/AM(K)                                            000645
00455  152*            IF (RH(K) .GT. 0.0)  RH(K) = WP(K)/RH(K)                       000650
00457  153*            DO 215 J=1,L                                                   000662
00462  154*            BOP(J,K)=BOP(J,K)/WP(K)                                        000662
```

```
00463  155.          IF(V(J) .LT. 0.)VMIN(K) = VMIN(K)+BOP(J,K)*V(J)                    000664
00465  156.    215   IF (V(J) .GT. 0.0)  VPLS(K) = VPLS(K) + BOP(J,K)*V(J)             000673
00470  157.          IF(MOLES) GO TO 220                                                000705
00472  158.          DO 218 N=1,NREAC                                                   000712
00475  159.          IF((FOX(N).EQ.OX.AND.K.EQ.2).OR.(FOX(N).NE.OX.AND.K.EQ.1))GOTO218  000712
00477  160.          PECNT(N) = PECNT(N)/MP(K)                                          000732
00500  161.    218   CONTINUE                                                           000742
00502  162.    220   CONTINUE                                                           000742
00504  163.          NEWR=.TRUE.                                                        000742
00504  164.    C  ARE ELEMENTS SAME AS FOR  LAST SET OF REACTANTS, IF SO, NEWR=.FALSE.  4/23/70  000742
00505  165.          IF (L .NE. NLS .OR. NOMIT .NE. 0)  GO TO 226                       000744
00507  166.          DO 224 I=1,NLS                                                     000756
00512  167.          DO 222 J = 1,L                                                     000771
00515  168.          IF(LLMT(J).NE.LLMTS(I))  GO TO 222                                 000771
00517  169.          SBOP(I,1) = BOP(J,1)                                               000774
00520  170.          SBOP(I,2) = BOP(J,2)                                               000776
00521  171.          GO TO 224                                                          001000
00522  172.    222   CONTINUE                                                           001003
00524  173.          GO TO 226                                                          001003
00525  174.    224   CONTINUE                                                           001006
00527  175.          NEWR = .FALSE.                                                     001006
00530  176.          DO 225 I = 1,L                                                     001012
00533  177.          LLMT(I) = LLMTS(I)                                                 001012
00536  178.          BOP(I,1) = SBOP(I,1)                                               001013
00535  179.    225   BOP(I,2) = SBOP(I,2)                                               001015
00537  180.          GO TO 229                                                          001020
00540  181.    226   NLS = L                                                            001022
00541  182.          REWIND 9                                                           001023
00542  183.          DO 228 I = 1,L                                                     001026
00545  184.          SBOP(I,1) = BOP(I,1)                                               001033
00546  185.          SBOP(I,2) = BOP(I,2)                                               001034
00547  186.    228   LLMTS(I) = LLMT(I)                                                 001036
00551  187.    229   DO 230  N=1,NREAC                                                  001042
00554  188.          IF (DENS(N) .GT. 0.0)  GO TO 230                                   001046
00556  189.          RH(2) = 0.                                                         001050
00557  190.          RH (1) = 0.                                                        001051
00560  191.          RETURN                                                             001052
00561  192.    230   CONTINUE                                                           001057
00563  193.          RETURN                                                             001057
00564  194.          END                                                  RCTN0111      001110
```

END OF COMPILATION: NO DIAGNOSTICS.

aHDG,P RKTOUT

```
@FOR,S    RKTOUT,RKTOUT
HSA  S3 -10/15/80-13:07:33 (12,)

    SUBROUTINE RKTOUT    ENTRY POINT 000532

    STORAGE USED: CODE(1) 000541; DATA(0) 000122; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003   CONSTS 000006
     0004   POINTS 000335
     0005   SPECES 017106
     0006   INDX   000041
     0007   PERF   000166
     0010   OUPT   000073
     0011   CCC    000003
     0012   CFUEL  000001

    EXTERNAL REFERENCES (BLOCK, NAME)

     0013   MOVABS
     0014   OUT1
     0015   VARFNT
     0016   OUT2
     0017   GAMEFF
     0020   OUT3
     0021   OUT4
     0022   NWDUS
     0023   NIO2S
     0024   NIO1S
     0025   SQRT
     0026   NIO3S
     0027   NERR3S

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001   000063 1466      0000   000066 150F      0001   000074 1546      0001   000121 1706      0001   000150 2006
     0001   000202 200L      0000   000075 208F      0001   000422 220L      0001   000235 2226      0001   000263 2366
     0001   000316 2546      0001   000340 2666      0001   000350 2746      0001   000366 3056      0001   000511 312L
     0001   000416 3216      0001   000427 3266      0001   000445 3376      0001   000466 3506      0001   000505 3606
     0000   000006 37F       0000   000027 38F       0000   000056 40F       0001   000520 400L      0000   000047 737F
     0005   011052 A         0007 R 030150 AEAT      0007 R 000133 APP       0003 R 000000 ATMN      0000 R 000002 AW
     0006   000036 CALCH     0012 R 030000 CF        0005   000000 COEF      0006   000001 CONVG     0004   000032 CPR
     0000 R 000005 CSTR      0005   010624 DELN      0011   000002 DEMAND    0004   000064 DLVPT     000A   000047 DLVTP
     0005   009312 EN        0005   010150 ENLN      0007 L 000165 EQL       0010 R 000002 FA        0010   000003 FAP
     0010 R 000005 FB        0010 R 000006 FC        0010   000007 FCP       0010 R 000012 FCST      0010 R 000014 FCV
     0010 R 000015 FG        0010 R 000017 FGE       0010 R 000020 FGV       0010   000021 FH        0010 R 000023 FI
     0010 R 000025 FIV       0010   000027 FM        0010 R 000031 FMT       0010 R 000050 FN        0010 R 000052 FOUR
     0010 R 000053 FP        0010   000054 FS        0010   000056 FSV       0010   000057 FT        0010   000061 FTR
     0010   000063 FV        0010 R 000065 FVEL      0010 R 000001 F13       0010 R 000000 F9X       0004 R 000101 GAMMAS
     0003 R 000001 GMET      0011   000000 GRAPH     0006   000003 HP        0004 R 000000 HSUM      0005 R 010376 HO
     0000 I 000004 I         0006   000030 IC        0006   000000 IDEBUG    0006   000015 IMAT      0007   000105 INJPS
```

0006	000023	IONS	0006	000021	IP	0006	000037	IQSAVE	0006	000016	I01	0006	000005	ISV	
0006 I	000039	IT	0005	016266	IUSE	0006	000026	JLIO	0011 I	000001	JOUT	0006	000025	JSOL	
0006	000031	JS1	0000 I	000003	K	0006	000014	KMAT	0006	000000	LSAVE	0006	000006	MOLES	
0006	000024	NC	0006	000022	NEWR	0006	000035	NFZ	0006	000012	NLM	0006	000017	NOF	
0006	000020	NOMIT	0006	000007	NP	0006	000011	NPT	0006	000027	NREAC	0006	000013	NS	
0000 I	000000	NSPP1	0006	000010	NT	0010 R	000043	ONE	000A	000116	P	0003 R	000002	PATM	
0007	000000	PCP	0004 R	000217	PPP	0003	000003	RBAR	0003 R	000004	RBR	0003	000005	RVR	
0005	000064	S	0006	000033	SHOCK	0005	016664	SLN	0004 R	000251	SONVEL	0006	000000	SP	
0007 R	000047	SPIM	0006	000015	SSUM	0005	018364	SUB	0007	000101	SUBAR	0007	000116	SUPAR	
0004 R	000150	T	0000 R	000001	TEM	0005	016514	TEMP	0010 R	000070	THREE	0004	000320	TOTN	
0006	000002	TP	0004 R	000266	TTT	0010 R	000071	TWO	0004 R	000202	V	0007 R	000064	VACI	
0004	000103	VLM	0007 R	000032	VMOC	0006	000032	VOL	000A R	000234	W	0010	000072	ZERO	

```
00101      1•          SUBROUTINE RKTOUT (IGAM)                                                    000000
00101      2•    C                                                                                 000000
00101      3•    C  ROCKET PERFORMANCE PARAMETERS                                                  000000
00101      4•    C                                                                    ROUTOOO1     000000
00103      5•          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                    /CONSTS/     000000
00104      6•          COMMON/POINTS/MSUM(13),SSUM(13),CPR(13),,OLVTP(13),OLVPT(13)                000000
00104      7•         1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)            000000
00104      8•         2 ,VLM(13),IOIN(13)                                                          000000
00104      9•    C     COMMON/SPECES/COEF(7,150),S(150),EN(150,13),,NLW(150),HO(150)               000000
00104     10•    C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)             000000
00105     11•          INCLUDE SPECPR                                                               000000
00111     12•          COMMON /INDX/ IDEBUG,CONVG,TP,MP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,    /INDX/    000000
00111     13•         1              KMAT,IMAT,I01,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIO,  /INDX/    000000
00111     14•         2              NREAC,IC,JS1,VOL,SHOCK,II,NFZ,CA,CM,IQSAVE,LSAVE     /INDX/    000000
00112     15•          COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),        /PERF/    000000
00112     16•         1              SUPAR(13),APP(13),AEAT(13),EQL                       /PERF/    000000
00113     17•          COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),    /OUPT/    000000
00113     18•         1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FNT(18),FM(2),FOUR, /OUPT/    000000
00113     19•         2              FP,FS(2),FSV,FT(2),FTH(2),FV(2),FVEL(2),ONE,THREE,   /OUPT/    000000
00113     20•         3              TWO,ZERO                                             /OUPT/    000000
00113     21•    C                                                                                 000000
00114     22•          COMMON /CCC/ GRAPH,JOUT,DEMAND                                               000000
00114     23•    C                                                                                 000000
00115     24•          COMMON /CFUEL/CF                                                             000000
00116     25•          LOGICAL EQL                                                                  000000
00117     26•          CALL MOVABS(500,50)                                                          000000
00120     27•          IF(EQL) WRITE(JOUT,37)                                                       000003
00123     28•       37 FORMAT(1H1/29X,84HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRROCK0090   000012
00123     29•         1IUM COMPOSITION DURING EXPANSION         //)                               000012
00124     30•          IF (.NOT.EQL) WRITE(JOUT,38)                                                 000012
00127     31•       38 FORMAT(1H1,26X,78HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN CROCK0107   000023
00127     32•         1POSITION DURING EXPANSION         //)                          ROCK0108   000023
00130     33•          IF(TTT(1).EQ.T(IT)) WRITE(JOUT,737)                                          000023
00133     34•      737 FORMAT (52X,28HAT AN ASSIGNED TEMPERATURE      )                             000034
00134     35•          TEM = PATM*PPP(1)                                                            000034
00135     36•          AW = ATMN*PPP(1)                                                             000037
00136     37•          WRITE(JOUT,40) TEM,AW                                                        000042
00142     38•       40 FORMAT (5H PC =,F10.3,7H PSIA =,1PE13.6,7H N/M**2)                           000051
00143     39•          CALL OUT1                                                                    000051
00144     40•          K = NPT - 2                                                                  000053
```

```
00145   91.         DO 20 I = 1,K                                          000056
00150   92.      20 V(I) = WHEXIT                                          000063
00152   93.         WRITE(JOUT,150) (V(I), I = 1,K)                        000065
00160   94.   150   FORMAT (1HO,16X,16HCHAMBER   THRO,T,11(5X,A4))  RKT01590 000077
00160   95.   C     PRESSURE RATIOS                              OUTP0030  000077
00161   96.         FMT(3) = ONE                                           000077
00162   97.         CALL VARFMT (APP,NPT)                                  000101
00163   98.         WRITE(JOUT,FMT) FP,FB,FB,(APP(I), I = 1,NPT)           000105
00170   99.         CALL OUT2                                              000124
00175   100.        IF (NPT .LT. 2)  GO TO 312                             000126
00177   101.        DO 202 K=2,NPT                               ROUT0028  000136
00202   102.        SPIM(K) = SQRT(2.0*RBR*(HSUM(1) - HSUM(K)))/GMET       000150
00202   103.  C  AM (A/M) IN UNITS OF SEC/ATM                              000150
00203   104.        AM = RBR*TTT(K)/(PPP(K)*WM(K)*SPIM(K)*GMET**2)         000161
00204   105.        IF (K.NE.2)GO TO 200                         ROUT0031  000171
00206   106.        CSTR = GMET*AM*PPP(1)                                  000174
00207   107.        AEAT(2) = 1.                                           000177
00210   108.     200 VACI(K)=SPIM(K)+PPP(K)*AM                             000202
00211   109.        IF (SONVEL(K) .GT. 0.0)  VMOC(K) = GMET*SPIM(K)/SONVEL(K)  000205
00213   110.     202 V(K) = GMET*SPIM(K)                                   000214
00215   111.        V(1) = 0.0                                             000221
00216   112.        WRITE(JOUT,FMT) FGV,FVEL,(V(I), I = 1,NPT)             000222
00216   113.  C   MACH NUMBER                                  ROUT0040  000222
00226   114.        FMT(4) = FOUR                                          000240
00227   115.        VMOC(1)=0.                                   ROUT0042  000242
00230   116.        IF (GAMMAS(2) .LE. 0.0)  VMOC(2) = 0.0                 000243
00232   117.        WRITE(JOUT,FMT) FN,FB,(VMOC(I), I = 1,NPT)             000247
00242   118.        WRITE(JOUT,208)                                        000266
00244   119.     208 FORMAT (1H )                                 ROUT0048  000273
00244   120.  C   AREA RATIO                                     ROUT0062  000273
00245   121.        CALL VARFMT (AEAT,NPT)                                 000273
00246   122.        FMT(3) = F9X                                           000301
00247   123.        WRITE(JOUT,FMT) FA,FB,FB,(AEAT(I), I = 2,NPT)          000303
00247   124.  C     CSTAR                                                  000303
00260   125.        FMT(4) = F13                                           000321
00261   126.        FMT(5) = TWO                                           000323
00262   127.        WRITE(JOUT,FMT) FCST,FB,(CSTR, I = 2,NPT)              000325
00262   128.  C   CF - THRUST COEFICIENT                        ROUT0055  000325
00272   129.        FMT(5) = FOUR                                          000343
00273   130.        DO 212  I=2,NPT                              ROUT0057  000350
00276   131.     212 V(I) = GMET*SPIM(I)/CSTR                              000350
00300   132.        WRITE(JOUT,FMT) FC,FB,FB,(V(I), I = 2,NPT)             000354
00311   133.        IF (IGAM .EQ. 0)  GO TO 220                            000371
00311   134.  C     EFFECTIVE GAMMA                                        000371
00313   135.        CALL GAMEFF (V,GAMMAS,APP,NPT,MO)                      000373
00314   136.        WRITE(JOUT,FMT) FGE(1),FGE,FB,(MO(I), I = 2,NPT)       000402
00314   137.  C     VACUUM THRUST COEFFICIENT                  RKT01050    000402
00325   138.     220 DO 230 I = 2,NPT                                      000422
00330   139.     230 V(I) = GMET*VACI(I)/CSTR                              000427
00332   140.        WRITE(JOUT,FMT) FCV,FB,FB,(V(I), I = 2,NPT)            000433
00332   141.  C   VACUUM IMPULSE                                 ROUT0067  000433
00343   142.        FMT(5) = THREE                                         000450
00344   143.        WRITE(JOUT,FMT) FIV,FB,(VACI(I), I = 2,NPT)            000452
00344   144.  C   SPECIFIC IMPULSE                              ROUT0071  000452
00350   145.        WRITE(JOUT,FMT) FI,FB,(SPIM(I), I = 2,NPT)             000471
00350   146.  C     FROZEN MOLE FRACTION OUTPUT MOVED TO SUBROUTINE OUT3   000471
```

```
00364    97.          312 CALL OUT3                                    000511
00365    98.              IF (CF+1.0) .400.                            000512
00370    99.              CALL OUT4                                    000515
00371   100.          400 CONTINUE                                     000520
00372   101.              RETURN                                       000520
00373   102.              END                                          000540
```

END OF COMPILATION: NO DIAGNOSTICS.

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$HDR.P    ROCKET
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@FOR,S    ROCKET,ROCKET
HSA  E3 -10/15/80-13:07:36 (10.)

      SUBROUTINE ROCKET    ENTRY POINT 001310

      STORAGE USED: CODE(1) 001317; DATA(0) 000231; BLANK COMMON(2) 000000

       COMMON BLOCKS:

       0003   CONSTS  000006
       0004   POINTS  000335
       0005   MISC    001701
       0006   INDX    000041
       0007   PERF    000166
       0010   CCC     000003

      EXTERNAL REFERENCES (BLOCK, NAME)

       0011   NEWOF
       0012   FROZEN
       0013   EQLBRM
       0014   RKTOUT
       0015   SAVE
       0016   NWDUS
       0017   NIO2S
       0020   NRNLS
       0021   NWNLS
       0022   XPRR
       0023   ALOG
       0024   EXP
       0025   XPDR
       0026   SQRT
       0027   NERR3S

      STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

       0001   000013 1256      0001   000162 1332L     0001   000035 1046      0001   000054 1566      0000   000104 1811F
       0001   000302 194L      0001   000420 192L      0000   000101 194F      0001   000261 195L      0001   000126 2036
       0000   000065 302F      0001   000026 303L      0001   000045 306L      0001   000103 321L      0001   000122 322L
       0001   000153 331L      0001   000160 332L      0001   000175 333L      0001   000213 334L      0001   000610 799L
       0001   000536 800L      0001   000763 802L      0001   000640 805L      0001   000703 809L      0001   000653 810L
       0001   001007 820L      0000   000125 821F      0001   001015 830L      0001   001043 834L      0001   001053 835L
       0001   001055 859L      0001   001061 860L      0000   000137 862F      0000   000166 865F      0001   001121 870L
       0001   001135 880L      0001   000457 899L      0001   000477 900L      0000   000073 923F      0001   000416 925L
       0001   001171 990L      0001   001232 997L      0001   001264 999L      0007 R 000150 AEAT      0000 R 000037 AEATL
       0005   000640 AM        0005   000705 AM1       0005   001135 ANUM      0007 R 000133 APP       0000 R 000035 APPL
       0000 R 000033 ARATIO    0000 L 000005 AREA      0000 D 000001 ASQ       0003   000000 ATMN      0005   000004 ATOM
       0000 R 000030 AWT       0005   000514 BO        0005   000545 BOP       0006   000036 CALCH     0006   000001 CONV6
       0004 R 000032 CPR       0000 R 000023 CPRF      0005   000706 CPR1      0005 R 000634 CPSUM     0005   000654 DATA
       0010   000002 DEMAND    0005   001560 DENS      0000 R 000026 DH        0000 R 000032 DLNP      0000 R 000040 DLNPE
       0000 R 000027 DLT       0004   000064 DLVPT     0004 R 000047 DLVTF     0000 R 000034 ELN       0005   001700 ENLSAV
       0005 R 000000 ENN       0005   001676 ENNL      0005   001677 ENSAVE     0005   001414 ENTH      0007 L 000165 EQL
```

0005	000636	EQRAT	0005	001445	FAZ	0005	001527	FOX	0000 L	000006	FROZ	0004 R	000101	GAMMAS
0003	000001	GMET	0010	000000	GRAPH	0006 L	000003	HP	0005	000642	HPP	0005	000637	HSUB0
0004 R	000000	HSUM	0000 I	000012	I	0006	000030	IC	0000 I	000000	ICASE	0006 I	000000	IDEBUG
0000 I	000011	IGAM	0006	000015	IMAT	0000	000215	INJPS	0000 I	000016	IOF	0005	000023	IONS
0006 I	000021	IP	0000 I	000022	IPP	0006	000037	IQSAVE	0006	000016	IQ1	0000 I	000020	ISUB
0000 I	000021	ISUP	0006 I	000005	ISV	0006 I	00003A	IT	0000 I	000017	ITNUM	0000 I	000025	ITROT
0006	000026	JLIQ	0010 I	000001	JOUT	0006 I	000025	JSOL	0006	000031	JS1	0006	000014	KMAT
0005	000463	LLMT	0006	000040	LSAVE	0006	000006	MOLES	0005	000707	NAME	0006	000024	NC
0006	000022	NEWR	0006 I	000035	NFZ	0006	000012	NLM	0006 I	000017	NOF	0006	000020	NOMIT
0006 I	000007	NP	0000 I	000013	NPP	0006 I	000011	NPT	0006	000027	NREAC	0006	000013	NS
0000 I	000014	NSUB	0000 I	000015	NSUP	0006 I	000010	NT	0005 R	000635	OF	0005 R	001644	OXF
0004 R	000116	P	0003	000002	PATM	0007 R	000000	PCP	0000 R	000031	PCPLT	0005	001363	PECNT
0005 R	000633	PP	0004 R	000217	PPP	0003	000003	RBAR	0003 R	000004	RBR	0005	000644	RH
0005	001611	RHOP	0000	000041	RKTINP	0005	001612	RMW	0005	001476	RTEMP	0003	000005	RVR
0000 L	000007	SEQL	0006	000033	SHOCK	0004	000251	SONVEL	0006 L	000004	SP	0007	000017	SPIM
0004 R	000015	SSUM	0007 R	000101	SUBAR	0005	000001	SUMN	0007 R	000116	SUPAR	0005 R	000003	SO
0004 R	000150	T	0000 L	000010	THI	0005	000632	THIGH	0005	001643	TLN	0005	000630	TLOW
0005	000627	TM	0000 R	000024	TMELT	0005	000631	TMID	0000 R	000036	TOL	0004	000320	TOTN
0006 L	000002	TP	0005 R	000002	TT	0004 R	000266	TTT	0000 D	000003	USQ	0004	000202	V
0007	000064	VACI	0004	000303	VLM	0005	000646	VMIN	0007	000032	VMOC	0006	000032	VOL
0005	000650	VPLS	0004 R	000234	WM	0005	000652	WP						

```
00101     1*          SUBROUTINE ROCKET                                                ROCK0002   000000
00101     2*    C                                                                      ROCK0001   000000
00101     3*    C     ROCKET PERFORMANCE                                               ROCK0004   000000
00101     4*    C                                                                                 000000
00103     5*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                      /CONSTS/   000000
00104     6*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)               000000
00104     7*         1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)          000000
00104     8*         2 ,VLM(13),TOTM(13)                                                       000000
00105     9*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),                 000000
00105    10*         1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,           000000
00105    11*         2              HSUB0,AM(2),HPP(2),RM(2),VMIN(2),VPLS(2),WP(2),  /MISC/   000000
00105    12*         3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECNT(25),        000000
00105    13*         4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,         000000
00105    14*         5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                    000000
00106    15*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,  /INDX/   000000
00106    16*         1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/   000000
00106    17*         2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE    /INDX/   000000
00107    18*          COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),      /PERF/   000000
00107    19*         1              SUPAR(13),APP(13),AEAT(13),EQL                     /PERF/   000000
00107    20*    C                                                                                 000000
00110    21*             COMMON /CCC/ GRAPH,JOUT,DEMAND                                         000000
00110    22*    C                                                                                 000000
00111    23*          DATA ICASE/0/                                                             000000
00113    24*          DOUBLE PRECISION ASQ,USQ                                                  000000
00114    25*          LOGICAL AREA,EQL,FROZ,HP,SEQL,SP,THI,TP                                   000000
00114    26*    C                                                                                 000000
00115    27*          NAMELIST /RKTINP/ EQL,FROZ,IGAM,PCP,SUBAR,SUPAR                  /RKTINP/   000000
00115    28*    C                                                                                 000000
00116    29*          NFZ = 1                                                                   000000
00117    30*          APP(1) = 1.                                                               000001
00120    31*          IF (ICASE .GT. 0)  GO TO 303                                              000003
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00122   32*           ICASE = 1                                          000006
00123   33*           IGAM = 0                                           000007
00124   34*           DO 300 I=1,26                                      000013
00127   35*           PCP(I)= 0.                                         000013
00130   36*    300    SUBAR(I) = 0.0                                     000013
00132   37*           EQL = .TRUE.                                       000015
00133   38*           FROZ = .FALSE.                                     000017
00134   39*           WRITE (6,302)                                      000020
00136   40*    302    FORMAT (' BEGIN NAMELIST RKTINP INPUT')            000026
00137   41*    303    READ (5,RKTINP)                                    000026
00142   42*           NPP = 0                                            000031
00143   43*           DO 305 I = 1,26                                    000035
00146   44*           IF (PCP(I) .LE. 0.0)  GO TO 306                    000035
00150   45*    305    NPP = I                                            000040
00152   46*    306    NPP = NPP*2                                        000045
00153   47*           NSUB = 0                                           000047
00154   48*           NSUP = 0                                           000050
00155   49*           DO 320  I=1,13                                     000054
00160   50*           IF (SUBAR(I) .GT. 0.0)  NSUB = NSUB + 1            000054
00162   51*    320    IF (SUPAR(I) .GT. 0.0)  NSUP = NSUP + 1            000061
00165   52*           WRITE(JOUT,RKTINP)                                 000071
00170   53*           SEQL = EQL                                         000075
00171   54*           IOF = 0                                            000077
00172   55*           II = 3000.                                         000100
00172   56*    C      LOOP FOR EACH O/F                                  000100
00173   57*      321  IT = 1                                             000103
00174   58*           IOF = IOF + 1                                      000104
00175   59*           OF = OXF(IOF)                                      000107
00176   60*           CALL NEWOF                                         000111
00177   61*           IF (T(I) .LE. 0.0)  GO TO 322                      000113
00201   62*           TT = T(IT)                                         000117
00201   63*    C      LOOP FOR CHAMBER PRESSURES                         000117
00202   64*      322  DO 998 IP = 1,NP                                   000122
00205   65*           ITNUM = 0                                          000126
00206   66*           AREA = .FALSE.                                     000127
00207   67*           IF (T(1) .LE. 0.0)  HP = .TRUE.                    000130
00211   68*           IF (T(1) .GT. 0.0)  TP = .TRUE.                    000135
00213   69*           SP = .FALSE.                                       000142
00214   70*           EQL = .TRUE.                                       000143
00215   71*           ISUB = 1                                           000145
00216   72*           ISUP = 1                                           000146
00217   73*           PP = P(IP)                                         000147
00220   74*           IPP = 1                                            000151
00220   75*    C      LOOP FOR PRESSURE RATIOS                           000151
00221   76*      331  IF(EQL)  GO TO 332                                 000153
00223   77*           CALL FROZEN                                        000154
00224   78*           GO TO 1332                                         000156
00225   79*      332  CALL EQLBRM                                       000160
00225   80*    C      TT = 0 IF NO CONVERGENCE                           000160
00226   81*    1332   IF (TT .GT. 0.0)  GO TO 333                       000162
00230   82*           IF (NPT .LT. 2)  RETURN                            000164
00232   83*           GO TO 900                                          000173
00233   84*      333  IF(IPP.GT.1) GO TO 195                            000175
00233   85*    C      COMBUSTION CHAMBER                        ROCK0060 000175
00235   86*           EQL = SEQL                                         000200
00236   87*           TP = .FALSE.                              ROCK0062 000202
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00237   88*          HP = .FALSE.                                          ROCK0063   000203
00238   89*          SP = .TRUE.                                           ROCK0064   000204
00241   90*          SO = SSUM(1)                                                     000206
00242   91*          CPRF = CP SUM                                                    000210
00243   92*      334 TMELT=0.                                                         000213
00244   93*          ITROT = 3                                                        000213
00245   94*          THI = .FALSE.                                                    000215
00246   95*          APP(2)=((GAMMAS(1)+1.)/2.)**(GAMMAS(1)/(GAMMAS(1)-1.))  ROCK0066 000216
00247   96*          IF(EQL)  WRITE(JOUT,194) APP(2)                                  000234
00253   97*          PP = PPP(1)/APP(2)                                               000244
00254   98*          TT = 2.*TT/(GAMMAS(1)+1.)                                        000247
00255   99*          ISV = 1                                                          000255
00256  100*          GO TO 870                                                        000257
00257  101*      195 USQ = 2.0*RBR*(HSUM(1) - HSUM(NPT))                              000261
00260  102*          IF (IPP.GT.2) GO TO 900                                          000271
00260  103*    C     THROAT                                                ROCK0073   000271
00262  104*          IF (.NOT. THI)  GO TO 191                                        000275
00264  105*          GAMMAS(2) = 0.                                                   000277
00265  106*          GO TO 899                                                        000300
00264  107*      191 ASQ = RBR*GAMMAS(2)*TT*ENN                                       000302
00267  108*          IF(IDEBUG.EQ.1.OR.IDEBUG.EQ.2)  WRITE(JOUT,923)USQ,ASQ           000311
00274  109*      923 FORMAT(5HUSQ=,E15.8,5X,4HASQ=,E15.8)                             000334
00275  110*          DH = (USQ-ASQ)/ASQ                                               000336
00276  111*          IF(DH.LT.0.) DH=-DH                                              000341
00300  112*          IF(DH.LE.0.5E-5.OR.ITROT.EQ.0)  GO TO 899                        000346
00302  113*          IF (JSOL .NE. 0)  GO TO 925                                      000361
00304  114*          IF (TMELT .LE. 0.0)  GO TO 192                                   000363
00306  115*          DLT = ALOG(TMELT/TT)                                             000366
00307  116*          PP = PP*EXP(DLT*CPR(2)/(ENN*DLVTP(2)))                           000375
00310  117*          APP(2) = P(IP)/PP                                                000407
00311  118*          THI = .TRUE.                                                     000412
00312  119*          GO TO 331                                                        000414
00313  120*      925 TMELT = TT                                                       000416
00314  121*      192 APP(2) = APP(2)/(1.0 + (USQ - ASQ)/(ENN*(GAMMAS(2) + 1.0)*RBR*TT))  000420
00315  122*          PP = P(IP)/APP(2)                                                000437
00316  123*          ITROT = ITROT-1                                       ROCK0079   000442
00317  124*          IF(EQL)  WRITE(JOUT,194) APP(2)                                  000445
00323  125*      194 FORMAT(7H PC/PT=,F9.6)                                           000455
00324  126*          GO TO 331                                                        000455
00325  127*      899 AMT =ENN*TT/(PP*USQ**.5)                                         000457
00326  128*          PCPLT = ALOG(APP(2))                                             000472
00327  129*      900 ISV =0                                                           000477
00330  130*          IF (TT .LE. 0.0)  GO TO 860                                      000500
00332  131*          AEAT(NPT) = ENN*TT/(PP*USQ**.5*AMT)                              000503
00333  132*          IF(AREA)  GO TO 800                                              000521
00335  133*          IF(IPP.LT.NPP)  GO TO 859                                        000523
00337  134*          IF((NSUB+NSUP).EQ.0)  GO TO 860                                  000527
00341  135*          AREA = .TRUE.                                                    000533
00341  136*    C     PCP ESTIMATES FOR AREA RATIOS                                    000533
00342  137*      800 IF(ITNUM.NE.0)  GO TO 810                                        000536
00344  138*          DLNP = 1.                                                        000541
00345  139*          ITNUM = 1                                                        000543
00346  140*          ARATIO = SUBAR(ISUB)                                             000545
00347  141*          IF(NSUB.LE.0)  ARATIO=SUPAR(ISUP)                                000551
00351  142*          ELN = ALOG(ARATIO)                                               000557
00352  143*          IF(NSUB.LE.0)  GO TO 799                                         000563
```

```
00354  144*          APPL = PCPLT/(SUBAR(ISUB)+(10.587*ELN**2-9.454)*ELN)                    000566
00355  145*          IF(ARATIO.LT.1.09)  APPL=.9*APPL                                        000577
00357  146*          GO TO 859                                                               000606
00360  147*      799 IF(SUPAR(ISUP).LT.2.)  GO TO 805                                        000610
00362  148*          IF(ISUP.GT.1.AND.SUPAR(ISUP-1).GE.2.)  GO TO 802                        000614
00364  149*          APPL = GAMMAS(2)*ELN+1.0                                                000632
00365  150*          GO TO 859                                                               000636
00366  151*      805 APPL = SQRT(ELN*(1.535+3.294*ELN))+PCPLT                                000640
00367  152*          GO TO 859                                                               000651
00370  153*      810 IF (IDEBUG .LE. 0 .OR. NPT .LT. IDEBUG)  GO TO 809                      000653
00372  154*          WRITE(JOUT,1811) ITNUM,ARATIO,AEAT(NPT),APP(NPT),DLNP                   000667
00401  155*     1811 FORMAT (6HOITER=,I2,5X,15HASSIGNED AE/AT=,F15.8,5X,6HAE/AT=,F15.8,     000703
00401  156*         15X,5HPC/P=,F15.8,5X,11HDELTA LN P=,F15.8)                               000703
00402  157*      809 TOL = 1.0E-5                                                            000703
00403  158*          IF (ARATIO .GE. 10.0)  TOL = 4.0E-5                                     000706
00405  159*          IF (ABS(AEAT(NPT) - ARATIO)/ARATIO .LE. TOL)  GO TO 830                 000710
00407  160*          IF (ABS(DLNP) .LT. 4.0E-6)  GO TO 830                                   000724
00411  161*          AEATL = ALOG(AEAT(NPT))                                                 000730
00412  162*          ITNUM = ITNUM + 1                                                       000736
00413  163*          IF (ITNUM .GT. 25)  GO TO 820                                           000741
00415  164*          ASQ = RBR*GAMMAS(NPT)*ENN*TT                                            000744
00416  165*          DLNPE = GAMMAS(NPT)*USQ/(USQ-ASQ)                                       000754
00417  166*      802 DLNP = DLNPE*ELN-DLNPE*AEATL                                            000763
00420  167*          APPL = APPL + DLNP                                                      000771
00421  168*          IF(ITNUM.EQ.1)  GO TO 859                                               000773
00423  169*          APP(NPT) = EXP(APPL)                                                    000776
00424  170*          PP = P(IP)/APP(NPT)                                                     001002
00425  171*          GO TO 33                                                                001005
00426  172*      820 WRITE(JOUT,821) ARATIO                                                  001007
00431  173*      821 FORMAT (/10X,40HROCKET DID NOT CONVERGE FOR AREA RATIO =,F11.6/)        001015
00432  174*      830 ITNUM = 0                                                               001015
00433  175*          AEAT(NPT) = ARATIO                                                      001016
00434  176*          IF(NSUB.LE.0)  GO TO 834                                                001020
00436  177*          ISUB = ISUB+1                                                           001023
00437  178*          IF (ISUB .LE. NSUB)  GO TO 800                                          001026
00441  179*          ISUB = 1                                                                001031
00442  180*          NSUB = -NSUB                                                            001033
00443  181*          IF(ISUP.LE.NSUP)  GO TO 800                                             001035
00445  182*          GO TO 835                                                               001041
00446  183*      834 ISUP = ISUP+1                                                           001043
00447  184*          IF(ISUP.LE.NSUP)  GO TO 800                                             001045
00451  185*          ISUP = 1                                                                001050
00452  186*      835 AREA = .FALSE.                                                          001053
00453  187*          GO TO 860                                                               001053
00454  188*      859 ISV = NPT                                                               001055
00455  189*          IF(NPT.NE.13)  GO TO 870                                  ROCK0088      001056
00457  190*      860 CALL RKTOUT (IGAM)                                                      001061
00460  191*          IF (TT .LE. 0.0)  ISV = 0                                               001063
00462  192*          IF (.NOT. EOL .AND. TT .LE. 0.0)  WRITE(JOUT,862)                       001067
00465  193*      862 FORMAT (//2X,125HCALCULATIONS WERE STOPPED IN ROCKET BECAUSE NEXT       001104
00465  194*         1POINT IS MORE THAN 50 DEGREES BELOW TEMPERATURE RANGE OF A CONDENS      001104
00465  195*         2ED SPECIES)                                                             001104
00466  196*          IF (ISV.EQ.0) GO TO 990                                                 001104
00470  197*          IDEBUG = IDEBUG-13                                                      001106
00471  198*          WRITE(JOUT,865)                                                         001111
00473  199*      865 FORMAT(1H1)                                                             001116
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00474   200*          NPT = 2                                                  001116
00475   201*    870   NPT = NPT + 1                              ROCK0121      001121
00476   202*          IF(.NOT.EQL)  GO TO 880                                  001123
00500   203*          IF(ISV.EQ.1)  ISV = -1                                   001125
00502   204*          CALL SAVE                                                001132
00503   205*    880   IPP = IPP+1                                             001136
00504   206*          IF(NPT.EQ.2)  GO TO 331                                  001140
00506   207*          IF(.NOT.AREA)  APP(NPT)=PCP(IPP-2)                       001143
00510   208*          IF(AREA)  APP(NPT)=EXP(APPL)                             001154
00512   209*          PP = P(IP)/APP(NPT)                                      001163
00513   210*          GO TO 331                                                001167
00514   211*    990   IF(IDEBUG.LT.0)  IDEBUG=IDEBUG+13                       001171
00516   212*          IF(NSUB.LT.0)  NSUB=-NSUB                                001176
00520   213*          IF (.NOT.FROZ.OR..NOT.EQL)  GO TO 997                    001203
00522   214*          CPR(1) = CPRF                                            001206
00523   215*          GAMMAS(1) = CPRF/(CPRF-1./WM(1))                         001210
00524   216*          TT = TTT(1)                                              001215
00525   217*          IPP = 1                                                  001217
00526   218*          NPT = 1                                                  001221
00527   219*          CALL SAVE                                                001222
00530   220*          EQL = .FALSE.                                            001224
00531   221*          ENN = 1./WM(1)                                           001226
00532   222*          GO TO 334                                                001230
00533   223*    997   NPT = 1                                                  001232
00534   224*          WRITE(JOUT,865)                                          001233
00536   225*          IF (SEQL)  CALL SAVE                                     001240
00540   226*    998   TT = TTT(1)                                             001244
00542   227*          IF(IT.GE.NT)  GO TO 999                                  001250
00544   228*          IT = IT+1                                                001254
00545   229*          TT = T(IT)                                               001260
00546   230*          GO TO 322                                                001262
00547   231*    999   IF (IOF .GE. NOF)  RETURN                               001264
00551   232*          GO TO 321                                                001272
00552   233*          END                                      ROCK0129        001316

        END OF COMPILATION:        NO  DIAGNOSTICS.

@HDG,P      RREAD
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@FOR,S    RREAD,RREAD
HSA  E3 -10/15/80-13:07:40 (26,)

     SUBROUTINE RREAD     ENTRY POINT 001330

     STORAGE USED: CODE(1) 001345; DATA(0) 001373; BLANK COMMON(2) 000000

      COMMON BLOCKS:

      0003   CFUEL   000001

     EXTERNAL REFERENCES (BLOCK, NAME)

      0004   RDYES
      0005   PAGII
      0006   CHRSIZ
      0007   GOUT
      0010   NNCOD$
      0011   RDATAI
      0012   RDATAF
      0013   DMMRTF
      0014   RDCHAR
      0015   NREW$
      0016   NRBU$
      0017   NIO2$
      0020   NIO1$
      0021   NERR2$
      0022   NWBU$
      0023   NWEF$
      0024   NERR3$

     STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

      0001   000014 10L      0001   000277 100L     0001   000375 106L     0001   000437 110L     0001   000517 120L
      0001   000551 130L     0001   000605 140L     0001   000623 150L     0001   000644 160L     0001   000662 170L
      0001   000041 176G     0001   000703 200L     0001   000045 202G     0001   000116 232G     0001   000134 242G
      0001   000747 300L     0001   001032 310L     0001   000326 322G     0001   001062 330L     0001   001110 340L
      0001   000366 344G     0001   001127 350L     0001   001144 360L     0001   000454 365G     0001   001163 370L
      0001   000501 376G     0001   001201 400L     0001   001216 408L     0001   001305 420L     0001   000716 450G
      0001   000717 453G     0001   000070 50L      0001   000770 501G     0001   001015 512G     0001   001210 565G
      0001   001231 602G     0001   001235 606G     0001   001276 635G     0001   000177 70L      0000   001276 802F
      0001   000240 90L      0001   000274 95L      0000 R 000226 ANUM     0003 R 000000 CF       0000 R 000702 DENS
      0000 R 000536 ENTH     0000 R 001125 EXMP1A    0000 R 001140 EXMP1B    0000 R 001150 EXMP2     0000 R 001156 EXMP2B
      0000 R 001163 EXMP3    0000 R 001170 EXMP3B    0000 R 001177 EXMP4     0000 R 001203 EXMP5     0000 R 001207 EXMP6
      0000 R 001214 EXMP7    0000 R 000567 FAZ       0000 R 000651 FOX       0000 I 001252 I         0000 I 001257 ICHNG
      0000   001347 INJPS    0000 I 001250 IO        0000 I 001255 IOPT      0000 I 001023 IOUT      0000 I 001220 IREACT
      0000 I 001253 J        0000 I 001236 LINE0     0000 I 000733 LINE1     0000 I 000760 LINE2     0000 I 001003 LINE3
      0000 I 001050 MODIFY   0000 I 001065 MODMEN    0000 I 000535 MOLE      0000 I 001256 N         0000 I 000000 NAME
      0000 I 001254 NAST     0000 I 001260 NDUMMY    0000 I 001251 NREAC     0000 I 001246 N3        0000 I 001247 N8
      0000 R 000454 PECWT    0000 R 001224 RDUM      0004 L 000000 RDYES     0000 R 000620 RTEMP
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00101     1*            SUBROUTINE RREAD(FIRST)                                          000000
00103     2*            LOGICAL FIRST,RDYES                                              000000
00103     3*      C                                                                      000000
00103     4*      C     USE MIPS INPUT ROUTINES TO READ REACTANT CARDS (STORE ON FILE 8) 000000
00103     5*      C                                                                      000000
00103     6*      C     DATA ARRAYS FOR REACTANT CARDS                                   000000
00104     7*          DIMENSION NAME(25,6),ANUM(25,6),PECWT(25),MOLE(25),ENTH(25),     000000
00104     8*         X  FAZ(25),RTEMP(25),FOX(25),DENS(25)                               000000
00104     9*      C                                                                      000000
00105    10*            COMMON /CFUEL/CF                                                 000000
00105    11*      C     ARRAYS FOR DATA MENU'S                                           000000
00106    12*            DIMENSION LINE1(21),LINE2(19),LINE3(16),IOUT(21),MODIFY(13)      000000
00107    13*            DIMENSION MODMEN(9,8),EXMP1A(11),EXMP1B(8),EXMP2(6),EXMP2B(5),   000000
00107    14*         1  EXMP3(5),EXMP3B(7),EXMP4(9),EXMP5(9),EXMP6(5),EXMP7(8),       000000
00107    15*         2  IREACT(9),ROUM(10),LINED(8)                                      000000
00107    16*      C                                                                      000000
00107    17*      C     SET DATA ARRAYS FOR MENUS                                        000000
00110    18*            DATA LINED,6HTYPE  ,6HYES  T,6HO READ,6H IN PR,6HEVIOUS,         000000
00110    19*         1  6H REACT,6HANT SE,6HT     /                                    000000
00112    20*            DATA LINE1/6H INDEX,4*6H      ,6HREACTA,6HNT(*) ,3*6H      ,   000000
00112    21*         1  6H     R,6HEL WT/,6H   MOL,6HE  ENT,6HHALPY/,6H   PHA,6HSE  TE,  000000
00112    22*         2  6HMP,K  ,6H FUEL/,6H  DENS,6HITY  /                             000000
00114    23*            DATA LINE2/10*6H     ,6H    N,6HO MOLE,6HS     ,6H   INT,      000000
00114    24*         1  6H ENERG,6HY     ,2*6H      ,6H OXID /                         000000
00116    25*            DATA LINE3/8*6H      ,6H  *   ,6H   IND,6HICATES,6H ENTHA,      000000
00116    26*         1  6HLPY TO,6H BE CA,6HLCULAT,6HED     /                          000000
00120    27*            DATA MODMEN/24H 1-REACTANT FORMULA     ,                        000000
00120    28*         1  24H 2-REL WT/NO MOLES      ,24H 3-ENTHALPY/ENERGY//CALC ,      000000
00120    29*         2  24H 4-PHASE (S-L-G)        ,24H 5-TEMPERATURE (K)       ,      000000
00120    30*         3  24H 6-FUEL,OXIDIZER (F/O)  ,24H 7-DENSITY (G/CM3)       ,      000000
00120    31*         4  24H RETURN TO CONTINUE     /                                   000000
00122    32*            DATA EXMP1A/36H TYPE CHEMICAL FORMULA THIS REACTANT,             000000
00122    33*         1  3OH, HOLLERITH CODE FOR SYMBOLS /                             000000
00124    34*           DATA EXMP1B/48H EXAMPLE CARBON TETRACHLORIDE  1HC 1. 2HCL 4.   / 000000
00126    35*            DATA EXMP2/36H TYPE REL WEIGHT/NUMBER OF MOLES    /           000000
00130    36*            DATA EXMP2B/30H TYPE YES IF VALUE IS MOLES   /                  000000
00132    37*            DATA EXMP3/30H TYPE ENTHALPY/INTERNAL ENERGY/                   000000
00134    38*            DATA EXMP3B/42H TYPE YES IF ENTHALPY TO BE CALCULATED    /      000000
00136    39*            DATA EXMP4/24H TYPE PHASE (S-L-G)     /                         000000
00140    40*            DATA EXMP5/24H TYPE TEMPERATURE (K)   /                         000000
00142    41*            DATA EXMP6/30H TYPE FUEL/OXIDIZER (F/O)    /                    000000
00144    42*            DATA EXMP7/24H TYPE DENSITY (G/CC)    /                         000000
00146    43*            DATA MODIFY/6H TYPE ,6H 1, 2,,6HOR 3  ,6HTO MOD,6HIFY, D,       000000
00146    44*         1  6HELETE,,6H OR AD,6HD A RE,6HACTANT,6H (RETU,6HRN TO ,          000000
00146    45*         2  6HCONTIN,6HUE)   /                                            000000
00150    46*            DATA IREACT/24H TYPE REACTANT NUMBER   /                        000000
00152    47*          DATA N3/8/,N8/12/                                                 000000
00152    48*      C                                                                      000000
00155    49*           CALL PAGIT                                                       000000
00156    50*            IO=N3                                                           000001
00157    51*        6   NREAC=0                                                        000003
00157    52*      C                                                                      000003
00157    53*      C     FOR FIRST PASS DO NOT CHECK SAVED DATA                           000003
00160    54*            IF(.NOT.FIRST) GO TO 10                                         000004
00162    55*            IF(.NOT.RDYES(LINED,43)) GO TO 50                               000006
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00162    56*     C                                                              000006
00162    57*     C       READ IN PRESENT CASE                                   000006
00164    58*      10     CONTINUE                                               000014
00165    59*             IF (IO.EQ.N3) REWIND IO                                000014
00167    60*             READ (IO) NREAC,CF                                     000021
00173    61*             IF(NREAC.LT.1) GO TO 50                                000027
00175    62*             DO 25 I=1,NREAC                                        000033
00200    63*             READ (IO) (NAME(I,J),ANUM(I,J),J=1,5),PECNT(I),MOLE(I),  000041
00200    64*         X   ENTH(I),NAME(I,6),ANUM(I,6),FAZ(I),RTEMP(I),FOX(I),DENS(I)  000041
00220    65*      25     CONTINUE                                               000070
00220    66*     C                                                              000070
00220    67*     C       DISPLAY PRESENT SET OF REACTANTS (ADD IF NONE EXIST)   000070
00222    68*      50     CONTINUE                                               000070
00223    69*             CALL PAGIT                                             000070
00224    70*             CALL CHRSIZ(4)                                         000071
00225    71*          IF (NREAC.LT.1) GO TO 70                                  000074
00227    72*             CALL GOUT(LINE1,125)                                   000100
00230    73*             CALL GOUT(LINE2,114)                                   000104
00231    74*             DO 60 I=1,NREAC                                        000116
00234    75*             NAST=1H                                                000116
00235    76*             IF (NAME(I,6).EQ.2H00) NAST=1H*                        000120
00237    77*             ENCODE(802,IOUT,1) (NAME(I,J),ANUM(I,J),J=1,5),PECNT(I),MOLE(I),  000125
00237    78*         X   ENTH(I),NAST,FAZ(I),RTEMP(I),FOX(I),DENS(I)            000125
00257    79*             CALL GOUT(IOUT,125)                                    000153
00260    80*      60     CONTINUE                                               000162
00262    81*          CALL GOUT(' ',1)                                          000162
00263    82*             CALL GOUT(LINE3,92)                                    000166
00264    83*          CALL GOUT(' ',1)                                          000172
00265    84*      70     CONTINUE                                               000177
00266    85*             CALL GOUT(MODIFY,75)                                   000177
00267    86*             IOPT=0                                                 000202
00270    87*             CALL RDATAI(1,IOPT,$70)                                000203
00271    88*             IF(IOPT.LT.0 .OR. IOPT.GT.3) GO TO 70                  000210
00273    89*             IF(IOPT.EQ.0) GO TO 400                                000225
00275    90*             GO TO(90,90,300),IOPT                                  000227
00275    91*     C                                                              000227
00275    92*     C       SELECT REACTANT NUMBER                                 000227
00276    93*      90     CONTINUE                                               000240
00277    94*             N=1                                                    000240
00300    95*             IF(NREAC.EQ.1) GO TO 95                                000241
00302    96*             N=0                                                    000243
00303    97*             CALL GOUT(IREACT,29)                                   000246
00304    98*             CALL RDATAI(1,N,$90)                                   000250
00305    99*             IF(N.LT.1 .OR. N.GT.NREAC) GO TO 90                    000255
00307   100*      95     CONTINUE                                               000274
00310   101*             IF(IOPT.EQ.2) GO TO 200                                000274
00310   102*     C                                                              000274
00310   103*     C       SELECT MODIFICATION OPTIONS                            000274
00312   104*     100     CONTINUE                                               000277
00313   105*             CALL PAGIT                                             000277
00314   106*             NAST=1H                                                000300
00315   107*             IF (NAME(I,6).EQ.2H00) NAST=1H*                        000302
00317   108*             ENCODE(802,IOUT,N) (NAME(N,J),ANUM(N,J),J=1,5),PECNT(N),MOLE(N),  000312
00317   109*         X   ENTH(N),NAST,FAZ(N),RTEMP(N),FOX(N),DENS(N)            000312
00337   110*             CALL GOUT(LINE1,125)                                   000343
00340   111*             CALL GOUT(LINE2,114)                                   000347
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00341  112*            CALL BOUT(IOUT,125)                                  000353
00342  113*          CALL GOUT(' ',1)                                       000357
00343  114*            DO 105 I=1,8                                         000366
00346  115*            CALL GOUT(MODMEN(1,I),2H)                            000366
00347  116*  105       CONTINUE                                             000375
00351  117*  106       CONTINUE                                             000375
00352  118*            ICHNG=0                                              000375
00353  119*            CALL RDATAI(1,ICHNG,$106)                            000376
00356  120*            IF(ICHNG .EQ. 0) GO TO 50                            000402
00360  121*            IF(ICHNG.LT.1 .OR. ICHNG.GT.7) GO TO 106             000404
00361  122*            GO TO (110,120,130,140,150,160,170),ICHNG            000422
00362  123*  110       CONTINUE                                             000437
00363  124*            CALL GOUT(EXMP1A,66)                                 000437
00364  125*            CALL GOUT(EXMP1B,98)                                 000492
00367  126*            DO 112 I=1,5                                         000454
00370  127*            J=(I-1)*2 + 1                                        000454
00371  128*            RDUM(J)=2H                                           000461
00372  129*            RDUM(J+1)=0.                                         000464
00374  130*  112       CONTINUE                                             000467
00375  131*            CALL RDATAF(10,RDUM,$110)                            000467
00400  132*            DO 114 I=1,5                                         000501
00401  133*            J=(I-1)*2 + 1                                        000503
00402  134*            FLD(0,36,NAME(N,I))=FLD(0,36,RDUM(J))                000507
00403  135*  C       CALL CHECKNAME(N,I)                                    000507
00405  136*            ANUM(N,I)=RDUM(J+1)                                  000511
00405  137*  114       CONTINUE                                             000515
00406  138*            GO TO 100                                            000515
00406  139*  C                                                              000515
00407  140*  120       CONTINUE                                             000517
00410  141*            CALL DMWRTF(EXMP2,36,PECNT(N),6)                     000517
00411  142*            CALL RDATAF(1,PECNT(N),$120)                         000527
00412  143*            MOLE(N)=1H                                           000536
00413  144*            IF(.NOT.RDYES(EXMP2B,30)) GO TO 100                  000540
00415  145*            MOLE(N)=1HM                                          000545
00415  146*            GO TO 100                                            000547
00415  147*  C                                                              000547
00416  148*  130       CONTINUE                                             000551
00417  149*            CALL DMWRTF(EXMP3,30,ENTH(N),5)                      000551
00420  150*            CALL RDATAF(1,ENTH(N),$130)                          000561
00421  151*            NAME(N,6)=2H                                         000570
00422  152*            IF (RDYES(EXMP3B,92)) NAME(N,6)=2HOO                 000573
00424  153*            GO TO 100                                            000603
00424  154*  C                                                              000603
00425  155*  140       CONTINUE                                             000605
00426  156*            CALL GOUT(EXMP4,24)                                  000605
00427  157*            CALL RDCHAR(FAZ(N),1,1,$140)                         000611
00430  158*            GO TO 100                                            000621
00430  159*  C                                                              000621
00431  160*  150       CONTINUE                                             000623
00432  161*            CALL DMWRTF(EXMP5,24,RTEMP(N),$150)                  000623
00433  162*            CALL RDATAF(1,RTEMP(N),$150)                         000633
00434  163*            GO TO 100                                            000642
00434  164*  C                                                              000642
00435  165*  160       CONTINUE                                             000644
00436  166*            CALL GOUT(EXMP6,30)                                  000644
00437  167*            CALL RDCHAR(FOX(N),1,1,$160)                         000650
```

```
00440  169*          60 TO 100                                          000660
00440  169*    C                                                        000660
00441  170*  170     CONTINUE                                           000662
00442  171*          CALL DMWRTF(EXMP7,24,DENS(N),5)                    000662
00443  172*          CALL RDATAF(1,DENS(N),$170)                        000672
00444  173*          GO TO 100                                          000701
00444  174*    C                                                        000701
00444  175*    C     DELETE A REACTANT                                  000701
00445  176*  200     CONTINUE                                           000703
00446  177*          NREAC=NREAC-1                                      000703
00447  178*          DO 220 I=N,NREAC                                   000707
00452  179*          DO 210 J=1,6                                       000717
00455  180*              NAME(I,J)=NAME(I+1,J)                          000717
00456  181*              ANUM(I,J)=ANUM(I+1,J)                          000720
00457  182*  210     CONTINUE                                           000723
00461  183*          PECNT(I)=PECNT(I+1)                                000723
00462  184*          MOLE(I)=MOLE(I+1)                                  000725
00463  185*          ENTH(I)=ENTH(I+1)                                  000727
00464  186*          FAZ(I)=FAZ(I+1)                                    000731
00465  187*          RTEMP(I)=RTEMP(I+1)                                000733
00466  188*          FOX(I)=FOX(I+1)                                    000735
00467  189*          DENS(I)=DENS(I+1)                                  000737
00470  190*  220     CONTINUE                                           000745
00472  191*          GO TO 50                                           000745
00472  192*    C                                                        000745
00472  193*    C     ADD A REACTANT                                     000745
00473  194*  300     CONTINUE                                           000747
00474  195*          NREAC=NREAC+1                                      000747
00475  196*          N=NREAC                                            000751
00476  197*          CALL GOUT(EXMP14,66)                               000762
00477  198*          CALL GOUT(EXMP18,48)                               000756
00500  199*          DO 305 I=1,6                                       000770
00503  200*          J=(I-1)*2 + 1                                      000770
00504  201*          RDUM(J)=2H                                         000775
00505  202*          RDUM(J+1)=0.                                       001000
00506  203*  305     CONTINUE                                           001003
00510  204*          CALL RDATAF(10,RDUM,$300)                          001009
00511  205*          DO 307 I=1,5                                       001015
00514  206*          J=(I-1)*2 + 1                                      001015
00515  207*          FLD(0,36,NAME(N,I))=FLD(0,36,RDUM(J))              001023
00515  208*    C     CALL CHECK(NAME(N,I))                              001023
00516  209*          ANUM(N,I)=RDUM(J+1)                                001025
00517  210*  307     CONTINUE                                           001032
00521  211*  310     CONTINUE                                           001032
00522  212*          CALL GOUT(EXMP2,36)                                001032
00523  213*          PECNT(N)=0.                                        001036
00524  214*          CALL RDATAF(1,PECNT(N),$310)                       001037
00525  215*  320     CONTINUE                                           001046
00526  216*          MOLE(N)=1H                                         001046
00527  217*          IF(ROYES(EXMP28,30)) MOLE(N)=1HM                   001051
00531  218*  330     CONTINUE                                           001062
00532  219*          CALL GOUT(EXMP3,30)                                001062
00533  220*          ENTH(N)=0.                                         001066
00534  221*          CALL RDATAF(1,ENTH(N),$330)                        001067
00535  222*          IF (ROYES(EXMP38,42)) NAME(N,6)=2HOO               001077
00537  223*  340     CONTINUE                                           001110
```

```
00540   220*            CALL GOUT(EXMP8,24)                                    001110
00541   225*            FAZ(N)=1HS                                             001114
00542   226*            CALL RDCHAR(FAZ(N),1,-1,$340)                          001116
00543   227*      380   CONTINUE                                               001127
00544   228*            CALL GOUT(EXMP5,24)                                    001127
00545   229*            RTEMP(N)=0.                                            001133
00546   230*            CALL RDATAF(1,RTEMP(N),$350)                           001134
00547   231*      360   CONTINUE                                               001144
00550   232*            CALL GOUT(EXMP6,30)                                    001144
00551   233*            FOX(N)=1HF                                             001150
00552   234*            CALL RDCHAR(FOX(N),1,-1,$360)                          001152
00553   235*      370   CONTINUE                                               001163
00554   236*            CALL GOUT(EXMP7,24)                                    001163
00555   237*            DENS(N)=0.                                             001167
00556   238*            CALL RDATAF(1,DENS(N),$370)                            001170
00557   239*            GO TO 50                                               001177
00557   240*      C                                                            001177
00557   241*      C     STORE CASE TO FILE 8                                   001177
00560   242*      400   CONTINUE                                               001201
00561   243*            REWIND IO                                              001201
00562   244*            IF (IO.NE.N8) GO TO 408                                001203
00564   245*            DO 406 I=1,5                                           001210
00567   246*            READ (IO) NDUMMY                                       001210
00572   247*      406   CONTINUE                                               001216
00576   248*      408   CONTINUE                                               001216
00578   249*            WRITE (IO) NREAC,CF                                    001216
00601   250*            DO 410 I=1,NREAC                                       001231
00604   251*            WRITE (IO) (NAME(I,J),ANUM(I,J),J=1,6),PECNT(I),MOLE(I),  001231
00604   252*         X  ENTH(I),NAME(I,6),ANUM(I,6),FAZ(I),RTEMP(I),FOX(I),DENS(I)  001231
00624   253*      410   CONTINUE                                               001257
00626   254*            IF (IO.EQ.N8) GO TO 420                                001257
00630   255*            IF (.NOT.RDYES('TYPE YES TO EDIT COAL REACTANT DATA',35))  001262
00630   256*         X     GO TO 420                                           001262
00632   257*            IO=N8                                                  001267
00633   258*            REWIND IO                                              001271
00636   259*            DO 412 I=1,5                                           001276
00637   260*            READ (IO) NDUMMY                                       001303
00642   261*      412   CONTINUE                                               001303
00644   262*            GO TO 10                                               001305
00645   263*      420   ENDFILE IO                                             001307
00646   264*            RETURN                                                 001308
00647   265*      802 FORMAT(1X,I2,2X,5(A2,F8.4,2X),F10.6,2X,A1,F13.4,A1,3X,A1,F12.3,  001308
00647   266*         1  3X,A1,F12.5,1X)                                        001308
00650   267*            END                                                    001308

      END OF COMPILATION:       NO  DIAGNOSTICS.

@HOG,P      SAVE
```

```
@FOR,S   SAVE,SAVE
HSA  E3 -10/15/80-13:07:45 (13.)

    SUBROUTINE SAVE      ENTRY POINT 000501
               NEWOF     ENTRY POINT 000504

    STORAGE USED: CODE(1) 000507; DATA(0) 000104; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003   CONSTS 000004
     0004   MOLCON 000010
     0005   SPECES 017106
     0006   MISC   001701
     0007   INDX   000041
     0010   CCC    000001
     0011   CFUEL  000004

    EXTERNAL REFERENCES (BLOCK, NAME)

     0012   MCALC
     0013   EXP
     0014   NWDUS
     0015   NIO2S
     0016   NIO1S
     0017   NERR3S

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001    000137 100L      0001    000056 13L       0001    000042 1326      0001    000073 15L       0001    000112 20L
     0001    000172 200L      0001    000161 201G      0001    000207 2106      0001    000326 2526      0001    000241 302L
     0001    000435 317G      0001    000127 50L       0000    000019 730F      0000    000017 732F      0001    000311 7##L
     0001    000322 745L      0001    000356 750L      0001    000365 760L      0000    000035 770F      0000    000045 780F
     0000    000050 785F      0005    011052 A         0006    000640 AM        0006    000705 AM1       0006    001135 AMUM
     0003    000000 ATMN      0006    000004 ATOM      0006 R  000514 BO        0006 R  000545 CNP       0007 L  000036 CALCM
     0011 R  000000 CF        0005    000000 COEF      0000 R  000006 COF       0007    000001 CONVG     0006    000706 CPR1
     0006    000634 CPSUM     0006    000654 DATA      0005    01062* DELN      0010    000002 DEMAND    0006    001560 DENS
     0005 R  009312 EN        0004    000000 END       0005 R  01015D ENLN      0006 R  001700 ENLSAV    0006 R  000000 ENN
     0006 R  001676 ENNL      0006 R  001677 ENSAVE    0006    001414 ENTH      0006 R  000636 EORAT     0006    001445 FAZ
     0000 R  000003 FCAL      0000 R  000013 FF        0000 R  000002 FHH       0006    001527 FOX       0000 R  000001 FUU
     0004    000001 GAS       0003    000001 GMET      0010    000000 GRAPH     0011    000001 HHVV      0007    000003 HP
     0006 R  000642 HPP       0000 R  000012 HS        0006 R  000637 HSUBO     0005    010376 HO        0007 I  000030 IC
     0007    000000 IDEBUG    0004 I  000002 IE        0007    000015 IMAT      0000    000057 INJPS     0007 L  000023 IONS
     0007    000021 IP        0007 I  000037 IQSAVE    0007 I  000016 IQ1       0007 I  000005 ISV       0007    000034 IT
     0005 I  016266 IUSE      0004    000003 IZERO     0000 I  000005 J         0007 I  000026 JLIQ      0010 I  000001 JOUT
     0007 I  000025 JSOL      0007    000031 JS1       0007    000014 KMAT      0004 I  000004 LANR      0006 I  000463 LLMT
     0000 I  000004 LL1       0007 I  000040 LSAVE     0004    000005 MOL       0007    000006 MOLES     0006    0007#7 NAMF
     0007    000024 NC        0007    000022 NEWR      0007    000035 NFZ       0007 I  000012 NLM       0007    000017 NOF
     0007    000020 NOMIT     0007    000007 NP        0007 I  000011 NPT       0007    000027 NREAC     0007 I  000013 NS
     0000 I  000000 NSPP1     0007    000010 NT        0006 R  000635 OF        0004    000006 OI        0006    061444 OXF
     0003    000002 PATM      0006    001363 PFCNT     0011 R  000003 PER       0006    000633 PP        0003 R  000003 RBAR
     0003    000004 RBR       0006 R  000644 RH        0006 R  001611 RHOP      0006    001612 RHW       0006    001476 RTEMP
```

0003	000003	RVR	0005	000064	S	0007	06_333	SHOCK	0005	R 016660	SLN	0007	000004	SP	
0005	015369	SUB	0000	R 000007	SUM	0006	000001	SUMN	0006	000003	SB	0005	016814	TEMP	
0006	000632	T_H	I_{GH}	0006	001643	T_{LN}	0006	000630	TLOW	0006	000627	TM	0006	000631	TMID
0007	000002	TP	0006	000002	TT	0006	R 000646	VMIN	0007	L 000032	VOL	0006	R 000650	VPLS	
0000	R 000011	V_1	0000	R 000010	V2	0011	R 000002	WC_R	0006	000652	WP	0004	000007	ZERO	

```
00101     1*          SUBROUTINE SAVE                                                    000000
00101     2*    C                                                                        000000
00101     3*    C  SAVES OR USES COMPOSITIONS FROM PREVIOUS POINT AS INITIAL ESTIMATES   000000
00101     4*    C                                                                        000000
00103     5*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR              /CONSTS/  000000
00104     6*          COMMON /MOLCON/ EM,GAS,IE,IZERO,LANK,MOL,OX,ZERO         /MOLCON/  000000
00106     7*    C     COMMON/SPECES/CREF(2,7,150),S(150),EN(150,13),ENLN(150),NO(150)    000000
00106     8*    C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)    000000
00105     9*          INCLUDE SPECBK                                                     000000
00111    10*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),          000000
00111    11*         1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,     000000
00111    12*         2              MSUBO,AM(2),MPP(2),RM(2),VMIN(2),VPLS(2),WP(2),  /MISC/  000000
00111    13*         3              DATA(25),AMI,CPRI,NAME(25,6),ANUM(25,6),PECNT(25),  000000
00111    14*         4              ENTH(25),FAZ(25),TEMP(25),FOX(25),DENS(25),RHOP,    000000
00111    15*         5              RMM(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV              000000
00112    16*          COMMON /INDX/ IDEBUG,CONVG,TP,MP,SP,ISV,MOLES,MP,MT,MPT,MLM,MS,  /INDX/  000000
00112    17*         1              KMAT,IMAT,IQI,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ, /INDX/  000000
00112    18*         2              NREAC,IC,JS1,VOL,SHOCK,IT,NF2,CALCM,IOSAVE,LSAVE    /INDX/  000000
00112    19*    C                                                                        000000
00113    20*          COMMON /CCC/ GRAPH,JOUT,DEMAND                                     000000
00114    21*          COMMON /CFUEL/CF,HHYY,WGR,PER                                      000000
00114    22*    C                                                                        000000
00115    23*          DATA FUU/0HU, C/,FMM/0HM, C/,FCAL/0HAL/0/                          000000
00121    24*          LOGICAL CALCM,IONS,VOL                                             000000
00121    25*    C                                                                        000000
00122    26*          IF(ISV)100,10,200                                                  000000
00122    27*    C  NEXT POINT FIRST T IN SCHEDULE, USE PREVIOUS COMPOSITIONS FOR THIS T  000000
00125    28*       10 IQI = IOSAVE                                                       000003
00126    29*          ENN = ENSAVE                                                       000005
00127    30*          ENNL = ENLSAV                                                      000007
00130    31*          LL1 = NLM                                                          000011
00131    32*          DO 50 J = 1,MS                                                     000042
00134    33*          IF (.NOT. IONS .OR. LLMT(NLM) .EQ. LSAVE) GO TO 15                 000042
00136    34*          IF(LLMT(NLM).EQ.IE)  GO TO 13                                      000043
00140    35*          IF(IUSE(J).NE.-10000)  GO TO 15                                    000046
00142    36*          IUSE(J) = 0                                                        000051
00143    37*          LL1  = NLM+1                                                       000052
00144    38*          GO TO 20                                                           000054
00145    39*       13 IF(SLN(J).NE.0..OR.IUSE(J).NE.0)  GO TO 15                         000056
00147    40*          LL1 = NLM-1                                                        000065
00150    41*          IUSE(J) = -10000                                                   000067
00151    42*          GO TO 50                                                           000071
00152    43*       15 IF (IUSE(J).EQ.0) GO TO 20                                         000073
00154    44*          EN (J,NPT) = SLN(J)                                                000074
00155    45*          IF(IUSE(J).GT.0) IUSE(J) = - IUSE(J)                               000076
00157    46*          IF (EN(J,NPT) .GT. 0.0)  IUSE(J) = - IUSE(J)                       000103
00161    47*          GO TO 50                                                           000110
```

```
00162   48*        20 EN(J,NPT) = 0.                                                    000112
00163   49*           ENLN(J) = SLN(J)                                                  000112
00164   50*           IF (ENLN(J) + 18.50 .LE. ENNL)  GO TO 50                          000114
00166   51*           EN(J,NPT) = EXP(ENLN(J))                                          000120
00167   52*        50 CONTINUE                                                          000131
00171   53*           NLM = LL1                                                         000131
00172   54*           RETURN                                                            000133
00172   55*     C  FIRST T--SAVE COMPOSITIONS FOR FUTURE POINTS WITH THIS T             000133
00173   56*       100 ISV = -ISV                                                        000137
00174   57*           IQSAVE = IQ1                                                      000140
00175   58*           ENSAVE = ENN                                                      000142
00176   59*           ENLSAV = ENNL                                                     000144
00177   60*           LSAVE = LLMT(NLM)                                                 000146
00200   61*           DO 150 J = 1,NS                                                   000161
00203   62*           SLN(J) = ENLN(J)                                                  000161
00204   63*       150 IF (IUSE(J) .NE. 0)  SLN(J) = EN(J,ISV)                           000162
00204   64*     C  USE COMPOSITIONS FROM PREVIOUS POINT                                 000162
00207   65*       200 DO 300 J = 1,NS                                                   000172
00212   66*       300 EN(J,NPT) = EN(J,ISV)                                             000207
00214   67*           RETURN                                                            000211
00214   68*     C  CALCULATE NEW VALUES OF BO AND HSUBO FOR NEW OF RATIO                000211
00215   69*           ENTRY NEWOF                                                       000214
00216   70*           WRITE(JOUT,730) OF                                                000214
00221   71*       730 FORMAT(6HCOF = ,F10.6)                                            000222
00222   72*           IF (CF+1.0) ,302,                                                 000222
00225   73*           COF=OF/CF                                                         000225
00226   74*           WRITE (JOUT,732) COF,WCR,PER                                      000230
00233   75*       732 FORMAT (21X,'OXIDIZER/COAL=',F8.4,5X,'WATER/COAL=',F8.4,          000241
00233   76*          X   5X,'CARBON CONVERSION=',F8.4)                                  000241
00234   77*       302 CONTINUE                                                          000241
00235   78*           SUM = OF + 1.                                                     000241
00236   79*           V2 =   (OF*VMIN(1)+VMIN(2))/SUM                                   000243
00237   80*           V1 =   (OF*VPLS(1)+VPLS(2))/SUM                                   000250
00240   81*           IF (V2 .LT. 0.0)  EQRAT = ABS(V1/V2)                              000255
00242   82*           IF (RH(1) .GT. 0.0 .AND. RH(2) .GT. 0.0)  GO TO 744               000264
00244   83*           RHOP = RH(2)                                                      000300
00245   84*           IF (RHOP .LE. 0.0)  RHOP = RH(1)                                  000302
00247   85*           GO TO 745                                                         000307
00250   86*       744 RHOP =  (OF+1.)*RH(1)*RH(2)/(RH(1)+ OF *RH(2))                    000311
00251   87*       745 DO 747 J = 1,NLM                                                  000322
00254   88*       747 BO(J) = (BOP(J,2) + BOP(J,1)*OF)/SUM                              000326
00256   89*           NPT = 1                                                MAIN0139   000333
00257   90*           IF(.NOT.CALCH)  GO TO 750                                         000335
00261   91*           CALL HCALC                                                        000337
00262   92*           CALCH = .FALSE.                                                   000341
00263   93*           IF (OF .GT. 0.0)  HPP(1) = SUM*HPP(1)/OF                          000342
00265   94*           HPP(2) = SUM*HPP(2)                                               000351
00266   95*           GO TO 760                                                         000354
00267   96*       750 HSUBO = (HPP(2) + HPP(1)*OF)/(RBAR*SUM)                           000356
00270   97*       760 IC = 0                                                            000365
00271   98*           JSOL = 0                                                          000365
00272   99*           JLIQ = 0                                                          000366
00273  100*           HS = RBAR*HSUBO                                                   000367
00274  101*           WRITE(JOUT,770)                                                   000372
00276  102*       770 FORMAT (1HO,17X,4HFUEL ,13X,7HOXIDANT  ,12X,7HMIXTURE  //)  MAIN0124  000377
00277  103*       780 FORMAT (1H 2A4,3E18.8/)                                  MAIN012   000377
```

```
00300   104*          FF = FHH                                                    000377
00301   105*          IF(VOL)FF = FUU                                             000401
00303   106*          WRITE(JOUT,780) FF,FCAL ,HPP(2),HPP(1),HS                   000405
00312   107*          WRITE(JOUT,785)                                             000421
00314   108*      785 FORMAT (12H KG-ATOMS/KG)                                    000426
00315   109*          WRITE(JOUT,780) (LLMT(J),LANK,BOP(J,2),BOP(J,1),BOL(J),J = 1,NLM1  000426
00327   110*          RETURN                                                      000494
00330   111*          END                                                         000506
```

END OF COMPILATION: NO DIAGNOSTICS.

```
@HDG,P      SEARCH
```

```
@FOR,S    SEARCH,SEARCH
HSA  E3 -10/15/80-13:07:48 (16.)

SUBROUTINE SEARCH    ENTRY POINT 000445

STORAGE USED: CODE(1) 000461; DATA(0) 000121; BLANK COMMON(2) 000000

 COMMON BLOCKS:

 0003   HOLCON 000010
 0004   SPECES 017106
 0005   MISC   001701
 0006   INDX   000041
 0007   CCC    000003

EXTERNAL REFERENCES (BLOCK, NAME)

 0010   MOVABS
 0011   HOLDIT
 0012   PAGIT
 0013   GOUT
 0014   NREW$
 0015   NROU$
 0016   NIO2$
 0017   NIO1$
 0020   NWOU$
 0021   NERR3$

STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

 0000   000022 10F      0001   000021 125G     0001   000022 130G     0001   000310 145L     0001   000050 146G
 0001   000102 154G     0001   000313 170L     0001   000128 171G     0001   000326 171L     0000   000045 172F
 0001   000126 173G     0000   000055 176F     0000   000030 20F      0001   000144 204G     0001   000154 207G
 0001   000204 220G     0001   000211 225G     0001   000222 233G     0001   000276 254G     0001   000346 277G
 0001   000376 306G     0000   000020 5F       0001   000042 7L       0001   000167 805L     0001   000171 810L
 0001   000225 820L     0001   000234 825L     0000   000032 871F     0004 R 011052 A        0005   000640 AM
 0005   000705 AM1      0005   001135 ANUM     0005   000004 ATOM     0000 R 000001 B        0005   000514 BO
 0005   000545 BOP      0006   000036 CALCH    0004 R 000000 COEF     0006   000001 CONVG    0005   000706 CPR1
 0005   000634 CPSUM    0005   000654 DATA     0004 R 004312 DATE     0004   010624 DELN     0007   000002 DEMAND
 0005   001560 DENS     0004   004312 EN       0003 I 000000 END      0004   010150 ENLN     0005   001700 ENLSAV
 0005   000000 ENN      0005   001676 ENNL     0005   001677 ENSAVE   0005   001414 ENTH     0005   000636 EQRAT
 0005   001445 FAZ      0005   001527 FOX      0003 I 000001 GAS      0007   000000 GRAPH    0006   000003 HP
 0005   000642 HPP      0005   000637 HSUBO    0004   010376 HO       0000 I 000013 I        0006   000030 IC
 0006   000000 IDEBUG   0003   000002 IE       0006   000015 IMAT     0000   000073 INJP$    0006   000023 IONS
 0006   000021 IP       0006   000037 IQSAVE   0006   000016 IO1      0006   000005 ISV      0006   000034 IT
 0004 I 016266 IUSE     0000 I 000012 IX       0003   000003 IZERO    0000 I 000014 J        0006   000026 JLIO
 0007 I 000001 JOUT     0006   000025 JSOL     0006   000031 JS1      0000 I 000017 K        0006   000014 KMAT
 0006 I 000012 L        0003   000004 LANK     0005 I 000463 LLMT     0006   000040 LSAVE    0003   000005 MOL
 0006   000006 MOLES    0000 I 000005 MT       0005   000707 NAME     0006 I 000024 NC       0006 L 000022 NEWP
 0006   000035 NFZ      0006   000017 NOF      0006 I 000020 NOMIT    0006   000007 NP       0006   000011 NPT
 0006   000027 NREAC    0006 I 000013 NS       0000 I 000000 NSPP1    0006   000010 NT       0005   000635 OF
 0004 I 010150 OMIT     0003   000006 OX       0005   001644 OXF      0005   001363 PECWT    0000 I 000011 PHAZ
```

0005	000633	PP	0005	000644	RH	0005	001611	RHOP	0005	001612	RMW	0005	001476	RTEMP
0004	004064	S	0006	000033	SHOCK	0004	016660	SLN	0006	000004	SP	0004	I 015364	SUB
0005	000001	SUMN	0005	000003	SO	0004	R 016514	TEMP	0005	R 000632	THIGH	0005	001643	TLN
0005	R 000630	TLOW	0005	000627	TM	0005	R 000631	TMID	0006	000002	TP	0005	000002	TT
0000	R 000015	T1	0000	R 000016	T2	0005	000646	VMIN	0006	000032	VOL	0005	000650	VPLS
0005	000652	WP	0003	000007	ZERO									

```
00101     1*        SUBROUTINE SEARCH                                                    000000
00101     2*  C                                                                          000000
00101     3*  C  SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED               000000
00101     4*  C                                                                          000000
00103     5*        COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO          /HOLCON/ 000000
00103     6*  C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)     000000
00103     7*  C    1 ,DELN(150),A(15,150),SUB(15,3),IUSE(150),TEMP(50,2),SLN(150)      000000
00104     8*           INCLUDE SPECPK                                                   000000
00110     9*        COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(28),BO(25),          000000
00110    10*       1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,FQRAT,     000000
00110    11*       2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),DP(2),  /MISC/ 000000
00110    12*       3              DATA(25),AMI,CPRI,NAME(25,6),ANUM(25,6),PECNT(25),  000000
00110    13*       4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,   000000
00110    14*       5              RMW(25),ILN,QXF(26),ENNL,ENSAVE,ENLSAV              000000
00111    15*        COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,MP,NT,NPT,,,NS,    /INDX/ 000000
00111    16*       1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/ 000000
00111    17*       2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE    /INDX/ 000000
00111    18*  C                                                                          000000
00112    19*           COMMON /CCC/ GRAPH,JOUT,DEMAND                                   000000
00112    20*  C                                                                          000000
00113    21*        DIMENSION B(4),DATE(2,3),MT(4),OMIT(3,3)                           000000
00114    22*        EQUIVALENCE (DATE,EN),(ENLN,OMIT)                                  000000
00115    23*        INTEGER END,GAS,OMIT,PHAZ,SUB                                      000000
00116    24*        LOGICAL NEWR                                                       000000
00116    25*  C                                                                          000000
00116    26*  C     CHANGE WHEN CHANGE SPECIES SIZE                                    000000
00117    27*        NSPP1=150                                                          000000
00120    28*        NC= 0                                                              000001
00121    29*        IX= 0                                                              000002
00122    30*        SUB(1,1) = END                                                     000003
00123    31*        REWIND 4                                                           000011
00124    32*        DO 3 I=1,150                                                       000022
00127    33*        DO 3  J=1,L                                                        000022
00132    34*      3 A(J,I) = 0.0                                                       000022
00135    35*        READ(4,5)  TLOW,TMID,THIGH                                         000027
00142    36*      5 FORMAT (3F10.3)                                                    000037
00143    37*        NS = 1                                                             000037
00144    38*      7 READ    (4,10)(SUB(NS,I),I=1,3),DATE(1,NS),DATE(2,NS),(MT(J),B(J),  000042
00144    39*       1  J=1,4),PHAZ,T1,T2                                                000042
00164    40*       10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3)                          000112
00165    41*        IF(SUB(NS,1).EQ.END) GO TO 171                                     000112
00167    42*        READ      (4,20) (((COEF(I,J,NS),J=1,7),I=1,2)                     000115
00200    43*       20 FORMAT (5E15.8)                                                  000135
00201    44*        IF(NOMIT.EQ.0) GO TO 810                                           000135
00203    45*        DO 805 I=1,NOMIT                                                   000137
00206    46*        DO 804 J=1,3                                                       000156
```

```
00211   47*      805  IF (OMIT(J,I) .NE. SUB(NS,J))  GO TO 805                    000154
00214   48*           GO TO 7                                                      000165
00215   49*       805 CONTINUE                                                     000171
00217   50*       810 DO 820 K=1,4                                                 000171
00222   51*           IF(B(K),EQ.0.) GO TO 825                                     000204
00224   52*           DO 168 I=1,L                                                 000211
00227   53*       168 IF (ILMT(I) .EQ. MT(K))  GO TO 820                           000211
00232   54*           DO 819 J=1,L                                                 000222
00235   55*       819 A(J,NS) = 0.                                                 000222
00237   56*           GO TO 7                                                      000223
00240   57*       820 A(I,NS)= B(K)                                                000225
00242   58*       825 IUSE(NS) = 0                                                 000234
00243   59*           IF(PHAZ.EQ.GAS) GO TO 170                                    000235
00245   60*           NC= NC+1                                                     000240
00246   61*           TEMP(NC,1)= T1                                               000243
00247   62*           TEMP(NC,2)= T2                                               000246
00250   63*           IX= IX+1                                                     000250
00251   64*           IF(IUSE(NS-1).EQ.0 .OR. NC.EQ.1) GO TO 145                   000263
00253   65*           DO 830 I=1,L                                                 000276
00256   66*       830 IF (A(I,NS) .NE. A(I,NS-1))  GO TO 145                       000276
00261   67*           IX= IX-1                                                     000304
00262   68*       145 IUSE(NS)= -IX                                                000310
00263   69*       170 NS= NS+1                                                     000313
00264   70*           IF (NS.LE.NSPP1) GO TO 7                                     000315
00266   71*           WRITE (JOUT,871)                                             000320
00270   72*       871 FORMAT (//20X,54HDIMENSIONS IN /SPECES/ FOUND TO BE TOO SMALL IN S  000326
00270   73*          1EARCH/)                                                      000326
00271   74*       171 NS= NS-1                                                     000326
00272   75*           NEWR= .FALSE.                                                000330
00273   76*           WRITE(JOUT,172)                                              000335
00275   77*       172 FORMAT(42HOSPECIES BEING CONSIDERED IN THIS SYSTEM    )      000346
00276   78*           DO 174 I=1,NS,5                                              000346
00301   79*           K = I + 4                                                    000351
00302   80*           IF (NS .LT. K)  K = NS                                       000354
00304   81*       174 WRITE(JOUT,176)(DATE(1,J),DATE(2,J),SUB(J,1),SUB(J,2),SUB(J,3),  000362
00304   82*          1   J=I,K)                                                    000362
00317   83*       176 FORMAT(5(5X,2A3,2X,3A4))                                     000407
00320   84*           CALL MOVABS(500,50)                                          000407
00321   85*           CALL HOLDIT                                                  000413
00322   86*           CALL PABIT                                                   000415
00323   87*           CALL GOUT(' ',1)                                             000417
00324   88*           RETURN                                                       000423
00325   89*           END                                                          000460

        END OF COMPILATION:        NO  DIAGNOSTICS.

@HD6,P      SHCK
```

```
@FOR,S    SHCK.SHCK
HSA  E3 -10/15/80-13:07:51 (12.)

     SUBROUTINE SHCK      ENTRY POINT 001367

     STORAGE USED: CODE(1) 001401; DATA(0) 000263; BLANK COMMON(2) 000000

      COMMON BLOCKS:

     0003   CONSTS 000006
     0004   HOLCON 000010
     0005   POINTS 000335
     0006   SPECES 017106
     0007   MISC   001701
     0010   DOUBLE 001560
     0011   INDX   000091
     0012   PERF   000166
     0013   OUPT   000073
     0014   CCC    000003

     EXTERNAL REFERENCES (BLOCK, NAME)

     0015   RDYES
     0016   PAGIT
     0017   CHRSIZ
     0020   GOUT
     0021   NEWOF
     0022   HCALC
     0023   OUT1
     0024   OUT2
     0025   EOLBRM
     0026   SAVE
     0027   OUT3
     0030   NWNLS
     0031   NRNLS
     0032   NWDUS
     0033   NIO2S
     0034   SQRT
     0035   NIO3S
     0036   NIO1S
     0037   ALOG
     0040   EXP
     0041   NERR3S

     STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0000   000143 125F    0001   000211 14L     0001   000011 10SG    0001   000221 15L     0001   001001 150L
     0000   000165 152F    0001   000022 156G    0000   000101 16F     0001   001112 161L    0001   000126 17L
     0001   000143 19L     0001   000073 204G    0001   000114 21L     0001   000136 223G    0001   000147 231G
     0001   000245 30L     0001   000356 323G    0001   000376 334G    0001   000520 361G    0001   000534 40L
     0001   001125 431L    0001   000320 44L     0001   000325 45L     0000   000137 46F     0001   001057 461G
     0001   000412 47L     0001   000547 50L     0001   001201 520G    0001   001232 536G    0001   001247 547G
```

0001	001266	5616	0001	001303	5706	0000	000176	58F	0001	001322	6046	0001	001345	6206
0000	000202	68F	0001	000750	75L	0000	000111	861F	0000	000122	862F	0000	000131	863F
0001	001106	880L	0006	011052	A	0007	000640	AM	0007 R	000705	AM1	0007	001135	ANUM
0003	000000	ATMR	0007	000004	ATOM	0000 R	000036	AX	0000 R	000037	AXX	0000 R	000024	A1
0007	000514	B0	0007	000545	BOP	0011	000036	CALCH	0006	000000	COEF	0011	000001	CONVG
0005 R	000032	CPR	0007 R	000706	CPR1	0007	00063A	CPSUM	0007	000654	DATA	0006	010624	DELN
0019	000002	DEMAND	0007	001560	DENS	0005 R	000064	DLVPT	0005 R	000047	DLVTP	0006 R	004312	EN
0004	000000	END	0006 R	010150	ENLN	0007	001700	ENLSAV	0007	000000	ENN	0007	001676	ENNL
0007	001677	ENSAVE	0007	001414	ENTH	0012 L	000165	EQL	0007	000636	EQRAT	0013	000002	FA
0013	000003	FAP	0007	001445	FAZ	0013 R	000005	FB	0013	000006	FC	0013	000007	FCP
0013	000012	FCST	0013	000014	FCV	0013	000015	FG	0013	000017	FGE	0013	000020	FGV
0013	000021	FH	0013	000023	FI	0013	000025	FIV	0013	000027	FM	0000 R	000001	FMM
0013 R	000031	FMT	0013 R	000050	FN	0013 R	000052	FOUR	0007	001527	FOX	0013	000053	FP
0000 R	000002	FPP	0000 R	000003	FRA	0000 R	000009	FRB	0013	000084	FS	0013	000086	FSV
0013	000057	FT	0013	000061	FTK	0000 R	000005	FTT	0000 R	000006	FU1	0000 R	000007	FU2
0013	000063	FV	0013 R	000065	FVEL	0000 R	000010	FV21	0000 R	000011	FV22	0000 R	000012	FV23
0013 R	000001	F13	0013	000000	F9X	0010 D	000000	G	0005 R	000101	GAMMAS	0000 R	000020	GAMMA1
0004	000001	GAS	0010 D	001516	GG	0003	000001	GMET	0014	000000	GRAPH	0011	000003	HP
0007	000642	HPP	0000 R	000030	HS	0007 R	000637	HSUBO	0005 R	000000	HSUM	0006	010376	HO
0000 I	000022	I	0011	000030	IC	0011 I	000000	IDEBUG	0004	000002	IE	0011	000015	IMAT
00C0 L	000013	INCODE	0000 L	000014	INCOFZ	0000	000233	INJP	0000 I	000021	IOF	0011	000023	IONS
0011	000021	IP	0011	000037	IQSAVE	0011	000016	IQ1	0011 I	000005	ISV	0011	000034	IT
0006 I	016266	IUSE	0004 I	000003	IZERO	0000 I	000025	J	0011	000026	JLIQ	0019 I	000001	JOUT
0011	000025	JSOL	0011	000031	JS1	0000 I	000040	K	0011	000014	KMAT	0004	000004	LANK
0007	000463	LLMT	0011	000040	LSAVE	0012 R	000116	MACH1	0004	000005	MOL	0011	000006	MOLES
0000 R	000017	MU12RT	0000 R	000016	M1	0012 R	000150	M2M1	0007 I	000707	NAME	0011	000024	NC
0011	000022	NEWR	0011	000035	NFZ	0011	000012	NLM	0011 I	000017	NOF	0011	000020	NOMIT
0011	000007	NP	0011 I	000011	NPT	0011 I	000027	NREAC	0011 I	000013	NS	0000 I	000023	NSK
0000 I	000000	NSPP1	0011	000010	NT	0007 R	000635	OF	0013	000067	ONE	0004	000006	OX
0007 R	001644	OXF	0005 R	000116	P	0003	000002	PATM	0012 R	000000	PCP	0007	001363	PECWT
0007 R	000633	PP	0005 R	000217	PPP	0000 R	000026	P1	0000 R	000031	P21	0000 R	000033	P21L
0003	000003	RBAR	0003 R	000004	RBR	0015 L	000000	RDYES	0007	000644	RH	0007	001611	RHOP
0000 R	000035	RHO12	0007	001612	RHW	0012 R	000133	RRHO	0007 R	001476	RTEMP	0003	000005	RVR
0006	00406*	S	0000 L	000015	SEQL	0000	000041	SHKINP	0011	000033	SHOCK	0006	016660	SLN
0005	000251	SONVEL	0011	000004	SP	0005 R	000015	SSUM	0006	015364	SUB	0007	000001	SUMN
0007	000003	SQ	0005 R	000150	T	0006	016514	TEMP	0007	000632	THIGH	0013 R	000070	THREE
0007 R	001643	TLN	0007	000630	TLOW	0007	000627	TM	0007	000631	TMID	0005	000320	TOTN
0011 L	000002	TP	0007 R	000002	TT	0005 R	000266	TTT	0013 R	000071	TWO	0000 R	000027	T1
0012 R	000047	T2T1	0000 R	000032	T21	0000 R	000034	T21L	0005 R	000303	UTWO	0012 R	000101	U1
0012 R	000064	U1U2	0005	000202	V	0007	000646	VMIN	0012	000032	VMOC	0011	000032	VOL
0007	000650	VPLS	0005 R	000234	WM	0007	000652	WP	0010 D	001510	X	0004	000007	ZERO
0013	000072	ZEROF												

```
00101      1*          SUBROUTINE SHCK                                                                  000000
00101      2*    C                                                                                      000000
00103      3*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                        /CONSTS/      000000
00104      4*          COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO                  /HOLCON/      000000
00105      5*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                      000000
00105      6*         1 ,GAMMAS(13),P(26),T(26),V(13),Ppp(13),WM(13),SONVEL(13),TTT(13)                 000000
00105      7*         2 ,UTWO(13),TOTN(13)                                                              000000
00105      8*    C     COMMON/SPECES/COEF(2,7,15),S(15),EN(150,13),ENLN(150),NO(150)                    000000
00105      9*    C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                   000000
00106     10*          INCLUDE SPECPK                                                                    000000
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00112    11*          COMMON /MISC/ ENN,SUMN,TT,SD,ATOM(3,101),LLMT(25),BO(25),
00112    12*         1              BDP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,
00112    13*         2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),      /MISC/
00112    14*         3              DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECWT(25),
00112    15*         4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,
00112    16*         5              RHW(25),ILM,OXF(26),ENML,ENSAVE,ENLSAV
00113    17*          COMMON /DOUBLE/ G(20,21), X(20)
00114    18*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,      /INDX/
00114    19*         1              KMAT,IMAT,IO1,NOF,NOMIT,IP,NEVR,IONS,NC,JSOL,JLIQ,  /INDX/
00114    20*         2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE     /INDX/
00115    21*          COMMON /PERF/ PCP(26),VMOC(13),T2T1(13),U1U2(13),U1(13),           /PERF/
00115    22*         1              MACH1(13),RRHO(13),M2M1(13),EQL                      /PERF/
00116    23*          COMMON /OUPT/ FOX,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),    /OUPT/
00116    24*         1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/
00116    25*         2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,   /OUPT/
00116    26*         3              TWO,ZEROF                                            /OUPT/
00116    27*     C
00117    28*              COMMON /CCC/ GRAPH,JOUT,DEMAND
00117    29*     C
00120    30*          DATA FMM/6HM2  /M1  /,FPP/6HP2/P1  /,FRA/6HRHO2/R/,FRB/6HHO1    /,
00120    31*         1     FTT/6HP2/P1  /,FU1/6HU1  VE/,FU2/6HU2  VE/,FV21/6HV2(U1-/,
00120    32*         2     FV22/6HU2/M/S/,FV23/2HEC/
00133    33*          DOUBLE PRECISION G,GG,X
00133    34*          EQUIVALENCE (X(9),GG)
00135    35*          LOGICAL EQL,INCDEQ,INCDFZ,SEQL,TP
00135    36*     C
00136    37*              LOGICAL ROYES
00136    38*     C
00137    39*          REAL M1,MACH1,M2M1,MU12RT
00137    40*     C
00140    41*          NAMELIST /SHKINP/ GAMMA1,INCDEQ,INCDFZ,MACH1,U1                    /SHKINP/
00140    42*     C
00141    43*          IOF = 0
00142    44*          TP=.TRUE.
00143    45*          CPR1 = 0.
00144    46*          DO 10 I=1,13
00147    47*          MACH1(I)=0.
00150    48*       10 U1(I) = 0.0
00152    49*          GAMMA1 = 0.
00153    50*          INCDEQ = .TRUE.
00154    51*          INCDFZ = .TRUE.
00155    52*          DO 18 I = 1,NREAC
00160    53*       18 NAME(I,6)=IZERO
00162    54*             CALL PAGIT
00163    55*             CALL CHRSIZ(1)
00164    56*             IF(ROYES('TYPE YES FOR PRESENT VALUES OF SHKINP NAMELIST',46))
00164    57*            1   WRITE(6,SHKINP)
00170    58*             CALL CHRSIZ(8)
00171    59*             CALL GOUT('TYPE NAMELIST  SHKINP HERE.',21)
00172    60*          READ (5,SHKINP)
00175    61*          WRITE(JOUT,SHKINP)
00200    62*          SEQL = INCDEQ
00201    63*          IF (T(1) .LE. 0.0)  T(1) = RTEMP(1)
00203    64*          DO 20 I = 1,13
00206    65*          IF (MACH1(I) .LE. 0.0 .AND. U1(I) .LE. 0.0)  GO TO 21
00210    66*       20 NSK = I
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00212   67*        21 IOF = IOF+1                                                    000114
00213   68*           OF = DXF(IOF)                                                  000117
00214   69*           CALL NEWOF                                                     000121
00215   70*           INCDEQ = .FALSE.                                               000123
00216   71*        17 PP = P(1)                                                      000126
00217   72*           II = I(1)                                                      000127
00220   73*           IF (INCDEQ) GO TO 19                                           000131
00220   74*     C  FROZEN                                                            000131
00222   75*           DO 118 I = 1,13                                                000136
00225   76*           DLVTP(I) = 1.0                                                 000136
00226   77*       118 DLVPT(I) = -1.0                                                000137
00230   78*        19 DO 35 NPT=1,NSX                                                000143
00233   79*           PPP(NPT) = P(NPT)                                              000147
00234   80*           TTT(NPT) = T(NPT)                                              000151
00235   81*           IF(NPT.EQ.1) GO TO 14                                          000153
00237   82*           IF (PPP(NPT) .LE. 0.0)  PPP(NPT) = PPP(NPT-1)                  000156
00241   83*           IF (TTT(NPT) .LE. 0.0)  TTT(NPT) = TTT(NPT-1)                  000163
00243   84*           SSUM(NPT) = SSUM(NPT-1)                                        000170
00244   85*           HSUM(NPT) = HSUM(NPT-1)                                        000172
00245   86*           IF(TTT(NPT).EQ.TT.AND.PPP(NPT).EQ.PP) GO TO 15                 000176
00247   87*        14 PP = PPP(NPT)                                                  000211
00250   88*           TT = TTT(NPT)                                                  000212
00251   89*           CALL HCALC                                                     000214
00252   90*           HSUM(NPT) = HSUB0                                              000216
00253   91*        15 IF (CPR1 .GT. 0.0)  GAMMA1 = CPR1/(CPR1 - 1.0/AM1)            000221
00255   92*           IF (GAMMA1 .GT. 0.0)  GO TO 30                                 000231
00257   93*           WRITE(JOUT,16)                                                 000234
00261   94*        16 FORMAT (//20X,34HMISSING GAMMA1 OR CP VALUE IN SHCK/)          000241
00262   95*           RETURN                                                         000241
00263   96*        30 A1 = SQRT(RBR*GAMMA1*TT/AM1)                                   000245
00264   97*           IF (U1(NPT) .LE. 0.0)  U1(NPT) = A1*MACH1(NPT)                 000255
00266   98*           IF (MACH1(NPT) .LE. 0.0)  MACH1(NPT) = U1(NPT)/A1              000263
00270   99*           WM(NPT) = AM1                                                  000271
00271  100*           CPR(NPT) = CPR1                                                000273
00272  101*        35 GAMMAS(NPT) = GAMMA1                                           000275
00274  102*           EQL = .FALSE.                                                  000301
00274  103*     C  OUTPUT--1ST CONDITION                                             000301
00275  104*           WRITE(JOUT,861)                                                000302
00277  105*        861 FORMAT(1H1,43X,39HINCIDENT SHOCK WAVE PARAMETERS ASSUMING    ) 000307
00300  106*           IF(.NOT.INCDEQ)  GO TO 44                                      000307
00302  107*                    WRITE(JOUT,862)                                       000311
00304  108*        862 FORMAT (1H ,51X,23HEQUILIBRIUM COMPOSITION //)                000316
00305  109*           GO TO 45                                                       000316
00306  110*        44                 WRITE(JOUT,863)                             000320
00310  111*        863 FORMAT (1H ,53X,18HFROZEN COMPOSITION //)                     000325
00311  112*        45 CALL OUT1                                                      000325
00312  113*           WRITE(JOUT,46)                                                 000326
00314  114*        46 FORMAT (16H INITIAL GAS (1) )                                  000336
00315  115*           FMT(3) = F13                                                   000336
00316  116*           FMT(4) = FOUR                                                  000340
00317  117*           WRITE(JOUT,FMT) FN,FB,(MACH1(J), J = 1,NPT)                    000342
00327  118*           FMT(4) = TWO                                                   000361
00330  119*           WRITE(JOUT,FMT) FU1,FVEL,(U1(J), J = 1,NPT)                    000363
00340  120*           CALL OUT2                                                      000401
00340  121*     C     BEGIN CALCULATIONS FOR 2ND CONDITION                           000401
00341  122*           IF(INCDEQ)   EQL = .TRUE.                                      000403
```

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00343   123.        NPT = 1                                                    000407
00344   124.     47 GAMMA1 = GAMMAS(NPT)                                       000412
00345   125.        M1 = WM(NPT)                                               000414
00346   126.        P1 = PPP(NPT)                                              000416
00347   127.        T1 = TTT(NPT)                                              000420
00350   128.        HS = HSUM(NPT)                                             000422
00351   129.        P21 = (2.*GAMMA1*MACH1(NPT)**2-GAMMA1+1.)/(GAMMA1+1.)      000424
00352   130.        T21 = P21*(2./MACH1(NPT)**2+GAMMA1-1.)/(GAMMA1+1.)         000436
00353   131.        IF((T1*T21).GT.2000..AND. EQL) T21 = .7*T21 + 600./T1      000453
00355   132.        MU12RT = AM1*U1(NPT)**2/(RBR*T1)                           000473
00356   133.        P21L=ALOG(P21)                                             000503
00357   134.        T21L=ALOG(T21)                                             000507
00360   135.        DO 100 I = 1,8                                             000520
00363   136.        TT=T21*T1                                                  000520
00364   137.        PP=P21*P1                                                  000523
00365   138.        IF (.NOT.EQL) GO TO 40                                     000526
00367   139.        CALL EQLBRM                                                000530
00370   140.        GO TO 50                                                   000532
00370   141.     C  FROZEN                                                     000532
00371   142.     40 TLN = ALOG (TT)                                            000534
00372   143.        CALL HCALC                                                 000537
00373   144.        HSUM(NPT) = HSUBO                                          000542
00374   145.        CPR(NPT) = CPR1                                            000544
00375   146.     50 RHO12 = M1*T21/(WM(NPT)*P21)                               000547
00376   147.        GG=RHO12*MU12RT                                            000554
00377   148.        G(1,1)=-GG*DLVPT(NPT)-P21                                  000564
00400   149.        G(1,2)=-GG*DLVTP(NPT)                                      000572
00401   150.        G(1,3)=P21-1.+MU12RT*(RHO12-1.)                            000576
00402   151.        GG = (U1(NPT)*RHO12)**2/RBR                                000605
00403   152.        G(2,1)=-GG*DLVPT(NPT)+TT*(DLVTP(NPT)-1.)/WM(NPT)           000613
00404   153.        G(2,2)=-GG*DLVTP(NPT)-TT*CPR(NPT)                          000626
00405   154.        G(2,3) = HSUM(NPT) - HS - U1(NPT)**2*(1.0 - RHO12**2)/(2.0*RBR)  000636
00406   155.        X(3)=G(1,1)*G(2,2)-G(1,2)*G(2,1)                           000652
00407   156.        X(1)=(G(1,3)*G(2,2)-G(2,3)*G(1,2))/X(3)                    000661
00410   157.        X(2)=(G(1,1)*G(2,3)-G(2,1)*G(1,3))/X(3)                    000671
00411   158.        AX = X(1)                                                  000701
00412   159.        AXX = X(2)                                                 000703
00413   160.        IF(AX.LT.0.) AX = -AX                                      000705
00415   161.        IF (AXX.LT.0.) AXX = -AXX                                  000712
00417   162.        IF (AXX.GT.AX)  AX = AXX                                   000717
00421   163.        IF(AX.LT..00005)  GO TO 150                                000725
00423   164.        AX = AX/.4054652                                           000731
00424   165.        IF(AX.LE.1.)  GO TO 75                                     000734
00426   166.        X(1) = X(1)/AX                                             000737
00427   167.        X(2) = X(2)/AX                                             000743
00430   168.     75 P21L=P21L+X(1)                                             000750
00431   169.        T21L=T21L+X(2)                                             000753
00432   170.        P21=EXP(P21L)                                              000757
00433   171.   100  T21 = EXP(T21L)                                            000763
00435   172.        WRITE(JOUT,125) U1(NPT)                                    000771
00440   173.     125 FORMAT(25HODID NOT CONVERGE FOR U1=,F8.2,66H   ANSWERS PROBABLY NO  001001
00440   174.       1T RELIABLE, SOLUTION PROBABLY DOES NOT EXIST)               001001
00441   175.     150 RRHO(NPT) = 1./RHO12                                       001001
00442   176.        M2M1(NPT) = WM(NPT)/AM1                                    001004
00443   177.        PCP(NPT) = P21                                             001007
```

```
00445  179*          IF (NPT .GE. IDEBUG .AND. IDEBUG .NE. 0) WRITE(JOUT,152) I,T21,P21          001013
00453  180*      152 FORMAT(10H0ITR NO.= ,I1,7X,7HT2/T1 =,F9.2,7X,7HP2/P1 =,F9.2 )            001036
00454  181*          UTWO(NPT) = U1(NPT)*RHO12                                                001036
00455  182*          U1U2(NPT) = U1(NPT)-UTWO(NPT)                                            001042
00456  183*          IF(.NOT.EQL) GO TO 16                                                    001044
00460  184*          DO 880 K=1,NS                                                            001047
00463  185*          IF(IUSE(K).LT.0) GO TO 880                                               001057
00465  186*          IF(ENLN(K).GT.-87..AND.ENLN(K).LT.87.) EN(K,NPT) = EXP(ENLN(K))          001061
00467  187*      880 CONTINUE                                                                 001110
00471  188*          GO TO 43                                                                 001110
00471  189*      C  FROZEN                                                                    001110
00472  190*      161 PPP(NPT) = PP                                                            001112
00473  191*          TTT(NPT) = TT                                                            001114
00474  192*          GAMMAS(NPT) = CPR(NPT)/(CPR(NPT) - 1.0/AM1)                              001116
00475  193*       43 ISV = 0                                                                  001125
00476  194*          IF(NPT.LT.NSK) ISV=NPT                                                   001126
00500  195*          IF(NPT.EQ.1) ISV=-1                                                      001133
00502  196*          NPT = NPT+1                                                              001140
00503  197*          IF(EQL) CALL SAVE                                                        001146
00505  198*          IF(NPT.LE.NSK) GO TO 47                                                  001147
00507  199*          NPT = NSK                                                                001153
00507  200*      C  OUTPUT--2ND CONDITION                                                     001153
00510  201*          WRITE(JOUT,58)                                                           001156
00512  202*       58 FORMAT (16HOSHOCKED GAS (2) )                                            001162
00513  203*          FMT(8) = TWO                                                             001162
00514  204*          WRITE(JOUT,FMT) FU2,FVEL,(UTWO(J),J = 1,NPT)                             001164
00520  205*          CALL OUT2                                                                001204
00525  206*          WRITE(JOUT,68)                                                           001206
00527  207*       68 FORMAT (26HOINCIDENT SHOCK PARAMETERS  )                                 001216
00530  208*          FMT(8) = THREE                                                           001216
00531  209*          WRITE(JOUT,FMT) FPP,FB,FB,(PCP(J), J = 1,NPT)                            001220
00542  210*          WRITE(JOUT,FMT) FTT,FB,FB,(T2T1(J), J = 1,NPT)                           001235
00553  211*          FMT(8) = FOUR                                                            001252
00554  212*          WRITE(JOUT,FMT) FMM,FB,FB,(M2M1(J), J = 1,NPT)                           001254
00565  213*          WRITE(JOUT,FMT) FRA,FRB,FB,(RRHO(J), J = 1,NPT)                          001271
00576  214*          FMT(8) = TWO                                                             001306
00577  215*          WRITE(JOUT,FMT) FV21,FV22,FV23,(U1U2(J), J = 1,NPT)                      001310
00610  216*          CALL OUT3                                                                001325
00611  217*          INCODE = .FALSE.                                                         001327
00612  218*          IF(INCOFZ.AND.EQL) GO TO 17                                              001330
00614  219*          IF(IOF.LT.NOF) GO TO 21                                                  001333
00616  220*          TP = .FALSE.                                                             001341
00617  221*          DO 999 K = 1,NREAC                                                       001345
00622  222*      999 RTEMP(K) = T(1)                                                          001345
00624  223*          RETURN                                                                   001347
00625  224*          END                                                                      001400
```

END OF COMPILATION: NO DIAGNOSTICS.

@MOD,P THERMP

```
@FOR,S   THERMP,THERMP
HASP EJ -10/15/80-13:07:55 ,19,)

    SUBROUTINE THERMP    ENTRY POINT 000427

    STORAGE USED: CODE(1) 000437; DATA(0) 000117; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003   CONSTS  000006
     0004   POINTS  000335
     0005   MISC    001701
     0006   INDX    000041
     0007   OUPT    000073
     0010   CCC     000003
     0011   CFUEL   000002

    EXTERNAL REFERENCES (BLOCK, NAME)

     0012   NEWOF
     0013   EQLORN
     0014   MOVABS
     0015   HOLDIT
     0016   PAGIT
     0017   GOUT
     0020   OUT1
     0021   OUT2
     0022   OUT3
     0023   OUT4
     0024   SAVE
     0025   MWDUS
     0026   MIO2S
     0027   MIO1S
     0030   MERR3S

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0000   000021 10F      0000   000025 11F      0000   000033 12E      0001   000022 1256     0001   000044 1326
     0000   000041 20F      0000   000045 21F      0000   000054 22F      0001   000234 2256     0001   000261 2416
     0000   000006 5F       0001   000061 800L     0001   000111 860L     0001   000162 861L     0001   000207 862L
     0000   000062 863F     0001   000265 869L     0000   000070 858F     0001   000354 870L     0001   000403 871L
     0001   000276 902L     0001   000006 95L      0005   000640 AM       0005   000705 AM1      0005   001135 ANUM
     0003   000000 ATMN     0005   000004 ATOM     0005   000514 BO       0005   000545 BOP      0006   000036 CALCM
     0011 R 000000 CF       0006   000001 CONVG    0004   000032 CPR      0005   000706 CPR1     0005   000634 CPSUM
     0005   000654 DATA     0010   000002 DEMAND   0005   001560 DENS     0004   000064 DLVPT    0004   000047 DLVTP
     0005   001700 ENLSAV   0005   000000 ENM      0005   001676 ENML     0005   001677 ENSAVE   0005   001414 ENTM
     0005   000636 EORAT    0007   000002 FA       0007   000003 FAP      0005   001445 FA2      0007 R 000005 FB
     0007   000006 FC       0007   000007 FCP      0007   000012 FCST     0007   000014 FCV      0007   000015 FG
     0007   000017 FGE      0007   000020 FGV      0007   000021 FH       0007   000023 FI       0007   000025 FIV
     0007   000027 FM       0007 R 000031 FMT      0007   000050 FN       0007   000052 FOUR     0005   001527 FOX
     0007   000053 FP       0007   000054 FS       0007   000056 FSV      0007   000057 FT       0007   000061 FTK
     0000 R 000000 FUA      0000 R 000001 FUB      0007   000063 FV       0007   000065 FVEL     0007   000001 F13
```

```
0007   000000 F9X      0004   000101 GAMMAS   0003   000001 GMZT     0010   000000 GRAPH    0011   000001 HHVV
0006 L 000003 HP       0005   000642 HPP      0004 R 000637 HSUBO    0004   000000 HSUM     0000 I 000003 I
0006   000030 IC       0006 I 000000 IDEBUG   0006   000015 IMAT     0000   000100 INJPS    0000 I 000002 IOF
0006   000023 IONS     0006 I 000021 IP       0006   000037 IOSAVE   0006   000016 IO1      0006 I 000005 ISV
0006 I 000034 IT       0006   000026 JLIO     0010 I 000001 JOUT     0006   000025 JSOL     0006   000031 JS1
0006   000014 KMAT     0005   000463 LLMI     0006   000040 LSAVE    0004   000004 MOLES    0004   000707 NAME
0006   000024 NC       0006   000022 NEVR     0006   000035 NFZ      0006   000012 NLM      0006 I 000017 NOF
0006   000020 NOMIT    0006 I 000007 NP       0006 I 000011 NPT      0006   000027 NREAC    0006   000013 NS
0006 I 000010 NT       0005 R 000635 OF       0007 R 000067 ONE      0005 R 001644 OXF      0004 R 000116 P
0003   000002 PATM     0005   001363 PECUT    0005 R 000633 PP       0004   000217 PPP      0003 R 000003 RBAR
0003   000004 RBR      0005   000644 RM       0005   001611 RHOP     0005   001612 RMW      0005   001476 RTEMP
0003   000005 RYR      0006   000033 SHOCK    0004   000251 SONVEL   0004 L 000004 SP       0004   000015 SSUM
0005   000001 SUMN     0005   000003 SO       0004 R 000150 T        0005   000632 THIGH    0007   000070 THREE
0005   001643 TLN      0005   000630 TLOW     0005   000627 TM       0005   000631 TMID     0004   000320 TOTN
0006 L 000002 TP       0005 R 000102 TT       0004   000266 TTT      0007 R 000071 TWO      0004 R 000202 V
0004 R 000303 VLM      0005   000646 VMIN     0004 L 000032 VOL      0005   000650 VPLS     0004   000234 WM
0005   000652 WP       0007   000072 ZERO
```

```
00101         SUBROUTINE THERMP                                                      000000
00101   C                                                                  MOLI0001  000000
00103         COMMON /CONSIS/ ATMM,GMEI,P,IM,RBAR,RBR,RYR                  /CONSIS/  000000
00104         COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)              000000
00104        1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)        000000
00104        2 ,VLM(13),TOTN(13)                                                        000000
00105         COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMI(25),BO(25),                 000000
00105        1              BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,             000000
00105        2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),   /MISC/   000000
00105        3              DATA(25),AM3,CPR1,NAME(25,6),ANUM(25,6),PECUT(25),         000000
00105        4              ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,          000000
00105        5              RMW(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                     000000
00106         COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,   /INDX/   000000
00106        1              KMAT,IMAT,IO1,NOF,NOMIT,IP,NEVR,IONS,NC,JSOL,JLIO,   /INDX/   000000
00106        2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCM,IOSAVE,LSAVE     /INDX/   000000
00107         COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),   /OUPT/   000000
00107        1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR,  /OUPT/   000000
00107        2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,   /OUPT/   000000
00107        3              TWO,ZERO                                            /OUPT/   000000
00107   C                                                                                000000
00110           COMMON /CCC/ GRAPH,JOUT,DEMAND                                           000000
00110   C                                                                                000000
00111         COMMON /CFUEL/CF,HHVV                                                      000000
00112         DATA FUA/6HU CAL//,FUB/6HGRAM  /                                           000000
00115         LOGICAL HP,SP,TP,VOL                                                       000000
00115   C                                                                                000000
00116         IF (T(1) .LE. 0.0)  T(1) = 3800.0                                          000000
00120         IOF = 0                                                                    000004
00121      95 IOF = IOF+1                                                                000004
00122         OF = OXF(IOF)                                                              000011
00123         CALL NEWOF                                                                 000013
00123   C     SET ASSIGNED P OR VOLUME                                                   000013
00124         DO 871 IP = 1,NP                                                           000015
00127         PP = P(IP)                                                                 000035
00130         VLM(NPT) = P(IP)                                                           000037
```

```
00130   38.     C     SET ASSIGNED T                                    MOLID016   000037
00131   39.           DO 871 IT = 1,NT                                             000044
00134   38.           TT = T(IT)                                        MOLID019   000044
00135   39.           CALL EOLBRM                                       MOLID025   000046
00136   40.           IF (TT .GT. 0.0)  GO TO 800                                  000050
00140   41.           IF (NPT .EQ. 0)  RETURN                                      000053
00142   42.     800   ISV = 0                                                      000061
00143   43.           IF (IP .EQ. NP .AND. IT .EQ. NT .OR. TT .LE. 0.0)  GO TO 860 000061
00145   44.           ISV = NPT                                                    000104
00146   45.           IF(NPT.NE.13)  GO TO 870                          MOLID030   000106
00150   46.     860   CONTINUE                                                     000111
00151   47.           CALL MOVABS(500,50)                                          000114
00152   48.           CALL HOLDIT                                                  000114
00153   49.           CALL PAGIT                                                   000116
00154   50.           CALL GOUT(' ',1)                                             000120
00155   51.           WRITE (JOUT,5)                                               000129
00157   52.         5 FORMAT(1H1,41X,9HTHERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNEDMOLID032 000131
00157   53.          1)                                                          000134
00160   54.           IF(.NOT.VOL)  GO TO 861                                      000131
00162   55.           IF (HP)  WRITE(JOUT,10)                                      000133
00165   56.        10 FORMAT(1H0,62X,7H VOLUME /)                                  000142
00166   57.           IF (TP)  WRITE(JOUT,11)                                      000142
00171   58.        11 FORMAT(1H0,54X,22HTEMPERATURE AND VOLUME/)                   000151
00172   59.           IF (SP)  WRITE(JOUT,12)                                      000151
00175   60.        12 FORMAT(1H0,56X,18HENTROPY AND VOLUME/)                       000160
00176   61.           GO TO 862                                                    000160
00177   62.     861   IF(HP)  WRITE(JOUT,20)                                       000162
00202   63.        20 FORMAT(1H0,62X,10H PRESSURE  /)                            000170
00203   64.           IF(TP)  WRITE(JOUT,21)                                       000170
00206   65.        21 FORMAT(1H0,53X,29HTEMPERATURE AND PRESSURE/)                 000177
00207   66.           IF(SP)  WRITE(JOUT,22)                                       000177
00212   67.        22 FORMAT(1H0,55X,20HENTROPY AND PRESSURE/)                     000207
00213   68.     862   CALL OUT1                                                    000207
00214   69.           WRITE(JOUT,863)                                              000210
00216   70.     863   FORMAT (25HOTHERMODYNAMIC PROPERTIES//)                      000223
00217   71.           IF(.NOT.VOL)  GO TO 864                                      000223
00221   72.           FMT(3) = ONE                                                 000225
00222   73.           IF (.NOT. HP)  GO TO 864                                     000227
00224   74.           DO 63 I=1,NPT                                                000230
00227   75.           FMT(I+2) = TWO                                               000230
00230   76.           IF (I .EQ. 13)  FMT(15) = 5HF9.2)                            000236
00232   77.     63    V(I) = RBAROHSUB0                                            000243
00234   78.           WRITE(JOUT,FMT) FUA,FUB,FB,(V(I), I = 1,NPT)                 000247
00245   79.     864   CALL OUT2                                                    000265
00246   80.           CALL OUT3                                                    000266
00247   81.           IF (CF+1.0) ,902,                                            000270
00252   82.     900   CALL OUT4                                                    000273
00253   83.     902   CONTINUE                                                     000276
00254   84.           CALL MOVABS(500,50)                                          000276
00255   85.           CALL HOLDIT                                                  000301
00256   86.           CALL PAGIT                                                   000303
00257   87.           IF (ISV .EQ. 0 .AND. IOF .EQ. NOF)  RETURN                   000305
00261   88.           IF(IDEBUG.GT.13)  IDEBUG=IDEBUG-13                           000322
00263   89.           WRITE(JOUT,868)                                              000331
00265   90.     868   FORMAT(1H1)                                                  000336
00266   91.           IF(NT.EQ.1.AND.NP.EQ.1)  GO TO 95                            000336
```

```
00270    92*          NPT = 0
00271    93*      870 NPT = NPT + 1                                  000352
00272    94*          IF(.NOT.TP)  T(1)=TT                MOLI0037  000354
00274    95*          IF(TP.EQ.1.AND.IT.EQ.1)  ISV=-ISV              000356
00276    96*          IF(NT.EQ.1)  GO TO 871                 12-22   000362
00300    97*          IF(IT.EQ.NT)  ISV=0                    12-22   000373
00302    98*      871 CALL SAVE                                      000376
00305    99*          GO TO 95                                       000403
00306   100*          END                                            000410
                                                            MOLI0045 000436
```

END OF COMPILATION: NO DIAGNOSTICS.

```
@MDS,P     VARFMT
```

```
@FOR,S    VARFMT,VARFMT
HSA  E3 -10/15/80-13:07:58 (7,)

    SUBROUTINE VARFMT    ENTRY POINT 000115

    STORAGE USED: CODE(1) 000124; DATA(0) 000023; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003  OUPT  000073

    EXTERNAL REFERENCES (BLOCK, NAME)

     0004   NERR3S

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001   000006 1146      0001   000046 ADL       0001   000100 AS        0003   000002 FA        0003   000003 FAP
     0003   000005 FB        0003   000006 FC        0003   000007 FCP       0003   000012 FCST      0003   000014 FCV
     0000 R 000000 FFOUR     0003   000015 FG        0003   000017 FGE       0003   000020 FGV       0003   000021 FH
     0003   000023 FI        0003   000025 FIV       0003   000027 FM        0003 R 000031 FMT       0003   000050 FN
     0000 R 000001 FONE      0003 R 000052 FOUR      0003   000053 FP        0003   000054 FS        0003   000056 FSV
     0003   000057 FT        0000 R 000002 FTHREE    0003   000061 FTK       0000 R 000003 FTWO      0003   000063 FV
     0003   000065 FVEL      0000 R 000004 FZERO     0003   000001 F13       0003   000008 F9X       0000 I 000000 I
     0000   000012 INJPS     0003 R 000067 ONE       0003 R 000070 THREE     0003 R 000071 TWO       0003 R 000072 ZERO

00101      1*          SUBROUTINE VARFMT(V,NPT)                                                    000006
00101      2*    C
00103      3*          COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),     /OUPT/   000006
00103      4*         1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/   000006
00103      5*         2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,   /OUPT/   000006
00103      6*         3              TWO,ZERO                                             /OUPT/   000006
00103      7*    C                                                                                  000006
00104      8*          DATA FFOUR/5HF9.4)/,FONE/5HF9.1)/,FTHREE/5HF9.3)/,FTWO/5HF9.2)/,            000006
00104      9*         1     FZERO/5HF9.0)/                                                         000006
00112     10*          DIMENSION V(13)                                                             000006
00112     11*    C                                                                                  000006
00113     12*          DO 45 I = 1,NPT                                                             000006
00116     13*          IF (I .GE. 13)  GO TO 40                                                    000006
00120     14*          FMT(I+2) = FOUR                                                             000012
00121     15*          IF (V(I) .GE. 10.0)  FMT(I+2) = THREE                                       000016
00123     16*          IF (V(I) .GE. 100.0)  FMT(I+2) = TWO                                        000022
00125     17*          IF (V(I) .GE. 1.0E4)  FMT(I+2) = ONE                                        000030
00127     18*          IF (V(I) .GE. 1.0E6)  FMT(I+2) = ZERO                                       000036
00131     19*          GO TO 45                                                                    000040
00132     20*       40 FMT(15) = FFOUR                                                             000046
00133     21*          IF (V(I) .GE. 10.0)  FMT(15) = FTHREE                                       000047
00135     22*          IF (V(I) .GE. 100.0)  FMT(15) = FTWO                                        000055
00137     23*          IF (V(I) .GE. 1.0E4)  FMT(15) = FONE                                        000063
```

```
00141    24*          IF (V(I) .GE. 1.0E6)  FMT(15) = 'ZERO
00143    25*     45   CONTINUE                                          000102
00145    26*          RETURN                                            000102
00146    27*          END                                               000123
```

END OF COMPILATION: NO DIAGNOSTICS.

$NO
$END IGNORED - IN CONTROL MODE

$FIN

RUNID: LEWIST ACCT: 1HPA01R5002 PROJECT: SEVI6M0IN20

LOAD 15753 11/0 PUR -1 LEWIST

TIME: SUPS: 00:02:51.912 CBSUPS: 057007923

CPU: 00:00:38.729 I/O: 00:01:29.681

CC/ER: 00:00:43.501 WAIT: 00:00:00.065

IMAGES READ: 61 PAGES: 118

START: 13:09:96 OCT 15,1980 FIN: 13:08:01 OCT 15,1980

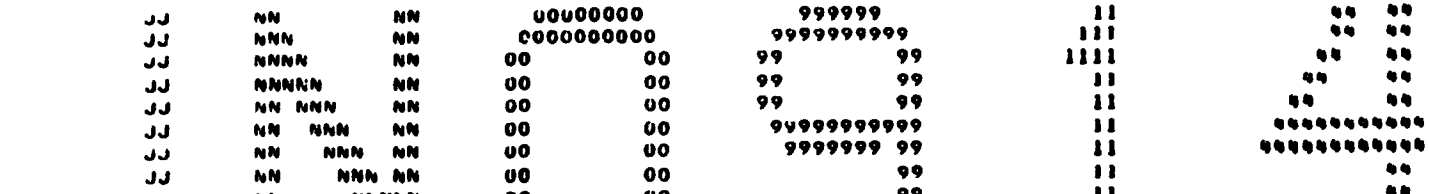
THE 1108 (HOST2) WILL BE POWERED OFF NO LATER THAN NOV 15 1980

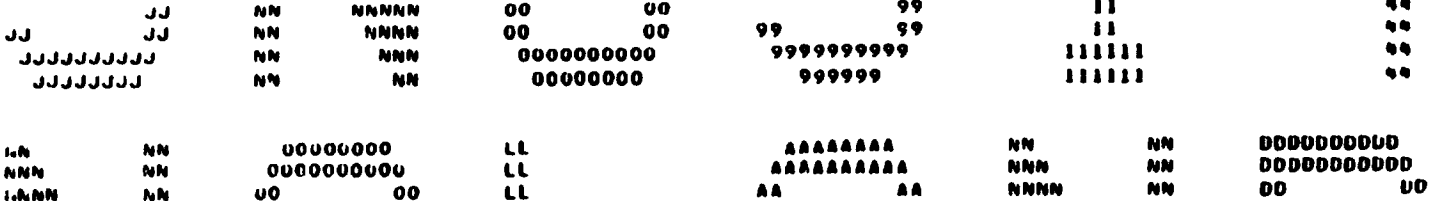
* * * * * * UNIVAC 1100 TIME/SHARING EXEC ACCOUNT NUMBER * IMPAGES 2 VER. EM 33R3MOST2 SITE * MOST 2 * * * * * *

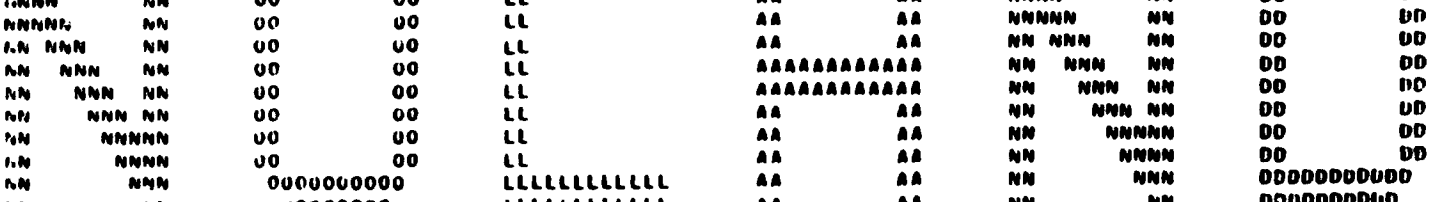
APPENDIX C

SOURCE LISTING OF PROGRAM ELEMENTS WITHOUT MODIFICATIONS

This is a printout of the Lewis Chemical Equilibrium Program without the modifications necessary for coal gasification data. There have been intermediate changes, principally to make the program an interactive one.







C-1

• • • • • • UNIVAC 1100 TIME/SHARING EXEC ACCOUNT NUMBER • IMPDU13K0000 VER. CR 33R3M0S11 SITE • HOST 1 • • • • • •

USER ID • JNOV19 USER ID • PART NUMBER • 01 INPUT DEVICE • DTR00A OUTPUT DEVICE • PR2

FILE NAME • PRT CREATED AT: 17:37:49 OCT 25,1979 PRINTED AT: 17:43:59 OCT 25,1979

(1) SPECIES DIMENSIONS CHANGED TO 150,
(2) MAIN PROGRAM MODIFIED TO PREVENT PAGE RESET

```
MTOK,S LEWIS.BLOCK1,LEWIS.BLOCKB
MSA  13 -10/25/79-17:37:58 (0,)

  BLOCK DATA

  STORAGE USED: CODE(1) 000000; DATA(0) 000000; BLANK COMMON(2) 000000

   COMMON BLOCKS:

    0003   CONSTS 000006
    0004   MOLCON 000010
    0005   MISC   001264
    0006   OUPT   000073


  STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

  0005   000570 AM       0005   000624 AM1      0005   000741 ANUM     0005 R 000004 ATAM     0006 R 000235 ATEM
  0003 R 000000 ATMN     0005   000004 ATOM     0005   000502 BO       0005   000521 BUP      0005   000625 CPR1
  0005   000564 CPSUM    0005   000604 DATA     0005   001167 DENS     0004 R 000000 ENU      0005   001263 ENLSAV
  0005   000000 ENN      0005   001261 ENNL     0005   001262 ENSAVE   0005   001073 ENNM     0005   000566 EQRAT
  0006 R 000002 FA       0006 R 000003 FAP      0005   001132 FAZ      0006 R 000005 FB       0006 R 000004 FC
  0006 R 000007 FCP      0006 R 000012 FCST     0006 R 000014 FCV      0006 R 000015 FG       0006 R 000017 FGE
  0006 R 000020 FGV      0006 R 000021 FH       0006 R 000023 FI       0006 R 000025 FIV      0006 R 000027 FM
  0006 R 000031 FMT      0006 R 000050 FN       0006 R 000052 FOUR     0005   001150 FOX      0006 R 000053 FP
  0006 R 000054 FS       0006 R 000056 FSV      0006 R 000057 FT       0006 R 000061 FTK      0006 R 000063 FV
  0006 R 000065 FVEL     0006 R 000001 F13      0006 R 000000 F9X      0004 R 000001 GAS      0003 R 000001 GMET
  0005   000572 HPP      0005   000567 HSUBU    0004 I 000002 IE       0004 I 000003 IZERO    0004 I 000004 LANN
  0005   000463 LLMT     0004 I 000005 MOL      0005   000626 NAME     0005   000565 OF       0006 R 000067 ONE
  0004 R 000006 OX       0005   001227 OXF      0003 R 000002 PAIN     0005   001054 PECWT    0005   000563 PP
  0003 R 000003 RBAR     0003 R 000004 RBR      0005   000574 RH       0005   001206 RHOP     0005   001207 RMW
  0005   001131 RTEMP    0003 R 000005 RVR      0005   000001 SUMN     0005   000003 SO       0005   000562 THIGH
  0006 R 000070 THREE    0005   001226 TLN      0005   000560 TLOW     0005   000557 TM       0005   000561 TMID
  0005   000002 TT       0006 R 000071 TWO      0005   000576 VMIN     0005   000600 VPLS     0005   000602 WP
  0004 R 000007 ZERO     0006 R 000072 ZEROF


 00101          BLOCK DATA                                                           ATMOU00I     000000
 00101      C                                                                                     000000
 00102          COMMON /CONSTS/ ATMN,GMET,PAIN,RBAR,RBR,RVR                           /CONSTS/     000000
 00103          COMMON /MOLCON/ ENU,GAS,IE,IZERO,LANN,MOL,OX,ZERO                     /MOLCON/     000000
 00104          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),              /MISC/       000000
 00104     1                 BUP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,          /MISC/       000000
 00104     2                 HSUBU,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),          /MISC/       000000
 00104     3                 DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15),       /MISC/       000000
 00104     4                 ENNM(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,        /MISC/       000000
 00104     5                 RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                   /MISC/       000000
 00105          COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),        /OUPT/       000000
 00105     1                 FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR,     /OUPT/       000000
 00105     2                 FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,       /OUPT/       000000
 00105     3                 TWO,ZEROF                                                /OUPT/       000000
 00105      C                                                                                     000000
 00106          DIMENSION ATAM(3,51),ATEM(3,50)                                                   000000
 00107          EQUIVALENCE (ATOM(1,1),ATAM),(ATOM(1,52),ATEM)                                    000000
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ORIGINAL PAGE IS
OF POOR QUALITY

```
      180      C
      190      C  ATOMIC SYMBOLS, WEIGHTS, AND VALENCES                                                    000000
      200            DATA AIAM/2HH ,1.00797,1.0,2HHE,4.0026,0.0,2HLI,6.939,1.0,2HBE,                      000000
      210           1 9.0122,2.0,2HB ,10.811,3.0,2HC ,12.0115,4.0,2HN ,14.0067,0.0,                      000000
      220           2 2HO ,15.9994,-2.0,2HF ,18.9984,-1.0,2HNE,20.183,0.0,2HNA,22.9898,                  000000
      230           3 1.0,2HMG,24.312,2.0,2HAL,26.9815,3.0,2HSI,28.086,4.0,2HP ,30.9738                  000000
      240           4,5.0,2HS ,32.064,4.0,2HCL,35.453,-1.0,2HAR,39.948,0.0,2HK ,39.102,                  000000
      250           5 1.0,2HCA,40.080,2.0,2HSC,44.956,3.0,2HTI,47.90,4.0,2HV ,50.942,                    000000
      260           6 5.0,2HCR,51.996,3.0,2HMN,54.9380,2.0,2HFE,55.847,3.0,2HCO,58.9332                  000000
      270           7,2.0,2HNI,58.710,2.0,2HCU,63.540,2.0,2HZN,65.370,2.0,2HGA,69.720,                   000000
      280           8 3.0,2HGE,72.590,4.0,2HAS,74.9216,3.0,2HSE,78.960,4.0,2HBR,79.909,                  000000
      290           9 -1.0,2HKR,83.80,0.0,2HRB,85.47,1.0,2HSR,87.620,2.0,2HY ,88.905,                   000000
      300           A 3.0,2HZR,91.220,4.0,2HNB,92.906,5.0,2HMO,95.94,6.0,2HTC,99.0,7.0,                  000000
      310           B 2HRU,101.070,3.0,2HRH,102.905,3.0,2HPD,106.40,2.0,2HAG,107.870,                    000000
      320           C 1.0,2HCD,112.40,2.0,2HIN,114.820,3.0,2HSN,118.690,4.0,2HSB,                        000000
      330           D 121.750,3.0/                                                                       000000
      340            DATA AIEM/2HTE,127.60,4.0,2HI ,126.9044,-1.0,2HXE,131.30,0.0,2HCS,                  000000
      350           1 132.905,1.0,2HBA,137.340,2.0,2HLA,138.918,3.0,2HCE,140.120,3.0,                    000000
      360           2 2HPR,140.907,3.0,2HND,144.240,3.0,2HPM,145.0,3.0,2HSM,150.350,3.0                  000000
      370           3,2HEU,151.960,3.0,2HGD,157.250,3.0,2HTB,158.924,3.0,2HDY,162.50,                    000000
      380           4 3.0,2HHO,164.930,3.0,2HER,167.260,3.0,2HTM,168.934,3.0,2HYB,                       000000
      390           5 173.040,3.0,2HLU,174.997,3.0,2HHF,178.490,4.0,2HTA,180.948,5.0,                    000000
      400           6 2HW ,183.850,6.0,2HRE,186.20,7.0,2HOS,190.20,4.0,2HIR,192.20,4.0,                  000000
      410           7 2HPT,195.090,4.0,2HAU,196.967,3.0,2HHG,200.590,2.0,2HTL,204.370,                   000000
      420           8 1.0,2HPB,207.190,2.0,2HBI,208.980,3.0,2HPO,210.0,2.0,2HAT,210.0,                   000000
      430           9 0.0,2HRN,222.0,0.0,2HFR,223.0,1.0,2HRA,226.0,2.0,2HAC,227.0,3.0,                   000000
      440           A 2HTH,232.038,4.0,2HPA,231.0,5.0,2HU ,238.030,6.0,2HNP,237.0,5.0,                   000000
      450           B 2HPU,242.0,4.0,2HAM,243.0,3.0,2HCM,247.0,3.0,2HBK,249.0,3.0,2HCF,                  000000
      460           C 251.0,3.0,2HES,254.0,0.0,2HFM,253.0,0.0,U,2HD ,2.014102,1.0/                       000000
      470      C     INFORMATION USED IN VARIABLE OUTPUT FORMAT                                          000000
      480            DATA F9X/3H9X,/,F13/2H13/,FA/6HAE/AT /,FB/6H      /,FC/6HCF    /,  /OUPT/         000000
      490           1     FCV/6HCF yAC/,FG/12HGAMMA (S)   /,FI/12HISP SECONDS /,        /OUPT/         000000
      500           2     FIV/12HIVAC SECONDS/,FM/12HM MOL WEIGHT/,FMT/6HIJH ,2.       /OUPT/         000000
      510           3     6HA6,A2,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,    /OUPT/         000000
      520           4     5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1,,5HF9.1)/,    /OUPT/         000000
      530           5     FN/12HMACH NUMBER /,FOUR/5HF9.4,/,FP/6HPC/P  /,              /OUPT/         000000
      540           6     FT/12HIDLV/DLP) T /,FV/12HIDLV/DLT) P /,ONE/5HF9.1,/,        /OUPT/         000000
      550           7     THREE/5HF9.3,/,TWO/5HF9.2,/,ZEROF/5HF9.0,/,FAP/12HPRESS N/M**                000000
      560           82/,FCP/12HCP CAL/(G)(K,2H) /,FCST/12HCSTAR M/SEC /,FGE/6HIEFF) /,                   000000
      570           9 FGV/6HGAS VE/,FH/12HENTH CAL/G  /,FS/12HS CAL/(G)(K)/,FSV/6HSON V                  000000
      580           AE/,FTM/12HTEMP DEG. K /,FVEL/6HL M/SE,2HC /                                         000000
      590            DATA END/3HEND/,BAS/1HG/,IE/1HE/,IZERO/2H00/,LANR/2H  /,MOL/1HM/                    000000
      600           1 ,UX/1HO/,ZERO/1HO/,ATMM/101325.0/,RVR/82.05544997/                                 000000
      610           3 ,GMLT/9.8066S6/,PATM/14.696U060/,RBAR/1.9871650/,RBR/8314.298360/                  000000
      620            END                                                                  ATM000060     000000
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.FOR,S LEWIS.CPHS,LEWIS.CPHS
H.A  E:  -10/25/79-17:37:57 (9,)


    SUBROUTINE CPHS       ENTRY POINT 000567


    STORAGE USED: CODE(1) 000603; DATA(0) 000160; BLANK COMMON(2) 000000

     COMMON BLOCKS:

      0003   SPECES 01.320
      0004   MISC   001264
      0005   INDX   000041
      0006   LOWTH  001201
      0007   CCC    000003


    EXTERNAL REFERENCES (BLOCK, NAME)

      0010   NW0015
      0011   .I02S
      0012   ALOG
      0013   .I01S
      0014   NERR36


    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

      0001    000031 10L        0001    000207 171G       0001    000217 174G       0001    000043 20L        0001    000351 221G
      0001    000462 254G       0001    0C0065 30L        0001    000067 31L        0001    000157 32L        0000    000041 3333F
      0001    000164 40L        0001    000176 60L        0001    000230 70L        0001    000233 80L        0001    000412 87L
      0001    000060 66F        0001    000472 69L        0001    000531 90L        0000    000103 904F       0003    006034 A
      0004    000570 AM         0004    000624 AM1        0004    000741 ANUM       0004    000004 ATOM       0004    000502 B0
      0004    000571 B0P        0005    000036 CALCH      0003 R  000000 COEF       0005    000001 CONVG      0006 R  000361 CPL
      0004    000625 CPM1       0004 R  000564 CPSUM      0000 R  000040 CPUSED     0000 R  000035 CPX        0000 R  000007 CPXX
      0004    000604 DATA       0003    005670 DELN       0007    000002 DEMAND     0004    001167 DENS       0003 R  002734 EN
      0004    005360 ENLN       0004    001263 ENLSAV     0004    000000 ENN        0004    001261 ENNL       0004    001262 ENSAVE
      00      001073 ENTH       0004    000566 EQRAT      0004    001112 FAZ        0004    001150 FOX        0007    000000 GRAPH
      0006 R  000551 HL         0005    000003 HF         0004    000572 HPP        0004    000567 HSUBU      0000 R  000034 HX
      0000 R  000013 HXX        0001 R  005524 HO         0000 I  000037 I          0005    000030 IC         0005    000000 IDEBUG
      0000 I  000001 IER        0000 I  000023 IEXTND     0006 I  001131 ILSP       0005    000015 IMAT       0000 I  000002 IMSG
      0000    000132 INJFB      0005    000023 IONS       0005    000021 IP         0005    000037 IQSAVE     0005    000016 IQ1
      0005    000035 ISW        0005    000034 IT         0003 I  011444 IUSE       0000 I  000026 IX         0005 I  000031 J
      0005    000026 JCIQ       0007 I  000001 JOUT       0005    000025 JSOL       0000 I  000024 K          0000 I  000025 KK
      0005    000014 KMAT       0000 I  000027 KX         0004    000463 LLMT       0005    000040 LSAVL      0000 I  000036 M
      0005    000006 MOLES      0004    000626 NAME       0005    000024 NC         0005    000022 NEWR       0005    000035 NFZ
      0005    000012 NLM        0006 I  000000 NLTSP      0005    000017 NOF        0005    000020 NOMIT      0005    000007 NP
      0007 I  000011 NPI        0005    000027 NREAC      0005 I  000013 NS         0000 I  000000 NSPPI      0005    000010 NT
      0000 I  000030 NTOP       0004    000565 OF         0004    001227 OXF        0004    001054 PECWT      0004    000563 PP
      0004    000479 RH         0004    001206 RHOP       0004    001207 RMW        0004    001131 RTEMP      0003 R  002570 S
      0005    000033 SHOCK      0006 R  000741 SL         0003    011754 SLN        0005    000004 SP         0003 I  010770 SUB
      0004 I  000001 SUELI      0004    000001 SUMN       0000 R  000033 SX         0000 R  000017 SXX        0004    000003 SO
      0003    011610 TEMP       0004    000562 THIGH      0006 R  000171 TL         0004 R  001226 TLN        0000 R  000032 TLNS
      0004 R  000561 TLOW       0004    000557 TM         0004 R  000561 TMID       0005    000002 TP         0004 R  000002 TT
      0006 R  000031 TTS        0000 R  000033 TXX        0004    000576 VMIN       0005    000032 VOL        0004    000600 VPLS
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      SUBROUTINE CPHS                                                                  000002
C                                                                                      000002
C     CALCULATES THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES                       000002
C                                                                                      000002
C     COMMON/SPECES/COEFF(2,7,ISO),S(ISO),EN(ISO,13),ENLN(ISO),HO(ISO)                 000002
C    . ,DELN(ISO),A(15,ISO),SUB(ISO,3),IUSE(ISO),TEMP(ISO,2),SLN(ISO)                 000002
      INCLUDE SPECPH                                                                   000002
      COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,IO1),LLMT(15),BO(15),          /MISC/        000002
     1              BUP(15,2),TM,TLOW,TMID,TMIGH,PP,CPSUM,OF,EQRAT,      /MISC/        000002
     2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),UP(2),      /MISC/        000002
     3              DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),PECWT(15),   /MISC/        000002
     4              LNTM(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,    /MISC/        000002
     5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV               /MISC/        000002
      COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,MP,NT,NPT,NLM,NS,     /INDX/        000002
     1              AMAT,IMAT,IOI,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,   /INDX/        000002
     2              AREAC,IC,J,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE       /INDX/        000002
      COMMON /LOWTM/ NLTSP,SUBLT(40,3),TL(40,3),CPL(40,3),HL(40,3),      /LOWTM/        000002
     1               SL(40,3),ILSP(40)                                   /LOWTM/        000002
C                                                                                      000002
C        COMMON /CCC/ GRAPH,JOUT,DEMAND                                                000002
C                                                                                      000002
      DATA ILP/0/,IMSG/-1/                                                             000002
      DIMENSION TX(40),CPXX(40),HXX(40),SXX(40)                          CPHS  20      000002
      INTEGER SUM,SUBLT                                                                000002
C                                                                                      000002
      IEXIND = 0                                                         CPHS 190      000030
      IF(TT.LT.TLOW) IEXIND = 1                                          CPHS 200      000033
      IF(IEXIND.NE.0) IMSG = IMSG + 1                                    R FEB-3       000011
      IF(IMSG.NE.0) GO TO 10                                             R FEB-3       000016
      IF(IEXIND.NE.0) WRITE(JOUT,3333) TT                                              000020
 3333 FORMAT (///25X,48HLOW TEMPERATURE THERMO EXTENSION IN CPHS AT TT =,              000031
     1        F12.6,15H DEGREES KELVIN//)                                             000031
                                                                                       000031
   10 N = 1                                                                            000032
      IF (TT.LE.TMID) N=2                                                CPHS 240      000040
      AA=0                                                               CPHS 250      000040
      CPSUM=0.                                                           CPHS 260      000041
   20 IF (COEFF(N,1,JJ).NE.0.) GO TO 30                                  CPHS 270      000043
      IF (IUSE(JJ).LT.0) GO TO 40                                        CPHS 280      000047
      AA=A                                                               CPHS 290      000053
      N=1                                                                CPHS 300      000058
      IF (AA.EQ.1) N=2                                                   CPHS 310      000057
   30 IF (IEXIND .NE. 0)  GO TO 60                                                     000065
   31 S(JJ) = ((((COEFF(N,5,JJ)/4.0)*TT + COEFF(N,4,JJ)/3.0)*TT + COEFF(N,3,JJ)       000067
     1       /2.0)*TT + COEFF(N,2,JJ))*TT + COEFF(N,1,JJ)*TLN + COEFF(N,7,JJ)        000067
      HH(JJ)=(((((COEFF(N,5,JJ)/5.0*TT+COEFF(N,4,JJ)/4.0)*TT+COEFF(N,3,JJ)/3.0)*TTCPHS 370      000110
     1+COEFF(N,2,JJ)/2.0)*TT+COEFF(N,1,JJ))*COEFF(N,6,JJ)/TT                   CPHS 380      000114
      CPSUM=CPSUM+(((((COEFF(N,5,JJ)*TT+COEFF(N,4,JJ))*TT+COEFF(N,3,JJ))*TT+COECPHS 390      000140
     1F(N,2,JJ))*TT+COEFF(N,1,JJ))*ENL(JJ,NPT)                                 CPHS 400      000140
   32 IF (AA .EQ. 0)  GO TO 40                                                         000157
      A=2                                                                CPHS 430      000160
      N=2                                                                CPHS 440      000162
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C-5

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      60  IF (J .EQ. NSJ)  RETURN                                                  000360
      530       J=J+1                                                  CPHS  480  000370
      540       GO TO 20                                               CPHS  490  000380
      550   60  IF (NLISP .EQ. 0)  GO TO 31                                       000390
      560       DO 70 II= 1,NLISP                                      CPHS  500  000400
      570       DO 65 KK = 1,3                                                    000410
      580   65  IF (ISUBJ,KK) .NE. SUBLT(IX,KK))  GO TO 70                       000420
      590       GO TO 80                                               CPHS  510  000430
      600   70  CONTINUE                                               CPHS  520  000440
      610       GO TO 31                                               CPHS  530  000450
      620   80  NTUP = ILSP(IX)                                                   000460
      630       IF(TT.LT.TLI(IX,1)) GO TO 90                           CPHS  540  000470
      640       TTS = TT                                               CPHS  550  000480
      650       TLNS= TLN                                              CPHS  560  000490
      660       TT = TLOW                                              CPHS  570  000500
      670       TLN= ALOG(TT)                                          CPHS  580  000510
      680       KK = 2                                                 CPHS  590  000520
      690       SK =(((((COEF(IX,5,J)/5.)*TT+COEF(IX,4,J))/4.)*TT+COEF(IX,3,J))/3.)*TT+COEF(IX,2,J)  CPHS  600  000530
      700      1     *TT+COEF(IX,1,J))*TT+COEF(IX,0,J)                        CPHS  610  000540
      710       HK =(((((COEF(IX,5,J)/5.)*TT+COEF(IX,4,J))/4.)*TT+COEF(IX,3,J))/3.)  CPHS  620  000550
      720      1     *TT+COEF(IX,2,J))/2.)*TT+COEF(IX,1,J))*COEF(IX,6,J))/RT  CPHS  630  000560
      730       CPK=(((((COEF(IX,5,J)*TT+COEF(IX,4,J))*TT+COEF(IX,3,J))*TT  CPHS  640  000570
      740      1     *COEF(IX,2,J))*TT+COEF(IX,1,J)                           CPHS  650  000580
      750       DO 86 KK = 1,NTUP                                                 000590
      760       TKK(KK) = TL(IX,KK)                                               000600
      770       CPKK(KK) = CPL(IX,KK)                                             000610
      780       HKK(KK) = HL(IX,KK)                                               000620
      790   86  SKK(KK) = SL(IX,KK)                                              000630
      800       TKK(NTUP+1) = TT                                       CPHS  660  000640
      810       CPKK(NTUP+1) = CPK                                     CPHS  670  000650
      820       HKK(NTUP+1) = HK                                       CPHS  680  000660
      830       SKK(NTUP+1) = SK                                       CPHS  690  000670
      840       TT = TTS                                               CPHS  700  000680
      850       TLN = TLNS                                             CPHS  710  000690
      860       M = 1                                                             000700
      870       I = 1                                                             000710
      880       IF (TT .LT. TKK(M))  I = -1                                       000720
      890   87  IF (TT .GE. TKK(M) .AND. TT .LE. TKK(M+1))  GO TO 89              000730
      900       M = M + I                                                         000740
      910       IF (M .LT. NTUP + 1 .AND. M .GT. 0)  GO TO 87                     000750
      920       WRITE (IOUT,88) TT,M,NTUP,(I,TKK(I), I = 1,6)                    000760
      930   88  FORMAT (///5OX,23H*CPHS* VARIABLE OUTSIDE TABLE//45X,6HTT =,1PE15.8  000770
      940      1,5H  M =,I2,2H  NTUP =,I2///5OX,6HTKK(I,3I,3H) =,E15.8))         000780
      950       GO TO 31                                                          000790
      960   89  SI(J) = SKK(M) + (SKK(M+1)-SKK(M))*(TT-TKK(M))/(TKK(M+1)-TKK(M))  000800
      970       HU(J) = HKK(M) + (HKK(M+1)-HKK(M))*(TT-TKK(M))/(TKK(M+1)-TKK(M))  000810
      980       CPUSED = (CPKK(M)+(CPKK(M+1)-CPKK(M))*(TT-TKK(M))/(TKK(M+1)-TKK(M))  000820
      990       CPSUM = CPSUM + CPUSED * ENI(J,NPI)                    CPHS  720  000830
     1000       GO TO 32                                               CPHS  730  000840
     1010   90  IF (IEN .LT. 1)  WRITE (IOUT,91) TT                             000850
     1020  91   FORMAT (///25X,'ODE&ROR DURING LOW TEMPERATURE THERMO EVALUATION IN  000860
     1030      1 CPHS, TT =,F12.6,1H DEGREES KELVIN///)                          000870
     1040       IEN = 1                                                          000880
     1050       GO TO 31                                                         000890
     1060   99  END                                                              000900
```

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```
@FOR,S LEWIS.DETON,LEWIS.DETGN
FOR  L3 -10/25/79-17:38:09 (V,0)

   SUBROUTINE DETON      ENTRY POINT 001331

   STORAGE USED: CODE(1) 001347; DATA(0) 000201; BLANK COMMON(2) 000000

    COMMON BLOCKS:

     0003    CONSTS 000006
     0004    HOLLOW 000010
     0005    POINTS 000335
     0006    MISC   001264
     0007    INDA   000041
     0010    PERF   000166
     0011    OUPT   000073
     0012    CCC    000003

   EXTERNAL REFERENCES (BLOCK, NAME)

     0013    NEWOF
     0014    NCALC
     0015    OUTI
     0016    ECLDAM
     0017    OUT2
     0020    OUT3
     0021    SAVE
     0022    NXOUI
     0023    NIO2$
     0024    XPRN
     0025    EXP
     0026    SQRT
     0027    NIO1$
     0030    NIO3$
     0031    NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001    001305 1000L     0000    000035 11F       0001    000005 1306      0001    000040 1466      0001    000566 150L
     0001    000053 154G      0000    000044 190F      0000    000053 203F      0001    000255 205L      0001    000176 2146
     0000    000055 300       0001    000451 3416      0001    000672 3526      0001    000711 3626      0001    000717 3676
     0001    000563 40L       0001    000750 4016      0001    000767 4116      0001    001004 4226      0001    001024 4336
     0001    001055 451G      0000    000114 46F       0001    001100 4646      0001    001115 4756      0000    000102 5F
     0001    001123 502G      0001    001142 5146      0001    001157 5256      0001    001176 5356      0001    001216 5465
     0000    000120 5AF       0000    000123 60F       0001    000016 7L        0001    000615 860L      0000    000130 860F
     0001    001051 870L      0001    001270 902L      0000 R  000032 ALAM      0000 R  000017 ALFA      0006    000570 AM
     0006 R  000020 A11       0006    000701 ANUM      0010    000133 APP       0003    000000 AIMN      0006    000004 ATOM
     0000 R  000022 A11       0000 R  000023 A12       0000 R  000024 A21       0000 R  000025 A22       0006    000502 B0
     0006    000521 [illegible]  0000 R  000026 B1    0000 R  000027 B2        0007    000036 CALCN     0007    000001 CONV6
     0000 R  000030 CP        0000 R  000032 CFR       0006 R  000625 CPH1      0006    000564 CPSUM     0012    000002 DEMAND
     0006    001167 [illegible]  0000 R  [illegible] CLVFI  0005 R  000047 DLVIP  0004   000000 END    0006    001243 ENGSAV
     0006    000000 [illegible]  0000  001261 ENGL  0006    001262 ENSAVE     0006    001073 ENTH      0010 L  000145 EOL
```

```
0006   000546 EQRAT     0011   000002 FA        0011   000003 FAP       0006   001112 FAZ       0011 R 000005 FB
0011   000006 FC        0011 R 000007 FCP       0011   000012 FCST      0011   000014 FCV       0011   000015 FG
0011   000017 FGL       0011   000020 FGV       0000 R 000009 FGI       0011 R 000021 FH        0011   000023 FI
0011   000025 FIV       0011 R 000027 FM        0000 R 000001 FMM       0011 R 000031 FMT       0011   000050 FN
0011 R 000052 FOUR      0006   001150 FOX       0011   000053 FP        0000 R 000003 FPP       0000 R 000002 FPI
0000 R 000004 FRA       0000 R 000005 FRB       0011   000054 FS        0011 R 000056 FSV       0011 R 000057 FT
0011   000061 FIX       0000 R 000006 FTI       0000 R 000007 FUO       0011   000063 FV        0011 R 000065 FVEL
0011 R 000001 F13       0011   000000 F9X       0000 R 000014 GAM       0005 R 000101 GAMMAS    0004   000001 GAS
0005   000001 GMLT      0010 R 000150 GMI       0012   000000 GRAPH     0007 L 000003 HP        0006   000572 HPP
0006 R 000567 HSUBO     0005 R 000000 HSUM      0010 R 000064 HI        0007   000030 IC        0007 I 000000 IDEBUG
0004   000002 IE        0000 I 000011 II        0007   000015 IMAT      0000   000143 INJPS     0000 I 000010 IOF
0007   000023 IONS      0007 I 000021 IP        0007   000037 IOSAVE    0007   000016 IQI       0007 I 000034 IT
0000 I 000012 ITR       0004 I 000003 IZERO     0000 I 000034 J         0007   000026 JLIQ      0012 I 000001 JOUT
0007   000025 JSOL      0007   000031 JST       0007 I 000005 K         0007   000014 KMAT      0004   000004 LANK
0004   000463 LLMT      0007   000040 LSAVE     0004   000005 MOL       0007   000006 MOLES     0006 I 000626 NAME
0007   000024 NC        0007   000022 NEWR      0007   000035 NFZ       0007   000012 NLM       0007 I 000017 NOF
0007   000020 NOMIT     0007 I 000007 NP        0007 I 000011 NPT       0007 I 000027 NREAL     0007   000013 NS
0007 I 000010 NT        0006 R 000565 OF        0011 R 000067 ONE       0004   000006 OX        0006 R 001227 OXF
0005 R 000116 P         0003   000002 PATM      0010 R 000000 PCP       0006   001054 PECWT     0006 R 000563 PP
0005 R 000217 PPP       0000 R 000013 PPI       0010 R 000101 PUB       0003 R 000003 RBAR      0003 R 000004 RBR
0006   000574 RH        0006   001206 RHOF      0000 R 000020 RK        0006   001207 RMW       0010 R 000047 RRHO
0000 R 000021 RRI       0006 R 001131 RTEMP     0003   000005 RVR       0007   000033 SHOCK     0005 R 000251 SONVEL
0007   000304 SP        0005   000015 SSUM      0006   000001 SUMN      0006   000063 SO        0005 R 000157 T
0000 R 000016 TEM       0006   000562 THIGH     0011 R 000070 THREE     0006   001226 TLN       0006   000560 TLOW
0006   000557 TM        0006   000561 TMID      0005   000320 TOIN      0007 L 000002 TP        0006 R 000002 TT
0005 R 000266 TTT       0000 R 000015 TTI       0010 R 000116 TUB       0011 R 000071 TWO       0000 R 000033 UD
0000 R 000002 V         0005   000303 VLM       0006   000576 VMIN      0010 R 000032 VMOC      0007   000032 VOL
0006   000600 VPLS      0005 R 000234 WM        0006   000602 WP        0000 R 000030 X1        0000 R 000031 X2
0004   000007 ZERO      0012   000072 ZEROF
```

```
00101            SUBROUTINE DETON                                                          000000
00101      C                                                                 00343900     000000
00101      C     CHAPMAN-JOUGUET DETONATIONS                                 00344000     000000
00101      C                                                                              000000
00103            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                  /CONSTS/     000000
00104            COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO            /HOLCON/     000000
00105            COMMON/POINTS/PSUM(,3),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)               000000
00105          1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)           000000
00105          2 ,VLM(13),TOTN(13)                                                         000000
00106            COMMON /MISC/ LNN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),    /MISC/       000000
00106          1               BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT, /MISC/      000000
00106          2               HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2), /MISC/      000000
00106          3               CP(16),AMI,CPRI,NAKE(15,5),ANUM(15,5),PECWT(15), /MISC/     000000
00106          4               ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOF, /MISC/    000000
00106          5               RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV         /MISC/       000000
00107            COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,K,MOLES,NP,NT,NPT,NLM,NS, /INDX/      000000
00107          1               KMAT,IMAT,IQI,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ, /INDX/   000000
00107          2               NREAL,IC,JST,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE /INDX/     000000
00110            COMMON /PERF/ FCP(26),VMOC(13),RRHO(13),HI(13),PUB(13),      /PERF/       000000
00110          1               TUB(13),APP(13),GMI(13),EQL                    /PERF/       000000
00111            COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2), /OUPT/    000000
00111          1               FGL,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/ 000000
00111          2               FP,FS(2),FSV,FT(2),FIX(2),FV(2),FVEL(2),ONE,THREE, /OUPT/   000000
```

```
      3                TWO,ZEROF                                                /OUPT/
C
      COMMON /CCC/ GRAPH,JOUT,DEMAND
C
      LOGICAL EQL,HP,TP
      DATA FG1/6HGAMMA1/,FMM/6HM/M1  /,FP1/6HP1 ATM/,FPP/6HP/P1  /,
     1 FRA/6HR BAR/RA/,FRB/6HQ1    /,FTT/6HT/T1  /,FUD/6HDET VE/
C
      XX(A,X,B,Y,C,D) = (A*X-B*Y)/(A*C-B*D)
C
      IOF = 0
      DO 4 II = 1,NREAC
    4 NAME(II,5) = IZERO
      TT = 0.
      IF (T(1) .LE. 0.0)  T(1) = RTEMP(1)
    7 IOF = IOF+1
      OF = OXF(IOF)
      CALL NEWOF
      WRITE(JOUT,11)
   11 FORMAT(33HDETONATION VELOCITY CALCULATIONS)
      DO 902 IT = 1,NT
      TT = T(IT)
      CALL HCALC
      CALL OUT1
      DO 902 IP=1,NP
      H1(NPT) = RBAR*HSUBO
      TUB(NPT) = T(IT)
      PUB(NPT) = P(IP)
      CP(NPT) = RBAR*CPR1
      ITR= 0
      TT= 3800.
      PP1= 15.
      PP = PP1*P(IP)
      HSUBO = H1(NPT)/RBAR + 0.750*T(IT)*PP1/AM1
      TP = .FALSE.
      HP= .TRUE.
      CALL EQLBRM
      HSUBO = H1(NPT)/RBAR
      HP= .FALSE.
      IF (TT .LE. 0.0)  GO TO 902
      GAM= GAMMAS(NPT)
      TT1 = TT/T(IT)
      II= 0
      TEM=TT1-.75*PP1/(CPR(NPT)*AM1)
      WRITE(JOUT,190)TT
  190 FORMAT(8HOT EST.=,F8.2/11X,4HP/P1,17X,4HT/T1)
      WRITE(JOUT,203) II,PP1,TT1
      DO 202 II = 1,3
      ALFA = WM(NPT)/AM1/TT1
      PP1= (1.+GAM)*(1.+(1.-4.*GAM*ALFA/(1.+GAM)**2)**.5)/(2.*GAM*ALFA)
      RK=PP1*ALFA
      TT1= TEM+.5*PP1*GAM*(RK*RK-1.)/(AM1*CPR(NPT)*RK)
  202 WRITE(JOUT,203) II,PP1,TT1
  203 FORMAT (I5,2E26.8)
      IP= .TRUE.
      TT = TT1*T(IT)
```

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ORIGINAL PAGE IS
OF POOR QUALITY

```
                205 ITR= ITR+1                                                  000255
                    PP = PP1*P(IP)                                              000257
                    CALL EQLBRM                                                 000262
                    IF (NPT.EQ.0) GO TO 1000                                    000264
                    IF (TT .LE. 0.0)  GO TO 860                                 000266
                    GAM= GAMMAS(NPT)                                            000272
                    RR1 = PP1*WM(NPT)/AM1/TT1                                   000274
                    A11= 1./PP1 + GAM*RR1*DLVPT(NPT)                            000302
                    A12= GAM*RR1*DLVTP(NPT)                                     000310
                    A21= .5*GAM*(RR1**2-1.-DLVPT(NPT)*(1.+RR1**2))+DLVTP(NPT)-1.  000314
                    A22=-.5*GAM*DLVTP(NPT)*(RR1**2+1.)-WM(NPT)*CPR(NPT)         000330
                    B1= 1./PP1-1.+GAM*(RR1-1.)                                  000343
                    B2 = WM(NPT)*(HSUM(NPT) - H1(NPT)/RBAR)/TT - 0.5*GAM*(RR1**2 - 1.)  000353
                    X1 = XX(A22,B1,A12,B2,A11,A21)                              000370
                    X2 = XX(A11,B2,A21,B1,A22,A12)                              000400
                    ALAM= 1.                                                    000412
                    TEM = X1                                                    000414
                    IF(TEM.LT.0.)  TEM = -TEM                                   000416
                    IF(X2.GT.TEM)  TEM=X2                                       000423
                    IF (-X2.GT.TEM) TEM = -X2                                   000431
                    IF(TEM.GT.0.4) ALAM=.4/TEM                                  000437
                    PP1= PP1*EXP(X1*ALAM)                                       000446
                    TT1= TT1*EXP(X2*ALAM)                                       000456
                    TT = TT1*T(IT)                                              000466
                    UD = RR1*SQRT(RBR*GAM*TT/WM(NPT))                           000470
                    WRITE(JOUT,30)ITR,PP1,TT1,RR1,X1,X2                         000503
                 30 FORMAT(7HOITER =,I2,5X,6HP/P1 =,E15.8,5X,6HT/T1 =,E15.8,5X,10HRHO/  000516
                   1RHO1 =,E15.8/7X,13HDEL LN P/P1 =,E15.8,5X,13HDEL LN T/T1 =,E15.8)  000516
C                   CONVERGENCE TEST                                            000516
                    IF(ITR.LE.10 .AND. TEM.GT.0.5E-04)  GO TO 205               000516
                    RRHO(NPT)=RR1                                               000534
                    IF (CP(NPT) .LE. 0.0)  GO TO 40                             000536
                    GM1(NPT) = CP(NPT)/(CP(NPT) - RBAR/AM1)                     000541
                    VMOC(NPT) = UD/SQRT(RBR*GM1(NPT)*T(IT)/AM1)                 000547
                    GO TO 150                                                   000561
                 40 GM1(NPT) = 0.                                               000563
                    VMOC(NPT) = 0.                                              000564
                150 K = 0                                                       000566
                    IF (IP .EQ. NP .AND. IT .EQ. NT .OR. TT .LE. 0.0)  GO TO 860  000566
                    K = NPT                                                     000610
                    IF(NPT.NE.13)  GO TO 870                                    000612
C  OUTPUT                                                                       000612
                860 WRITE(JOUT,5)                                               000615
                  5 FORMAT(1H1,42X,46HDETONATION PROPERTIES OF AN IDEAL REACTING GAS )  000621
                    CALL OUT1                                                   000621
                    WRITE(JOUT,46)                                              000623
                 46 FORMAT(13H UNBURNED GAS//)                                  000633
                    FMT(3) = F13                                                000633
                    FMT(4) = FOUR                                               000635
                    WRITE(JOUT,FMT) PP1,FB,FB,(PUR(J), J = 1,NPT)               000637
                    FMT(4) = T=0                                                000654
                    WRITE(JOUT,FMT) TT,FB,(TUR(J), J = 1,NPT)                   000656
                    WRITE(JOUT,FMT) FH,FB,(H1(J), J = 1,NPT)                    000675
                    DO 56 J = 1,NPT                                             000717
                    V(J) = AM1                                                  000717
                 56 SONVEL(J) = SQRT(RBR*GM1(J)*TUR(J)/AM1)                     000720
```

```
00374    136*          FMT(4) = THREE                                                  000732
00375    137*          WRITE(JOUT,FMT) FM,FB,(V(J), J = 1,NPT)                         000734
00405    138*          FMT(4) = FOUR                                                   000753
00406    139*          WRITE(JOUT,FMT) FCP,(CP(J), J = 1,NPT)                          000755
00415    140*          WRITE(JOUT,FMT) FG1,FB,FB,(GM1(J), J = 1,NPT)                   000772
00426    141*          FMT(4) = ONE                                                    001007
00427    142*          WRITE(JOUT,FMT) FSV,FVEL,(SONVEL(J), J = 1,NPT)                 001011
00437    143*          WRITE(JOUT,58)                                                  001027
00441    144*       58 FORMAT(11HOBURNED GAS//)                                        001034
00442    145*          FMT(3) = ONE                                                    001039
00443    146*          CALL OUT2                                                       001036
00444    147*          WRITE(JOUT,68)                                                  001040
00446    148*       68 FORMAT(22HODETONATION PARAMETERS //)                            001050
00447    149*          FMT(4) = THREE                                                  001050
00450    150*          DO 70 J = 1,NPT                                                 001055
00453    151*          V(J) = PPP(J)/PUB(J)                                            001055
00454    152*          PCP(J) = TTT(J)/TUB(J)                                          001057
00455    153*       70 SONVEL(J) = SONVEL(J)*RRHO(J)                                   001062
00457    154*          WRITE(JOUT,FMT) FPP,FB,FB,(V(J), J = 1,NPT)                     001066
00470    155*          WRITE(JOUT,FMT) FTT,FB,FB,(PCP(J), J = 1,NPT)                   001103
00501    156*          DO 73 J = 1,NPT                                                 001123
00504    157*       73 V(J) = WM(J)/AM1                                                001123
00506    158*          FMT(4) = FOUR                                                   001126
00507    159*          WRITE(JOUT,FMT) FMM,FB,FB,(V(J), J = 1,NPT)                     001130
00520    160*          WRITE(JOUT,FMT) FRA,FRB,FB,(RRHO(J), J = 1,NPT)                 001145
00531    161*          WRITE(JOUT,FMT) FM,FB,(VMOC(J), J = 1,NPT)                      001162
00541    162*          FMT(4) = ONE                                                    001201
00542    163*          WRITE(JOUT,FMT) FUD,FVEL,(SONVEL(J), J = 1,NPT)                 001203
00552    164*          EQL=.TRUE.                                                      001221
00553    165*          CALL OUT3                                                       001223
00554    166*          IF (K .EQ. 0 .AND. IOF .EQ. NOF)  GO TO 1000                    001225
00556    167*          IDEBUG = IDEBUG-13                                              001237
00557    168*          WRITE(JOUT,868)                                                 001242
00561    169*       868 FORMAT(1H1)                                                    001247
00562    170*          NPT = 0                                                         001247
00563    171*       870 NPT = NPT + 1                                                  001251
00564    172*          IF (K .EQ. 1)  K = -1                                           001253
00566    173*          CALL SAVE                                                       001260
00567    174*          WRITE(JOUT,868)                                                 001262
00571    175*       902 CONTINUE                                                       001270
00574    176*          IF(IOF.GE.NOF)  GO TO 1000                                      001270
00576    177*          IDEBUG = IDEBUG+13                                              001300
00577    178*          GO TO 7                                                         001303
00600    179*       1000 IF = .FALSE.                                                  001305
00601    180*          RETURN                                                          001305
00602    181*          END                                                             001306
END FOR
```

```
CFOR,S LEWIS.EQLBRM,LEWIS.EQLBRM
DCA 'ES' -10/25/79-17:38:12 (9,)


    SUBROUTINE EQLBRM    ENTRY POINT 003112


    STORAGE USED: CODE(1) 003130; DATA(0) 000440; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003   CONSTS 00000
     0004   HOLLOW 001310
     0005   POINTS 000335
     0006   SPECES 01.120
     0007   MISC   001264
     0010   DOUBLE 001560
     0011   INDX   000041
     0012   PERF   000166
     0013   CCC    000003


    EXTERNAL REFERENCES (BLOCK, NAME)

     0014   CPHS
     0015   MATRIX
     0016   GAUSS
     0017   ALOG
     0020   %0001
     0021   %1019
     0022   %1023
     0023   EXP
     0024   NERR3%

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    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001   001202 100L      0001   001211 101L      0001   002164 1023G     0001   002214 1033G     0000   000201 110F
     0001   001452 111L      0001   001575 1115L     0001   001633 1116L     0001   001517 113L      0001   002475 1130G
     0001   002503 1134G     0001   001513 114L      0001   001542 115L      0001   002543 1150G     0001   001660 116L
     0001   002616 1160L     0001   002446 1165L     0001   002710 1171L     0000   000202 1183F     0001   002636 1201G
     0001   002670 1217G     0001   002733 1240G     0001   002046 13L       0001   001747 130L      0000   000300 136F
     0001   002652 143L      0000   000236 144F      0001   002255 147L      0001   002262 148L      0001   000116 151G
     0001   002510 153L      0001   002304 154L      0000   000244 156F      0001   002334 157L      0001   002373 158L
     0001   002431 159L      0001   002144 160L      0000   000256 161F      0001   000151 165G      0001   002622 165L
     0001   002642 166L      0000   000266 168F      0001   002610 169L      0001   002613 170L      0001   002717 171L
     0001   002677 172L      0001   000430 174L      0001   002002 183L      0001   003005 186L      0000   000153 1929F
     0001   002774 199L      0000   000305 201F      0001   001561 2115L     0001   000244 221G      0001   000277 232G
     0000   000040 244F      0001   000325 245G      0001   000332 251G      0001   000374 270G      0001   000406 277G
     0000   000206 304F      0001   000464 315G      0001   000517 324G      0001   000131 33L       0001   000613 360G
     0000   000071 373F      0001   002695 40L       0001   000721 416G      0001   000732 422G      0001   000155 43L
     0001   001003 445G      0001   001141 477G      0001   000125 49L       0001   001172 506G      0001   001452 531G
     0001   001413 600F      0001   000413 62L       0001   000251 63L       0001   001464 631G      0001   000302 67L
     0001   001425 673G      0001   001642 704G      0001   000342 72L       0001   001722 726G      0000   000075 73F
     0000   000126 74F       0001   001750 744G      0000   000303 771F      0000   000063 772F      0001   000412 773L
     0001   000524 774L      0001   000536 775L      0000   000132 776F      0001   000747 80L       0001   000766 83L
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0001    001023 84L      0001    001036 85L      0001    000571 871L     0001    003063 873L     0000    000105 874F
0001    001332 917L     0000    000134 923F     0000    000157 924F     0000    000176 925F     0001    000603 966L
0001    000622 968L     0001    001632 969L     0001    001111 97L      0001    000635 970L     0001    000644 971L
0000    000220 973F     0001    000654 997L     0006 R  006034 A        0000 R  000047 AA       0012    000150 AEAT
0007    000570 AM       0000 R  000042 AMBDA    0000 R  000043 AMBDA1   0007    000624 AM1      0007    000741 ANUM
0012 R  000133 APP      0003    000000 ATMN     0007    000004 ATOM     0007 R  000502 BD       0007    000521 BDP
0011    000036 CALCH    0006    000000 COEF     0011 L  000001 CONVG    0005 R  000032 CPR      0007    000625 CPR1
0007 R  000564 CPSUM    0000 R  000026 CRITV    0007    000604 DATA     0000 R  000055 DELF     0006 R  005670 DELN
0013    000002 DEMAND   0007    001167 DENS     0000 R  000041 DLNT     0005 R  000064 DLVPT    0005 R  000047 DLVTP
0006 R  002734 EN       0004    000000 END      0000 R  000025 ENL      0006 R  005360 ENLN     0007    001263 ENLSAV
0007 R  000000 ENN      0007 R  001261 ENNL     0007    001262 ENSAVE   0000 R  000033 ENSOL    0007    001073 ENTH
0012    000165 EQL      0007 R  000566 EQRAT    0007    001112 FAZ      0000 R  000045 FNEG1    0000 R  000046 FNEG2
0007    001150 FOX      0010 D  000000 G        0005 R  000101 GAMMAS   0004    000001 GAS      0003    000001 GMET
0013    000000 GRAPH    0011 L  000003 HP       0007    000572 HPP      0007    000567 HSUBU    0005 R  000000 HSUM
0006 R  005524 HO       0000 I  000032 I        0011 L  000030 IC       0011 I  000000 IDEBUG   0004 I  000002 IE
0011 I  000015 IMAT     0000 I  000051 INC      0000    000400 INJPS    0011 L  000023 IONS     0011    000021 IP
0011    000037 IQSAVE   0011 I  000016 IQ1      0000 I  000035 IQ2      0000 L  000022 ISING    0011    000005 ISV
0011    000034 IT       0000 I  000030 ITNUMR   0006 I  011444 IUSE     0004    000003 IZERO    0000 I  000031 J
0000 I  000056 JDELF    0000 I  000037 JJ       0000 I  000053 JKG      0011 I  000026 JLIQ     0013 I  000001 JOUT
0011 I  000025 JSOL     0011 I  000031 JSI      0000 I  000052 KG       0011 I  000014 KMAT     0011 I  000012 L
0004    000004 LANK     0007 I  000463 LLMT     0000 L  000023 LOGV     0011    000040 LSAVE    0004    000005 MOL
0011    000006 MOLES    0007    000626 NAME     0011 I  000024 NC       0000 I  000040 NEN      0011    000022 NEWR
0011    000035 NFZ      0011    000017 NOF      0011    000020 NOMIT    0011    000007 NP       0011 I  000011 NPT
0011    000027 NREAC    0011 I  000013 NS       0000 I  000000 NSPP1    0011    000010 NT       0000 I  000036 NTZERO
0000 I  000034 NUMR     0007    000565 OF       0004    000006 OX       0007    001227 OXF      0005    000116 P
0003    000002 PATM     0012    000000 PCP      0007    001054 PECWT    0007 R  000563 PP       0005 R  000217 PPP
0000 R  000001 PROW     0003    000003 RBAR     0003    000004 RBR      0007    000574 RH       0007    001206 RHOP
0000 L  000024 RITE     0007    001207 RMW      0007    001131 RTEMP    0003 R  000005 RVR      0006 R  002570 S
0011 L  000033 SHOCK    0000 R  000027 SIZEF    0006    011754 SLN      0005    000251 SONVEL   0011 L  000004 SP
0012    000047 SPIM     0000 R  000050 SS       0005 R  000015 SSUM     0006 R  010770 SUB      0012    000101 SUBAR
0000 D  000020 SUM      0007 R  000001 SUMN     0000 R  000044 SUM1     0012    000116 SUPAR    0007 R  000003 SO
0005 R  000150 T        0006 R  011610 TEMP     0007 R  000562 THIGH    0007 R  001226 TLN      0007 R  000560 TLOW
0007 R  000557 TM       0000 R  000054 TMELT    0007    000561 TMID     0000 R  000057 TN       0005 R  000320 TOTN
0011 L  000002 TP       0007 R  000002 TT       0005 R  000266 TTT      0005    000202 V        0012    000064 VACI
0005 R  000203 VLM      0007    000576 VMIN     0012    000032 VMOC     0011 I  000032 VOL      0007    000600 VPLS
0006 R  000234 WM       0007    000602 WP       0010 D  001510 X        0004    000007 ZERO
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0001        1*          SUBROUTINE EQLBRM                                                   EQLNUD02    000000
0001        2*     C                                                                                   000000
0001        3*     C  ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES          EQLNUD03    000000
0001        4*     C                                                                       EQLNUD04    000000
0003        5*           COMMON /CONSTS/ AIMN,GMET,PATM,RBAR,RBR,RVR                       /CONSTS/    000000
0004        6*           COMMON /MOLCON/ ENN,GAS,IE,IZERO,LANK,MOL,OX,ZERO                 /MOLCON/    000000
0005        7*           COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                   000000
0006        8*          1 ,GAMMAS(13),R(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)              000000
0006        9*          2 ,VLM(13),TOTN(13)                                                            000000
0007       10*     C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)               000000
0008       11*     C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)               000000
0008       12*           INCLUDE SPECPR                                                                000000
0012       13*           COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BD(15),         /MISC/      000000
0012       14*          1              DP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,     /MISC/      000000
0014       15*     C                   HSUB0,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),    /MISC/      000000
0014       16*     C                   DATA(16),AMI,CPSI,NAME(15,5),ANUM(15,5),PECWT(15),  /MISC/     000000
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      4                ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,     /MISC/      000000
      5                RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                /MISC/      000000
       COMMON /DOUBLE/ G(20,21), X(20)                                      EQLNU013    000000
       COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,        /INDX/      000000
      1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,   /INDX/      000000
      2              NREAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE     /INDX/      000000
       COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),         /PERF/      000000
      1              SUPAR(13),APP(13),AEAT(13),EVL                       /PERF/      000000
C                                                                                     000000
C          COMMON /CCC/ GRAPH,JOUT,DEMAND                                             000000
C                                                                                     000000
C                                                                                     000000
       DIMENSION PROW(15)                                                           000000
       DOUBLE PRECISION G,SUM,X                                                     000000
       LOGICAL CONVG,HP,IC,IONS,ISING,LOGV,RITE,SHOCK,SP,TP,VOL                     000000
C                                                                                     000000
       ENL = ENNL                                                                   000000
       RITE = .FALSE.                                                               000001
       IF(IDEBUG.GT.0.AND.NPT.GE.IDEBUG)  RITE=.TRUE.                               000002
       CRITV = 5.0E-6                                                               000021
       SIZEF = 0.                                                                   000023
       ISING = .FALSE.                                                              000024
       LOGV = .FALSE.                                                               000025
       IF (VOL)  PP = RVR*ENN*TT/VLM(NPT)                                           000026
       TLN = ALOG(TT)                                                               000040
       CONVG = .FALSE.                                                              000044
       ITNUMB = 100                                                                 000045
       JSI = 1                                                                      000047
       CALL CPHS                                                                    000051
       TM = ALOG(PP/ENN)                                                            000053
C      IF(IC) PREVIOUS POINT HAD SINGULAR MATRIX                                    000053
       IF(IC)  GO TO 966                                                            000062
       IF (E.NOT.IONS.OR.IE.EQ.LLMT(L)) GO TO 33                                    000064
       L = L+1                                                                      000102
       IQ1 = IQ1+1                                                                  000105
       DO 499 J = 1,NS                                                              000116
       IF (A(L,J) .EQ.0.) GO TO 499                                                 000116
       ENJ(J,NPT) = 1.E-8                                                           000117
       ENLN(J) = -18.4206810                                                        000121
       IUSE(J) = 0                                                                  000123
  499 CONTINUE                                                                      000131
   33 IF(NPT.EQ.1.AND..NOT.SHOCK)  WRITE(JOUT,244)(LLMT(I),I=1,L)                   000131
  244 FORMAT (4HOPT ,14(5X,A4))                                                     000155
C      BEGIN ITERATION                                                            000155
   43 IF(IC)  GO TO 1171                                                          000156
       IF (.NOT.CONVG)  GO TO 62                                                    000166
       SUM = ENN                                                                    000170
       IF(JSOL.EQ.0)  GO TO 6.                                                      000172
       ENSOL = ENJ(JSOL,NPT)                                                        000174
       ENJ(JSOL,NPT) = ENJ(JSOL,NPT)+ENJ(JLIQ,NPT)                                  000200
       IUSE(JLIQ) = -IUSE(JLIQ)                                                     000202
       IQ1 = IQ1-1                                                                  000205
       DLVTP(NPT) = 0.                                                              000206
       DPR(NPT) = 0.                                                                000207
       GAMMAS(NPT) = 0.                                                             000210
       LOGV = .TRUE.                                                                000211
   62 CALL MATRIX                                                       EQLNU048
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                NUMP = IQ1 - ITNUMB                                                  000214
                IQ2 = IQ1 + 1                                                        000217
                IF(.NOT.CONVG)    GO TO 67                                           000222
                IF (LOGV.AND.JSOL.EQ.0) GO TO 63                                     000224
                DO 162  I=1,L                                          EQLN0140      000244
                PROW(I) = G(IQ1,I)                                                   000244
                IF (.NOT.LOGV) GO TO 67                                              000246
      C         LOGV = .TRUE.-- SET UP MATRIX TO SOLVE FOR DLVPT                     000246
             63 G(IQ1,IQ2) = ENN                                                     000251
                J = IQ1 - 1                                                          000260
                DO 777 I = 1,J                                                       000270
              777  G(I,IQ2) = G(I,IQ1)                                              000277
               67 IF(.NOT.RITE)  GO TO 72                                            000302
                WRITE(JOUT,772) NUMB                                                 000303
              772 FORMAT (11HOITERATION  ,I3,6X,7HMATRIX ///)                        000325
                DO 911 I=1,IMAT                                        EQLN0051      000325
              911  WRITE(JOUT,73) (G(I,J), J = 1,KMAT)                              000325
               72 IF(CONVG)  IMAT=IMAT-1                                             000342
                J = IMAT                                                             000346
                CALL GAUSS                                                           000350
                IF (J .NE. IMAT)  GO TO 774                                          000352
                IF(.NOT.RITE)  GO TO 773                                             000355
                WRITE(JOUT,373)(LLMT(I),I=1,L)                                       000363
              373 FORMAT (7HOPI     ,9(A9,10X))                                      000377
                WRITE(JOUT,73)(X(I),I=1,IMAT)                                        000377
               73 FORMAT (9E14.6)                                      EQLN0062      000412
              773 IF(.NOT.CONVG)  GO TO 85                                           000412
                IF(.NOT.LOGV)  GO TO 174                                             000413
                IF(JLIQ.NE.0) EN(JSOL,NPT)=ENSOL                                     000421
                GO TO 171                                                            000426
              174 SUM = 0.                                             EQLN0148      000430
                DO 175 J=1,L                                           EQLN0149      000431
              175  SUM = SUM + PROW(J)*X(J)                                          000464
                DLVIP(NPT) = 1.+G(IQ2,IQ1)/ENN-SUM/ENN  - X(IQ1)       EQLN0151      000470
                CPR(NPT) = G(IQ2,IQ2)                                  EQLN0152      000502
                DO 176 J=1,IQ1                                         EQLN0153      000512
              176  CPR(NPT) = CPR(NPT) - G(IQ2,J)*X(J)                              000512
                LOGV = .TRUE.                                          EQLN0155      000520
                GO TO 62                                                             000522
      C   SINGULAR MATRIX                                                           000522
             774 IF(.NOT.CONVG)  GO TO 775                                           000524
      C         IF(ISING)  SINGULAR ONCE                                           000524
      C         IF(IC)     SINGULAR TWICE                                          000524
                WRITE(JOUT,172)                                                      000525
              172 FORMAT(28HODERIVATIVE MATRIX SINGULAR )                            000532
                IC = .TRUE.                                                          000532
                GO TO 1171                                                           000534
              775 IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.IT.GT.100.)  GO TO 871       000536
                WRITE(JOUT,874)                                                      000562
              874 FORMAT(96HOLOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE   000567
                 1BEEN INCLUDED ON AN INSERT CARD, RESTART )                         000567
                GO TO 873                                                            000571
              871 WRITE(JOUT,74)                                                     000575
               74 FORMAT(16HOSINGULAR MATRIX)                                        000575
                IF(IC)  GO TO 873                                                    000577
                IF (ISING) GO TO 997
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00356    1290          NTZERO = 0                                                                  000601
00357    1300      966 DO 970 JJ = 1, NS                                                           000603
00362    1310          IF(IUSE(JJ)) 970,968,967                                                    000613
00365    1320      967 IF (EN(JJ,NPT))  969,873,969                                                000616
00370    1330      968 IF (EN(JJ,NPT) .GT. 0.0)  GO TO 969                                         000622
00372    1340          EN(JJ,NPT) = 1.0E-6                                                         000629
00373    1350          ENLN(JJ) = -13.815511                                                       000626
00374    1360          GO TO 970                                                                   000630
00375    1370      969 NTZERO = NTZERO+1                                                           000632
00376    1380      970 CONTINUE                                                                    000637
00400    1390          IF(.NOT.IC)  GO TO 971                                                      000637
00402    1400          IC = .FALSE.                                                                000641
00403    1410          GO TO 43                                                                    000642
00404    1420      971 ISING = .TRUE.                                                              000644
00405    1430          WRITE(JOUT,776)                                                             000645
00407    1440      776 FORMAT (8HORESTART)                                                         000652
00410    1450          GO TO 43                                                                    000652
00411    1460      997 IF(NTZERO.NE.L-1.OR.EQRAT.GT.1.00001.OR.EQRAT.LT..99999) GO TO 873          000658
00413    1470          ENN=0.                                                                      000710
00414    1480          NEN = 0                                                                     000711
00415    1490          DO 83  I=1,L                                                                000721
00420    1500          JJ = 0                                                                      000724
00421    1510          DO 80  J=1,NS                                                               000732
00424    1520          IF (EN(J,NPT) .EQ. 0.0 .OR. A(I,J) .EQ. 0.0)  GO TO 80                      000732
00426    1530          IF (JJ .NE. 0)  GO TO 83                                                    000742
00430    1540          JJ = J                                                                      000744
00431    1550       80 CONTINUE                                                                    000752
00433    1560          NEN = NEN+1                                                                 000752
00434    1570          EN(JJ,NPT) = BO(I)/A(I,JJ)                                                  000755
00435    1580       83 CONTINUE                                                                    000767
00437    1590          IF(NEN.LT.NTZERO)  GO TO 873                                                000767
00441    1600          CONVG = .TRUE.                                                              000773
00442    1610          IC = .TRUE.                                                                 000775
00443    1620          HSUM(NPT) = 0.                                                              000776
00444    1630          DO 84  J=1,NS                                                               001003
00447    1640          IF (EN(J,NPT) .LE. 0.0)  GO TO 84                                           001003
00451    1650          ENN = EN(J,NPT)+ENN                                                         001005
00452    1660          ENLN(J) = ALOG(EN(J,NPT))                                                   001010
00456    1670          HSUM(NPT) = HSUM(NPT) + EN(J,NPT)*HO(J)                                     001016
00460    1680       84 CONTINUE                                                                    001025
00461    1690          TM = ALOG(PP/ENN)                                                           001025
00457    1700          GO TO 43                                                                    001034
00460    1710       85 ITNUMB= ITNUMB-1                                                 EQLN0068    001036
00461    1720          IF (ITNUMB .LT. 30)  CRITV = CRITV * 2.50E-7                                001040
00461    1730      C       OBTAIN CORRECTIONS TO THE ESTIMATES                          EQLN0070    001040
00463    1740          JJ = L + 1                                                                  001047
00464    1750          IF(VOL)  X(IG2)=X(IG1)                                                      001060
00466    1760          IF(TP)  X(IG2)=0.                                                           001066
00470    1770          DLNT= X(IG2)                                                        EQLN0072    001073
00471    1780          SUM = X(IG1)                                                                001076
00472    1790          IF(.NOT.VOL) GO TO 97                                                       001101
00474    1800          X(IG1) = 0.                                                                 001103
00475    1810          SUM =   -DLNT                                                               001105
00476    1820       97 DO 101 J=1,NS                                                               001111
00501    1830          IF (IUSE(J)) 101,98,100                                                     001145
00504    1840       98 DELX(J) = HO(J)*DLNT-HO(J)*X(J)-ENLN(J)-TM*SUM                              001151
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00505   185*          DO 99 I = 1,L                                                    001172
00510   186*       99 DELN(J) = DELN(J) + A(I,J)*X(I)                                  001172
        187*          GO TO 101                                                        001200
00513   188*      100 DELN(J) = X(JJ)                                                  001202
00514   189*          JJ = JJ + 1                                                      001205
00515   190*      101 CONTINUE                                              EQLNU079   001213
00517   191*          AMBDA= 1.                                             EQLNU080   001213
00520   192*          AMBDA1= 1.                                            EQLNU081   001215
00521   193*          SUM = X(IQ1)                                                     001216
00522   194*          IF(SUM.LT.0.)  SUM=-SUM                                          001222
00524   195*          IF(DLNT.GT.SUM)  SUM=DLNT                                        001230
00526   196*          IF(-DLNT.GT.SUM)  SUM=-DLNT                                      001236
00530   197*          DO 917 J=1,NS                                             EQLNU084   001252
00533   198*          IF (IUSE(J).NE.0) GO TO 917                                      001252
00535   199*          IF (ENL(J,NPT) .GT. 0.0 .AND. DELN(J) .GT. SUM)  SUM = DELN(J)   001253
00537   200*          IF (ENL(J,NPT) .GT. 0.0 .OR. DELN(J) .LE. 0.0)  GO TO 917        001272
00541   201*          SUM1 = (-9.212-ENLN(J)+ ENL)/(DELN(J)-X(IQ1))                    001306
00544   202*          IF(SUM1.LT.0.)  SUM1=-SUM1                                       001316
00549   203*          IF (SUM1.LT.AMBDA1) AMBDA1 = SUM1                                001323
00546   204*       917 CONTINUE                                             EQLNU089   001339
00550   205*          IF(SUM.GT.2.)AMBDA=2./SUM                             EQLNU090   001339
00552   206*          IF (AMBDA1.LT.AMBDA) AMBDA = AMBDA1                              001349
00554   207*          IF(.NOT.RITE)  GO TO 111                                         001352
00556   208*          WRITE(JOUT,923) TT,ENN, ENL,PP,TM,AMBDA                          001359
00562   209*       923 FORMAT (3HOT=,E15.8,6H  ENN=,E15.8,7H  ENNL=E15.8,5H  PP=,E15.8,  001367
00566   210*         1 9H  LN P/N=E15.8,8H  AMBDA=E15.8 )                             001367
00567   211*          IF(VOL)  WRITE(JOUT,1924) VLM(NPT)                               001367
00573   212*      1924 FORMAT(8H VOLUME=,E15.8,2HCC)                                   001401
00574   213*          WRITE(JOUT,924)                                                  001401
00576   214*       924 FORMAT(1HO,18X,2HNI,12X,5HLN NI,8X,9HDEL LN NI,10X,4HH/RT,9X,4HSO/  001413
00576   215*         1R,12X,6H-GO/RT,9X,5H-G/RT  )                                    001413
00577   216*          DO 926 J=1,NS                                                    001413
00602   217*          FNEG1 = S(J)-HO(J)                                               001413
00603   218*          FNEG2 = FNEG1                                                    001415
00604   219*          IF(IUSE(J).EQ.0)  FNEG2=FNEG2-ENLN(J)-TM                         001416
00606   220*       926  WRITE(JOUT,925) SUB(J,1),SUB(J,2),SUB(J,3),ENL(J,NPT),ENLN(J),  001429
00610   221*         A                 DELN(J),HO(J),S(J),FNEG1,FNEG2                 001429
00615   222*       925 FORMAT (1X,3A4,7E15.6)                                         001444
00624   223*          WRITE(JOUT,110)                                                  001444
00626   224*       110 FORMAT(1HO)                                                     001452
00626   225*     C     APPLY CORRECTIONS TO ESTIMATES                          EQLNU096   001452
00627   226*       111 SUM = 0.                                                       001452
00630   227*          DO 113 J=1,NS                                           EQLNU099   001453
00633   228*          IF (IUSE(J)) 113,112,114                                         001464
00636   229*       112 ENLN(J)=ENLN(J)+AMBDA*DELN(J)                          EQLNU100   001467
00637   230*          ENL(J,NPT) = 0.                                         EQLNU101   001473
00640   231*          IF (ENLN(J) + 18.4206810 .LE. ENL)  GO TO 113                    001474
00642   232*          ENL(J,NPT) = EXP(ENLN(J))                                        001500
00643   233*          SUM = SUM+ENL(J,NPT)                                             001506
00644   234*          GO TO 113                                                        001511
00645   235*       114 ENL(J,NPT) = ENL(J,NPT) + AMBDA * DELN(J)                       001513
00646   236*       113 CONTINUE                                                       001521
00650   237*          SUMN = SUM                                                       001521
00651   238*          IF (ITP) GO TO 115                                      EQLNU104   001523
00653   239*          TLN= TLN+AMBDA*DELN                                     EQLNU105   001525
00654   240*          TT      = EXP(TLN)                                      EQLNU106   001531
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00655   2410          JS1 = 1                                                                  001535
00656   2420          CALL CPHS                                                                001537
00657   2430    115   IF(VOL) GO TO 2115                                                       001542
00661   2440          ENL = ENL+AMBDA*X(IQ1)                                                   001543
00662   2450          ENN = EXP(ENL)                                                           001553
00663   2460          GO TO 1115                                                               001557
00664   2470   2115   ENN = SUMN                                                               001561
00665   2480          ENNL = ALOG(ENN)                                                         001562
00666   2490          PP = RVR*TT*ENN/VLM(NPT)                                                 001566
00667   2500   1115   TM = ALOG(PP/ENN)                                                        001575
00670   2510          IF (ELMT(L).NE.IE) GO TO 116                                             001603
00670   2520    C     CHECK ON REMOVING IONS                                                   001603
00672   2530          DO 1116 J = 1,NS                                                         001625
00675   2540          IF (A(L,J).EQ.0.) GO TO 1116                                             001625
00677   2550          IF (EN(J,NPT).GT.0.) GO TO 116                                           001627
00701   2560   1116   CONTINUE                                                                 001642
00702   2570          DO 1118  J=1,NS                                                          001642
00706   2580   1118   IF (A(L,J) .NE. 0.0)  IUSE(J) = - 10000                                 001642
00711   2590          L = L-1                                                                  001650
00712   2600          IQ1 = IQ1-1                                                              001653
00713   2610          GO TO 43                                                                 001656
00713   2620    C     TEST FOR CONVERGENCE                                          EQLNU110   001656
00714   2630     116  IF (ITNUMB.EQ.0) GO TO 13                                     EQLNU112   001660
00716   2640          IF (AMBDA.LT.1.) GO TO 43                                     EQLNU113   001661
00720   2650          SUM = (ENN-SUMN)/ENN                                                     001674
00721   2660          IF (SUM.LT.0.) SUM = -SUM                                                001709
00723   2670          IF (SUM .GT. CRITV)  GO TO 43                                            001712
00725   2680          DO 130 J=1,NS                                                 EQLNU115   001722
00730   2690          IF (IUSE(J).LT.0) GO TO 130                                              001722
00732   2700          AA= DELN(J)/SUMN                                                         001725
00733   2710          IF(AA.LT.0.)  AA=-AA                                                     001730
00735   2720          IF (IUSE(J).EQ.0) AA = AA*EN(J,NPT)                                      001735
00737   2730          IF (AA .GT. CRITV)  GO TO 43                                             001742
00741   2740     130  CONTINUE                                                                 001751
00741   2750    C     CALCULATE ENTROPY, CHECK ON DELTA S FOR SP PROBLEMS                      001751
00743   2760          TOTN(NPT) = 0.                                                           001751
00744   2770          SSUM(NPT) = 0.                                                           001753
00745   2780          DO 183 J=1,NS                                                 EQLNU133   001760
00750   2790          IF(IUSE(J).LT.0)  GO TO 183                                              001760
00752   2800          TOTN(NPT) = TOTN(NPT) + EN(J,NPT)                                        001762
00753   2810          SS = S(J)                                                                001765
00754   2820          IF(IUSE(J).EQ.0)  SS=SS-ENLN(J)-TM                                       001767
00756   2830          SSUM(NPT) = SSUM(NPT)+SS*EN(J,NPT)                                       001775
00757   2840     183  CONTINUE                                                      EQLNU136   002004
00761   2850          IF(.NOT.SP.OR.NPT.EQ.1)  GO TO 13                                        002004
00763   2860          SS = SSUM(NPT) -S0                                                       002019
00764   2870          IF(SS.LT.(-0.00005).OR.SS.GT.0.00005)  GO TO 43                          002020
00766   2880          IF(WRITE)  WRITE(JOUT,1183)  SS                                          002035
00772   2890   1183   FORMAT(1H0,DELTA S/R =,E15.8)                                            002046
00773   2900     13   CONVG = .TRUE.                                                EQLNU117   002046
00774   2910          IF(T(     .LT.TLOW.OR.T(     .GT.THIGH)WRITE(JOUT,306)TT,NPT           002047
01001   2920    306   FORMAT(1H0,THE TEMPERATURE=E12.4,26H IS OUT OF RANGE FOR POINT,I5)EQLNU119 002074
01002   2930          IF(ITNUMB.NE.0) GO TO 160                                                002074
01004   2940          WRITE(JOUT,977) NPT                                                      002076
01007   2950    977   FORMAT (27H0,4PHIGO ITERATIONS DID NOT SATISFY THE CONVERGENCE REQ       002134
01007   2960         1UIREMENTS FOR POINT,I3/)                                                002104
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      IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 873
      WRITE(JOUT,874)
      TT = T(1)
      RETURN
C     CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES.
  160 IF(NC.EQ.0) GO TO 143
      SIZEF = 0.
      INC = 0
      DO 170 J = 1,NS
      IF (IUSE(J).EQ.0 .OR. IUSE(J).EQ.-10000) GO TO 170
      INC = INC + 1
      IF(PRITE)  WRITE(JOUT,144)(SUB(J,I),I=1,3),TEMP(INC,1),TEMP(INC,2),
     1IUSE(J),EN(J,NPT)
  144 FORMAT (1H0,3A4,2F10.3,3X,5HIUSE=,I4,E15.7)
      IF (EN(J,NPT))  146,148,169
  146 IF (J.NE.JSOL .AND. J .NE.JLIQ) GO TO 147
      JSOL = 0
      JLIQ = 0
  147 IQI = IQI - 1
      EN(J,NPT) = 0.
      GO TO 166
  148 KG = 1
      IF(IUSE(J).EQ.-IUSE(J+1)) GO TO 154
      IF (J .EQ. 1 .OR. IUSE(J) .NE. -IUSE(J-1))  GO TO 153
      KG = -1
  154 JKG = J + KG
      IF (EN(JKG,NPT).LT.0.) GO TO 170
      TMELT = TEMP(INC,1)
      IF (TMELT .EQ. TEMP(INC*KG,2))  GO TO 158
      TMELT = TEMP(INC,2)
      IF (TMELT .EQ. TEMP(INC*KG,1))  GO TO 157
      WRITE(JOUT,156)
  156 FORMAT (50H03 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER  )
C  JTH SPECIES A SOLID (EN=0), (J+KG)TH SPECIES A LIQUID (EN IS +)
  157 IF (TT .GT. TMELT .OR. (TP .AND. TT .EQ. TMELT))  GO TO 169
      IF (TP .OR. TT .LE. TMELT - 15).0)  GO TO 1165
      JSOL = J
      JLIQ = JKG
      GO TO 159
C  JTH SPECIES A LIQUID(EN=0), (J+KG)TH SPECIES A SOLID (EN IS +)
  158 IF (TT .LT. TMELT .OR. (TP .AND. TT .EQ. TMELT))  GO TO 169
      IF (TP .OR. TT .GE. TMELT + 150.0)  GO TO 1165
      JSOL = JKG
      JLIQ = J
  159 TLN = ALOG (TMELT)
      TT = TMELT
      EN(JKG,NPT) = .5 * EN(JKG,NPT)
      EN(J,NPT) = EN(JKG,NPT)
      GO TO 165
C  WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH EN
 1165 EN(J,NPT) = EN (JKG, NPT)
      IUSE(J) = -IUSE(J)
      IUSE (JKG) = -IUSE(JKG)
      EN(JKG,NPT)= 0.
      WRITE(JOUT,161) (SUB(JKG,I), I = 1,3),(SUB(J,I), I = 1,3)
  161 FORMAT (1H ,,22HPHASE CHANGE, REPLACE ,3A4,6H WITH ,3A4)
```

```
                  GO TO 90                                                                  002506
  153 IF ((TT.LT.TEMP(INC,1) .AND.TEMP(INC,1).NE.TLOW) GO TO 169                            002510
      IF ((TT.GT.TEMP(INC,2)) GO TO 169                                                     002525
      SUM = 0.                                                                              002534
      DO 167 I = 1,L                                                                        002543
  167 SUM = SUM + A(I,J)*X(I)                                                               002543
      DELF = HO(J)-S(J)-SUM                                                                 002547
      IF(WRITE)  WRITE(JOUT,168)DELF,SIZEF                                                  002555
  168 FORMAT (17H GO-SUM(AIJ*PI) =E15.7,10X,18HPREVIOUS DELTA G =,E15.7)                    002566
      IF(DELF.GE.SIZEF .OR. DELF.GE.0.) GO TO 169                                           002566
      SIZEF = DELF                                                                          002603
      JDELF = J                                                                             002605
  169 IF(INC.EQ.NC) GO TO 1160                                                              002610
  170 CONTINUE                                                                              002616
 1160 IF (SIZEF.EQ.0.) GO TO 143                                                            002616
      J = JDELF                                                                             002617
  165 IQI = IQI + 1                                                                         002627
      WRITE(JOUT,136) (SUB(J,I), I = 1,3)                                                   002629
  136 FORMAT (10X,9HADD ,3A4)                                                               002642
  166 IUSE(J) = - IUSE(J)                                                                   002642
   90 CONVG = .FALSE.                                                                       002645
      JSI = 1                                                                               002645
      CALL CPHS                                                                             002647
  143 IN = NUMB                                                                             002652
      IF (.NOT. SHOCK)  WRITE(JOUT,771) NPT,(X(I), I = 1,L),IN                              002659
  771 FORMAT (I5,1PE9.3)                                                                    002675
      JSI = 1                                                                               002675
      IF(TP.AND.CONVG)  CALL CPHS                                                           002677
      ITNUMB = 100                                                                          002704
      GO TO 93                                                                  EQLNU126    002706
C     CALCULATE EQUILIBRIUM PROPERTIES                                          EQLNU128    002706
 1171 DLVPT(NPT) = -1.                                                                      002710
      DLVTP(NPT) = 1.                                                                       002712
      CPR(NPT) = CPSUM                                                                      002715
      GO TO 199                                                                             002717
  171 SUM = 0.                                                                  EQLNU167    002720
      DO 179 J = 1,L                                                                        002733
  179 SUM = SUM + PRO(J)*X(J)                                                   EQLNU170    002737
      DLVPT(NPT) = -1.+SUM/ENN* X(IQI)                                                      002746
      IF (JLIQ .EQ. 0)  GO TO 199                                                           002750
      IUSE(JLIQ) = -IUSE(JLIQ)                                                              002753
      HSUM(NPT) = HSUM(NPT)+EN(JLIQ,NPT)*(HO(JLIQ)-HO(JSOL))                                002764
      IQI = IQI+1                                                                           002767
      GAMMAS(NPT) = -1./DLVPT(NPT)                                                          002772
      GO TO 186                                                                             002774
  199 GAMMAS(NPT) = -1./(DLVPT(NPT)+(DLVTP(NPT)**2)*ENN/CPR(NPT))               EQLNU171    003005
  186 TT(NPT) = T                                                               EQLNU178    003007
      ENNL = ENN                                                                            003011
      PP(NPT) = P                                                                           003013
      VLM(NPT) = RVP*ENN*T/PP                                                               003020
      HSUM(NPT) = HSUM(NPT)*T                                                               003023
      WM(NPT) = 1./ENN                                                          EQLNU180    003027
      IF (.NOT. WRITE)  RETURN                                                              003039
      WRITE(JOUT,,101) NOT,APP(NPT),PP,T,HSUM(NPT),SSUM(NPT),WM(NPT),                      003059
     1 T(NPT),DLVPT(NPT),DLVTP(NPT),GAMMAS(NPT),VLM(NPT)                                    003059
  101 FORMAT (2H0,POINT ,I2,3X,9HPCP/P=E13.6,3X,4HP =E15.6,3X,2HT=E13.6,3X,4H               003062
```

```
      IN/R=E13.6,3X,4HS/R=E13.6//3X,3HMW=E13.6,3X,5HCP/R=E13.6,3X,6HDLVPT   003057
     2=E13.6,3X,6HDLVTP=E13.6,3X,9HGAMMA(S)=E13.6,3X,2HV=,E1' .6)           003057
      RETURN                                                                003057
C     ERROR, SET TT=0                                                       003057
  673 TT=0.                                                                 003063
      NPT = NPT-1                                                           003063
      RETURN                                                                003066
      END                                                                   003127
```

```
.FOR,S LL,IS.FROZEN,LEWIS.FROZEN
HSA  LS -10/25/79-17:38:28 (8,)

   SUBROUTINE FROZEN     ENTRY POINT 000345

   STORAGE USED: CODE(1) 000360; DATA(0) 000041; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003    CONSTS 000006
    0004    POINTS 000335
    0005    SPECES 012120
    0006    MISC   001264
    0007    INDX   000041

   EXTERNAL REFERENCES (BLOCK, NAME)

    0010    CPRS
    0011    ALOG
    0012    EXP
    0013    NERR36

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001    000066 135G      0001    000251 207G      0001    000022 51L       0001    000050 55L       0001    000120 60L
    0001    000165 81L       0001    000313 901L      0001    000321 903L      0005    006034 A         0006    000570 AM
    0006    000624 AM1       0006    000741 ANUM      0003    000000 ATMN      0006    000004 ATOM      0006    000502 BO
    0006    000521 BOP       0007    000036 CALCH     0000 R  000005 CC        0005    000000 COEF      0007 L  000001 CONVG
    0004 R  000032 CPR       0006    000625 CPR1      0006 R  000564 CPSUM     0006    000604 DATA      0005    005670 DELN
    0006    001167 DENS      0000 R  000007 DLNT      0004 R  000064 DLVPT     0004 R  000047 DLVTP     0005 R  007734 EN
    0005    005360 ENLN      0006    001263 ENLSAV    0006    000000 ENN       0006    001261 ENNL      0006    001262 ENSAVE
    0006    001073 ENTH      0006    000566 EQRAT     0006    001112 FAZ       0006    001150 FOX       0004 R  000101 GAMMAS
    0004    000001 GMLT      0007 L  000003 HP        0006    000572 HPP       0006 R  000567 HSUBU     0004 R  000000 HSUM
    0005 R  005524 HO        0007    000030 IC        0007    000000 IDEBUG    0007    000015 IMAT      0000 I  000010 INC
    0000    000015 INJPS     0007    000023 IONS      0007    000021 IP        0007    000037 IQSAVE    0007    000016 IQ1
    0007    000005 ISV       0007    000034 IT        0005 I  011444 IUSE      0000 I  000004 J         0007    000026 JL1Q
    0007    000025 JSOL      0007 I  000031 JS1       0007    000014 KMAT      0006    000463 LLMT      0007    000040 LSAVE
    0007    000006 MOLES     0006    000626 NAME      0007 I  000024 NC        0007    000022 NEWR      0007 I  000035 NF2
    0007    000012 NLM       0007    000017 NOF       0007    000020 NOMIT     0007    000007 NP        0007 I  000011 NPT
    0007    000027 NREAC     0007 I  000013 NS        0005 I  000000 NSPPI     0007    000010 NT        0006    000565 OF
    0006    001227 OXF       0004    000116 P         0003    000002 PATM      0006    001054 PECWI     0006 R  000563 PP
    0004 R  000417 PPP       0003    000003 RBAR      0003    000004 RBR       0006    000574 RH        0006    001206 RHOP
    0006    001207 RMW       0000 R  000001 RNV       0006    001131 RTEMP     0003 R  000005 RVR       0005 R  002570 S
    0007    000033 SHOCK     0005    011754 SLN       0004    000251 SONVEL    0007 L  000004 SP        0000 R  000006 SS
    0004 R  000015 SSUM      0005    010770 SUB       0000 R  000003 SUMH      0006    000001 SUMN      0000 R  000002 SUMS
    0005 R  000003 SU        0004    000150 T         0005 R  011610 TEMP      0006    000562 THIGH     0006 R  001226 TLN
    0006 R  000563 TLOW      0006    000557 TM        0006    000561 TMID      0004 R  000320 TOTN      0007    000002 TP
    0006 R  000570 TT        0004 R  000266 TTT       0004    000202 V         0004 R  000303 VLM       0006    000576 VMIN
    0007 L  000032 VOL       0006    001200 VPLS      0004 R  000234 WM        0006    000602 WP
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C-22

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00101      1*            SUBROUTINE FROZEN                                                    FROZ0002    000000
00101      2*      C                                                                          FROZ0001    000000
00101      3*      C     (FROZEN COMPOSITION EXPANSION ONLY)                                  FROZ0004    000000
00101      4*      C                                                                          FROZ0005    000000
00102      5*            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                          /CONSTS/    000000
00103      6*            COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                      000000
00104      7*           1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)                 000000
00104      8*           2 ,VLM(13),TOIN(13)                                                               000000
00104      9*      C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)                   000000
00104     10*      C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                    000000
00105     11*            INCLUDE SPLCPK                                                                    000000
00111     12*            COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),            /MISC/       000000
00111     13*           1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,       /MISC/       000000
00111     14*           2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),       /MISC/       000000
00111     15*           3              DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15),    /MISC/       000000
00111     16*           4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,     /MISC/       000000
00111     17*           5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                /MISC/       000000
00112     18*            COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,      /INDX/       000000
00112     19*           1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,    /INDX/       000000
00112     20*           2              NREAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE      /INDX/       000000
00112     21*      C                                                                                       000000
00113     22*            LOGICAL CONVG,HP,SP,VOL                                                           000000
00113     23*      C                                                                                       000000
00114     24*            CONVG = .FALSE.                                                                   000000
00115     25*            TLN = ALOG(TT)                                                                    000000
00116     26*            IF (VOL)  RNV = RVR/(VLM(NPT)*WM(NFZ))                                            000004
00120     27*         51 SUMS=0.                                                                           000022
00121     28*            SUMH = 0.                                                                         000022
00122     29*            JSI = 1                                                                           000023
00123     30*            J = NPT                                                                           000025
00124     31*            NPT = NFZ                                                                         000027
00125     32*            CALL CPHS                                                                         000031
00126     33*            CC = CPSUM                                                                        000033
00127     34*            IF(.NOT.VOL)  GO TO 55                                                            000035
00131     35*            CC = CPSUM-1./WM(NFZ)                                                             000037
00132     36*            PP = RNV*TT                                                                       000046
00133     37*         55 NPT = J                                                                           000050
00134     38*            DO 60 J = 1,NS                                                                    000051
00137     39*            IF (EN(J,NFZ) .LE. 0.0)  GO TO 60                                                 000066
00141     40*            SS = S(J)                                                                         000070
00142     41*            IF(IUSE(J).EQ.0)  SS=SS-ALOG(EN(J,NFZ)*PP*WM(NFZ))                               000072
00144     42*            SUMS = SUMS+SS*EN(J,NFZ)                                                          000105
00145     43*            IF (CONVG.OR.HP)  SUMH=SUMH+HO(J)*EN(J,NFZ)                                       000111
00147     44*         60 CONTINUE                                                             FROZ0058    000122
00151     45*            IF (CONVG) GO TO 81                                                  FROZ0059    000122
00153     46*            IF(SP)  DLNT=(SUMS-SO)/CC                                                        000124
00155     47*            IF(HP)  DLNT=(SUMH-HSUBO/TT)/CC                                                  000132
00157     48*            TLN=TLN-DLNT                                                         FROZ0061    000141
00160     49*            IF(DLNT.LT.0.) DLNT=-DLNT                                                        000144
00162     50*            IF(DLNT.LT.0.5E-4)  CONVG=.TRUE.                                                 000151
00164     51*            TT = EXP(TLN)                                                                    000157
00165     52*            GO TO 51                                                             FROZ0063    000163
00166     53*         81 TTT(NPT)= TT                                                                     000165
00167     54*            SSUM(NPT)= SUMS                                                                  000167
00170     55*            HSUM(NPT)= TT*SUMH                                                               000171
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00171     569           GAMMAS(NPT)= CPSUM/(CPSUM-1./WM(NFZ))                                    000173
00172     570           VLM(NPT) = RVR*TT/(WM(NFZ)*PP)                                           000202
00173     580           WM(NPT) = WM(NFZ)                                                        000210
00174     590           DLVPT(NPT) = -1.                                                         000212
00175     600           DLVTP(NPT) = 1.                                                          000214
00176     610           IOIN(NPT) = IOIN(NFZ)                                                    000215
00177     620           PPP(NPT) = PP                                                            000217
00200     630           CPR(NPT)= CPSUM                                                          000221
00201     640           IF (TT.LT.(TLOW-150.))GO TO 903                                          000223
00203     650           IF (NC .EQ. 0)  RETURN                                                   000230
00205     660           INC =0                                                                   000244
00206     670           DO 901 J = 1,NS                                                          000251
00211     680           IF (IUSE(J) .EQ. 0 .OR. IUSE(J) .EQ. - 10000)  GO TO 901                 000251
00213     690           INC = INC+1                                                              000263
00214     700           IF (EN(J,NFZ) .LE. 0.0)  GO TO 901                                       000267
00216     710           IF (TT.LT.TEMP(INC,1)-50. .OR. TT.GT.TEMP(INC,2)+50.)  GO TO 903         000272
00220     720       901 CONTINUE                                                                 000315
00222     730           RETURN                                                                   000315
00223     740       903 TT=0.                                                                    000321
00224     750           NPT= NPT-1                                                               000321
00225     760           RETURN                                                                   000324
00226     770           END                                                    FROZ0084          000357
END PGM
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FOR,S LEWIS.GAMEFF,LEWIS.GAMEFF
HASP FS -10/25/79-17:38:33 (2.)

   SUBROUTINE GAMEFF     ENTRY POINT 000176

   STORAGE USED: CODE(1) 000217; DATA(0) 000044; BLANK COMMON(2) 003000

   EXTERNAL REFERENCES (BLOCK, NAME)

    0003    XPRR
    0004    SQRT
    0005    NERR36

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001   000036 10L        0001   000025 1056       0001   000132 20L        0001   000152 50L        0000 R 000002 ANK
    0000 R 000006 CFA        0000 R 000005 CGAM       0000 R 000001 G          0000 R 000004 GM         0000 R 000003 GP
    0000 I 000000 1          0000   000014 INJP$
```

```
00101      10*          SUBROUTINE GAMEFF (V,GAMMAS,A,N,H)                                    000025
00102      20*          DIMENSION A(13),GAMMAS(13),H(13),V(13)                                000025
00103      30*    C                                                                           000025
00104      40*          DO 50 I = 2,N                                                         000025
00107      50*          G = GAMMAS(I)                                                         000026
00110      60*          ANK = +1.0                                                            000030
00111      70*          IF (G .GT. 1.0)  GO TO 10                                             000033
00113      80*          G = 1.0010                                                            000036
00114      90*       10 GP = G + 1.0                                                          000040
00115      100*         GM = G - 1.0                                                          000043
00116      110*         CGAM = SQRT(G)*(2.0/GP)**(GP/(2.0*GM))                                000063
00117      120*         CFA = CGAM*SQRT(2.0*G*(1.0 - (1.0/A(I))**(GM/G)))/GM)                 000110
00100      130*         IF (ABS(V(I) - CFA) .LE. 5.0E-5)  GO TO 50                            000115
00122      140*         IF (G .LT. 2.0)  GO TO 20                                             000121
00124      150*         IF (ANK .LT. 0.0)  GO TO 50                                           000124
00126      160*         ANK = -1.0                                                            000126
00130      170*         G = GAMMAS(I)                                                         000130
00131      180*         GO TO 10                                                              000132
00132      190*      20 G = G + ANK*(V(I) - CFA)                                              000136
00134      200*         IF (G .GT. 1.0)  GO TO 10                                             000141
00136      210*         IF (ANK .LT. 0.0)  GO TO 50                                           000144
00137      220*         ANK = -1.0                                                            000146
00140      230*         G = GAMMAS(I)                                                         000150
00141      240*         GO TO 10                                                              000152
00143      250*      50 H(I) = G                                                              000157
00144      260*         RETURN                                                                000216
00145      270*          END
END FOR
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@FOR,S LEWIS.GAUSS,LEWIS.GAUSS
HSA  E  -10/25/79-17:38:38 (7,)

   SUBROUTINE GAUSS      ENTRY POINT 000411

  STORAGE USED: CODE(1) 000431; DATA(0) 000126; BLANK COMMON(2) 000000

   COMMON BLOCKS:

   0003    DOUBLE 001560
   0004    INDX   000041

  EXTERNAL REFERENCES (BLOCK, NAME)

   0005    NERR3$

  STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

   0001      000107 10L       0001     000011 110G      0001     000043 120G      0001     000062 127G      0001     000130 152G
   0001      000161 167G      0001     000204 177G      0001     000115 18L       0001     000256 210G      0001     000257 213G
   0001      000141 22L       0001     000361 23L       0001     000333 231G      0001     000167 31L       0001     000275 4EL
   0001      000303 47L       0001     000340 51L       0001     000020 8L        0001     000101 9L        0004     000036 CALCH
   0000 D 000000 COEFX     0004     000001 CONVG     0003 D 000000 G        0004     000003 HP        0000 I 000056 I
   0004      000030 IC        0004     000000 IDEBUG    0000     000071 INJP$     0004     000023 IONS      0004     000021 IP
   0004      000037 IOSAVE    0004     000016 IQ1       0004     000005 ISV       0004     000034 IT        0004 I 000015 IUSE
   0000 I 000054 IUSE1     0000 I 000057 J          0004     000026 JLIQ      0004     000025 JSOL      0004     000031 JS1
   0000 I 000061 K         0004     000014 KMAT      0004     000040 LSAVE     0004     000006 MOLES     0004     000024 NC
   0004      000022 NEWR      0004     000035 NFZ       0004     000012 NLM       0000 I 000055 NN       0004     000017 NOF
   0004      000020 NOMIT     0004     000007 NP        0004     000011 NPT       0004     000027 NREAC     0004     000013 NS
   0004      000010 NT        0004     000033 SHOCK     0004     000004 SP        0000 D 000050 SUM      0000 R 000060 TEMP
   0004      000002 TP        0004     000032 VOL       0003 D 001510 X        0000 D 000052 Z


 00101      1*           SUBROUTINE GAUSS                                                              000000
 00103      2*           COMMON/DOUBLE/G(20,21),X(20)                                                  000000
 00104      3*           COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,    /INDX/    000000
 00104      4*          1              KMAT,IUSE,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/    000000
 00104      5*          2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE    /INDX/    000000
 00105      6*           DOUBLE PRECISION COEFX(20),G,SUM,X,Z                                          000000
 00105      7*     C     BEGIN ELIMINATION OF NNTH VARIABLE                             00205000   000000
 00106      8*           IUSE1=IUSE+1                                                   00203600   000000
 00107      9*           DO 45 NN = 1,IUSE                                                         000002
 00112     10*           IF (NN .NE. IUSE)  GO TO 8                                                000011
 00114     11*           IF (G(NN,NN))  31,23,31                                                   000014
 00114     12*     C     SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW                     00205600   000014
 00117     13*         8 DO 15 I=NN,IUSE                                                           000020
 00122     14*           COEFX(I) = 1.0E38                                                         000047
 00123     15*           IF(G(I,NN).EQ.0.)  GO TO 18                                               000051
 00125     16*           COEFX(I) = 0.                                                             000054
 00126     17*           DO 10 J=NN,IUSE1                                                          000062
```

```
00131    190          SUM = G(I,J)                                                    000062
00132    200          IF(SUM.LT.0.)  SUM=-SUM                                         000064
00134    210          IF(J.NE.NN)  GO TO 9                                            000072
00136    220          Z = SUM                                                         000075
00137    230          GO TO 10                                                        000077
00140    240        9 IF(SUM.GT.COEFX(I))  COEFX(I)=SUM                               000101
00142    250       10 CONTINUE                                                        000111
00144    260          COEFX(I) = COEFX(I)/Z                                           000111
00145    270       18 CONTINUE                                                        000121
00147    280          TEMP = 1.0E38                                                   000121
00150    290          I=0                                                  00207200   000123
00151    300          DO 22 J = NN,IUSE                                               000130
00154    310          IF (COEFX(J) .GE. TEMP)  GO TO 22                               000130
00156    320          TEMP = COEFX(J)                                                 000134
00157    330          I=J                                                  00207600   000136
00160    340       22 CONTINUE                                             00207700   000143
00162    350          IF (I .EQ. 0)  GO TO 23                                         000143
00162    360    C     INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH     00208200   000143
00162    370    C     VARIABLE FROM THE REMAINING EQUATIONS                           00208300   000143
00162    380    C      INTERCHANGE EQUATIONS I AND NN                                 00208500   000143
00164    390          IF (NN .EQ. I)  GO TO 31                                        000145
00166    400          DO 30 J = NN,IUSE1                                              000150
00171    410          Z=G(I,J)                                                        000161
00172    420          G(I,J)=G(NN,J)                                       00208900   000162
00173    430       30 G(NN,J) = Z                                          00209000   000164
00175    440    C     DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH    00209300   000164
00175    450    C     VARIABLE FROM THE REMAINING EQUATIONS                           00209400   000164
00175    460       31 K = NN + 1                                                    00209600   000167
00176    470          DO 36 J = K, IUSE1                                           00209700   000171
00201    480          IF(G(NN,NN).EQ.0.)  GO TO 23                                    000204
00203    490       36 G(NN,J) = G(NN,J)/G(NN,NN)                                      000207
00205    500          IF (K .EQ. IUSE1)  GO TO 45                                     000214
00207    510          DO 44 I = K,IUSE                                                000217
00212    520          DO 44 J = K,IUSE1                                               000257
00215    530       44 G(I,J) = G(I,J) - G(I,NN)*G(NN,J)                               000257
00220    540       45 CONTINUE                                                 00210500   000300
00220    550    C     BACKSOLVE FOR THE VARIABLES                             00210700   000300
00222    560          K = IUSE                                                00211000   000300
00223    570       47 J = K + 1                                               00211100   000303
00224    580          X(K) = 0.000                                            00203800   000305
00225    590          SUM = 0.0                                               00211200   000312
00226    600          IF (IUSE .LT. J)  GO TO 51                                      000313
00230    610          DO 50 I = J,IUSE                                                000316
00233    620       50 SUM = SUM + G(K,I)*X(I)                                         000333
00235    630       51 X(K) = G(K,IUSE1) - SUM                                         000340
00236    640          K = K - 1                                               00211800   000350
00237    650          IF (K .NE. 0)  GO TO 47                                         000353
00241    660          RETURN                                                          000355
00242    670       23 IUSE = IUSE-1                                                   000361
00243    680          RETURN                                                          000363
00244    690          END                                                             000430
```

```
@FOR,S LEWIS.HCALC,LEWIS.HCALC
H.A  E:  -10/25/79-17:38:44  (9,)


   SUBROUTINE HCALC      ENTRY POINT 000526

   STORAGE USED: CODE(1) 000542; DATA(0) 000066; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   CONSTS 000006
    0004   HOLLOW 000010
    0005   POINTS 000101
    0006   SPECES 01.120
    0007   MISC   001264
    0010   INDX   000041
    0011   CCC    000003


   EXTERNAL REFERENCES (BLOCK, NAME)

    0012   CPHS
    0013   ALOG
    0014   SWPOS
    0015   910Z6
    0016   NERR3$


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001    000070 143G       0001    000107 15L        0001    000131 16L        0001    000145 165G       0001    000154 172G
    0001    000162 177G       0001    000204 210G       0001    000275 227G       0001    000170 30L        0001    000026 4L
    0001    000177 50L        0001    000432 500L       0001    000251 55L        0001    000265 56L        0001    000307 70L
    0001    000447 75L        0000    000010 76F        0001    000477 80L        0000    000024 85F        0001    000037 9L
    0001    000312 90L        0006 R  006034 A          0004 I  000001 AG         0007 R  000570 AM         0007 R  000624 AM1
    0000 R  000002 ANN        0007 R  000741 ANUM       0003    000000 ATMN       0007    000004 ATOM       0004 I  000004 BLK
    0007    000502 BO         0007    000521 BOP        0010 L  000036 CALCH      0006    000000 COEF       0010    000001 CONVG
    0005    000032 CPH        0007 R  000625 CPR1       0007 R  000564 CPSUM      0007 R  000604 DATA       0006    005670 DELN
    0011    000002 DEMAND     0007    001167 DENS       0005    000064 DLVPT      0005    000047 DLVTP      0006 R  002734 EN
    0004    000000 END        0000 R  000007 ENJ        0006    005360 ENLN       0007    001263 ENLSAV     0007    000000 ENN
    0007    001261 ENNL       0007    001262 ENSAVE     0007 R  001073 ENTH       0007    000566 EQRAT      0007 I  001112 FAZ
    0007 I  001150 FOX        0003    000001 GMET       0011    000000 GRAPH      0010    000003 HP         0007 R  000572 HPP
    0007 R  000567 HSUBO      0005    000000 HSUM       0006 R  005524 HO         0000 I  000005 I          0010    000030 IC
    0010    000000 IDEBUG     0004    000002 IE         0010    000015 IMAT       0000    000044 INJP1      0010    000023 IONS
    0010    000021 IP         0010    000037 IQSAVE     0010    000016 IQ1        0000 I  000006 IS         0010    000005 ISV
    0010    000034 IT         0006 I  011444 IUSE       0004 I  000003 IZERO      0010 I  000031 J          0010    000026 JL10
    0011 I  000001 JOUT       0010    000025 JSOL       0000 I  000004 K          0010    000014 KMAT       0010 I  000012 L
    0007 I  000463 LLMT       0010    000040 LSAVE      0004    000005 MOL        0010 L  000006 MOLES      0000 I  000003 N
    0007 I  000626 NAME       0010    000024 NC         0010    000022 NEWR       0010    000035 NFZ        0010    000017 NOF
    0011    000020 NOMIT      0010    000007 NP         0010 I  000011 NPT        0010 I  000027 NREAC      0010 I  000013 NS
    0000 I  000000 NSPP1      0010    000010 NT         0007 I  000741 NUM        0007 R  000565 OF         0004 I  000006 OX
    0007    001227 OXF        0003    000002 PATM       0007 R  001054 PFCNT      0007 R  000563 PP         0003 R  000003 RBAR
    0007    000004 RBR        0007    000574 RH         0007    001206 RHOP       0007 R  001207 RHOW       0007 R  001131 RTEMP
    0010    000001 RVW        0004 R  002370 S          0010 L  000033 SHOCK      0006    011754 SLN        0010    000004 SP
    0006 R  010001 SSUM       0006    011770 SUB        0007    000001 SUMN       0007    000003 SO         0006 R  011610 TEMP
```

```
0007 R 000562 THIGH     0007 R 001226 TLN       0007 R 000560 TLOW      0007 R 000557 TM        0007   000561 TMID
0010   000002 IF        0000 R 000001 TSAVE     0007 R 000002 TT        0007   000576 VMIN      0010 L 000032 VOL
0007   000600 VPLS      0007 R 000602 WP        0004   000007 ZERO
```

```
00101      10*          SUBROUTINE HCALC                                                                  000000
00101      20*    C  CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS                                  000000
00103      30*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                    /CONSTS/           000000
00104      40*          COMMON /HOLCON/ END,AG,IE,IZERO,BLK,MOL,OX,ZERO                /HOLCON/           000000
00105      50*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                       000000
00105      60*    C     COMMON/SPECIES/COLF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)                  000000
00105      70*    C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                    000000
00106      80*          INCLUDE SPECPR                                                                    000000
00112      90*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,10),LLMT(15),BO(15),       /MISC/             000000
00112     100*         1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,  /MISC/             000000
00112     110*         2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),  /MISC/             000000
00112     120*         3              DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15),/MISC/            000000
00112     130*         4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,/MISC/             000000
00112     140*         5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV           /MISC/             000000
00113     150*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,   /INDX/             000000
00113     160*         1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,/INDX/            000000
00113     170*         2              NREAC,IC,J,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE   /INDX/             000000
00113     180*    C                                                                                      000000
00114     190*              COMMON /CCC/ GRAPH,JOUT,DEMAND                                             000000
00114     200*    C                                                                                      000000
00115     210*          DIMENSION NUM(15,5)                                                            000000
00116     220*          EQUIVALENCE (ANUM,NUM)                                                         000000
00117     230*          INTEGER AG,BLK,FAZ,FOX,OX                                                      000000
00120     240*          LOGICAL CALCH,MOLES,SHOCK,VOL                                                  000000
00121     250*          TSAVE = TT                                                                     000000
00122     260*          IF (AM(1) .GT. 0.0 .AND. AM(2) .GT. 0.0)  GO TO 4                              000001
00124     270*          AM1= AM(2)                                                                     000015
00125     280*          IF (AM(2) .LE. 0.0)  AM1 = AM(1)                                               000017
00127     290*          GO TO 9                                                                        000024
00130     300*        4 AM1=(OF+1.)*AM(1)*AM(2)/(AM(1)+OF*AM(2))                                       000026
00131     310*        9 TM = 0.                                                                        000037
00132     320*          IF(PP.GT.0.) TM = ALOG(PP*AM1)                                                 000037
00134     330*          SSUM(NPT) = 0.                                                                 000051
00135     340*          HPP(1) = 0.                                                                    000053
00136     350*          HPP(2) = 0.                                                                    000054
00137     360*          HSUBO = 0.                                                                     000055
00140     370*          CPR1 = 0.                                                                      000056
00141     380*          ANN = (1.+OF)                                                                  000057
00141     390*    C     LOOP ON REACTANTS. IF OXIDANT, K = 1, IF FUEL, K = 2.                          000057
00142     400*          DO 700 N=1,NREAC                                                               000070
00143     410*          K=2                                                                            000070
00146     420*          IF(FOX(N).EQ.OX)K=1                                                            000072
00150     430*          IF(NAME(N,5).NE.IZERO)  GO TO 90                                               000077
00152     440*          IF(.NOT.CALCH)  GO TO 15                                                       000102
00154     450*          TT = RTEMP(N)                                                                  000104
00154     460*    C  15 TT IN RANGE                                                                    000104
00155     470*       15 IF (SHOCK)  GO TO 16                                                           000107
00157     480*          IF (TT .LT. TLOW - 100.0 .OR. TT .GT. THIGH + 1000.0)  GO TO 75                000117
00161     490*       16 J = ANUM(N,5)                                                                  000131
```

```
00162     500           IF (J.NE.0)  GO TO 90                                                                  000136
00164     510           DO 10 J=1,L                                                                            000145
00167     520       10  DATA(J) = 0.0                                                                         000145
00171     530           DO 30 I = 1,4                                                                          000154
00174     540           IF (ANUM(N,I) .LE. 0.0)  GO TO 50                                                      000154
00176     550           DO 20 J=1,L                                                                            000162
00201     560       20  IF (LLMT(J) .EQ. NAME(N,I))  GO TO 30                                                  000162
00204     570       30  DATA(J) = DATA(J) + ANUM(N,I)                                                          000170
00206     580        50 IS=0                                                                                   000177
00207     590           DO 70 J=1,NS                                                                           000177
00212     600           IF(IUSL(J).EQ.0)GO TO 55                                                               000204
00214     610           IS = IS+1                                                                              000206
00215     620           IF(FAZ(N).EQ.AG)GO TO 70                                                               000212
00217     630           IF(TT.GT.TEMP(IS,2).AND.TEMP(IS,2).NE.THIGH)  GO TO 70                                 000215
00221     640           IF(TT.LT.TEMP(IS,1).AND.TEMP(IS,1).NE.TLOW)  GO TO 70                                  000232
00223     650           GO TO 56                                                                               000247
00224     660        55 IF(FAZ(N).NE.AG.AND.FAZ(N).NE.BLK)  GO TO 70                                           000251
00226     670        56 DO 60 I=1,L                                                                            000265
00231     680       60  IF (A(I,J) .NE. DATA(I))  GO TO 70                                                    000275
00234     690           NUM(N,5) = J                                                                           000303
00235     700           GO TO 90                                                                               000305
00236     710        70 CONTINUE                                                                               000310
00240     720           GO TO 80                                                                               000310
00241     730        90 IF (MOLES)        ENJ = PECWT(N)/WP(K)                                                 000312
00243     740           IF (.NOT.MOLES)        ENJ = PECWT(N)/RMW(N)                                           000325
00245     750           ENJ = ENJ/ANN                                                                          000332
00246     760           IF(K.EQ.1)  ENJ = ENJ*DF                                                               000335
00250     770           IF(NAME(N,5).NE.IZERO)GO TO 500                                                        000343
00252     780           I = NS                                                                                 000346
00253     790           NS = J                                                                                 000350
00254     800           TLN = ALOG(TT)                                                                         000352
00255     810           IF(.NOT.CALCH)  ENTH(J,NPT) = ENJ                                                      000356
00257     820           CALL CPHS                                                                              000363
00260     830           NS = I                                                                                 000366
00261     840           IF (HO(J).GT.-.01 .AND. HO(J).LT..01) HO(J) = 0.                                       000371
00263     850           RTEMP(N) = TT                                                                          000411
00264     860           IF(VOL) HO(J)=HO(J)-1.                                                                 000413
00266     870           ENTH(N) = RBAR*TT*HO(J)                                                                000421
00267     880           CPRI = CPR1 + CPSUM                                                                    000426
00270     890       500 HSUBO = HSUBO + ENTH(N)*ENJ                                                            000432
00271     900           HPP(K) = HPP(K)+ENTH(N)*ENJ                                                            000440
00272     910       900 SSUM(NPT) = SSUM(NPT) + ENJ*(S(J) - ALOG(ENJ) - TM)                                    000444
00274     920           TT = TSAVE                                                                             000456
00275     930           HSUBO = HSUBO/RBAR                                                                     000460
00276     940           RETURN                                                                                 000463
00277     950        75 WRITE(JOUT,76)                                                                         000467
00301     960        76 FORMAT (///20X,57HREACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA                      000473
                     1IN HCALC/)                                                                              000473
00332     980           RETURN                                                                                 000473
00333     990        80 WRITE(JOUT,85) N                                                                       000477
00336    1000        85 FORMAT (///20X,I2,42H TH REACTANT IS NOT IN THERMO DATA IN HCALC/)                      000504
00507    1010           RETURN                                                                                 000504
00510    1020           END                                                                                    000541
```

```
-FOR,S LEWIS.LTCPHS,LEWIS.LTCPHS
HASP ES -107,5779-17:38:51 (2,)


    SUBROUTINE LTCPHS    ENTRY POINT 000205


    STORAGE USED: CODE(1) 000221; DATA(0) 000130; BLANK COMMON(2) 00000


     COMMON BLOCKS:

     0003   CONSTS 00000
     0004   LOWTH  001201


    EXTERNAL REFERENCES (BLOCK, NAME)

     0005   PAUSE
     0006   THRSIZ
     0007   GOTO
     0010   RDATA1
     0011   RDCHAR
     0012   WRCODS
     0013   RDATAF
     0014   NIOIS
     0015   NIOZS
     0016   NERR3S


    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001   000006 IOL       0000   000072 IOUF      0001   000025 124G      0001   000045 132G      0001   000111 144G
     0001   000113 147G      0001   000124 156G      0001   000026 20L       0001   000051 30L       0001   000122 46L
     0002   000000 ATMN      0004 R 000361 CPL       0003   000001 GMET      0004 R 000551 HL        0000 I 000066 I
     0004 I 001131 ILSP      0000 I 000024 IMN       0000   000107 INJPS     0000 I 000000 INLTMN    0000 I 000012 ISNMN
     0000 I 000015 ITMPMN    0000 I 000067 J         0000 I 000071 K         0004 I 000000 NLTSP     0000 I 000070 NT
     0003   000002 PATM      0003 R 000003 RBAR      0003   000004 RBR       0000 R 000062 RDUM      0003   000005 RVR
     0004 R 000741 SL        0004 R 000601 SUBLT     0004 R 000171 TL


00101      1S          SUBROUTINE LTCPHS                                                    LTCP  10    000000
00101      2S    C                                                                                      000000
00101      3S    C       PROCESS LOW TEMPERATURE  CP,H,S  (VIA MIPS I/O)                              000000
00101      4S    C                                                                                      000000
00101      5S    C       DIMENSION MIPS OUTPUT ARRAYS                                                 000000
00103      6S            DIMENSION INLTMN(10),ISNMN(3),ITMPMN(7),IMN(5,6),RDUM(4)                     000000
00103      7S    C                                                                                      000000
00104      8S            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                          /CONSTS/  000000
00105      9S            COMMON /LOWTH/ NLTSP,SUBLT(40,3),TL(40,3),CPL(40,3),HL(40,3),        /LOWTH/  000000
00105     10S           1               SL(40,3),ILSP(40)                                     /LOWTH/  000000
00105     11S    C                                                                                      000000
00105     12S    C       SET DATA FOR MIPS OUTPUT                                                     000000
00106     13S            DATA INLTMN/24HTYPE THE NUMBER OF LOW T,                                     000000
00120     14S           1   24HTEMPERATURE SPECIES TO BE ENTERED    /                               000000
```

```
      DATA ISNMN/18HTYPE SPECIES NAME /                                 000000
      DATA ITMPMN/42HTYPE NUMBER OF TEMPERATURES,THIS SPECIES=4/        000000
      DATA IMN/36HTYPE   TL,CPL,HL,SL   WHERE -                        ,000000
     1          36H   TL-TEMPERATURE                                   ,000000
     2          36H CPL-CONSTANT PRESSURE SPECIFIC HEAT,               000000
     3          36H   HL-ENTHALPY                                      ,000000
     4          36H   SL-ENTROPY                                       /000000
C                                                                       000000
      NLTSP=0                                                           000000
      CALL PAGIT                                                        000000
      CALL CHRSIZ(3)                                                    000002
   10 CALL GOUT(INLTMN,56)                                              000006
      CALL RDATAI(1,NLTSP,$10)                                          000011
C                                                                       000011
C     LOOP FOR EACH SPECIES                                             000011
      DO 60 I=1,NLTSP                                                   000016
   20 CALL GOUT(ISNMN,17)                                               000026
      CALL RDCHAR(RDUM,2,-1,$20)                                        000031
      DECODE(100,RDUM) (SUBLT(I,J),J=1,3)                               000037
   30 CALL GOUT(ITMPMN,42)                                              000051
      CALL RDATAI(1,NT,$30)                                             000056
      IF(NT.LT.1 .OR. NT.GT.3) GO TO 30                                 000069
      ILSP(I)=0                                                         000102
C                                                                       000102
C          LOOP FOR EACH TEMPERATURE                                    000102
           DO 50 K=1,NT                                                 000103
           DO 45 J=1,5                                                  000113
           CALL GOUT(IMN(J,1),36)                                       000113
   45      CONTINUE                                                     000129
   46      CONTINUE                                                     000129
           DO 48 J=1,4                                                  000129
           RDUM(J)=0.                                                   000129
   48      CONTINUE                                                     000125
           CALL RDATAF(4,RDUM,$46)                                      000125
           TL(I,K)=RDUM(1)                                              000132
           CPL(I,K)=RDUM(2)                                             000134
           HL(I,K)=RDUM(3)                                              000136
           SL(I,K)=RDUM(4)                                              000140
           ILSP(I)=ILSP(I)+1                                            000142
           CPL(I,K)=CPL(I,K)/RBAR                                       000145
           HL(I,K)=HL(I,K)/(TL(I,K)*RBAR)                               000147
           SL(I,K)=SL(I,K)/RBAR                                         000152
   50      CONTINUE                                                     000163
C                                                                       000163
C     END SPECIES LOOP                                                  000163
   60 CONTINUE                                                          000163
C                                                                       000163
      RETURN                                                            000163
C                                                                       000220
  100 FORMAT(8A4)                                                       000220
C                                                                       000220
      END                                                               000220
```

```
»FOR,S LL=IS.MAIN.LL=IS.MAIN
N%A  ES -10/25/79-17:38:58 (12.)

   MAIN PROGRAM

   STORAGE USED: CODE(1) 001235; DATA(0) 000424; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   CONSTS 000006
    0004   HOLCOM 000010
    0005   POINTS 000335
    0006   SPECES 012120
    0007   MISC   001264
    0010   INDX   000041
    0011   PERF   000166
    0012   CCC    000003


   EXTERNAL REFERENCES (BLOCK, NAME)

    0013   RDYES
    0014   MESINT
    0015   PAGIT
    0016   CHRSIZ
    0017   GOUT
    0020   RDATAI
    0021   REACT
    0022   LIBPHS
    0023   RDCHAR
    0024   NBCODE
    0025   SEARCH
    0026   THERMP
    0027   DETON
    0030   ROCKET
    0031   SHOCK
    0032   MESTRM
    0033   NINTRS
    0034   NWDUS
    0035   NIOCS
    0036   NERR2S
    0037   NALLOC
    0040   NRDUS
    0041   NIOIS
    0042   NIOTS
    0043   NWNLS
    0044   NRNLS
    0045   ALOG
    0046   NSTOP,


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001   000006 IL      0003   000271 I0F     0001   000406 I0BL    0001   000211 I1L     0001   000576 I305L
    0001   000015 I41S    0004   000419 I61L    0000   000330 Z0F     0001   000064 Z03L    0001   000441 Z05L
    0001   000447 Z06L    0005   000340 Z07F    0001   000474 Z08L    0000   000306 Z1F     0001   000502 Z10L
```

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0000   000350 211F      0000   000312 22F       0001   000233 240G      0001   000403 25L       0001   001227 3L
0001   001175 301L      0001   001177 302L      0001   000605 304L      0001   000367 320G      0001   000643 322L
0001   000702 323L      0001   000740 333L      0001   000243 39L       0000   000147 400F      0001   000553 414G
0001   001112 434L      0001   000607 4336      0001   000645 450G      0001   000657 457G      0000   000267 5F
0000   000255 52F       0001   001016 526G      0001   001060 543G      0001   001133 565G      0001   001145 570G
0001   001157 575G      0001   000655 722L      0000   000356 724F      0001   000746 745L      0001   001003 746L
0001   001030 748L      0001   001201 749L      0001   001211 791L      0001   001225 800L      0001   000246 90L
0001   000277 97L       0006 R 000034 A         0011   000150 AEAT      0007   000570 AM        0007   000624 AMI
0007   000741 ANUM      0011   000133 APP       0003 R 000000 ATMN      0007   000004 ATOM      0004 I 000004 BLANK
0007   000502 BD        0007 R 000521 BOP       0010 L 000036 CALCH     0006   000000 COEF      0010   000001 CONVG
0005   000052 CPR       0007   000625 CPRI      0007   000564 CPSUM     0007 I 000604 DATA      0006   005670 DELN
0012   000002 DEMAND    0007   001167 DENS      0000 L 000013 DETN      0005   000064 DLVPI     0005   000047 DLVTP
0006 R 002734 EN        0004 I 000000 END       0006 R 005360 ENLN      0007   001263 ENLSAV    0007 R 000000 ENN
0007 R 001461 ENNL      0007   001262 ENSAVE    0006 I 005670 ENSERT    0007   001073 ENTH      0011 L 000165 EQL
0007 R 000566 EQRAT     0000 L 000014 ERATIO    0000 L 000015 FA        0007   001112 FAZ       0000 L 000026 FIRST
0007   001150 FOR       0000 L 000016 FPCT      0005   000101 GAMMAS     0004   000001 GAS       0003   000001 GMET
0012   000000 GRAPH     0010 L 000003 HP        0007   000572 HPP       0007   000567 HSUBU     0005   000000 HSUM
0006   005524 HO        0000 I 000027 I         0010   000030 IC        0000 I 000030 ICARD     0010 I 000000 IDEBUG
0004 I 000002 IE        0010   000015 IMAT      0000   000035 INPTZ     0000 I 000003 INSERT    0010 L 000023 IONS
0010   000021 IP        0010   000037 IQSAVE    0010 I 000016 IQI       0000 I 000034 IST       0010   000005 ISV
0010 I 000034 IT        0006 I 011444 IUSE      0004 I 000003 IZ        0000 I 000032 J         0010   000026 JLIQ
0012 I 000001 JOUT      0010   000025 JSOL      0010   000031 JSI       0010   000014 KMAT      0010 I 000012 L
0007 I 000463 LLMT      0010   000040 LSAVE     0000 I 000004 MIT       0007 R 001227 MIX       0000 I 000006 MLOW
0000 L 000017 MMHG      0004   000005 MOL       0010 L 000006 MOLES     0007 I 000626 NAME      0010 I 000024 NC
0000 I 000007 NCO       0010 L 000022 NEWR      0010   000035 NFZ       0000 I 000005 NMLT      0010 I 000017 NOF
0010 I 000020 NOMIT     0010 I 000007 NP        0010   000011 NPT       0010 I 000027 NREAC     0010 I 000013 NS
0000 I 000031 NSERT     0000 I 000000 NSPPI     0000 L 000020 NSUM      0010 I 000010 NT        0007 L 000565 OF
0004 I 005360 OMIT      0004   000006 OX        0007 R 001227 OXF       0007 R 000565 OXFL      0005 R 000116 P
0003 R 000002 PATM      0011   000000 PCP       0007   001054 PECWT     0007   000563 PP        0005   000217 PPP
0000 L 000021 PSIA      0003 R 000003 RBAR      0003   000004 RBR       0000 R 000033 RDUM      0013 L 000000 RDYES
0000 I 000001 REAC      0007   000574 RH        0007 R 001206 RHOP      0000 L 000022 RMT       0007   001207 RMW
0007   001131 RTEMP     0003   000005 RVR       0006   002570 S         0010 L 000033 SHOCK     0006   011754 SLN
0007 R 000003 SP        0005   000251 SONVEL    0010 L 000004 SP        0011   000047 SPIM      0005   000015 SSUM
0006 I 010770 SUB       0011   000101 SUBAR     0007 R 000031 SUMN      0011   000116 SUPAR     0000 L 000023 SV
0007 R 000003 SP        0005 R 000150 T         0006   011610 TEMP      0007 R 000562 THIGH     0000 I 000002 THRM
0007   001126 TLN       0007 R 000560 TLOW      0007   000557 TM        0007 R 000561 TMID      0005   000320 TOTN
0010 L 000002 TP        0007   000004 TT        0005   000266 TTT       0000 L 000024 TV        0000 L 000025 UV
0005 R 000032 V         0011   000064 VACI      0005   000303 VLM       0007 R 000576 VMIN      0011   000032 VMOC
0010 L 000052 VOL       0007 R 000600 VPLS      0005   000234 WM        0007 R 000602 WP        0004   000007 ZERO
```

```
0100       10      C  MAIN PROGRAM                                                                  MAIN0002   000000
0100       20      C                                                                                             000000
0101       30            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                              /CONSTS/   000000
0103       40            COMMON /HOLCON/ END,GAS,IE,IZ,BLANK,MOL,OX,ZERO                          /HOLCON/   000001
0104       50            COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPI(13)                         000001
0109       60           1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)                    000001
0109       70           2 ,VLM(13),TOTN(13)                                                                  000001
0109       80      C     COMMON/SPECES/COEF(2,7,150),ST(150),EN(150,13),ENLN(150),HO(150)                     000001
0109       90      C    1 ,DELN(150),AT(5,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                       000001
0115      100            INCLUDE SPECPR                                                                       000001
0111      110            COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,10I),LLMT(15),BO(15),              /MISC/      000001
0111      120           1              BOP(15,2),IM,TLOW,IMID,THIGH,PP,CPSUM,OF,EQRAT,         /MISC/      000001
0111      130           2              HSUBU,AM(2),HPP(2),WM(2),VMIN(2),VPLS(2),WP(2),         /MISC/      000001
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0111    140          3              DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),PECWT(15),    /MISC/    000001
0111    150          4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,     /MISC/    000001
0111    160          5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                /MISC/    000001
0111    170           COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,       /INDX/    000001
0112    180          1              KMAT,IMAT,IQI,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,    /INDX/    000001
0112    190          2              NREAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE      /INDX/    000001
0113    200           COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),         /PERF/    000001
0113    210          1              SUPAR(13),APP(13),AEAT(13),EQL                        /PERF/    000001
0113    220 C                                                                                        000001
0114    230               COMMON /CCC/ GRAPH,JOUT,DEMAND                                         000001
0115    240           INTEGER BLANK,DATA,END,ENSERT,OMIT,REAC,SUB,THRM                           000001
0116    250           DATA INSERT,MIT,NMLT,REAC,THRM/4HINSE,4HOMIT,4HNAME,4HREAC,4HTHER/         000001
0124    260           DATA MLOW/4HLOW /                                                          000001
0126    270           DIMENSION ENSERT(3,[illegible]),NCO(4),OMIT(3,[illegible])                 000001
0127    280           EQUIVALENCE (DELN,ENSERT),(ENLN,OMIT),(MIX,OXF),(OF,OXF[illegible]),(SO,SO)  000001
0130    290           LOGICAL CALCH,DEIN,EQL,ERATIO,FA,FPCT,HP,IONS,MMHG,MOLES,NEWR,             000001
0130    300          1         NSOM,OF,PSIA,RKT,SHOCK,SP,SV,TP,TV,UV,VOL                       000001
0130    310 C                                                                                    000001
0131    320               LOGICAL ROYES,FIRST                                                    000001
0131    330 C                                                                                    000001
0132    340           REAL MIX(26)                                                               000001
0132    350 C                                                                                    000001
0133    360           NAMELIST /INPT2/ DEIN,ERATIO,FA,FPCT,HP,IDEBUG,IONS,MIX,MMHG,NSOM,  /INPT2/  000001
0133    370          1                 OF,P,PSIA,RKT,SO,SHOCK,SO,SP,SV,T,TP,TV,UV,V       /INPT2/  000001
0138    380 C                                                                                    000001
0139    390           FIRST=.TRUE.                                                               000001
0135    400              CALL MPSINT                                                             000003
0136    410           1 WRITE(JOUT,900)                                                          000006
0140    420             DO 300 I=1,26                                                            000015
0143    430             MIX(I) = 0.0                                                             000015
0144    440             P(I)= 0.                                                    ODE  115     000015
0145    450             T(I)= 0.                                                    ODE  116     000016
0146    460      300    V(I) = 0.0                                                               000017
0150    470             TP = .FALSE.                                                ODE  123     000021
0151    480             HP=.FALSE.                                                  ODE  124     000022
0152    490             TV = .FALSE.                                                             000023
0153    500             UV = .FALSE.                                                             000024
0154    510             SV = .FALSE.                                                             000025
0155    520             RKT = .TRUE.                                                             000026
0156    530             SHOCK = .FALSE.                                             ODE  129     000030
0157    540             DEIN = .FALSE.                                              ODE  130     000031
0160    550             MMHG   = .FALSE.                                            ODE  133     000032
0161    560             PSIA = .TRUE.                                                            000033
0162    570             NSOM = .FALSE.                                                           000035
0163    580             IONS = .FALSE.                                                           000036
0164    590             IDEBUG = 0                                                               000037
0165    600             FA = .FALSE.                                                             000040
0166    610             OF = .TRUE.                                                              000041
0167    620             ERATIO = .FALSE.                                                         000043
0170    630             FPCT = .FALSE.                                                           000044
0171    640             EQL = .TRUE.                                                ODE  145     000045
0172    650             NEWR = .FALSE.                                              MAIN0022     000047
0173    660      900    FORMAT(1H1)                                                 MAIN0025     000050
0174    670                CALL PAGE1                                                            000050
0175    680                JOUT=6                                                                000052
0176    690                IF(IDEBUG.NE.0) WRITE(6,1500) JOUT=51                                 000054
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00200    700      203      CONTINUE                                                                  000064
00201    710               CALL PAGIT                                                                000064
00202    720               CALL CHRSIZ(1)                                                            000065
00203    730               CALL GOUTI'LEWIS CHEMICAL EQUILIBRIUM PROGRAM',34)                        000070
00204    740               CALL GOUTI' ',1)                                                          000074
00205    750               CALL GOUTI'          MAIN MENU',19)                                       000100
00206    760               CALL GOUTI' ',1)                                                          000104
00207    770               CALL GOUTI' 1 - READ THERMODYNAMIC DATA FROM CARDS',39)                   000110
00210    780               CALL GOUTI' 2 - READ LOW TEMP EXTENSION THERMO DATA',40)                  000114
00211    790               CALL GOUTI' 3 - SELECT REACTANTS',21)                                     000120
00212    800               CALL GOUTI' 4 - OMIT SPECIES FROM THERMO DATA',34)                        000124
00213    810               CALL GOUTI' 5 - INSERT CONDENSED SPECIES',29)                             000130
00214    820               CALL GOUTI' 6 - BEGIN NAMELIST INPUT',25)                                 000134
00215    830               CALL GOUTI' RETURN - TERMINATE PROGRAM',27)                               000140
00216    840                ICARD=0                                                                  000144
00217    850           CALL CHRSIZ(4)                                                                000145
00220    860               CALL RDATAI(1,ICARD,$203)                                                 000150
00221    870                IF(ICARD.EQ.0) GO TO 3                                                   000155
00223    880                IF(ICARD.LT.1 .OR. ICARD.GT.6) GO TO 203                                 000157
00225    890                GO TO(90,39,11,205,108,210),ICARD                                        000175
00225    900     C                                                                                   000175
00225    910     C         CALL SUBROUTINE TO READ REACTANT CARDS                                    000175
00226    920        11 NSERT = 0                                                    4/23/70          000211
00227    930           NOMIT = 0                                                                     000211
00230    940           MOLES = .FALSE.                                              MAIN0041         000212
00231    950           CALL REACT(FIRST)                                                             000213
00232    960           IF(L.EQ.0)  WRITE(JOUT,52)                                                    000216
00235    970        52 FORMAT(24HJERROR IN REACTANT CARDS)                                           000225
00236    980           CALCH = .FALSE.                                                               000225
00237    990           DO 755 I = 1,NREAC                                                            000233
00242   1000         755  IF (NAME(I,5) .EQ. 12)  CALCH = .TRUE.                                     000233
00245   1010           GO TO 203                                                     MAIN0053         000241
00245   1020    C                                                                                   000241
00245   1030    C         READ LOW TEMPERATURE EXTENSION THERMO DATA                                000241
00246   1040       39  CALL LTCPHS                                                                   000243
00247   1050           GO TO 203                                                                     000244
00247   1060    C                                                                                   000244
00247   1070    C         READ THERMO DATA FROM CARDS AND STORE ON  TAPE 4                          000244
00250   1080       90  NEWR = .TRUE.                                                                 000246
00251   1090           REWIND 4                                                                      000247
00252   1100               CALL GOUTI'ADD THERMO DATA HERE',20)                                       000252
00253   1110           READ(5,5) TLOW,TMID,THIGH                                                     000256
00260   1120         5 FORMAT (3F10.3)                                                               000266
00261   1130           WRITE (4,5) TLOW,TMID,THIGH                                                   000266
00266   1140        97  READ (5,10) DATA,NCD(1)                                                     000277
00272   1150        10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3,I15)                                   000310
00273   1160           IF(DATA(1).EQ.BLANK) DATA(1)=END                                           000310
00275   1170           WRITE (4,10) DATA                                                          000315
00300   1180           IF(DATA(1).EQ.END)  GO TO 203                                              000325
00302   1190           READ (5,20) (DATA(I), I = 1,5),NCD(2),(DATA(J), J = 6,10),NCD(3),          000330
00302   1200          1            (DATA(I), I = 11,14),NCD(4)                                     000330
00312   1210        20 FORMAT(5E15.8,I5/5E15.8,I5/4E15.8,I20)                                     000354
00313   1220           WRITE (4,21) (DATA(I), I = 1,14)                                           000354
00316   1230        21 FORMAT(5E15.8/5E15.8/4E15.8)                                               000367
00317   1240           DO 25  I=1,4                                                               000367
00322   1250           IF(NCD(I).EQ.I)  GO TO 25                                                  000367
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00324    126*          WRITE(JOUT,22) (DATA(J),J=1,3)                                    000372
00327    127*       22 FORMAT(28HOERROR IN ORDER OF CARDS FOR ,3A4)                       000404
00330    128*       25 CONTINUE                                                          000404
00332    129*          GO TO 97                                                          000404
00332    130*    C                                                                      000404
00332    131*    C     CHECK INSERT CARDS                                               000404
00333    132*      104     CONTINUE                                                     000406
00334    133*              CALL PAGIT                                                   000406
00335    134*              CALL GOUT('TYPE SPECIES TO INSERT(1 PER LINE)',34)           000407
00336    135*      181     CONTINUE                                                     000414
00337    136*              CALL RDCHAR(RDUM,2,-1,$203)                                  000414
00340    137*              NSERT=NSERT+1                                                000421
00341    138*              DECODE(207,RDUM) (ENSERT(1,NSERT),T=1,3)                     000424
00344    139*              GO TO 181                                                    000437
00344    140*    C                                                                      000437
00344    141*    C     CHECK OMIT CARDS                                               000437
00345    142*      205     CONTINUE                                                     000441
00346    143*              CALL PAGIT                                                   000441
00347    144*              CALL GOUT('TYPE SPECIES TO OMIT FROM THERMO DATA',37)        000442
00350    145*      206     CONTINUE                                                     000447
00351    146*              CALL RDCHAR(RDUM,2,-1,$208)                                  000447
00352    147*              NOMIT=NOMIT+1                                                000454
00353    148*              DECODE(207,RDUM) (OMIT(1,NOMIT),I=1,3)                       000457
00356    149*      207     FORMAT(3A4)                                                  000472
00357    150*              GO TO 206                                                    000472
00360    151*        208 CONTINUE                                          MAINU062   000474
00361    152*              NEWRS = .TRUE.                                               000474
00362    153*              REWIND 4                                                     000475
00363    154*              GO TO 203                                       MAINU063   000500
00363    155*    C                                                                      000500
00363    156*    C     BEGIN NAMELIST INPT2                              MAINU065   000500
00364    157*       210  RHOP = 0.0                                                    000502
00365    158*            SO = 0.0                                                     000502
00366    159*            SP=.FALSE.                                        ODE  125   000503
00367    160*            VOL = .FALSE.                                                000504
00370    161*            NT = 1                                                       000505
00371    162*                CALL PAGIT                                               000507
00372    163*                IF(RDYES('TYPE YES FOR PRESENT INPT2 NAMELIST',35))      000511
00372    164*           1    WRITE(6,INPT2)                                           000511
00376    165*               WRITE(6,211)                                              000522
00400    166*      211      FORMAT(' BEGIN NAMELIST INPT2 INPUT')                    000527
00401    167*               READ(5,INPT2)                                 MAINU086   000527
00404    168*                CALL PAGIT                                               000533
00405    169*               WRITE(JOUT,INPT2)                                         000535
00410    170*               IF(.NOT.TV.AND..NOT.UV.AND..NOT.SV)  GO TO 304            000541
00412    171*               VOL = .TRUE.                                              000546
00413    172*               DO 1304  I=1,26                                           000553
00416    173*               IF (P(I) .GT. 0.0)  P(I) = 1.0/P(I)                       000553
00420    174*               IF (V(I) .GT. 0.0)  P(I) = V(I)                           000561
00422    175*               IF (P(I) .LE. 0.0)  GO TO 1305                            000566
00424    176*        1304 NP = I                                                      000571
00426    177*        1305 IP = TV                                                     000576
00427    178*               NP = UV                                                   000577
00430    179*               SP = SV                                                   000601
00431    180*               GO TO 307                                                 000603
00432    181*         304   DO 305  I=1,26                                          000607
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00435   182*          IF (P(I) .LE. 0.0)  GO TO 322                                          000607
00437   183*          NP = I                                                          MAIN0090  000612
00440   184*          IF (MMHG) P(NP) = P(NP)/760.                                           000616
00442   185*          IF (PSIA)  P(NP) = P(NP)/PATM                                          000624
00444   186*      305 IF (NSQM)  P(NP) = P(NP)/ATMN                                          000632
00447   187*      322 DO 307 II = 1,26                                                       000645
00452   188*          IF (T(II) .LE. 0.0)  GO TO 722                                         000645
00454   189*      307 NT = II                                                                000650
00456   190*      722 DO 625 IST = 1,26                                                      000657
00461   191*          IF (MIX(IST) .GT. 0.0)  GO TO 323                                      000657
00463   192*          IF(IST.NE.1) GO TO 745                                                 000662
00465   193*          WRITE(JOUT,724)                                                        000665
00467   194*      724 FORMAT (//45X,40HNO INPT2 VALUE GIVEN FOR FA, FPCT, OR OF//)           000672
00470   195*          IF (WP(2) .GT. 0.0)  OXFL = WP(1)/WP(2)                                000672
00472   196*          GO TO 333                                                              000700
00473   197*      323 OXFL  = MIX(IST)                                                       000702
00474   198*          IF(FA) OXFL =1./   MIX(IST)                                            000703
00476   199*          IF(FPCT) OXFL =(100.-   MIX(IST))/   MIX(IST)                         000710
00500   200*          IF(.NOT.ERATIO)  GO TO 333                                             000716
00502   201*          EQRAT = MIX(IST)                                                       000720
00503   202*          IF(EQRAT.EQ.1.)  EQRAT = 1.000005                                      000722
00505   203*          OXFL  = (-EQRAT*VMIN(2)-VPLS(2))/(VPLS(1)+EQRAT*VMIN(1))               000727
00506   204*      333 OXF(IST) = OXFL                                                        000740
00507   205*      625 NOF = IST                                                              000741
00511   206*      745 IF (.NOT. IONS .OR. LLMT(L) .EQ. IE)  GO TO 746                        000746
00513   207*          L = L+1                                                                000756
00514   208*          IF(LLMT(L).NE.IE)  NEWR=.TRUE.                                         000761
00516   209*          REWIND 4                                                               000771
00517   210*          LLMT(L) = IE                                                           000774
00520   211*          BOP(L,1) = 0.                                                          000777
00521   212*          BOP(L,2) = 0.                                                          001000
00522   213*          GO TO 748                                                              001001
00523   214*      746 IF(LLMT(L).NE.IE)  GO TO 748                                           001003
00525   215*          DO 747  J=1,NS                                                         001006
00530   216*      747 IF (A(L,J) .NE. 0.0)  IUSE(J) = - 10000                                001016
00533   217*          L = L-1                                                                001024
00534   218*      748 IF(NEWR)  CALL SEARCH                                                  001030
00534   219*C     INITIAL ESTIMATES                                                          001030
00536   220*          SO = SO/REAR                                                           001033
00537   221*          ENN = .1                                                               001036
00540   222*          ENNL = -2.3025851                                                      001040
00541   223*          SUMN = ENN                                                      MAIN0141  001042
00542   224*          DO 432 J=1,NS                                                   MAIN0145  001060
00545   225*          IF(IUSE(J).GT.0)  IUSE(J)=-IUSE(J)                                     001060
00547   226*          IF(IUSE(J).EQ.-10000.AND.IONS)  IUSE(J) = 0                            001064
00551   227*          EN(J,1) = 0.                                                           001075
00552   228*          ENLN(J) = 0.                                                           001076
00553   229*          IF (IUSE(J).NE.0)  GO TO 432                                           001077
00555   230*          EN(J,1) = ENN/(NS - NC)                                                001101
00556   231*          ENLN(J) = ALOG(EN(J,1))                                                001103
00557   232*      432 CONTINUE                                                               001113
00561   233*          IC1= L+1                                                               001113
00562   234*          IF (INC.EQ.0.OR.NSERT.EQ.0) GO TO 790                                  001116
00564   235*          DO 302 I=1,NSERT                                                       001126
00567   236*          DO 301 J=1,NS                                                          001145
00572   237*          IF(IUSE(J).EQ.0) GO TO 301                                             001150
```

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00574    2380          DO 299 IST = 1,3                                                    001157
00577    2390      299 IF (SUB(J,IST) .NE. ENSERT(IST,I))  GO TO 301                       001157
0060.    2400          I01= I+1                                                            001166
0060.3   2410          IUSE(J)= -IUSE(J)                                                   001171
00604    2420          GO TO 302                                                           001173
00605    2430      301 CONTINUE                                                            001201
0060.    2440      302 CONTINUE                                                            001201
00611    2450      790 IF (.NOT. IP .AND. .NOT. HP .AND. .NOT. SP)  GO TO 791              001201
00615    2460          CALL THERMP                                                         001205
00619    2470          GO TO 800                                                           001207
00615    2480      791 IF (DETN)  CALL DETON                                               001211
00617    2490          IF(RKT) CALL ROCKET                                                 001214
00621    2500          IF(SHOCK)  CALL SHOK                                                001220
00623    2510      800 NSERT = 0                                                           001225
00624    2520          GO TO 1                                                 MAINU152    001225
00625    2530        3     CONTINUE                                                        001227
00626    2540              CALL MPSIRM                                                     001227
00627    2550              STOP                                                            001230
00630    2560          END                                                     MAINU153    001234
END FOR
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@FOR,S LEWIS.MATRIX,LEWIS.MATRIX
HASP ES -10/25/79-17:39:09 (8.)


   SUBROUTINE MATRIX     ENTRY POINT 001063


   STORAGE USED: CODE(1) 001107; DATA(0) 000116; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0001   POINTS 000335
    0004   SPECES 012120
    0005   MISC   001764
    0006   DOUBLE 001560
    0007   INDX   000041


   EXTERNAL REFERENCES (BLOCK, NAME)

    0010   NERR55


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001    000102 124G      0001    000103 127G      0001    000126 140G      0001    000215 154G      0001    000244 161G
    0001    000672 175L      0001    000677 185L      0001    000453 217G      0001    001011 230L      0001    000567 244G
    0001    000606 247G      0001    000623 257G      0001    001026 260L      0001    000757 303G      0001    001023 317G
    0001    000276 55L       0001    000346 59L       0001    000372 62L       0001    000376 64L       0001    000511 65L
    0001    000405 70L       0004 R  006034 A         0005    000570 AM        0005    000624 AM1       0005    000741 ANUM
    0005    000004 ATOM      0005 R  000502 BO        0005    000521 BOP       0007    000036 CALCH     0004    000000 COEF
    0007 L  000001 CONVG     0003    000032 CPR       0005    001625 CPR1      0005 R  000564 CPSUM     0005    000604 DATA
    0004    005670 DELN      0005    001167 DENS      0003    000064 DLVPT     0003    000047 DLVTP     0004 R  002734 EN
    0004 R  000013 ENERGY    0004 R  005360 ENLN      0005    001263 ENLSAV    0005 R  000000 ENN       0005    001261 ENNL
    0005    001262 ENSAVE    0005    001073 ENTH      0005    000566 EQRAT     0000 R  000010 F         0005    001112 FAZ
    0005    001150 FOX       0006 D  000000 G         0003    000101 GAMMAS    0007 L  000003 HP        0005    000572 HPP
    0005 R  000567 HSUBO     0003 R  000000 HSUM      0004 R  005524 HO        0000 I  000003 I         0007    000030 IC
    0007    000000 IDEBUG    0007 I  000015 IMAT      0000    000023 INJPS     0007    000023 IONS      0007    000021 IP
    0007    000037 IQSAVE    0007 I  000016 IQ1       0000 I  000001 IQ2       0000 I  000002 IQ3       0007    000005 ISV
    0007    000034 IT        0004 I  011444 IUSE      0000 I  000007 J         0007    000026 JLIQ      0007    000025 JSOL
    0007    000031 JSI       0000 I  000004 K         0000 I  000006 KK        0007 I  000014 KMAT      0007 I  000012 L
    0005    000463 LLMT      0007    000040 LSAVE     0007    000006 MOLES     0005    000626 NAME      0007    000024 NC
    0007    0000?  NEWR      0007    000035 NFZ       0007    000017 NOF       0007    000020 NOMIT     0007    000007 NP
    0007 I  000011 NPT       0007    000027 NREAC     0007 I  000013 NS        0000 I  000000 NSPP1     0007    000010 NT
    0005    000565 OF        0005    001227 OXF       0003    000116 P         0005    001054 PECWI     0005    000563 PP
    0005    000?17 PPP       0005    000574 RH        0005    001206 RHOP      0005    001207 RMW       0005    001131 RTEMP
    0004 R  002570 S         0007    000033 SHOCK     0004    011754 SLN       0003    000251 SONVEL    0007 L  000004 SP
    0000 R  000011 SS        0000 R  000005 SSS       0003    000015 SSUM      0004    010770 SUB       0005 R  000001 SUMN
    0005 R  000003 SO        0003    000150 T         0004    011610 TEMP      0000 R  000012 TERMI     0005    000562 THIGH
    0005    001226 TLN       0005    000560 TLOW      0005 R  000557 TM        0005    000561 TM10      0003    000320 TOTN
    0007 L  000002 IP        0005 R  000002 TT        0003    000266 TTT       0003    000202 V         0003    000303 VLM
    0005    000576 VMIN      0007 L  000032 VOL       0005    000600 VPLS      0003    000234 WM        0005    000602 WP
    0005 D  001510 X
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00101      1*            SUBROUTINE MATRIX                                                    MATX0001   000030
00101      2*      C                                                                                     000030
00103      3*            COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                   000030
00103      4*           1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)              000030
00103      5*           2 ,VLM(13),TOTN(13)                                                            000030
00103      6*      C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)               000030
00103      7*      C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                000030
00104      8*            INCLUDE SPECPK                                                                000030
00110      9*            COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,10),LLMT(15),BO(15),          /MISC/      000030
00110     10*           1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,    /MISC/      000030
00110     11*           2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),    /MISC/      000030
00110     12*           3              DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),PECWT(15),  /MISC/      000030
00110     13*           4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,   /MISC/      000030
00111     14*           5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV              /MISC/      000030
00111     15*            COMMON /DOUBLE/ G(20,21), X(20)                                  MATX0012   000030
00112     16*            COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,     /INDX/      000030
00112     17*           1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/      000030
00112     18*           2              NREAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE    /INDX/      000030
00112     19*      C                                                                                     000030
00113     20*            DOUBLE PRECISION G,X                                                          000030
00114     21*            LOGICAL CONVG,HP,SP,TP,VOL                                                    000030
00114     22*      C                                                                                     000030
00115     23*            IQ2 = IQ1 + 1                                                                 000030
00116     24*            IQ3 = IQ2 + 1                                                                 000033
00117     25*            KMAT = IQ3                                                         MATX0018   000035
00120     26*            IF(.NOT.CONVG.AND.TP) KMAT = IQ2                                   MATX0019   000036
00122     27*            IMAT = KMAT - 1                                                    MATX0020   000046
00122     28*      C     CLEAR MATRIX STORAGES TO ZERO                                      MATX0022   000046
00123     29*            DO 211 I=1,IMAT                                                               000057
00126     30*            DO 211 K=1,KMAT                                                               000103
00131     31*       211  G(I,K) = 0.000                                                                 000103
00134     32*            SSS = 0.                                                                      000111
00135     33*            HSUM(NPT) = 0.                                                                000112
00135     34*      C     BEGIN SET UP OF ITERATION MATRIX                                   MATX0028   000112
00136     35*            KK = L                                                                        000114
00137     36*            DO 65  J=1,NS                                                      MATX0031   000127
00142     37*            IF(IUSE(J).LT.0)  GO TO 65                                                    000141
00144     38*            IF(IUSE(J).GT.0)  GO TO 70                                                    000145
00146     39*            F = (HO(J)-S(J)+ENLN(J)+TM)*EN(J,NPT)                                         000150
00147     40*            SS = HO(J)*EN(J,NPT) - F                                                      000157
00150     41*            TERM1 = HO(J)*EN(J,NPT)                                                       000161
00151     42*            IF (KMAT .EQ. IQ2) TERM1 = F                                       MATX0037   000163
00152     43*            DO 55 I = 1, L                                                     MATX0038   000174
00153     44*      C     CALCULATE THE ELEMENTS  R(I,K)                                     MATX0040   000174
00156     45*            IF (A(I,J) .EQ. 0.) GO TO 55                                       MATX0042   000232
00160     46*            DO 15  K=I, L                                                      MATX0044   000234
00163     47*       15   G(I,K) = G(I,K) + A(K,J)*A(I,J)*EN(J,NPT)                                      000244
00165     48*            G(I,IQ1) = G(I,IQ1) + A(I,J)*EN(J,NPT)                                        000251
00166     49*            G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM1                                     MATX0048   000255
00167     50*            IF (CONVG .OR. TP) GO TO 55                                        MATX0049   000261
00171     51*            G(I,IQ3)= G(I,IQ3)+A(I,J)*F                                        MATX0050   000263
00172     52*            IF (SP) G(IQ2,I) = G(IQ2,I) + A(I,J)*SS                            MATX0051   000267
00174     53*       55  CONTINUE                                                            MATX0052   000305
00176     54*            IF (KMAT .EQ. IQ2) GO TO 69                                        MATX0053   000305
00200     55*            IF(CONVG.OR.HP) GO TO 59                                           MATX0054   000310
```

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00202      56*            G(IQ2,IQ1) = G(IQ2,IQ1) + SS                                    MATX0055    000323
00203      57*            G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*SS                                  MATX0056    000326
00204      58*            G(IQ2,IQ3) = G(IQ2,IQ3)+(S(J) - ENLN(J)-TM)*F                   MATX0057    000334
00205      59*            GO TO 62                                                        MATX0058    000344
00206      60*         59 G(IQ2,IQ2) = G(IQ2,IQ2) + HO(J)**2*EN(J,NPT)                                000346
00207      61*            IF (CONVG) GO TO 64                                             MATX0060    000362
00211      62*            G(IQ2,IQ3)=G(IQ2,IQ3)+HO(J)*F                                   MATX0061    000364
00212      63*         62 G(IQ1,IQ3)=G(IQ1,IQ3)+F                                         MATX0062    000372
00213      64*         64 G(IQ1,IQ2)=G(IQ1,IQ2)+TERM1                                     MATX0063    000376
00214      65*            GO TO 65                                                                   000403
00215      66*      C   CONDENSED SPECIES                                                            000403
00216      67*         70 KK = KK + 1                                                              000405
00221      68*            DO 75  I = 1,L                                                           000407
00222      69*            G(I,KK) = A(I,J)                                                         000453
00224      70*         75 G(I,KMAT) = G(I,KMAT) - A(I,J)*EN(J,NPT)                                 000456
00225      71*            G(KK,IQ2) = HO(J)                                                        000462
00226      72*            G(KK,KMAT) = HO(J) - S(J)                                                000465
00227      73*            HSUM(NPT) = HSUM(NPT) + HO(J)*EN(J,NPT)                                  000471
00231      74*            IF(.NOT.SP) GO TO 65                                                     000477
00232      75*            SSS = SSS + S(J)*EN(J,NPT)                                               000501
00233      76*            G(IQ2,KK) = S(J)                                                         000505
00235      77*         65 CONTINUE                                                     MATX0064    000520
00236      78*            SSS = SSS + G(IQ2,IQ1)                                                   000520
00237      79*            HSUM(NPT) = HSUM(NPT) + G(IQ1,IQ2)                                       000527
00241      80*            G(IQ1,IQ1) = SUMN - ENN                                                  000537
00242      81*      C     REFLECT SYMMETRIC PORTIONS OF THE MATRIX                        MATX0066    000537
00243      82*            K = IQ1                                                                  000543
00244      83*            IF (HP .OR. CONVG)  K = IQ2                                              000545
00246      84*            DO 102 I = 1,K                                                           000562
00247      85*            DO 102 J = I,K                                                           000606
00251      86*         102 G(J,I) = G(I,J)                                                         000606
00251      87*      C     COMPLETE THE RIGHT HAND SIDE                                    MATX0074    000606
00254      88*            IF(CONVG)  GO TO 175                                            MATX0076    000612
00256      89*            DO 145 I=1,L                                                    MATX0077    000623
00261      90*            X(I)=BO(I)-G(I,IQ1)                                                        000623
00262      91*         145 G(I,KMAT) = G(I,KMAT) + X(I)                                            000625
00264      92*            G(IQ1,KMAT) = G(IQ1,KMAT)+ENN-SUMN                              MATX0080    000630
00264      93*      C     COMPLETE ENERGY ROW AND TEMPERATURE COLUMN                      MATX0082    000630
00265      94*            IF (KMAT .EQ. IQ2) GO TO 185                                    MATX0084    000636
00267      95*            IF (SPIENERGY = SO+ENN-SUMN - SSS                                          000641
00271      96*            IF(HP)ENERGY=HSUBO/TT - HSUM(NPT)                                          000656
00273      97*            G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY                                              000665
00274      98*         175 G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM                                   MATX0088    000672
00275      99*         185 IF (.NOT. VOL .OR. CONVG)  RETURN                                         000677
00275     100*      C     CONSTANT VOLUME MATRIX                                                     000677
00277     101*            K = IQ1 - 1                                                                000704
00300     102*            IF(KMAT.EQ.IQ2) GO TO 230                                                  000707
00302     103*            DO 220 I = 1,K                                                             000721
00305     104*            G(IQ1,I) = G(IQ2,I)-G(IQ1,I)                                               000757
00306     105*            G(I,IQ1) = G(I,IQ2)-G(I,IQ1)                                               000761
00307     106*         220 G(I,IQ1) = G(I,IQ3)                                                       000764
00311     107*            G(IQ1,IQ1) = G(IQ2,IQ2)-G(IQ1,IQ2)-G(IQ2,IQ1)                              000767
00312     108*            G(IQ1,IQ2) = G(IQ2,IQ3)-G(IQ1,IQ3)                                         000774
00313     109*            IF (HP)  G(IQ1,IQ2) = G(IQ1,IQ2) + ENN                                     001001
00315     110*            GO TO 240                                                                  001007
00316     111*         230 DO 240 I = 1,K                                                            001011
```

```
                                                                  001023
                                                                  001026
                                                                  001027
                                                                  001031
                                                      MATX0090    001106
00321   1120      240  G(I,IQ1) = G(I,IQ2)
00323   1130      260 KMAT = IMAT
00329   1140          IMAT = IMAT-1
00325   1150          RETURN
00326   1160          END
END OF PA
```

```
FOR,S LEWIS.OUT1,LEWIS.OUT1
HSA  L: -10/25/79-17:39:20 (2,1)


   SUBROUTINE OUT1       ENTRY POINT 001137
              OUT2       ENTRY POINT 001142
              OUT3       ENTRY POINT 001145


   STORAGE USED: CODE(1) 001150; DATA(0) 000226; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   CONSTS 000000
    0004   HOLCOM 000010
    0005   POINTS 000335
    0006   SPECES 012120
    0007   MISC   001264
    0010   INOUT  000041
    0011   PERF   000166
    0012   OUPT   000073
    0013   CCC    000003


   EXTERNAL REFERENCES (BLOCK, NAME)

    0014   VARFMT
    0015   N600$
    0016   N101$
    0017   N102$
    0020   N103$
    0021   SQRT
    0022   NERR36


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000   000103 1F        0001   000034 10L       0001   000025 142G      0001   000043 152G      0001   000625 160L
    0001   000112 166G      0001   000651 170L      0001   000657 175L      0001   000726 177L      0001   000764 179L
    0001   000766 180L      0000   000062 20F       0001   001041 200L      0001   001076 210L      0001   001100 211L
    0001   000175 223G      0001   000205 230G      0000   000037 240F      0001   000233 241G      0001   000256 253G
    0001   000264 260G      0001   000303 270G      0001   000313 276G      0000   000112 280F      0000   000126 290F
    0001   00003  30L       0000   000154 300F      0001   000332 306G      0000   000156 310F      0001   000340 313G
    0000   000124 320F      0001   000356 322G      0001   000402 336G      0000   000116 340F      0001   000423 347G
    0001   000444 360G      0001   000452 365G      0001   000467 374G      0001   000506 404G      0001   000516 412G
    0001   000542 424G      0001   000602 441G      0001   000605 444G      0001   000065 45L       0001   000613 451G
    0001   000636 462G      0001   000645 467G      0001   000201 50L       0001   000664 501G      0001   000723 512G
    0001   000754 524G      0001   001002 546G      0001   001014 551G      0001   001036 560G      0001   001067 572G
    0000   000111 60F       0006   006034 A         0011   000150 ACAT      0007   000570 AM        0007   000624 AM1
    0007 R 000741 ANUM      0011   000133 APP       0003 R 000000 ATMN      0007   000004 ATOM      0007   000502 BU
    0007   000521 BUF       0010   000036 CALCH     0006   000000 COEF      0010   000001 CONVG     0005 R 000032 CPR
    0007   000625 CPR1      0007   000564 CPSUM     0007   000604 DATA      0006   005670 DELN      0013   000002 DEMAND
    0007 R 001167 DENS      0005 R 000064 DLVPT     0005 R 000047 DLVTP     0006 R 002734 EN        0004   000000 END
    0006   005360 ENLN      0007   001263 ENLSAV    0007   000000 ENN       0007   001261 ENNL      0007   001262 ENSAVE
    0007 R 001073 ENTH      0011 L 000165 EQL       0007 R 000566 EQRAT     0012   000002 FA        0012 R 000003 FAP
    0007 R 001114 FAZ       0012 R 000005 FC        0012   000006 FC        0012 R 000007 FCP       0012   000012 FCST
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0012   000014 FCV       0012   000015 FG        0012   000017 FGE       0012   000020 FGV       0012 R 000021 FM
0012   000023 FI        0012   000025 FIV       0012 R 000027 FM        0012 R 000031 FMT       0012   000053 FN
0012 R 000052 FOUR      0007 I 001150 FOX       0012   000053 FP        0000 R 000036 FPC       0012 R 000054 FS
0012 R 000056 FSV       0012 R 000057 FT        0012 R 000061 FTK       0012 R 000063 FV        0012 R 000065 FVEL
0000 R 000001 FVLM      0012 R 000001 F13       0012   000000 F9X       0005 R 000101 GAMMAS    0004   000001 GAS
0013   000001 GMET      0013   000000 GRAPH     0000 R 000003 HEAD      0010   000003 HP        0007   000572 HPP
0007   000567 HSUBO     0005 R 000000 HSUM      0006   005524 HO        0000 I 000035 I         0010   000030 IC
0010   000000 IDEBUG    0004   000002 IE        0010   000015 IMAT      0000   000207 INJPS     0010   000023 IONS
0010   000021 IP        0010   000037 IQSAVE    0010   000016 IQ1       0010   000005 ISV       0010   000034 IT
0006   011444 IUSE      0004   000003 IZ        0000 I 000034 J         0010   000026 JLIQ      0013 I 000001 JOUT
0010   000025 JSOL      0010   000031 JSI       0000 I 000032 K         0010   000014 KMAT      0004 I 000004 LANK
0007   000463 LLMT      0010   000040 LSAVE     0004   000005 MOL       0010 L 000006 MOLES     0000 I 000014 MW
0007 I 000626 NAME      0010   000024 NC        0000 I 000033 ND        0010   000022 NEWR      0010   000035 NFZ
0010   000012 NLM       0010   000017 NOF       0010   000020 NOMIT     0010   000007 NP        0010 I 000011 NPT
0010 I 000027 NREAC     0010 I 000013 NS        0000 I 000000 NSPP1     0010   000010 NT        0007 R 000565 OF
0012 R 000067 ONE       0004 I 000006 OX        0007   001227 OXF       0005   000116 P         0003   000002 PATM
0011   000000 PCP       0007 R 001054 PECWT     0007   000563 PP        0005 R 000217 PPP       0003 R 000003 RBAR
0003 R 000004 RBR       0007   000574 RH        0007 R 001206 RHOP      0007   001207 RMW       0007 R 001131 RTEMP
0003   000005 RVR       0006   002570 S         0010   000033 SHOCK     0006   011754 SLN       0005 R 000251 SONVEL
0010   000004 SP        0011   000047 SPIM      0005 R 000015 SSUM      0006 R 010770 SUB       0011   000101 SUBAR
0007   000001 SUMN      0011   000116 SUPAR     0007   000003 SO        0005   000150 T         0006   011610 TEMP
0007   000562 THIGH     0012   000070 THREE     0007   001226 TLN       0007   000560 TLOW      0007   000557 TM
0007   000561 TMID      0005 R 000320 TOTN      0010   000002 TP        0007   000002 TT        0005 R 000266 TTT
0012 R 000071 TWO       0005 R 000202 V         0011   000064 VACI      0005 R 000303 VLM       0007   000576 VMIN
0011   000032 VMOC      0010 L 000032 VOL       0007   000600 VPLS      0005 R 000234 WM        0007   000602 WP
0000 R 000020 YN        0000 R 000025 YX        0006 R 005524 Z         0004   000007 ZERO      0012   000072 ZEROF
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00101      1*          SUBROUTINE OUT1                                                    OUTPU001    000000
00101      2*    C                                                                                    000000
00103      3*          COMMON /CONSTS/ AIMN,GMET,PATM,RBAR,RBR,RVR                        /CONSTS/    000000
00104      4*          COMMON /MOLCON/ END,GAS,IE,IZ,LANK,MOL,OX,ZERO                     /MOLCON/    000000
00105      5*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                    000000
00105      6*         1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)               000000
00105      7*         2 ,VLM(13),TOTN(13)                                                             000000
00105      8*    C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)               000000
00105      9*    C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                000000
00106     10*          INCLUDE SPECPK                                                                  000000
00112     11*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),          /MISC/       000000
00112     12*         1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,     /MISC/       000000
00112     13*         2              HSUBO,AM(2),HFP(2),RH(2),VMIN(2),VPLS(2),WP(2),     /MISC/       000000
00112     14*         3              DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),PECWT(15),  /MISC/       000000
00112     15*         4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,   /MISC/       000000
00112     16*         5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV              /MISC/       000000
00113     17*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,    /INDX/       000000
00113     18*         1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/       000000
00113     19*         2              NREAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE    /INDX/       000000
00114     20*          COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),       /PERF/       000000
00114     21*         1              SUPAR(13),APP(13),AEAT(13),EQL                      /PERF/       000000
00115     22*          COMMON /OUPT/ FOX,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),   /OUPT/       000000
00115     23*         1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/       000000
00116     24*         2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,  /OUPT/       000000
00116     25*         3              TWO,ZEROF                                           /OUPT/       000000
00116     26*    C                                                                                    000000
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00116   270            COMMON /CCC/GRAPH,JOUT,DEMAND                                          000000
00116   280    C                                                                              000000
00117   290          DIMENSION FVLM(2),HEAD(9),MW(2,2),YN(5),YX(5),Z(10,3)                    000000
00120   300          EQUIVALENCE (Z,MU)                                                       000000
00121   310          INTEGER FOX,OX                                                           000000
00122   320          LOGICAL EQL,MOLES,VOL                                                    000000
00122   330    C                                                              OUTP0021        000000
00122   340    C     HEAD = (1XA6,2X5(A2,F8.5,3X), 5X,F7.5,F13.3,4X,A1,F10.2,F9.4)            000000
00122   350    C                                                                              000000
00123   360          DATA HEAD/6H(1XA6,,6H2X5(A2,6H,F8.4,,6H3X), 5,6HX,F7.5,6H,F13.3,         000000
00123   370         1     6H,4X,A1,6H,F10.2,6H,F9.4)/,YN/6H2X1(A2,6H2X2(A2,6H2X3(A2,         000000
00123   380         2     6H2X4(A2,6H2X5(A2/,YX/6H3X),57,6H3X),44,6H3X),31,6H3X),18,         000000
00123   390         3 6H3X), 5/,MW/24HWT FRACTION    MOLES    /,FVLM/12HVOLUME CC/G /       000000
00123   400    C                                                                              000000
00131   410          K = 1                                                                    000000
00132   420          IF (MOLES) K = 2                                                         000001
00134   430          WRITE(JOUT,240) MW(1,K),MW(2,K)                                          000005
00140   440      240 FORMAT (77X,2A6,3H ENTHALPY   STATE   TEMP   DENSITY/10X,               000025
00140   450         1       16HCHEMICAL FORMULA,65X,7HCAL/MOL,10X,6HDEG. K,3X,5HG/CM3)       000025
00141   460          DO 60 K = 1,NREAC                                                        000025
00144   470          IF (FOX(K) .NE. OX)  GO TO 10                                            000025
00146   480          ND = 6HOXIDNT                                                            000030
00147   490          GO TO 30                                                       OUT1 580  000032
00150   500       10 ND = 6HFUEL                                                              000036
00151   510       30 DO 40 J=1,5                                                 OUT1 610  000036
00154   520       40 IF(ANUM(K,J) .LE. 0. .OR. NAME(K,J) .EQ. LANK)  GO TO 45                 000043
00157   530          J=6                                                                      000062
00160   540       45 J=J-1                                                                    000065
00161   550          HEAD(2) = YN(J)                                                          000073
00162   560          HEAD(4) = YX(J)                                                          000075
00163   570       60 WRITE(JOUT,HEAD) ND,(NAME(K,I),ANUM(K,I),I = 1,J),PECWT(K),           000077
00163   580         1                 ENTH(K),FAZ(K),RTEMP(K),DENS(K)                      000077
00201   590          FPC = 100./(1.+OF)                                                       000126
00202   600          WRITE(JOUT,20)  OF  ,FPC,EQRAT,RHOP                                      000133
00210   610       20 FORMAT (1H0,15X, 4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,             000144
00210   620         1  19HEQUIVALENCE RATIO= ,F7.4,4X,8HDENSITY=,F8.4//)                     000144
00211   630          RETURN                                                                   000144
00211   640    C                                                                              000144
00212   650          ENTRY OUT2                                                               000147
00212   660    C     VOLUME                                                                   000147
00213   670          FMT(3) = ONE                                                             000151
00214   680          IF(.NOT.VOL)  GO TO 50                                                   000153
00216   690          CALL VARFMT(VLM,NPT)                                                     000157
00217   700          WRITE(JOUT,FMT) FVLM,FB,(VLM(I), I = 1,NPT)                              000157
00217   710    C   PRESSURE                                                      OUTP0038  000157
00227   720       50 DO 55 I = 1,NPT                                                          000201
00232   730       55 V(I) = ATMN*PPP(I)                                                       000205
00234   740          CALL VARFMT(V,NPT)                                                       000213
00235   750          WRITE(JOUT,FMT) FAP,FB,(V(J), J = 1,NPT)                                 000214
00235   760    C   TEMPERATURE                                                   OUTP0047  000214
00245   770          FMT(3) = F13                                                             000236
00246   780          FMT(4) = 1.0                                                             000240
00247   790          WRITE(JOUT,FMT) FTK,FB,(TTT(J), J = 1,NPT)                               000242
00247   800    C   ENTHALPY                                                      OUTP0056  000242
00257   810          DO 75 I=1,NPT                                                 OUTP0058  000264
00262   820       75 V(I) = PBAR*PSUM(I)                                                      000264
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0024   83*          WRITE(JOUT,FMT) FM,FB,(V(J), J = 1,NPT)                    000267
0264   84*    C   ENTROPY                                                      OUTPU064  000267
0274   85*          FM(4) = FOUR                                                         000306
0275   86*          DO 76 I = 1,NPT                                                      000313
0300   87*       76 V(I) = RBAR*SSUM(I)                                                  000313
0302   88*          WRITE(JOUT,FMT) FS,FB,(V(J), J = 1,NPT)                              000316
0302   89*    C     DENSITY                                                              000316
0312   90*          DO 70 I = 1,NPT                                                      000340
0315   91*       70 IF (VLM(I) .GT. 0.0)  V(I) = 1.0/VLM(I)                              000340
0320   92*          WRITE(JOUT,1) (V(J), J = 1,NPT)                                      000347
0326   93*       1  FORMAT (1X,14HDENSITY G/CC  ,1P13E9.3)                            000361
0327   94*          WRITE(JOUT,80)                                                       000361
0331   95*       80 FORMAT ( 1H )                                                 OUTPU070  000366
0331   96*    C   MOLECULAR WEIGHT                                               OUTPU072  000366
0332   97*          WRITE(JOUT,FMT) FM,FB,(WM(J), J = 1,NPT)                             000366
0332   98*    C   (DLV/DLP)T                                                     OUTPU078  000366
0342   99*          IF (EQL)  WRITE(JOUT,FMT) FT,FB,(DLVPT(J), J = 1,NPT)                000405
0342  100*    C   (DLV/DLT)P                                                     OUTPU083  000405
0353  101*          IF (EQL)  WRITE(JOUT,FMT) FV,FB,(DLVTP(J), J = 1,NPT)                000426
0353  102*    C   HEAT CAPACITY                                                  OUTPU087  000426
0364  103*          DO 85  I=1,NPT                                               OUTPU089  000452
0367  104*       85 V(I) = RBAR*CPR(I)                                                   000452
0371  105*          WRITE(JOUT,FMT) FCP,(V(J), J = 1,NPT)                                000455
0371  106*    C   GAMMA(S)                                                       OUTPU093  000455
0400  107*          WRITE(JOUT,FMT) FG,FB,(GAMMAS(J), J = 1,NPT)                         000472
0400  108*    C   SONIC VELOCITY                                                 OUTPU097  000472
0410  109*          FM(4) = TWO                                                          000511
0411  110*          DO 95 I = 1,NPT                                              OUTPU100  000516
0414  111*       95 SONVEL(I) = SQRT(RBAR*GAMMAS(I)*TTT(I)/WM(I))                        000516
0416  112*          WRITE(JOUT,FMT) FSV,FVEL,(SONVEL(J), J = 1,NPT)                      000527
0426  113*          RETURN                                                               000545
0426  114*    C                                                                OUTPU104  000545
0427  115*          ENTRY OUT3                                                           000550
0430  116*          WRITE(JOUT,80)                                                       000550
0432  117*          ND = 0                                                               000555
0432  118*    C     MOLE FRACTIONS EQUILIBRIUM OR FROZEN                       OUT12270  000555
0433  119*          WRITE(JOUT,280)                                                      000556
0435  120*    280   FORMAT (15HUMOLE FRACTIONS/)                                       000563
0436  121*          IF (.NOT. EQL)  GO TO 175                                            000563
0436  122*    C     EQUILBRIUM MOLE FRACTIONS                                          000563
0440  123*          DO 170 K=1,NS                                              OUT12330  000605
0443  124*          DO 140 I=1,NPT                                             OUT12340  000605
0444  125*       140 V(I) = ENK(K,I)/TOTN(I)                                             000605
0446  126*          DO 150 I=1,NPT                                             OUT12370  000613
0453  127*       150 IF (V(I) .GE. 5.0E-7)  GO TO 160                                    000613
0456  128*          ND = 1                                                               000621
0457  129*          GO TO 170                                                  OUT12400  000623
0460  130*       160 WRITE(JOUT,340) (SUB(K,J), J = 1,3),FB,(V(I), I = 1,NPT)           000625
0473  131*       340 FORMAT (1H ,3A4,A2,1P13E9.3)                                        000655
0474  132*       170 CONTINUE                                               OUT12430  000655
0474  133*    C     OUTPUT COMPLETE GO EXIT                                  OUT12590  000655
0476  134*          GO TO 411                                                OUT12600  000655
0476  135*    C     FROZEN MOLE FRACTIONS                                              000655
0477  136*       175 J = 0                                                               000657
0500  137*          DO 179 K = 1,NS                                            OUT12630  000657
0503  138*          V(J+1) = ENK(K,1)/TOTN(1)                                           000671
```

```
00504    1390*            IF (V(J+1) .LT. 5.0E-7)  ND = 1                                                  000675
00506    1400*            IF (V(J+1) .LT. 5.0E-7)  GO TO 177                                               000704
00508    1410*      C     OUTPUT VALUE ACCEPTED                                          OUT12660          000709
00510    1420*            J = J + 1                                                                        000711
00511    1430*            DO 176 I = 1,3                                                                   000714
00514    1440*       176  Z(J,I) = SUB(K,I)                                                                000723
00516    1450*       177  IF (J .NE. 4 .AND. K .NE. NS)  GO TO 179                                         000726
00520    1460*            IF (J .EQ. 0)  GO TO 180                                                         000741
00522    1470*            WRITE(JOUT,320) (Z(I,1),Z(I,2),Z(I,3),V(I), I = 1,J)                            000743
00533    1480*       320  FORMAT (1H ,4(3A4,F11.8,5X))                                                     000762
00534    1490*            J = 0                                                                            000762
00535    1500*       179  CONTINUE                                                       OUT12750          000766
00537    1510*       180  IF (ND .EQ. 0)  GO TO 211                                                        000765
00541    1520*            WRITE(JOUT,290)                                                                  000767
00543    1530*       290  FORMAT (///1X,116HADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHO             000774
00543    1540*           1SE MOLE FRACTIONS WERE LESS THAN 5.0E-7 FOR ALL ASSIGNED CONDITION              000774
00543    1550*           2S///)                                                                           000774
00544    1560*            J = 0                                                                            000774
00545    1570*            DO 210 K=1,NS                                                  OUT12780          001002
00550    1580*            DO 190 I=1,NPT                                                 OUT12790          001019
00553    1590*       190  IF ((EN(K,I)/TOTN(I)) .GE. (5.0E-7) ) GO TO 200                 OUT12800          001019
00556    1600*            J = J + 1                                                                        001029
00557    1610*            DO 195 I = 1,3                                                                   001027
00562    1620*       195  Z(J,I) = SUB(K,I)                                                                001036
00564    1630*       200  IF (J .NE. 10 .AND. K .NE. NS)  GO TO 210                                        001041
00566    1640*            IF (J .EQ. 0)  GO TO 211                                                         001059
00570    1650*            WRITE(JOUT,300) (Z(I,1),Z(I,2),Z(I,3), I = 1,J)                                  001056
00600    1660*       300  FORMAT (10(1X,3A4))                                            OUT13100          001079
00601    1670*            J = 0                                                                            001079
00602    1680*       210  CONTINUE                                                       OUT12900          001100
00604    1690*       211  IF (.NOT. MOLES)  WRITE(JOUT,310)                                               001100
00607    1700*       310  FORMAT (///1X,77HNOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND O             001106
00607    1710*           1F OXIDANT IN TOTAL OXIDANTS)                                                    001106
00610    1720*            RETURN                                                                           001106
00611    1730*            END                                                            OUTPU137          001197
END FOR
```

```
#FOR,S LEWIS.REACT,LEWIS.REACT
HSA  CS -10/25/79-17:39:27 (11.)


   SUBROUTINE REACT     ENTRY POINT 000714


   STORAGE USED: CODE(1) 000730; DATA(0) 000167; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   HOLLOW 000010
    0004   MISC   001264
    0005   INDX   000041
    0006   CCC    000003


   EXTERNAL REFERENCES (BLOCK, NAME)

    0007   #READ
    0010   NREAS
    0011   NRDUS
    0012   NIOCS
    0013   NIOIS
    0014   NWDUS
    0015   NERRMS


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0000   000107 10F       0001   000256 101L      0001   000003 121G      0001   000013 132G      0001   000053 154G
    0001   000104 177G      0001   000040 20L       0001   000355 200L      0000   000110 21F       0001   000414 210L
    0001   000551 218L      0001   000553 220L      0001   000615 222L      0001   000620 224L      0001   000635 226L
    0001   000657 229L      0001   000672 230G      0001   000673 230L      0001   000172 236G      0001   000205 245G
    0001   000227 260G      0001   000226 303G      0000   000123 31F       0001   000371 321G      0001   000411 335G
    0001   000432 344G      0001   000475 355G      0001   000155 37L       0001   000525 370G      0001   000601 405G
    0001   000604 410G      0001   000625 426G      0001   000650 441G      0001   000217 45L       0001   000663 450G
    0001   000224 46L       0001   000240 50L       0004 R 000570 AM        0004   000624 AMI       0004 R 000626 ANAME
    0004 R 000741 ANUM      0004 R 000004 ATOM      0004   000502 BD        0004 R 000521 BDX       0005   000036 CALCH
    0005   000001 CONVG     0004   000625 CPRI      0004   000564 CPSUM     0004 R 000604 DATA      0006   000002 DEMAND
    0004 R 001167 DENS      0003   000000 END       0004   001263 ENLSAV    0004   000000 ENN       0004   001261 ENNL
    0004   001262 ENSAVE    0004 R 001073 ENTH      0004   000566 EQRAT     0004 R 001112 FAZ       0004 I 001150 FOX
    0004   000001 GAS       0006   000000 GRAPH     0005   000003 HP        0004 R 000572 HPP       0004   000567 HSUBO
    0000 I 000102 I         0005   000030 IC        0005   000000 IDEBUG    0003   000002 IE        0005   000015 IMAT
    0000   000144 INJPR     0000 I 000075 IO        0005   000023 IONS      0005   000021 IP        0005   000037 IQSAVE
    0004   000016 IS1       0005   000005 ISV       0005   000034 IT        0003 I 000003 IZERO     0000 I 000077 J
    0000 I 000103 JJ        0005   000026 JLIQ      0006 I 000001 JOUT      0005   000025 JSOL      0005   000031 JS1
    0000 I 000076 K         0005   000014 KMAT      0005 I 000012 L         0003 I 000004 LANK      0004 I 000463 LLMT
    0000 I 000020 LLMTS     0005   000040 LSAVE     0003 I 000005 MOL       0000 I 000103 MOLE      0005 L 000006 MOLES
    0000 I 000101 N         0004 I 000626 NAME      0005   000020 NC        0005 L 000022 NEWP      0000 I 000100 NFUEL
    0005   000035 NFZ       0000 I 000000 NLS       0005   000017 NOF       0005 I 000020 NOMIT     0005   000007 NP
    0005   000011 NPI       0005 I 000027 NREAC     0005   000013 NS        0005   000010 NT        0004   000565 OF
    0004 I 000006 OX        0004   001227 OXF       0000 R 000106 PCWT      0004 R 001054 PECWT     0004   000563 PP
    0004 R 001574 PR        0004   001206 PROP      0000 R 000104 RM        0004 R 001207 RMW       0004 R 001131 RTEMP
    0004 R 000037 SHOF      0005   000033 SHOCK     0005   000004 SP        0006   000001 SUMN      0004   000003 SU
    0004   000562 THIGH     0004   001226 TLN       0004   000560 TLOW      0004   000557 TM        0004   000561 TMID
```

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 0005   000002 TP        0004   000602 TT        0000 R 000001 V         0004 R 000576 VMIN      0005   000032 VOL
 0004 R 000600 VPLS      0004 R 000602 WP        0003 I 000007 ZERO
```

```
 00101      10            SUBROUTINE REACT(FIRST)                                                          000003
 00101      20      C                                                                                      000003
 00103      30            COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO                  /HOLCON/      000003
 00104      40            COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),          /MISC/        000003
 00104      50           1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,    /MISC/        000003
 00104      60           2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),    /MISC/        000003
 00104      70           3              DATA(16),AM1,CPR1,NAME(35,5),ANUM(15,5),PECWT(15),  /MISC/       000003
 00104      80           4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,   /MISC/       000003
 00104      90           5              RMW(15),ILN,OXF(26),ENNL,ENSAVE,ENLSAV              /MISC/       000003
 00105     100            COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,      /INDX/        000003
 00105     110           1              KMAT,IMAT,IO1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/        000003
 00105     120           2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE    /INDX/        000003
 00105     130      C                                                                                      000003
 00106     140              COMMON /CLC/ GRAPH,JOUT,DEMAND                                               000003
 00106     150      C                                                                                      000003
 00107     160            DATA NLS/0/                                                                    000003
 00111     170            DIMENSION ANAME(15,5),V(15),LLMTS(15),SBOP(15,2)                               000003
 00112     180            EQUIVALENCE (NAME,ANAME)                                                       000003
 00113     190            INTEGER FOX,OX,ZERO                                                            000003
 00114     200            LOGICAL MOLES,NEWR                                                             000003
 00114     210      C                                                                                      000003
 00115     220              LOGICAL FIRST                                                                000003
 00116     230              DATA IO/8/                                                                   000003
 00116     240      C                                                                   RCTN0022   000003
 00120     250            DO 8 K = 1,2                                                                   000003
 00123     260            WP(K)=0.                                                                       000003
 00124     270            HPP(K)=0.                                                                      000004
 00125     280            RH(K)=0.                                                                       000005
 00126     290            VPLS(K)=0.                                                                     000006
 00127     300            VMIN(K)=0.                                                                     000007
 00130     310            AM(K)=0.                                                                       000013
 00131     320            DO 8 J=1,15                                                                    000013
 00134     330            LLMT(J)=0                                                                      000013
 00135     340          8 BOP(J,K) = 0.0                                                                 000017
 00140     350            NFUEL = 0                                                                      000020
 00141     360            K=1                                                                            000022
 00142     370            L=1                                                                            000022
 00142     380      C                                                                                      000022
 00142     390      C       CALL SUBROUTINE TO SET UP REACTANTS ON FILE 8                                  000023
 00143     400              CALL RREAD(FIRST)                                                            000027
 00143     410      C                                                                                      000023
 00143     420      C       READ REACTANTS FROM FILE 8                                                     000026
 00144     430              REWIND IO                                                                    000031
 00145     440              READ(IO,10) NREAC                                                            000040
 00150     450           10 FORMAT(I3)                                                                   000040
 00150     460      C                                                                                      000040
 00151     470           21    CONTINUE                                                                  000040
 00152     480            READ(8,21)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ(N)           000040
 00162     490           1 ,RTEMP(N),FOX(N),DENS(N)                                                     000040
 00170     500           21    FORMAT(2X,5(A2,F8.4,2X),/,F10.6,2X,A1,F13.4,4X,A1,F12.3,                 000067
```

```
      1    3X,A1,F12.5,1X)
           IF(NAME(N,1).EQ.LANK) GO TO 200
           IF(L.EQ.0)GO TO 23
           WRITE(OUT,21)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),
          1  FAZ(N),ELEMP(N),FOX(N),DENS(N)
       21  FORMAT(1X,5(A2,F8.4,2X),F10.6,2X,A1,F11.4,2X,A1,F11.3,2X,A1,F11.5)
           IF (MOLE .EQ. MOL)  MOLES = .TRUE.
           IF OXIDANT, M = 1; IF FUEL, M = 2.
           IF(FOX(N).EQ.ZERO)  FOX(N)=0X
           IF (PECWT(N) .LE. 0.0)  PECWT(N) = 1.0
           M = 1
           IF(FOX(N).EQ.0X)  GO TO 37
           M = 2
           NFUEL = NFUEL+1
           DO 36 J=1,15
       36  DATA(J) = 0.0
       37  AM=0.
           DO 100 JJ=1,5
           IF (ANUM(N,JJ) .LE. 0.0)  GO TO 101
           IF (NAME(N,JJ) .EQ. ZERO)  NAME(N,JJ) = 0X
           DO 41 J=1,15
           I = J
           IF(LLMT(J).EQ.0) GO TO 45
       41  IF (NAME(N,JJ) .EQ. LLMT(J))  GO TO 46
       45  L = 1
           LLMT(J)=NAME(N,JJ)
       46  DO 48 J = 1,101
       48  IF (ATOM(I,I) .EQ. ANAME(N,JJ))  GO TO 50
           L=0
           GO TO 40
       50  AM = AM + ANUM(N,JJ)*ATOM(2,I)
           V(J) = ATOM(3,I)
      100  DATA(J) = ANUM(N,JJ)
      101  PCWT=PECWT(N)
           IF(MOLES) PCWT=PCWT*AM
           WF(N)=WP(N) * PCWT
           IF (NAME(N,5) .NE. ZERO)  HPP(K) = HPP(K) + ENTH(N)*PCWT/AM
           AM(N)=AM(N)*PCWT/AM
           DO 110 J=1,L
      110  BOP(J,K) = DATA(J)*PCWT/AM + BOP(J,K)
           IF (DENS(N) .GT. 0.0)  RH(K) = RH(K) + PCWT/DENS(N)
           AMW(K) = AM
           N = N+1
           IF(N.NE.IE) GO TO 20
      200  NREAC =N-1
           IF(NFUEL.GT.0) GO TO 210
           TOO FEW OXIDANT, CALL REACTANTS FUEL
           DO 205  N=1,NREAC
           FOX(N) = 1.0M
      205  WF(N) = WP(N)
           AMW(2) = 0.
           HPP(2) = 0.
           RH(2) = 0.
           BOP(J,2) = 0.
           HPP(2) = HPP(1)
           RH(2) = RH(1)
           AM(2) = AM(1)
```

```
00354    107*          DO 208  J=1,L                                                                  000411
00357    108*      208 BOP(J,2) = BOP(J,1)                                                            000411
00341    109*      210 IF (L .EQ. 0)  RETURN                                                          000414
00343    110*          DO 220 K=1,2                                                                   000420
00346    111*          IF (WP(K) .LE. 0.0)  GO TO 220                                                 000452
00350    112*          HPP(K)=HPP(K)/WP(K)                                                            000455
00351    113*          AM(K) = WP(K)/AM(K)                                                            000460
00352    114*          IF (RH(K) .GT. 0.0)  RH(K) = WP(K)/RH(K)                                       000463
00354    115*          DO 215 J=1,L                                                                   000475
00357    116*          BOP(J,K)=BOP(J,K)/WP(K)                                                        000475
00360    117*          IF(V(J).LT.0.)VMIN(K)= VMIN(K)+BOP(J,K)*V(J)                                   000477
00362    118*      215 IF (V(J) .GT. 0.0)  VPLS(K) = VPLS(K) + BOP(J,K)*V(J)                          000506
00365    119*          IF(MOLES) GO TO 220                                                            000520
00367    120*          DO 218 N=1,NREAC                                                               000525
00372    121*          IF((FOX(N).EQ.0X.AND.K.EQ.2).OR.(FOX(N).NE.0X.AND.K.EQ.1))GOTO218              000525
00374    122*          PECWT(N) = PECWT(N)/WP(K)                                                      000545
00375    123*      218 CONTINUE                                                                       000555
00377    124*      220 CONTINUE                                                                       000555
00401    125*          NEWR=.TRUE.                                                                    000555
00401    126*      C  ARE ELEMENTS SAME AS FOR  LAST SET OF REACTANTS, IF SO, NEWR=.FALSE.  4/23/70   000555
00402    127*          IF (L .NE. NLS .OR. NOMIT .NE. 0)  GO TO 226                                   000557
00404    128*          DO 224 I=1,NLS                                                                 000571
00407    129*          DO 222 J = 1,L                                                                 000604
00412    130*          IF(LLMT(J).NE.LLMTS(I))  GO TO 222                                             000604
00414    131*          SBOP(I,1) = BOP(J,1)                                                           000607
00415    132*          SBOP(I,2) = BOP(J,2)                                                           000611
00416    133*          GO TO 224                                                                      000613
00417    134*      222 CONTINUE                                                                       000616
00421    135*          GO TO 226                                                                      000616
00422    136*      224 CONTINUE                                                                       000621
00424    137*          NEWR = .FALSE.                                                                 000621
00425    138*          DO 225 I = 1,L                                                                 000625
00430    139*          LLMT(I) = LLMTS(I)                                                             000625
00431    140*          BOP(I,1)  = SBOP(I,1)                                                          000626
00432    141*      225 BOP(I,2) = SBOP(I,2)                                                           000630
00434    142*          GO TO 229                                                                      000633
00435    143*      226 NLS = L                                                                        000635
00436    144*          NOMIT = 0                                                          4/23/70     000636
00437    145*          REWIND 4                                                                       000641
00440    146*          DO 228 I = 1,L                                                                 000650
00443    147*          SBOP(I,1) = BOP(I,1)                                                           000650
00444    148*          SBOP(I,2) = BOP(I,2)                                                           000651
00445    149*      228 LLMTS(I) = LLMT(I)                                                             000653
00447    150*      229 DO 230  N=1,NREAC                                                              000657
00452    151*          IF (QENS(N) .GT. 0.0)  GO TO 230                                               000663
00454    152*          RH(2) = 0.                                                                     000665
00455    153*          RH (1) = 0.                                                                    000666
00456    154*          RETURN                                                                         000667
00457    155*      230 CONTINUE                                                                       000674
00461    156*          RETURN                                                                         000674
00462    157*          END                                                            RCINDIII        000727
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@FOR,S LEWIS.RKTOUT,LEWIS.RKTOUT
FTN  E3 -10/25/79-17:39:33 (9,)

   SUBROUTINE RKTOUT     ENTRY POINT 000521

   STORAGE USED: CODE(1) 000530; DATA(0) 000120; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003     CONSTS 000006
    0004     POINTS 000335
    0005     SPECES 012120
    0006     INDX   000041
    0007     PERF   000166
    0010     OUPT   000073
    0011     CCC    000003

   EXTERNAL REFERENCES (BLOCK, NAME)

    0012     OUT1
    0013     VARFMT
    0014     OUT2
    0015     GAMEFF
    0016     OUT3
    0017     NWDU$
    0020     N102$
    0021     N101$
    0022     SQRT
    0023     N103$
    0024     NERR3$

   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001     000057 144G     0000     000066 150F     0001     000070 152G     0001     000115 166G     0001     000144 176G
    0001     000176 200L     0000     000075 208F     0001     000231 220G     0001     000416 220L     0001     000257 234G
    0001     000312 252G     0001     000334 264G     0001     000344 272G     0001     000362 303G     0001     000505 312L
    0001     000412 317G     0001     000423 324G     0001     000441 335G     0001     000462 346G     0001     000501 356G
    0000     000006 37F      0000     000027 38F      0000     000056 40F      0000     000047 737F     0005     006034 A
    0007 R   000150 ALAT     0007 R   000133 APP      0003 R   000000 ATMN     0000 R   000002 AW       0006     000036 CALCH
    0005     000000 COEF     0006     000001 CONVG    0004     000032 CPR      0000 R   000005 CSTR     0005     005670 DELN
    0011     000002 DEMAND   0004     000064 DLVPT    0004     000047 DLVTP    0005     002734 LN       0005     005360 ENLN
    0007 L   000165 EQL      0010 R   000002 FA       0010     000003 FAP      0010 R   000005 FB       0010 R   000006 FC
    0010     000007 FCF      0010 R   000012 FCST     0010 R   000014 FCV      0010 R   000015 FG       0010 R   000017 FGE
    0010 R   000020 FGV      0010     000021 FH       0010 R   000023 FI       0010 R   000025 FIV      0010     000027 FM
    0010 R   000031 FMT      0010 R   000050 FN       0010 R   000052 FOUR     0010 R   000053 FP       0010     000054 FS
    0010     000056 FSV      0010     000057 FT       0010     000061 FTK      0010     000063 FV       0010 R   000065 FVEL
    0011 R   000001 F13      0010 R   000000 F9X      0004 R   000101 GAMMAS   0003 R   000001 GMET     0011     000000 GRAPH
    0006     000003 HP       0004 R   000000 HSUM     0005 R   005524 HO       0000 I   000004 I        0006     000030 IC
    0006     000000 IDCHOL   0006     000015 IMAT     0000     000103 INJP$    0006     000023 IONS     0006     000021 IP
    0006     000037 ISSAVE   0006     000016 ICI      0006     000005 ISV      0006 I   000034 IT       0005     011444 IUSE
    0007     000026 JLIQ     0011 I   000001 JOUT     0006     000025 JSOL     0006     000031 JSI      0000 I   000003 K
    0006     000014 KMAT     0006     000040 LSAVE    0006     000006 MOLES    0006     000024 NC       0006     000022 NEWR
```

```
0006   000035 NFZ       0006   000012 NLM       0006   000017 NOF       0006   000020 NOMIT     0006   000007 NP
0006 I 000011 NPT       0006   000027 NREAC     0006   000013 NS        0000 I 000000 NSPPI     0006   000010 NT
0010 R 000067 ONE       0004   000116 P         0003 R 000002 PATM      0007   000000 PCP       0004 R 000217 PPP
0003   000003 RBAR      0003 R 000004 RBR       0003   000005 RVR       0005   002570 S         0006   000033 SHOCK
0005   011754 SLN       0004 R 000251 SONVEL    0006   000004 SP        0007 R 000047 SPIM      0004   000015 SSUM
0005   010770 SUB       0007   000101 SUBAR     0007   000116 SUPAR     0004 R 000150 T         0000 R 000001 TEM
0005   011610 TEMP      0010 R 000070 THREE     0004   000320 TOTN      0006   000002 TP        0004 R 000266 TTT
0010 R 000071 TWO       0004 R 000202 V         0007 R 000064 VACI      0004   000303 VLM       0007 R 000032 VMOC
0006   000032 VOL       0004 R 000234 WM        0010   000072 ZERO
```

```
00101      1*          SUBROUTINE RKTOUT (IGAM)                                                    000000
00101      2*    C                                                                                 000000
00101      3*    C  ROCKET PERFORMANCE PARAMETERS                                                  000000
00101      4*    C                                                                  ROUTU001       000000
00103      5*          COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                  /CONSTS/       000000
00104      6*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                 000000
00104      7*         1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)            000000
00104      8*         2 ,VLM(13),TOTN(13)                                                          000000
00104      9*    C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)             000000
00104     10*    C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)              000000
00105     11*          INCLUDE SPECPR                                                               000000
00111     12*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,    /INDX/    000000
00111     13*         1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/    000000
00111     14*         2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE    /INDX/    000000
00112     15*          COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),        /PERF/    000000
00112     16*         1              SUPAR(13),APP(13),AEAT(13),EQL                       /PERF/    000000
00113     17*          COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCSI(2),FCV,FG(2),    /OUPT/    000000
00113     18*         1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/    000000
00113     19*         2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,   /OUPT/    000000
00113     20*         3              TWO,ZERO                                             /OUPT/    000000
00113     21*    C                                                                                 000000
00114     22*          COMMON /CCC/ GRAPH,JOUT,DEMAND                                              000000
00114     23*    C                                                                                 000000
00115     24*          LOGICAL EQL                                                                 000000
00115     25*    C                                                                                 000000
00116     26*          IF(EQL) WRITE(JOUT,37)                                                      000000
00121     27*       37 FORMAT(1H1/24X,84HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRROCKU090  000006
00121     28*         1IUM COMPOSITION DURING EXPANSION        //)                               000006
00122     29*          IF (.NOT.EQL) WRITE(JOUT,38)                                                000006
00125     30*       38 FORMAT(1H1,26X,76HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN CROCKU107  000017
00125     31*         1OMPOSITION DURING EXPANSION        //)                          ROCKU10R  000017
00126     32*          IF(TTT(1).EQ.T(1)) WRITE(JOUT,737)                                          000017
00131     33*      737 FORMAT (52X,28HAT AN ASSIGNED TEMPERATURE       )                           000030
00132     34*          TEM = PATM*PPP(1)                                                           000030
00133     35*          AW = ATMN*PPP(1)                                                            000033
00134     36*          WRITE(JOUT,40) TEM,AW                                                       000036
00140     37*       40 FORMAT (5H PC =,F10.3,7H PSIA =,1PE13.6,7H N/M**2)                          000045
00141     38*          CALL OUT1                                                                   000045
00142     39*          K = NPT - 2                                                                 000047
00143     40*          DO 20 I = 1,K                                                               000052
00146     41*       20   V(I) = 9HEXIT                                                            000057
00150     42*          WRITE(JOUT,150) (V(I), I = 1,K)                                             000061
00156     43*      150   FORMAT (1HO,16X,14HCHAMBER   THROAT,11(5X,A4))                  RKTO1590  000073
```

```
00156     44*      C      PRESSURE RATIOS                                          OUTPU030   000073
00157     45*             FMT(3) = ONE                                                        000073
00160     46*             CALL VARFMT (APP,NPT)                                               000075
00161     47*             WRITE(JOUT,FMT) FP,FB,FB,(APP(I), I = 1,NPT)                        000101
00172     48*             CALL OUT2                                                           000120
00173     49*             IF (NPT .LT. 2)  GO TO 312                                          000122
00175     50*             DO 202 K=2,NPT                                           ROUTU028   000132
00200     51*             SPIM(K) = SQRT(2.0*RBR*(HSUM(1) - HSUM(K)))/GMET                    000144
00200     52*      C  AW (A/G) IN UNITS OF SEC/ATM                                            000144
00201     53*             AW = RBR*TTT(K)/(PPP(K)*WM(K)*SPIM(K)*GMET**2)                      000155
00202     54*             IF(K.NE.2)GO TO 200                                      ROUTU031   000165
00204     55*             CSTR = GMET*AW*PPP(1)                                               000170
00205     56*             AEAT(2) = 1.                                                        000173
00206     57*       200   VACI(K)=SPIM(K)+PPP(K)*AW                                         000176
00207     58*             IF (SONVEL(K) .GT. 0.0)  VMOC(K) = GMET*SPIM(K)/SONVEL(K)           000201
00211     59*       202   V(K) = GMET*SPIM(K)                                              000210
00213     60*             V(1) = 0.0                                                          000215
00214     61*             WRITE(JOUT,FMT) FGV,FVEL,(V(I), I = 1,NPT)                          000216
00214     62*      C    MACH NUMBER                                             ROUTU040   000216
00224     63*             FMT(4) = FOUR                                                       000234
00225     64*             VMOC(1)=0.                                              ROUTU042   000236
00226     65*             IF (GAMMAS(2) .LE. 0.0)  VMOC(2) = 0.0                              000237
00230     66*             WRITE(JOUT,FMT) FN,FB,(VMOC(I), I = 1,NPT)                          000243
00240     67*             WRITE(JOUT,208)                                                     000262
00242     68*       208   FORMAT (1H )                                             ROUTU048   000267
00242     69*      C    AREA RATIO                                              ROUTU062   000267
00243     70*             CALL VARFMT (AEAT,NPT)                                              000267
00244     71*             FMT(3) = F9X                                                        000275
00245     72*             WRITE(JOUT,FMT) FA,FB,FB,(AEAT(I), I = 2,NPT)                       000277
00245     73*      C      CSTAR                                                               000277
00256     74*             FMT(4) = F13                                                        000315
00257     75*             FMT(5) = TWO                                                        000317
00260     76*             WRITE(JOUT,FMT) FCST,FB,(CSTR, I = 2,NPT)                           000321
00260     77*      C    CF - THRUST COEFICIENT                                  ROUTU055   000321
00270     78*             FMT(5) = FOUR                                                       000337
00271     79*             DO 212  I=2,NPT                                         ROUTU057   000344
00274     80*       212   V(I) = GMET*SPIM(I)/CSTR                                         000344
00276     81*             WRITE(JOUT,FMT) FC,FB,FB,(V(I), I = 2,NPT)                          000350
00307     82*             IF (IGAM .EQ. 0)  GO TO 220                                         000365
00307     83*      C      EFFECTIVE GAMMA                                                     000365
00311     84*             CALL GAMEFF (V,GAMMAS,APP,NPT,HO)                                   000367
00312     85*             WRITE(JOUT,FMT) FG(1),FGE,FB,(HO(I), I = 2,NPT)                     000376
00312     86*      C      VACUUM THRUST COEFFICIENT                               RKTO1050   000376
00323     87*       220   DO 230 I = 2,NPT                                                   000416
00326     88*       230   V(I) = GMET*VACI(I)/CSTR                                          000423
00330     89*             WRITE(JOUT,FMT) FCV,FB,FB,(V(I), I = 2,NPT)                         000427
00330     90*      C    VACUUM IMPULSE                                          ROUTU067   000427
00341     91*             FMT(5) = THREE                                                      000444
00342     92*             WRITE(JOUT,FMT) FIV,FB,(VACI(I), I = 2,NPT)                         000446
00342     93*      C    SPECIFIC IMPULSE                                        ROUTU071   000446
00352     94*             WRITE(JOUT,FMT) FI,FB,(SPIM(I), I = 2,NPT)                          000465
00352     95*      C      FROZEN MOLE FRACTION OUTPUT MOVED TO SUBROUTINE OUT3    RKTO1480   000465
00362     96*       312   CALL OUT3                                                         000505
00363     97*             RETURN                                                              000506
00364     98*             END                                                                 000527
END FOR
```

```
@FOR,S LEWIS.ROCKET,LEWIS.ROCKET
HSA  FS -10/25/79-17:39:40 (8,)


   SUBROUTINE ROCKET    ENTRY POINT 001303


   STORAGE USED: CODE(1) 001312; DATA(0) 000222; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   CONSTS 000006
    0004   POINTS 000335
    0005   MISC   001264
    0006   INDX   000041
    0007   PERF   000166
    0010   CCC    000003


   EXTERNAL REFERENCES (BLOCK, NAME)

    0011   NEWOF
    0012   FROZEN
    0013   EQLBRM
    0014   RKTOUT
    0015   SAVE
    0016   NRNL$
    0017   NWNL$
    0020   XPRR
    0021   NWOU$
    0022   NIO2$
    0023   ALOG
    0024   EXP
    0025   XPOW
    0026   SQRT
    0027   NERR3$


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001   000013 1256      0001   000155 1332L     0001   000030 1416     0001   000047 1536     0000   000076 1811F
    0001   000275 1916      0001   000413 1926      0000   000073 1946     0001   000254 1956     0001   000121 2006
    0001   000021 3036      0001   000040 3066      0001   000076 3216     0001   000115 3226     0001   000146 3316
    0001   000153 3326      0001   000170 3336      0001   000206 3346     0001   000603 7996     0001   000531 8006
    0001   000756 8026      0001   000833 8056      0001   000676 8096     0001   000646 8106     0001   001002 8706
    0000   000117 821F      0001   001010 8306      0001   001036 8346     0001   001046 8356     0001   001050 8596
    0001   001054 8606      0000   000131 862F      0000   000160 865F     0001   001114 8706     0001   001130 8806
    0001   000452 8996      0001   000472 9006      0000   000065 923F     0001   000411 9256     0001   001164 9906
    0001   001225 9976      0001   001257 9996      0007 R 000150 AEAT     0000 R 000037 AEATL    0005   000570 AM
    0005   000624 AMI       0005   000741 ANUM      0007 R 000133 APP      0000 R 000035 APPL     0000 R 000033 APRATIO
    0000 L 000005 AREA      0000 D 000001 ASQ       0003   000000 ATMN     0005   000004 ATOM     0000 R 000030 AWT
    0005   000502 B0        0005   000521 BDP       0006   000036 CALCH    0006   000001 CONV6    0004 R 000032 CPR
    0000 R 000023 CPRF      0005   000625 CPR1      0005 R 000564 CPSUM    0005   000604 DATA     0010   000002 DEMAND
    0005   001167 DENS      0000 R 000026 DH        0000 R 000032 DLNP     0000 R 000040 DLNPE    0000 R 000027 DLT
    0004   000064 DLVPT     0004 E 000047 DLVTP     0000 R 000034 ELN      0005   001263 ENLSAV   0005 R 000000 ENN
    0007   001241 ENNL      0005   001262 ENSAVE     0005   001073 ENTH     0007 L 000165 EQL      0005   000566 EQRAT
```

```
0005   001112 FAZ      0005   001150 FOX      0000 L 000006 FROZ      0004 R 000101 GAMMAS    0003   000001 GMET
0010   000000 GRAPH    0006 L 000003 HP       0005   000572 HPP       0005   000567 HSUBO     0004 R 000000 HSUM
0000 I 000012 I        0006   000030 IC       0000 I 000000 ICASE     0006 I 000000 IDEBUG    0000 I 000011 IGAM
0006   000015 IMAT     0000   000206 INJPS    0000 I 000016 IOF       0006   000023 IONS      0006 I 000021 IP
0000 I 000022 IPP      0008   000037 IQSAVE   0006   000016 IQ1       0000 I 000020 ISUB      0000 I 000021 ISUP
0006 I 000005 ISV      0006 I 000034 IT       0000 I 000017 ITNUM     0000 I 000025 ITROT     0006   000026 JLIQ
0010 I 000001 JOUT     0006 I 000025 JSOL     0006   000031 JS1       0006   000014 KMAT      0005   000463 LLMT
0006   000040 LSAVE    0006   000006 MOLES    0005   000626 NAME      0006   000024 NC        0006   000022 NEWR
0006 I 000035 NFZ      0006   000012 NLM      0006 I 000017 NOF       0006   000020 NOMIT     0006 I 000007 NP
0000 I 000013 NPP      0006 I 000011 NPT      0006   000027 NREAC     0006   000013 NS        0000 I 000014 NSUB
0000 I 000015 NSUP     0006 I 000010 NT       0005 R 000565 OF        0005 R 001227 OXF       0004 R 000116 P
0003   000002 PATM     0007 R 000000 PCP      0000 R 000031 PCPLT     0005   001054 PECWT     0005 R 000563 PP
0004 R 000217 PPP      0003   000003 RBAR     0003 R 000004 RBR       0005   000574 RH        0005   001206 RHOP
0000   000041 RKTINP   0005   001207 RMW      0005   001131 RTEMP     0003   000005 RVR       0000 L 000007 SEQL
0006   000033 SHOCK    0004   000251 SONVEL   0006 L 000004 SP        0007   000047 SPIM      0004 R 000015 SSUM
0007 R 000101 SUBAR    0005   000001 SUMN     0007 R 000116 SUPAR     0005 R 000003 SO        0004 R 000150 T
0000 L 000010 THI      0005   000562 THIGH    0005   001226 TLN       0005   000560 TLOW      0005   000557 TM
0000 R 000024 TMELT    0005   000561 TMID     0000 R 000036 TOL       0004   000320 TOTN      0006 L 000002 TP
0005 R 000002 TT       0004 R 000266 TTT      0000 D 000003 USQ       0004   000202 V         0007   000064 VACI
0004   000303 VLM      0005   000576 VMIN     0007   000032 VMOC      0006   000032 VOL       0005   000600 VPLS
0004 R 000234 WM       0005   000602 WP
```

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C0101      1*          SUBROUTINE ROCKET                                                    ROCK0002   000000
C0101      2*    C                                                                          ROCK0001   000000
C0101      3*    C     ROCKET PERFORMANCE                                                   ROCK0004   000000
C0101      4*    C                                                                                     000000
C0103      5*          COMMON /CONSTS/ ATMN,GMEI,PATM,RBAR,RBR,RVR                          /CONSTS/   000000
C0104      6*          COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPI(13)                     000000
C0104      7*         1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)               000000
C0104      8*         2 ,VLM(13),TOTN(13)                                                             000000
C0105      9*          COMMON /MISC/ LNN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),            /MISC/     000000
C0105     10*         1              BOF(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,       /MISC/     000000
C0105     11*         2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),       /MISC/     000000
C0105     12*         3              DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),PECWT(15),    /MISC/     000000
C0105     13*         4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,     /MISC/     000000
C0105     14*         5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                /MISC/     000000
C0106     15*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,      /INDX/     000000
C0106     16*         1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,    /INDX/     000000
C0106     17*         2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE      /INDX/     000000
C0107     18*          COMMON /PERF/ PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),          /PERF/     000000
C0107     19*         1              SUPAR(13),APP(13),AEAT(13),EQL                        /PERF/     000000
C0107     20*    C                                                                                     000000
C0110     21*              COMMON /CCC/ GRAPH,JOUT,DEMAND                                            000000
C0110     22*    C                                                                                     000000
C0111     23*          DATA ICASE/0/                                                                   000000
C0113     24*          DOUBLE PRECISION ASQ,USQ                                                        000000
C0114     25*          LOGICAL AREA,EQL,FROZ,HP,SEQL,SP,THI,TP                                         000000
C0114     26*    C                                                                                     000000
C0115     27*          NAMELIST /RKTINP/ EQL,FROZ,IGAM,PCP,SUBAR,SUPAR                      /RKTINP/   000000
C0115     28*    C                                                                                     000000
C0116     29*          NFZ = 1                                                                         000000
C0117     30*          APP(1) = 1.                                                                     000001
C0120     31*          IF (ICASE .GT. 0)  GO TO 303                                                    000003
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```
                      ICASE = 1                                                 000006
                      IGAM = 0                                                  000007
                      DO 300 I=1,26                                             000013
                      PCP(I)= 0.                                                000013
                300   SUBAR(I) = 0.0                                            000013
                      EQL = .TRUE.                                              000015
                      FROZ = .FALSE.                                            000017
                303   READ (5,RKTINP)                                           000021
                      NPP = 0                                                   000029
                      DO 305 I = 1,26                                           000030
                      IF (PCP(I) .LE. 0.0)  GO TO 306                           000033
                305   NPP = I                                                   000033
                306   NPP = NPP*2                                               000040
                      NSUB = 0                                                  000042
                      NSUP = 0                                                  000043
                      DO 320  I=1,13                                            000047
                      IF (SUBAR(I) .GT. 0.0)  NSUB = NSUB + 1                   000047
                320   IF (SUPAR(I) .GT. 0.0)  NSUP = NSUP + 1                   000054
                      WRITE(JOUT,RKTINP)                                        000064
                      SEQL = EQL                                                000070
                      IOF = 0                                                   000072
                      TT = 3800.                                                000073
                C     LOOP FOR EACH O/F                                         000073
                321   IT = 1                                                    000076
                      IOF = IOF + 1                                             000077
                      OF = OXF(IOF)                                             000102
                      CALL NEWOF                                                000104
                      IF (TT(1) .LE. 0.0)  GO TO 322                            000106
                      TT = TT(IT)                                               000112
                C     LOOP FOR CHAMBER PRESSURES                                000112
                322   DO 998 IP = 1,NP                                          000115
                      ITNUM = 0                                                 000121
                      AREA = .FALSE.                                            000122
                      IF (TT(1) .LE. 0.0)  HP = .TRUE.                          000123
                      IF (TT(1) .GT. 0.0)  TP = .TRUE.                          000130
                      SP = .FALSE.                                              000135
                      EQL = .TRUE.                                              000136
                      ISUB = 1                                                  000140
                      ISUP = 1                                                  000141
                      PP = P(IP)                                                000147
                      IPP = 1                                                   000149
                C     LOOP FOR PRESSURE RATIOS                                  000149
                331   IF(EQL)  GO TO 332                                        000146
                      CALL FROZEN                                               000147
                      GO TO 1332                                                000151
                332   CALL EQLBRM                                               000153
                C     IT = 0 IF NO CONVERGENCE                                  000153
                1332  IF (IT .GT. 0.0)  GO TO 333                               000155
                      IF (NPT .LT. 2)  RETURN                                   000157
                      GO TO 900                                                 000166
                333   IF(IPP.GT.1) GO TO 195                                    000170
                C     COMBUSTION CHAMBER                                        000170
                      EQL = SEQL                                                000173
                      TP = .FALSE.                                              000175
                      HP = .FALSE.                                              000176
                      SP = .TRUE.                                               000177
```

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                SO = SSUM(I)                                                                    000201
                CPRF = CFSUM                                                                    000203
  334           IMELT=0.                                                                        000206
                ITROT = 3                                                                       000208
                THI = .FALSE.                                                                   000210
                APP(2)=((GAMMAS(1)+1.1/2.)**(GAMMAS(1)/(GAMMAS(1)-1.))          ROCK0066       000211
                IF(IEQL)  WRITE(JOUT,194) APP(2)                                                000227
                PP = PPP(1)/APP(2)                                                              000237
                TT = 2.*TT/(GAMMAS(1)+1.)                                                       000242
                ISV = 1                                                                         000250
                GO TO 870                                                                       000252
  195           USQ = 2.0*RBR*(HSUM(I) - HSUM(NPT))                                             000254
                IF (IPP.GT.2) GO TO 900                                                         000264
C               THROAT                                                           ROCK0073       000264
                IF (.NOT. THI)  GO TO 191                                                       000270
                GAMMAS(2) = 0.                                                                  000272
                GO TO 899                                                                       000273
  191           ASQ = RBR*GAMMAS(2)*TT*ENN                                                      000275
                IF(IDEBUG.EQ.1.OR.IDEBUG.EQ.2)  WRITE(JOUT,923)USQ,ASQ                          000304
  923 FORMAT(5HOUSQ=,E15.8,5X,4HASQ=,E15.8)                                                     000327
                DH = (USQ-ASQ)/ASQ                                                              000327
                IF(DH.LT.0.)  DH=-DH                                                            000334
                IF(DH.LE.0.4E-4.OR.ITROT.EQ.0)  GO TO 699                                       000341
                IF (JSOL .NE. 0)  GO TO 925                                                     000354
                IF (IMELT .LE. 0.0)  GO TO 192                                                  000356
                DLT = ALOG(IMELT/TT)                                                            000361
                PP = PP*EXP(DLT*CPR(2)/(ENN*DLVTP(2)))                                          000370
                APP(2) = P(IP)/PP                                                               000402
                THI = .TRUE.                                                                    000405
                GO TO 331                                                                       000407
  925           IMELT = TT                                                                      000411
  192           APP(2) = APP(2)/(1.0 + (USQ - ASQ)/(ENN*(GAMMAS(2) + 1.0)*RBR*TT))             000413
                PP = P(IP)/APP(2)                                                               000432
                ITROT = ITROT-1                                                  ROCK0079       000435
                IF(IEQL)  WRITE(JOUT,194) APP(2)                                                000440
  194 FORMAT(7H PC/PT=,F9.6)                                                                    000450
                GO TO 331                                                                       000450
  899           AWT =ENN*TT/(PP*USQ**.5)                                                        000452
                PCPLT = ALOG(APP(2))                                                            000465
  900           ISV =0                                                                          000472
                IF (TT .LE. 0.0)  GO TO 860                                                     000473
                AEAT(NPT) = ENN*TT/(PP*USQ**.5*AWT)                                             000476
                IF(AREA)  GO TO 800                                                             000514
                IF(IPP.LT.NPP)  GO TO 859                                                       000516
                IF(ENSUB+NSUP).EQ.0)  GO TO 860                                                 000522
                AREA = .TRUE.                                                                   000526
C               PCP ESTIMATES FOR AREA RATIOS                                                   000526
  800           IF(ITNUM.NE.0)  GO TO 810                                                       000531
                DLNP = 1.                                                                       000534
                ITNUM = 1                                                                       000536
                ARATIO = SUBAR(ISUB)                                                            000540
                IF(NSUB.LE.0)  ARATIO=SUPAR(ISUP)                                               000548
                ELN = ALOG(ARATIO)                                                              000552
                IF(NSUB.LE.0)  GO TO 799                                                        000556
                APPL = PCPLT/(SUBAR(ISUB)+(0.587*ELN**2+0.454)*ELN)                             000561
                IF(ARATIO.LT.1.04)  APPL=.9*APPL                                                000572
```

```
                      GO TO 859                                                          000601
  799 IF(SUPAR(ISUP).LT.2.)  GO TO 805                                                   000603
      IF(ISUP.GT.1.AND.SUPAR(ISUP-1).GE.2.)  GO TO 802                                   000607
      APPL = GAMMAS(2)*ELN*1.4                                                           000625
      GO TO 859                                                                          000631
  805 APPL = SQRT(ELN*(1.535*3.294*ELN))*PCPLT                                           000633
      GO TO 859                                                                          000644
  810 IF (IDEBUG .LE. 0 .OR. NPT .LT. IDEBUG)  GO TO 809                                 000648
      WRITE(JOUT,1811)ITNUM,ARATIO,AEAT(NPT),APP(NPT),DLNP                               000662
 1811 FORMAT (6HOITER=,I2,5X,15HASSIGNED AE/AT=,F15.8,5X,6HAE/AT=,F15.8,                 000676
     1 5X,5HPC/P=,F15.8,5X,11HDELTA LN P=,F15.8)                                        000676
  809 TOL = 1.0E-5                                                                       000676
      IF (ARATIO .GE. 10.0)  TOL = 4.0E-5                                                000701
      IF (ABS(AEAT(NPT) - ARATIO)/ARATIO .LE. TOL)  GO TO 830                            000707
      IF (ABS(DLNP) .LT. 4.0E-6)  GO TO 830                                              000717
      AEATL= ALOG(AEAT(NPT))                                                             000723
      ITNUM = ITNUM + 1                                                                  000731
      IF (ITNUM .GT. 25)  GO TO 820                                                      000734
      ASQ = WBR*GAMMAS(NPT)*ENN*TT                                                       000737
      DLNPE = GAMMAS(NPT)*USQ/(USQ-ASQ)                                                  000747
  802 DLNP = DLNPE*ELN-DLNPE*AEATL                                                       000756
      APPL = APPL + DLNP                                                                 000764
      IF(ITNUM.EQ.1)  GO TO 859                                                          000766
      APP(NPT) = EXP(APPL)                                                               000771
      PP = P(IP)/APP(NPT)                                                                000775
      GO TO 331                                                                          001000
  820 WRITE(JOUT,821) ARATIO                                                             001002
  821 FORMAT (//10X,40HROCKET DID NOT CONVERGE FOR AREA RATIO =,F11.6//)                 001010
  830 ITNUM = 0                                                                          001010
      AEAT(NPT) = ARATIO                                                                 001011
      IF(NSUB.LE.0)  GO TO 834                                                           001013
      ISUB = ISUB+1                                                                      001016
      IF (ISUB .LE. NSUB)  GO TO 800                                                     001021
      ISUB = 1                                                                           001024
      NSUB = -NSUB                                                                       001026
      IF(ISUP.LE.NSUP)  GO TO 800                                                        001030
      GO TO 835                                                                          001034
  834 ISUP = ISUP+1                                                                      001036
      IF(ISUP.LE.NSUP)  GO TO 800                                                        001040
      ISUP = 1                                                                           001043
  835 AREA = .FALSE.                                                                     001046
      GO TO 860                                                                          001046
  859 ISV = NPT                                                                          001050
      IF(NPT.NE.13)  GO TO 870                                          ROCKU088         001051
  860 CALL PRTOUT (IGAS)                                                                 001059
      IF (TT .LE. 0.0)  ISV = 0                                                          001056
      IF (.NOT. EQL .AND. TT .LE. 0.0)  WRITE(JOUT,862)                                  001062
  862 FORMAT (///2X,125HCALCULATIONS WERE STOPPED IN ROCKET BECAUSE NEXT                 001077
     1POINT IS MORE THAN 50 DEGREES BELOW TEMPERATURE RANGE OF A CONDENS                 001077
     2ED SPECIES)                                                                       001077
      IF (ISV.EQ.0) GO TO 990                                                            001077
      IDEBUG = IDEBUG-13                                                                 001101
      WRITE(JOUT,865)                                                                    001109
  865 FORMAT(1H1)                                                                        001111
      NPT = 2                                                                            001111
  870 NPT = NPT + 1                                                     ROCKU121         001114
```

```
      IF(.NOT.EQL) GO TO 880                                            001115
      IF(ISW.EQ.1) ISW = -1                                             001120
      CALL SAVE                                                         001125
  880 IPP = IPP+1                                                       001130
      IF(NPT.EQ.2) GO TO 331                                            001135
      IF(.NOT.ARLA) APPEND(PT)=PCP(IPP-2)                               001136
      IF(ARLA) APPEND(PT)=EXPIAPPL)                                     001147
      PP = PTPT/APP(NPT)                                                001156
      GO TO 331                                                         001162
  990 IF(IDEBUG.LT.0) IDEBUG=IDEBUG+13                                  001164
      IF(NSUB.LT.0) NSUB=-NSUB                                          001171
      IF (.NOT.FROZ.OR..NOT.EQL) GO TO 997                              001176
      CPRF(I) = CPRF                                                    001201
      GAMMAS(I) = (PRF/(CPRF-1./GM(I)))                                 001203
      II = IIII                                                         001210
      IPP = 1                                                           001212
      NPT = 1                                                           001214
      CALL SAVE                                                         001215
      EQL = .FALSE.                                                     001217
      ENN = 1./GM(I)                                                    001220
      GO TO 334                                                         001223
  997 NPT = 1                                                           001225
      WRITE(JOUT,865)                                                   001226
      IF (SEQL) CALL SAVE                                               001233
  998 II = IIII(I)                                                      001237
      IF(II.GE.NI) GO TO 999                                            001243
      II = II+1                                                         001247
      II = IIII                                                         001253
      GO TO 322                                                         001255
  999 IF (IOF .GE. NOF) RETURN                                          001257
      GO TO 321                                                         001265
      END                                                               001311
```

ROCKWELL

ORIGINAL PAGE IS
OF POOR QUALITY

```
@FOR,S LEWIS.RREAD,LEWIS.RREAD
FOR  E1 -10/25/79-17:37:49 (17,)

  SUBROUTINE RREAD      ENTRY POINT 001255

  STORAGE USED: CODE(1) 001273; DATA(0) 001031; BLANK COMMON(2) 000000

  EXTERNAL REFERENCES (BLOCK, NAME)

   0003    RDYES
   0004    PAGIT
   0005    CHRSIZ
   0006    GOUT
   0007    NNCODE
   0010    RDATAI
   0011    RDATAF
   0012    DMWRTF
   0013    RDCHAR
   0014    NRDW$
   0015    NRDU$
   0016    NIO2$
   0017    NIO1$
   0020    NERR2$
   0021    NRDU$
   0022    NWEF$
   0023    NERR3$

  STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

   0001     000010 10L       0001     000260 100L      0001     000343 106L      0001     000405 110L      0001     000470 120L
   0001     000522 130L      0001     000556 140L      0001     000574 150L      0001     000615 160L      0001     000633 170L
   0001     000032 172G      0001     000037 176G      0001     000654 200L      0001     000107 225G      0001     000116 232G
   0001     000720 300L      0001     000275 306G      0001     001003 310L      0001     000334 327G      0001     001033 330L
   0001     001061 340L      0001     000424 350G      0001     001100 350L      0001     001115 360L      0001     000452 361G
   0001     001134 370L      0001     001152 400L      0001     000667 433G      0001     000670 436G      0001     000741 464G
   0001     000766 475G      0001     000060 50L       0001     001170 551G      0001     001175 555G      0001     000160 70L
   0000     000722 800F      0000     000723 801F      0000     000736 802F      0000     000752 803F      0001     000221 90L
   0001     000255 95L       0000 R 000113 ANUM      0000 R 000360 DENS      0000 R 000264 ENTH      0000 R 000571 EXMP1A
   0000 R 000604 EXMP1B    0000 R 000614 EXMP2     0000 R 000622 EXMP2B    0000 R 000627 EXMP3     0000 R 000634 EXMP3B
   0000 R 000643 EXMP4     0000 R 000647 EXMP5     0000 R 000653 EXMP6     0000 R 000660 EXMP7     0000 R 000303 FAZ
   0000 R 000341 FOX       0000 I 000715 I         0000 I 000721 ICHNG     0000 I 000712 IDUM      0000     001006 INJP$
   0000 I 000713 IO        0000 I 000717 IOPT      0000 I 000467 IOUT      0000 I 000664 IREACT    0000 I 000716 J
   0000 I 000702 LINE0     0000 I 000377 LINE1     0000 I 000424 LINE2     0000 I 000447 LINE3     0000 I 000514 MODIFY
   0000 I 000531 MOUMLN    0000 I 000245 MOLE      0000 I 000720 N         0000 I 000000 NAME      0000 I 000714 NREAC
   0000 R 000226 PECWT     0000 R 000670 RDUM      0003 L 000000 RDYES     0000 R 000322 RTEMP


 00101      1*            SUBROUTINE RREAD(FIRST)                                                  000000
 00103      2*            LOGICAL FIRST,RDYES                                                      000000
 00103      3*                                                                                     000000
```

```
      C     USE MIFS INPUT ROUTINES TO READ REACTANT CARDS (STORE ON FILE 8)
      C
      C     DATA ARRAYS FOR REACTANT CARDS
            DIMENSION NAME(5,5),ANUM(15,5),PECWT(15),MOLE(15),ENTH(15),
     1      FAZ(15),RTEMP(15),FOX(15),DENS(15)
      C
      C     ARRAYS FOR DATA MENU'S
            DIMENSION LINE1(21),LINE2(19),LINE3(16),IOUT(21),MODIFY(13)
            DIMENSION MODMEN(4,8),EXMP1A(11),EXMP1B(8),EXMP2(6),EXMP2B(5),
     1      EXMP3(5),EXMP3B(7),EXMP4(4),EXMP5(4),EXMP6(5),EXMP7(4),
     .      IREACT(4),RNUM(10),LINE0(8)
      C
      C     SET DATA ARRAYS FOR MENUS
            DATA LINE0/6HTYPE  ,6HYES  ,6HNO READ,6H IN PR,6HEVIOUS,
     1      6H REACT,6HANT SE,6HT      /
            DATA LINE1/6H INDEX,4*6H       ,6HREACTA,6HNT(*) ,3*6H       ,
     1      6H     R,6HEL WT/,6H   MOL,6HE  ENT,6HHALPY/,6H   PHA,6HSE  TE,
     2      6HMP,K  ,6H FUEL/,6H  DENS,6HITY  /
            DATA LINE2/10*6H       ,6H     N,6HO MOLE,6HS      ,6H   INT,
     1      6H ENERG,6HY      ,2*6H       ,6H OXID /
            DATA LINE3/8*6H       ,6H  *  D,6HO  IND,6HICATES,6H ENTHA,
     1      6HLPY TO,6H BE CA,6HLCULAT,6HED      /
            DATA MODMEN/24H 1-REACTANT FORMULA      ,
     1      24H 2-REL WT/NO MOLES      ,24H 3-ENTHALPY/ENERGY//CALC ,
     2      24H 4-PHASE (S-L-G)        ,24H 5-TEMPERATURE (K)       ,
     3      24H 6-FUEL,OXIDIZER (F/O)  ,24H 7-DENSITY (G/CM3)       ,
     4      24H RETURN TO CONTINUE     /
            DATA EXMP1A/36H TYPE CHEMICAL FORMULA THIS REACTANT,
     1      30H, HOLLERITH CODE FOR SYMBOLS /
           DATA EXMP1B/48H EXAMPLE CARBON TETRACHLORIDE  1HC 1. 2HCL 4.   /
            DATA EXMP2/36H TYPE REL WEIGHT/NUMBER OF MOLES    /
            DATA EXMP2B/30H TYPE YES IF VALUE IS MOLES   /
            DATA EXMP3/30H TYPE ENTHALPY/INTERNAL ENERGY/
            DATA EXMP3B/42H TYPE YES IF ENTHALPY TO BE CALCULATED    /
            DATA EXMP4/24H TYPE PHASE (S-L-G)     /
            DATA EXMP5/24H TYPE TEMPERATURE (K)   /
            DATA EXMP6/30H TYPE FUEL/OXIDIZER (F/O)     /
            DATA EXMP7/24H TYPE DENSITY (G/CC)    /
            DATA MODIFY/6H TYPE ,6H 1. 2.,6HOR 3  ,6HTO MOD,6HIFY. 0.
     1      6HDELETE,,6H OR AD,6HD A RL,6HACTANT,6H (RETU,6HRN TO ,
     2      6HCONTIN,6HUE)   /
            DATA IREACT/24H TYPE REACTANT NUMBER   /
            DATA IRUM/1H /
            DATA IO/8/
      C
            NREAC=0
      C
      C     FOR FIRST PASS DO NOT CHECK SAVED DATA
            IF(.NOT.FIRST) GO TO 10
            IF(.NOT.ROYES(LINE0,4)) GO TO 50
      C
      C     REAL IN PRESENT CASE
     10   CONTINUE
            REWIND IO
            READ(IO,900) NREAC
            IF(NREAC.LT.1) GO TO 50
```

```
00171     60*                 DO 25 I=1,NREAC                                                    000024
00174     61*                 READ(10,801) (NAME(I,J),ANUM(I,J),J=1,5),PECWT(I),MOLE(I),         000032
00174     62*            1    ENTH(I),FAZ(I),RTEMP(I),FOX(I),DENS(I)                             000032
00212     63*       25        CONTINUE                                                           000060
00212     64*       C                                                                            000060
00212     65*       C         DISPLAY PRESENT SET OF REACTANTS (ADD IF NONE EXIST)               000060
00214     66*        50       CONTINUE                                                           000060
00215     67*                 FIRST=.FALSE.                                                      000060
00216     68*                 CALL PAGIT                                                         000060
00217     69*                 CALL CHRSIZ(4)                                                     000062
00220     70*                 IF(NREAC.LT.1) GO TO 300                                           000065
00222     71*                 CALL GOUT(LINE1,125)                                               000071
00223     72*                 CALL GOUT(LINE2,114)                                               000075
00224     73*                 DO 60 I=1,NREAC                                                    000107
00227     74*                 ENCODE(802,1OUT)I,(NAME(I,J),ANUM(I,J),J=1,5),PECWT(I),MOLE(I),    000107
00227     75*            1    ENTH(I),FAZ(I),RTEMP(I),FOX(I),DENS(I)                             000107
00240     76*                 CALL GOUT(IOUT,125)                                                000132
00247     77*        60       CONTINUE                                                           000143
00250     78*                 CALL GOUT(IDUM,1)                                                  000143
00252     79*                 CALL GOUT(LINE3,92)                                                000147
00253     80*                 CALL GOUT(IDUM,1)                                                  000153
00254     81*        70       CONTINUE                                                           000160
00255     82*                 CALL GOUT(MODIFY,75)                                               000160
00256     83*                 IOPT=0                                                             000163
00257     84*                 CALL RDATA(I,IOPT,$70)                                             000164
00260     85*                 IF(IOPT.LT.0 .OR. IOPT.GT.3) GO TO 70                              000171
00262     86*                 IF(IOPT.EQ.0) GO TO 400                                            000206
00264     87*                 GO TO(90,90,300),IOPT                                              000210
00264     88*       C                                                                            000210
00264     89*       C         SELECT REACTANT NUMBER                                             000210
00265     90*        90       CONTINUE                                                           000221
00266     91*                 N=1                                                                000221
00267     92*                 IF(NREAC.EQ.1) GO TO 95                                            000222
00271     93*                 N=0                                                                000224
00272     94*                 CALL GOUT(IREACT,24)                                               000225
00273     95*                 CALL RDATA(I,N,$90)                                                000231
00274     96*                 IF(N.LT.1 .OR. N.GT.NREAC) GO TO 90                                000236
00276     97*        95       CONTINUE                                                           000255
00277     98*                 IF(IOPT.EQ.2) GO TO 200                                            000255
00277     99*       C                                                                            000255
00277    100*       C         SELECT MODIFICATION OPTIONS                                        000255
00301    101*       100       CONTINUE                                                           000260
00302    102*                 CALL PAGIT                                                         000260
00303    103*                 ENCODE(802,1OUT)N,(NAME(N,J),ANUM(N,J),J=1,5),PECWT(N),MOLE(N),    000261
00303    104*            1    ENTH(N),FAZ(N),RTEMP(N),FOX(N),DENS(N)                             000261
00322    105*                 CALL GOUT(LINE1,125)                                               000311
00323    106*                 CALL GOUT(LINE2,114)                                               000315
00324    107*                 CALL GOUT(IOUT,125)                                                000321
00325    108*                 CALL GOUT(IDUM,1)                                                  000325
00326    109*                 DO 105 I=1,8                                                       000334
00331    110*                 CALL GOUT(MODMEN(1,I),24)                                          000334
00332    111*       105       CONTINUE                                                           000343
00334    112*       106       CONTINUE                                                           000343
00335    113*                 ICHNG=0                                                            000343
00336    114*                 CALL RDATA(I,ICHNG,$106)                                           000343
00337    115*                 IF(ICHNG .EQ. 0) GO TO 50                                          000357
```

```
      IF(ICHNG.LT.1 .OR. ICHNG.GT.7) GO TO 106
      GO TO (110,120,130,140,150,160,170),ICHNG
110   CONTINUE
      CALL GOUT(EXMP1A,66)
      CALL GOUT(EXMP1B,48)
      DO 112 I=1,5
      J=(I-1)*2 + 1
      FLD(0,36,RDUM(J))=FLD(0,36,NAME(N,I))
      RDUM(J+1)=ANUM(N,I)
112   CONTINUE
      CALL RDATAF(10,RDUM,$110)
      DO 114 I=1,5
      J=(I-1)*2 + 1
      FLD(0,36,NAME(N,I))=FLD(0,36,RDUM(J))
C     CALL CHECK(NAME(N,I))
      ANUM(N,I)=RDUM(J+1)
114   CONTINUE
      GO TO 100
C
120   CONTINUE
      CALL DMWRTF(EXMP2,36,PECWT(N),6)
      CALL RDATAF(1,PECWT(N),$120)
      MOLE(N)=1H
      IF(.NOT.RDYES(EXMP2B,30)) GO TO 100
      MOLE(N)=1HM
      GO TO 100
C
130   CONTINUE
      CALL DMWRTF(EXMP3,30,ENTH(N),5)
      CALL RDATAF(1,ENTH(N),$130)
      NAME(N,5)=2H
      IF(RDYES(EXMP3B,42)) NAME(N,5)=2HOO
      GO TO 100
C
140   CONTINUE
      CALL GOUT(EXMP4,24)
      CALL RDCHAR(FAZ(N),1,1,$140)
      GO TO 100
C
150   CONTINUE
      CALL DMWRTF(EXMP5,24,RTEMP(N),$150)
      CALL RDATAF(1,RTEMP(N),$150)
      GO TO 100
C
160   CONTINUE
      CALL GOUT(EXMP6,30)
      CALL RDCHAR(FOX(N),1,1,$160)
      GO TO 100
C
170   CONTINUE
      CALL DMWRTF(EXMP7,24,DENS(N),5)
      CALL RDATAF(1,DENS(N),$170)
      GO TO 100
C
C     DELETE A REACTANT
200   CONTINUE
```

```
00431    1720                NREAC=NREAC-1                                                  000654
00432    1730                DO 220 I=N,NREAC                                               000660
00435    1740                DO 210 J=1,5                                                   000670
00440    1750                     NAME(I,J)=NAME(I+1,J)                                     000670
00441    1760                     ANUM(I,J)=ANUM(I+1,J)                                     000671
00442    1770      210       CONTINUE                                                       000674
00444    1780                PECWT(I)=PECWT(I+1)                                            000674
00445    1790                MOLE(I)=MOLE(I+1)                                              000676
00446    1800                ENTH(I)=ENTH(I+1)                                              000700
00447    1810                FAZ(I)=FAZ(I+1)                                                000702
00450    1820                RTEMP(I)=RTEMP(I+1)                                            000704
00451    1830                FOX(I)=FOX(I+1)                                                000706
00452    1840                DENS(I)=DENS(I+1)                                              000710
00453    1850      220       CONTINUE                                                       000716
00455    1860                GO TO 50                                                       000716
00455    1870      C                                                                        000716
00455    1880      C         ADD A REACTANT                                                 000716
00456    1890      300       CONTINUE                                                       000720
00457    1900                NREAC=NREAC+1                                                  000720
00460    1910                N=NREAC                                                        000722
00461    1920                CALL GOUT(EXMP1A,66)                                           000723
00462    1930                CALL GOUT(EXMP1B,48)                                           000727
00463    1940                DO 305 I=1,5                                                   000741
00466    1950                J=(I-1)*2 + 1                                                  000741
00467    1960                RDUM(J)=2H                                                     000746
00470    1970                RDUM(J+1)=0.                                                   000751
00471    1980      305       CONTINUE                                                       000754
00473    1990                CALL RDATAF(10,RDUM,$300)                                      000754
00474    2000                DO 307 I=1,5                                                   000766
00477    2010                J=(I-1)*2 + 1                                                  000766
00500    2020                FLD(0,36,NAME(N,I))=FLD(0,36,RDUM(J))                          000774
00500    2030      C       CALL CHECK(NAME(N,I))                                          000774
00501    2040                ANUM(N,I)=RDUM(J+1)                                            000776
00502    2050      307       CONTINUE                                                       001003
00504    2060      310       CONTINUE                                                       001003
00505    2070                CALL GOUT(EXMP2,36)                                            001003
00506    2080                PECWT(N)=0.                                                    001007
00507    2090                CALL RDATAF(1,PECWT(N),$310)                                   001010
00510    2100      320       CONTINUE                                                       001017
00511    2110                MOLE(N)=1H                                                     001017
00512    2120                IF(RDYES(EXMP20,30)) MOLE(N)=1HM                               001022
00514    2130      330       CONTINUE                                                       001033
00515    2140                CALL GOUT(EXMP3,30)                                            001033
00516    2150                ENTH(N)=0.                                                     001037
00517    2160                CALL RDATAF(1,ENTH(N),$330)                                    001040
00520    2170                IF(RDYES(EXMP38,42)) NAME(N,5)=2HUO                            001050
00522    2180      340       CONTINUE                                                       001061
00523    2190                CALL GOUT(EXMP4,24)                                            001061
00524    2200                FAZ(N)=1HS                                                     001065
00525    2210                CALL RDCHAR(FAZ(N),1,-1,$340)                                  001067
00526    2220      350       CONTINUE                                                       001100
00527    2230                CALL GOUT(EXMP5,24)                                            001100
00530    2240                RTEMP(N)=0.                                                    001104
00531    2250                CALL RDATAF(1,RTEMP(N),$350)                                   001105
00534    2260      360       CONTINUE                                                       001115
00535    2270                CALL GOUT(EXMP6,30)                                            001115
```

```
                  FOX(N)=1HF                                                    001121
                  CALL RDCHAR(FOX(N),1,-1,$360)                                 001123
  370             CONTINUE                                                      001134
                  CALL GOUT(EAMF7,24)                                           001134
                  DENS(N)=0.                                                    001140
                  CALL RDATAF(1,DENS(N),$370)                                   001141
                  GO TO 50                                                      001150
C                                                                               001150
C       STORE CASE TO FILE 8                                                    001150
  410             CONTINUE                                                      001152
                  REWIND 10                                                     001152
                  WRITE(10,800) NREAC                                           001154
                  DO 410 I=1,NREAC                                              001170
                  WRITE(10,801) (NAME(I,J),ANUM(I,J),J=1,5),PECWT(I),MOLE(I),   001170
     1            ENTH(I),FAZ(I),ATEMP(I),FOX(I),DENS(I)                        001170
  410             CONTINUE                                                      001215
                  WRITE(10,803) IDUM                                            001215
                  WRITE(10,803) IDUM                                            001223
                  ENDFILE 10                                                    001251
                  RETURN                                                        001234
  800             FORMAT(I3)                                                    001272
  801             FORMAT(2X,5(A2,F8.4,2X),/,F10.6,2X,A1,F13.4,4X,A1,F12.3,      001272
     1            3X,A1,F12.5,1X)                                               001272
  802             FORMAT(1X,I2,2X,5(A2,F8.4,2X),F10.6,2X,A1,F13.4,4X,A1,F12.3,  001272
     1            3X,A1,F12.5,1X)                                               001272
  803             FORMAT(A1)                                                    001272
                  END                                                           001272
```

```
WFOR,S LE=IS.SAVE,LE=IS.SAVE
/JA  T  -10/25/79-17:40:00 (Y,T

    SUBROUTINE SAVE       ENTRY POINT 000463
               SE.OF      ENTRY POINT 000466


    STORAGE USED: CODE(I) 000471; DATA(D) 000065; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003   CONSTS 00000B
     0004   HOLLON 000010
     0005   SPECES 01,120
     0006   MISC   001264
     0007   INDX   000041
     0010   CCC    000003


    EXTERNAL REFERENCES (BLOCK, NAME)

     0011   $CALC
     0012   EXP
     0013   NADD$
     0014   MIO,$
     0015   MIOI$
     0016   NERR3$


    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0001   000137 100L      0001   000056 13L       0001   000042 131G      0001   000073 15L       0001   000112 20L
     0001   000161 200G      0001   000172 200L      0001   000207 207G      0001   000310 236G      0001   000417 303G
     0001   000127 50L       0000   000013 73UF      0001   000273 744L      0000   000304 745L      0001   000340 750L
     0001   000347 760L      0000   000016 770F      0000   000026 780F      0000   000031 785F      0005   000034 A
     0006   000570 AM        0006   000624 AM1       0006   000741 ANUM      0003   000000 ATMN      0006   000004 ATOM
     0006 R 000500 B0        0006 R 000521 B0P       0007 L 000036 CALCH     0005   000000 COEF      0007   000001 CONVG
     0006   000625 CPR1      0006   000564 CPSUM     0006   000604 DATA      0005   005670 DELN      0010   000002 DEMAND
     0006   001167 DENS      0005 R 002734 EN        0004   000000 END       0005 R 005360 ENLN      0006 R 001263 ENLSAV
     0006 R 000000 ENN       0006 R 001261 ENNL      0006 R 001262 ENSAVE    0006   001073 ENTM      0006 R 000566 EQRAT
     0006   001112 FAZ       0000 R 000003 FCAL      0000 R 000012 FF        0000 R 000002 FHH       0006   001150 FOX
     0000 R 000001 FOU       0004   000001 GAS       0003   000001 GMET      0010   000000 GRAPH     0007   000003 HP
     0006 R 000572 HPP       0000 R 000011 HS        0006 R 000567 HSUBO     0005   005524 HO        0007 I 000030 IC
     0007   000000 IDEBUG     0004 I 000002 IE        0007   000015 IMAT      0000   000040 INJPS     0007 L 000023 IONS
     0007   000021 IP        0007 I 000037 IQSAVE    0007 I 000016 IQ1       0007 I 000005 ISV       0007   000034 IT
     0005 I 011444 IUSE      0004   000003 IZERO     0000 I 000005 J         0007 I 000026 JLIQ      0010 I 000001 JOUT
     0007 I 000025 JSOL      0007   000031 JS1       0007   000014 KMAT      0004 I 000004 LANK      0006 I 000463 LLMT
     0000 I 000004 LLI       0007 I 000040 LSAVE     0004   000005 MOL       0007   000006 MOLES     0006   000626 NAME
     0007   000024 NC        0007   000022 NEWR      0007   000035 NFZ       0007 I 000012 NLM       0007   000017 NOF
     0007   000026 NOMIT     0007   000007 NP        0007 I 000011 NPT       0007   000027 NREAC     0007 I 000013 NS
     0000 I 000000 NSPPI     0007   000010 NT        0006 R 000565 OF        0004   000006 OX        0006   001227 OXF
     0007   000002 PATM      0006   001054 PECWT     0006   000563 PP        0003 R 000003 PRAR      0003   000004 PRP
     0006 R 000574 PH        0006 R 001206 PROP      0006   001207 PRW       0006   001131 PTEMP     0003   000005 PVR
     0005   002570 S         0007   000033 SHOCK     0005 R 011754 SLN       0007   000004 SP        0005   010770 SUB
     0010 R 000000 SUM       0006   000001 SUMN      0006   000003 SO        0005   011610 TEMP      0006   000562 THIGH
```

```
0005   001226 TLN      0006   000560 TLOW     0006   000557 TM       0006   000561 TMID     0007   000002 TP
0004   000002 TT       0006 R 000576 VMIN     0007 L 000032 VOL      0006 R 000600 VPLS     0000 R 000010 V1
0000 R 000007 V2       0006   000602 WP       0004   000007 ZERO
```

```
00101      1*          SUBROUTINE SAVE                                                                    000000
00101      2*    C                                                                                        000000
00101      3*    C  SAVES OR USES COMPOSITIONS FROM PREVIOUS POINT AS INITIAL ESTIMATES                   000000
00101      4*    C                                                                                        000000
00103      5*          COMMON /CONSTS/ ATMN,GMET,PAIM,RBAR,RBR,RVR                          /CONSTS/      000000
00109      6*          COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO                    /HOLCON/      000000
00109      7*    C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)                    000000
00109      8*    C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                     000000
00109      9*          INCLUDE SPECPR                                                                     000000
00111     10*          COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),             /MISC/       000000
00111     11*         1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,        /MISC/       000000
00111     12*         2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),        /MISC/       000000
00111     13*         3              DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),FECWT(15),     /MISC/       000000
00111     14*         4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,      /MISC/       000000
00111     15*         5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV                 /MISC/       000000
00112     16*          COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,      /INDX/       000000
00112     17*         1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,     /INDX/       000000
00112     18*         2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE       /INDX/       000000
00112     19*    C                                                                                        000000
00113     20*              COMMON /CCC/ GRAPH,JOUT,DEMAND                                               000000
00113     21*    C                                                                                        000000
00114     22*          DATA FOU/4HO, C/,FHH/4HH, C/,FCAL/4HAL/G/                                          000000
00120     23*          LOGICAL CALCH,IONS,VOL                                                             000000
00120     24*    C                                                                                        000000
00121     25*          IF(ISV)100,10,200                                                                  000000
00121     26*    C  NEXT POINT FIRST T IN SCHEDULE, USE PREVIOUS COMPOSITIONS FOR THIS T                  000000
00124     27*       10 IQ1 = IQSAVE                                                                       000003
00125     28*          ENN = ENSAVE                                                                       000005
00126     29*          ENNL = ENLSAV                                                                      000007
00127     30*          LL1 = NLM                                                                          000011
00130     31*          DO 50 J = 1,NS                                                                     000042
00133     32*          IF (.NOT. IONS .OR. LLMT(NLM) .EQ. LSAVE)  GO TO 15                                000042
00135     33*          IF(LLMT(NLM).EQ.IE)  GO TO 13                                                      000043
00137     34*          IF(IUSE(J).NE.-10000)  GO TO 15                                                    000046
00141     35*          IUSE(J) = 0                                                                        000051
00142     36*          LL1  = NLM+1                                                                       000052
00143     37*          GO TO 20                                                                           000054
00144     38*       13 IF(SLN(J).NE.0..OR.IUSE(J).NE.0)  GO TO 15                                         000056
00146     39*          LL1 = NLM-1                                                                        000065
00147     40*          IUSE(J) = -10000                                                                   000067
00150     41*          GO TO 50                                                                           000071
00151     42*       15 IF (IUSE(J).EQ.0) GO TO 20                                                         000073
00153     43*          EN (J,NPT) = SLN(J)                                                                000074
00154     44*          IF(IUSE(J).GT.0) IUSE(J) = - IUSE(J)                                               000076
00156     45*          IF (EN(J,NPT) .GT. 0.0)  IUSE(J) = - IUSE(J)                                       000103
00160     46*          GO TO 50                                                                           000110
00161     47*       20 EN(J,NPT) = 0.                                                                     000112
00162     48*          ENLEN(J) = SLN(J)                                                                  000117
00163     49*          IF (ENLEN(J) * 18.50 .LE. ENNL)  GO TO 50                                          000114
```

```
00165     50*          EN(J,NPT) = EXP(ENLN(J))                                                    000120
00166     51*       50 CONTINUE                                                                    000131
00170     52*          NLM = LLI                                                                   000131
00171     53*          RETURN                                                                      000133
00171     54*     C  FIRST T--SAVE COMPOSITIONS FOR FUTURE POINTS WITH THIS T                      000133
00172     55*      100 ISV = -ISV                                                                  000137
00173     56*          IQSAVE = IQI                                                                000140
00174     57*          ENSAVE = ENN                                                                000142
00175     58*          ENLSAV = ENNL                                                               000144
00176     59*          LSAVE = LLMT(NLM)                                                           000146
00177     60*          DO 150 J = 1,NS                                                             000161
00202     61*           ENLN(J) = ENLN(J)                                                          000161
00203     62*      150 IF (IUSE(J) .NE. 0)  SLN(J) = EN(J,ISV)                                     000162
00205     63*     C  USE COMPOSITIONS FROM PREVIOUS POINT                                          000162
00206     64*      200 DO 300 J = 1,NS                                                             000172
00211     65*      300 EN(J,NPT) = EN(J,ISV)                                                       000207
00213     66*          RETURN                                                                      000211
00213     67*     C  CALCULATE NEW VALUES OF BO AND HSUBO FOR NEW OF RATIO                         000211
00214     68*          ENTRY NEWOF                                                                 000214
00215     69*          WRITE(JOUT,730) OF                                                          000214
00220     70*      730 FORMAT(6H0OF = ,F10.6)                                                      000222
00221     71*          SUM = OF + 1.                                                               000222
00222     72*          V2 =    (OF*VMIN(1)+VMIN(2))/SUM                                            000225
00232     73*          V1 =    (OF*VPLS(1)+VPLS(2))/SUM                                            000232
00237     74*          IF (V2 .LT. 0.0)  EQRAT = ABS(V1/V2)                                        000237
00246     75*          IF (RH(1) .GT. 0.0 .AND. RH(2) .GT. 0.0)  GO TO 744                         000246
00256     76*          RHOP = RH(2)                                                                000262
00261     77*          IF (RHOP .LE. 0.0)  RHOP = RH(1)                                            000264
00263     78*          GO TO 745                                                                   000271
00264     79*      744 RHOF =  (OF+1.)*RH(1)*RH(2)/(RH(1)+ OF *RH(2))                              000273
00275     80*      745 DO 747 J = 1,NLM                                                            000304
00300     81*      747 BO(J) = (BOP(J,2) + BOP(J,1)*OF)/SUM                                        000310
00302     82*          NPT = 1                                                        MAIN0139     000315
00303     83*          IF(.NOT.CALCH)  GO TO 750                                                   000317
00305     84*          CALL HCALC                                                                  000321
00306     85*          CALCH = .FALSE.                                                             000323
00307     86*          IF (OF .GT. 0.0)  HPP(1) = SUM*HPP(1)/OF                                    000324
00321     87*          HPP(2) = SUM*HPP(2)                                                         000333
00322     88*          GO TO 760                                                                   000336
00323     89*      750 HSUBO = (HPP(2) + HPP(1)*OF)/(RBAR*SUM)                                     000340
00334     90*      760 IC = 0                                                                      000347
00335     91*          JSOL = 0                                                                    000347
00336     92*          JLIQ = 0                                                                    000350
00337     93*          HS = RBAR*HSUBO                                                             000351
00340     94*          WRITE(JOUT,770)                                                             000354
00342     95*      770 FORMAT (1H0,17X,4HFUEL ,13X,7HOXIDANT  ,12X,7HMIXTURE   ///)       MAIN0124 000361
00343     96*      780 FORMAT (1H 2A4,3E18.8/)                                            MAIN012  000361
00344     97*          FF = FMM                                                                    000361
00345     98*          IF(VOLIFF = F00                                                             000363
00347     99*          WRITE(JOUT,780) FF,FCAL ,HPP(2),HPP(1),HS                                   000367
00376    100*          WRITE(JOUT,785)                                                             000403
00300    101*      785 FORMAT (12H KG-ATOMS/KG)                                                    000410
00301    102*          WRITE(JOUT,780) (LLMT(J),LANK,BOP(J,2),BOP(J,1),BO(J), J = 1,NLM)           000413
00313    103*          RETURN                                                                      000426
00314    104*          END                                                                         000470
```

```
$LOAD,S LEWIS.SEARCH,LEWIS.SEARCH
M:A  E  -1072577?-17:40:07 (9.)


    SUBROUTINE SEARCH     ENTRY POINT 000424

    STORAGE USED: CODE(1) 000440; DATA(0) 000114; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003   HOLCOM 000010
     0004   SPECES 012120
     0005   MISC   001264
     0006   INDX   000041
     0007   CCC    000003

    EXTERNAL REFERENCES (BLOCK, NAME)

     0010   NABES
     0011   NIO2S
     0012   NIO1S
     0013   NWDUS
     0014   NERR36

    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0000    000022 10F        0001    000014 123G       0001    000015 126G       0001    000043 144G       0001    000303 145L
     0001    000075 152G       0001    000120 167G       0001    000306 170L       0001    000121 171G       0001    000321 171L
     0000    000045 172F       0000    000055 176F       0000    000030 20F        0001    000137 202G       0001    000147 205G
     0001    000177 216G       0001    000204 223G       0001    000215 231G       0001    000271 252G       0001    000341 275G
     0001    000371 304G       0000    000020 5F         0001    000035 7L         0001    000162 805L       0001    000164 810L
     0001    000220 820L       0001    000227 825L       0000    000032 871F       0004 R  006034 A          0005    000570 AM
     0005    000624 AMI        0005    000741 ANUM       0005    000004 ATOM       0000 R  000001 B          0005    000502 BD
     0005    000521 BOP        0006    000036 CALCH      0004 R  000000 COEF       0006    000001 CONVG      0005    000625 CPRI
     0005    000564 CPSUM      0005    000604 DATA       0004 R  002734 DATE       0004    005670 DELN       0007    000002 DEMAND
     0005    001167 DENS       0004    002734 EN         0003 I  000000 END        0004    005360 ENLN       0005    001263 ENLSAV
     0005    000000 ENN        0005    001261 ENNL       0005    001262 ENSAVE     0005    001073 ENTH       0005    000566 EQRAT
     0005    001112 FAZ        0005    001150 FOX        0003 I  000001 GAS        0007    000000 GRAPH      0006    000003 HP
     0005    000572 HPP        0005    000567 HSUBO      0004    005524 HO         0000 I  000013 I          0006    000030 IC
     0006    000000 IDEBUG     0003    000002 IE         0006    000015 IMAT       0000    000066 INJPS      0006    000023 IONS
     0006    000021 IP         0006    000037 IQSAVE     0006    000016 IQI        0006    000005 ISV        0006    000034 IT
     0004 I  011444 IUSE       0000 I  000012 IX         0003    000003 IZERO      0000 I  000014 J          0006    000026 JLIQ
     0007 I  000001 JOUT       0006    000025 JSOL       0006    000031 JSI        0000 I  000017 K          0006    000014 KMAT
     0006 I  000012 L          0003    000004 LANK       0005 I  000463 LLMT       0006    000040 LSAVE      0003    000005 MOL
     0006    000006 MOLES      0000 I  000005 MT         0005    000626 NAME       0006 I  000024 NC         0006 L  000022 NEWP
     0006    000035 NFZ        0006    000017 NOF        0006 I  000020 NOMIT      0006    000007 NP         0006    000011 NPT
     0006    000027 NREAC      0006 I  000015 NS         0000 I  000000 NSPPI      0006    000010 NT         0005    000565 OF
     0004 I  005360 OMIT       0003    000006 OX         0005    001227 OXF        0005    001054 PECWT      0000 I  000011 PMAZ
     0005    000583 PP         0005    000574 RH         0005    001206 RHOP       0005    001207 RHOW       0005    001131 RTEMP
     0004    002570 S          0006    000033 SHOCK      0004    011754 SLN        0006    000004 SP         0004 I  010770 SUB
     0005    000001 SUMA       0005    000603 SU         0004 R  011610 TEMP       0005 R  000562 THIGH      0005    001226 TLN
     0005 R  000560 TLOW       0005    000557 TM         0005 R  000561 TMID       0006    000002 TP         0005    000002 TT
     0000 R  000015 TI         0006 R  000016 T2         0005    000576 VMIN       0006    000032 VOL        0005    000600 VPLS
```

```
 G005    000602 =P        0003   000007 ZERO

      SUBROUTINE SEARCH                                                        000000
C                                                                              000000
C  SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED                    000000
C                                                                              000000
      COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO            /HOLCON/    000000
C     COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)          000000
C    1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)           000000
        INCLUDE SPECPK                                                         000000
      COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),    /MISC/      000000
     1              BOP(15,2),IM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT, /MISC/     000000
     2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2), /MISC/     000000
     3              DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15), /MISC/  000000
     4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP, /MISC/   000000
     5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV          /MISC/     000000
      COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS, /INDX/     000000
     1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ, /INDX/  000000
     2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE /INDX/    000000
C                                                                              000000
        COMMON /CCC/ GRAPH,JOUT,DEMAND                                         000000
C                                                                              000000
      DIMENSION B(4),DATE(2,3),MT(4),OMIT(3,3)                                 000000
      EQUIVALENCE (DATE,EN),(ENLN,OMIT)                                        000000
      INTEGER END,GAS,OMIT,PHAZ,SUB                                            000000
      LOGICAL NEWR                                                             000000
C                                                                              000000
      NC= 0                                                                    000000
      IX= 0                                                                    000000
      SUB(1,1) = END                                                           000001
      DO 3 I=1,150                                                             000015
      DO 3  J=1,L                                                              000015
    3 A(J,I) = 0.0                                                             000015
      READ(4,5)  TLOW,TMID,THIGH                                               000022
    5 FORMAT (3F10.3)                                                          000032
      NS = 1                                                                   000032
    7 READ    (4,10)(SUB(NS,I),I=1,3),DATE(1,NS),DATE(2,NS),(MT(J),B(J),       000035
     1  J=1,4),PHAZ,T1,T2                                                      000035
   10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3)                                  000105
      IF(SUB(NS,1).EQ.END) GO TO 171                                           000105
      READ      (4,20) ((COEF(I,J,NS),J=1,7),I=1,2)                            000110
   20 FORMAT (5E15.8)                                                          000130
      IF(NOMIT.EQ.0) GO TO 810                                                 000130
      DO 805 I=1,NOMIT                                                         000132
      DO 804 J=1,3                                                             000147
  804 IF (OMIT(J,I) .NE. SUB(NS,J))  GO TO 805                                 000147
      GO TO 7                                                                  000160
  805 CONTINUE                                                                 000164
  810 DO 820 K=1,4                                                             000164
      IF(B(K).EQ.0.) GO TO 825                                                 000177
      DO 168 I=1,L                                                             000204
  168 IF (LLMT(I) .EQ. MT(K))  GO TO 820                                       000204
      DO 819 J=1,L                                                             000215
```

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OF POOR QUALITY

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00233      53*          819 A(J,NS) = 0.                                                                  000215
00235      54*              GO TO 7                                                                       000216
00236      55*          820 A(I,NS)= B(K)                                                                 000220
00240      56*          825 IUSE(NS) = 0                                                                  000227
00241      57*              IF(PHAZ.EQ.GAS) GO TO 170                                                     000230
00243      58*              NC= NC+1                                                                      000233
00244      59*              TEMP(NC,1)= T1                                                                000236
00245      60*              TEMP(NC,2)= T2                                                                000241
00246      61*              IX= IX+1                                                                      000243
00247      62*              IF(IUSE(NS-1).EQ.0 .OR. NC.EQ.1) GO TO 145                                    000246
00251      63*              DO 830 I=1,L                                                                  000271
00254      64*          830  IF (A(I,NS) .NE. A(I,NS-1))  GO TO 145                                       000271
00257      65*              IX= IX-1                                                                      000277
00260      66*          145 IUSE(NS)= -IX                                                                 000303
00261      67*          170 NS= NS+1                                                                      000306
00262      68*              IF (NS .LT. NSPP1)  GO TO 7                                                   000310
00264      69*              WRITE (JOUT,871)                                                              000313
00266      70*          871  FORMAT (///20X,54HDIMENSIONS IN /SPECES/ FOUND TO BE TOO SMALL IN S       000321
                           1EARCH/)                                                                      000321
00267      71*          171 NS= NS-1                                                                      000321
00270      72*              NEWR= .FALSE.                                                                 000323
00271      73*              WRITE(JOUT,172)                                                               000330
00273      74*          172 FORMAT(42HOSPECIES BEING CONSIDERED IN THIS SYSTEM    )                       000341
00274      75*              DO 174 I=1,NS,5                                                               000341
00277      76*              K = I + 4                                                                     000344
00300      77*              IF (NS .LT. K)  K = NS                                                        000347
00302      78*          174  WRITE(JOUT,176)(DATE(1,J),DATE(2,J),SUB(J,1),SUB(J,2),SUB(J,3),          000355
                          1    J=I,K)                                                                   000355
00315      80*          176 FORMAT(5(5X,2A3,2X,3A4))                                                      000402
00316      81*              RETURN                                                                        000402
00317      82*              END                                                                           000437
END FOR
```

```
#RUN,S LEWIS,SHEK,LEWIS,SHEK
#A  T: -10/25/77,-17:40:16 (10,)


    SUBROUTINE SHEK       ENTRY POINT 001367


    STORAGE USED: CODE(1) 001401; DATA(D) 000263; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003   CONSTS 000006
     0004   HOLLOW 000010
     0005   POINTS 000335
     0006   SPECES 012120
     0007   MISC   001264
     0010   DOUBLE 001560
     0011   INDX   000041
     0012   PERF   000166
     0013   OUPT   000073
     0014   CCC    000003


    EXTERNAL REFERENCES (BLOCK, NAME)

     0015   RDYES
     0016   PAGIT
     0017   CHRSIX
     0020   SOUT
     0021   NEWOF
     0022   HEADC
     0023   OUT1
     0024   OUT2
     0025   ECLOSM
     0026   SAVE
     0027   OUT3
     0030   NONEW
     0031   NRNEW
     0032   NWEQU
     0033   N10.5
     0034   SQRT
     0035   N10J5
     0036   N1015
     0037   ALOG
     0040   EXP
     0041   NERR36


    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0000   0000143 125F      0001   000211 19L       0001   000011 1456      0001   000221 15L       0001   001001 150L
     0000   000165 152F       0001   000122 1566      0000   000101 16F       0001   001112 161L      0001   000126 17L
     0001   000193 19L        0001   000073 2046      0001   000114 21L       0001   000136 2236      0001   000147 2316
     0001   000245 30L        0001   000356 3736      0001   000376 3346      0001   000520 3616      0001   000534 40L
     0001   001123 411L       0001   000320 44L       0001   000325 45L       0000   000137 46F       0001   001057 4616
     0001   000412 47L        0001   000547 50L       0001   001201 5206      0001   001232 5366      0001   001247 5476
```

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0001   001276 5616      0001   001303 5726      0000   000176 5AF       0001   001322 6046      0001   001345 6206
0000   000252 A5        0001   000750 75L       0000   000111 B61F      0000   000122 B62F      0000   000131 B63F
0001   001106 ANGL      0006   006034 A         0007   000570 AM        0007 R 000624 AM1       0007   000741 AMUM
0005   000000 ATMN      0007   000004 ATOM      0000 R 000036 AX        0000 R 000037 AXX       0000 R 000024 A1
0007   000502 BP        0007 R 000625 CPR1      0011   000036 CALCH     0006   000000 COEF      0011   000001 CONVG
0005 R 000004 CPR       0007   000564 CPSUM     0007   000604 DATA      0005 R 000047 DLVTP     0006   005670 DELN
0019   000002 DEMAND    0007   001167 DENS      0005 R 000064 DLVPT     0006 R 002734 EN        0007   001261 ENNL
0009   000000 END       0006 R 005360 ENLN      0007   001263 ENLSAV    0007   000000 ENN       0013   000002 FA
0007   001262 ENSAVE    0013   001073 ENTH      0012 L 000165 EQL       0007   000566 EQRAT     0015   000007 FCP
0013   000003 FAP       0007   001112 FAZ       0013 R 000005 FB        0013   000006 FC        0015   000020 FGV
0015   000001 FCST      0013   000014 FCV       0013   000015 FG        0013   000017 FGE       0000 R 000001 FMM
0013   000021 FH        0013   000023 FI        0013   000025 FIV       0013   000027 FM        0013   000053 FP
0015 R 000031 FMI       0013 R 000050 FN        0013 R 000052 FOUR      0007   001150 FOX       0013   000056 FSV
000C R 000060 FPP       0000 R 000003 FRA       0000 R 000004 FRB       0013   000054 FS        0000 R 000006 FU1
0015   000057 FT        0013   000061 FTK       0000 R 000005 FTT       0000 R 000010 FV21      0000 R 000007 FU2
0015   000063 FV        0013 R 000065 FVEL      0000 R 000011 FV22      0000 R 000012 FV23      0000 R 000020 GAMMA1
0015 R 000001 FXS       0013   000000 F9X       0010 D 000000 G         0005 R 000101 GAMMAS     0000 R 000021 GAMMA2
0009   000001 GAS       0010 D 001516 GG        0003   000001 GMET      0014   000000 GRAPH     0011   000003 HP
0007   000572 HPP       0000 R 000030 HS        0007 R 000567 HSUBU     0005 R 000000 HSUM      0006   005524 HO
0010 I 000022 I         0011   000030 IC        0011 I 000000 IDEBUG    0004   000002 IE        0011   000015 IMAT
0000 L 000013 INCDEW    0000 L 000014 INCDFZ    0000   000233 INJPS     0000 I 000021 IOF       0011   000023 ION5
0011   000021 IP        0011   000037 IQSAVE    0011   000016 IQ1       0011 I 000005 ISV       0011   000034 IT
0004 I 011444 IUSP      0004 I 000033 IZERO     0000 I 000025 J         0011   000026 JLIQ      0014 I 000001 JOUT
0011   000025 JSOL      0011   000031 JS1       0000 1 000040 K         0011   000014 KMAT      0004   000004 LANK
0007   000463 LIMT      0011   000040 LSAVE     0012 R 000116 MACH1     0004   000005 MOL       0011   000006 MOLES
0000 R 000017 MOLSR1    0000 R 000016 MI        0012 R 000150 M2M1      0007 I 000626 NAME      0011   000024 NC
0011   000022 NFWD      0011   000035 NFZ       0011   000012 NLM       0011 I 000017 NOF       0011   000020 NOMIT
0011   000007 NP        0011 I 000011 NPT       0011 I 000027 NREAC     0011 I 000013 NS        0000 I 000023 NSR
0004 I 000000 NSPPT     0011   000010 NT        0007 R 000565 OF        0013   000067 ONE       0004   000006 OX
0007 R 001227 OXT       0005 R 000116 P         0003   000002 PATM      0012 R 000000 PCP       0007   001054 PECWT
0007 R 000563 PP        0005 R 000217 PPP       0000 R 000026 PI        0000 R 000031 P21       0000 R 000033 P21L
0003   000003 RBAR      0003 R 000004 RBR       0015 L 000000 ROYES     0007   000574 RH        0007   001206 RHOP
0000 R 000035 RHO12     0007   001207 RPM       0012 R 000133 RRHO      0007 R 001131 RTEMP     0003   000005 RVR
0006   002570 S         0000 L 000015 SEQL      0000   000041 SHKINP    0011   000033 SHOCK     0006   011754 SLN
0005   000251 SONVEL    0011   000004 SP        0005 R 000015 SSUM      0006   010770 SUB       0007   000001 SUMN
0007   000003 SQ        0005 R 000150 T         0006   011610 TEMP      0007   000562 THIGH     0013 R 000070 THREL
0007 R 001226 TLN       0007   000560 TLOW      0007   000557 TM        0007   000561 TMID      0005   000320 TOTN
0011 L 000002 TP        0007 R 000002 TT        0005 R 000266 TTT       0013 R 000071 TWO       0000 R 000027 TI
0013 R 000047 T21       0000 R 000032 T21L      0000 R 000034 T2IL      0005 R 000303 UTWO      0013 R 000101 U1
0013 R 000064 U102      0005   000202 V         0007   000576 VMIN      0012   000032 VMOC      0011   000032 VOL
0007   000600 WFLS      0005 R 000234 WM        0007   000602 WP        0010 D 001510 X         0004   000007 ZERO
0013   000072 ZERO1
```

```
00101        1*            SUBROUTINE SHCK                                                                          000000
00101        2*      C                                                                                              000000
00103        3*            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                                  /CONSTS/    000000
00104        4*            COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO                            /HOLCON/    000000
00105        5*            COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                              000000
00105        6*           1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)                         000000
00105        7*           . ,UTWO(13),TOTN(13)                                                                      000000
00105        8*            COMMON/SPECIES/COEF(2,7,150),S(150),ENT(150,13),ENLN(150),HO(150)                         000000
00105        9*           1 ,QLEN(150),ATIS,ISO),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)                           000000
                          INCLUDE SPECIES                                                                           000000
```

```
      COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),          /MISC/
     1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,     /MISC/
     2              HSUBU,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),     /MISC/
     3              DATA(16),AMI,CPRI,NAME(15,5),ANUM(15,5),PECWT(15),  /MISC/
     4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,   /MISC/
     5              AM=(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV              /MISC/
      COMMON /DOUBLE/ G(20,21), X(20)
      COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,    /INDX/
     1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIQ,  /INDX/
     2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE    /INDX/
      COMMON /PERF/ PCP(20),VMOC(13),T2T(13),U1U2(13),U1(13),           /PERF/
     1              MACH1(13),RRHO(13),M2M1(13),EQL                     /PERF/
      COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),   /OUPT/
     1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR,/OUPT/
     2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,  /OUPT/
     3              TWO,ZERO                                            /OUPT/
C
      COMMON /CCC/ GRAPH,JOUT,DEMAND
C
      DATA FMM/6HM2/M1 /,FPP/6HP2/P1 /,FRA/6HRHO2/R/,FRB/6HH01    /,
     1     FTT/6HT2/T1 /,FU1/6HU1  VE/,FU2/6HU2  VE/,FV21/6HV2(U1-/,
     2     FW22/6HW2/M/S/,FV23/2HEC/
      DOUBLE PRECISION G,GG,X
      EQUIVALENCE (X(4),GG)
      LOGICAL EQL,INCDEQ,INCDFZ,SEQL,TP
C
      LOGICAL ROYES
C
      REAL M1,MACH1,M2M1,MU12RT
C
      NAMELIST /SHKINP/ GAMMA1,INCDEQ,INCDFZ,MACH1,U1                   /SHKINP/
C
      IOF = 0
      IP=.TRUE.
      CPRI = 0.
      DO 10 I=1,13
      MACH1(I)=0.
   10 U1(I) = 0.0
      GAMMA1 = 0.
      INCDEQ = .TRUE.
      INCDFZ = .TRUE.
      DO 18 I = 1,NREAC
   18 NAME(I,5) = IZERO
         CALL PAGE
         CALL CHRSIZE(1)
         IF(ROYES('TYPE YES FOR PRESENT VALUES OF SHKINP NAMELIST',46))
     1   WRITE(6,SHKINP)
         CALL CHRSIZE(4)
         CALL GOUTE('TYPE NAMELIST  SHKINP HERE',21)
      READ (5,SHKINP)
      WRITE(JOUT,SHKINP)
      SEQL = INCDEQ
      IF (TEMP(1) .LE. 0.0)  T(1) = RTEMP(1)
      DO 20 I = 1,1
      IF (MACH1(I) .LE. 0.0 .AND. U1(I) .LE. 0.0)  GO TO 21
   20 NSH = I
```

```
      21 IOF = IOF+1                                                    000114
         OF = OXF(IOF)                                                  000117
         CALL NLWOF                                                     000121
         INCDEQ = SEQL                                                  000123
      17 PP = P(1)                                                      000126
         TT = T(1)                                                      000127
         IF (INCDEQ) GO TO 19                                           000131
C  FROZEN                                                              000131
         DO 118 I = 1,13                                                000136
         DLVTP(I) = 1.0                                                 000136
  118    DLVPT(I) = -1.0                                                000137
      19 DO 35  NPT=1,NSW                                               000143
         PPP(NPT) = P(NPT)                                              000147
         TTT(NPT) = T(NPT)                                              000151
         IF(NPT.EQ.1)  GO TO 14                                         000153
         IF (PPP(NPT) .LE. 0.0)  PPP(NPT) = PPP(NPT-1)                  000156
         IF (TTT(NPT) .LE. 0.0)  TTT(NPT) = TTT(NPT-1)                  000163
         SSUM(NPT) = SSUM(NPT-1)                                        000170
         HSUM(NPT) = HSUM(NPT-1)                                        000172
         IF(              TTT(NPT).EQ.TT.AND.PPP(NPT).EQ.PP)  GO TO 15  000174
      14 PP = PPP(NPT)                                                  000211
         TT = TTT(NPT)                                                  000212
         CALL HCALC                                                     000214
         HSUM(NPT) = HSUBO                                              000216
      15 IF (CPR1 .GT. 0.0)  GAMMA1 = CPR1/(CPR1 - 1.0/AM1)             000221
         IF (GAMMA1 .GT. 0.0)  GO TO 30                                 000231
         WRITE(JOUT,16)                                                 000234
      16 FORMAT (///20X,34HMISSING GAMMA1 OR CP VALUE IN SHOCK/)        000241
         RETURN                                                         000241
      30 A1 = SQRT(RBR*GAMMA1*TT/AM1)                                   000245
         IF (U1(NPT) .LE. 0.0)  U1(NPT) = A1*MACH1(NPT)                 000255
         IF (MACH1(NPT) .LE. 0.0)  MACH1(NPT) = U1(NPT)/A1              000263
         WM(NPT) = AM1                                                  000271
         CPR(NPT) = CPR1                                                000273
      35 GAMMAS(NPT) = GAMMA1                                           000275
         EQL = .FALSE.                                                  000301
C  OUTPUT--1ST CONDITION                                               000301
         WRITE(JOUT,861)                                                000302
  861 FORMAT(1H1,43X,39HINCIDENT SHOCK WAVE PARAMETERS ASSUMING   )     000307
         IF(.NOT.INCDEQ)  GO TO 44                                      000307
                  WRITE(JOUT,862)                                       000311
  862 FORMAT (1H ,51X,23HEQUILIBRIUM COMPOSITION  //)                   000316
         GO TO 45                                                       000316
      44                  WRITE(JOUT,863)                               000323
  863 FORMAT (1H ,51X,18HFROZEN COMPOSITION //)                         000325
      45 CALL OUT1                                                      000325
         WRITE(JOUT,96)                                                 000326
      96 FORMAT (16H INITIAL GAS (1) )                                  000336
         FMT(3) = F13                                                   000336
         FMT(4) = FOUR                                                  000340
         WRITE(JOUT,FMT) FN,FB,(MACH1(J), J = 1,NPT)                    000342
         FMT(4) = TWO                                                   000361
         WRITE(JOUT,FMT) FU1,FVEL,(U1(J), J = 1,NPT)                    000363
         CALL OUT2                                                      000401
C        BEGIN CALCULATIONS FOR 2ND CONDITION                           000401
         IF(INCDEQ)  EQL = .TRUE.                                       000403
```

```
                      NPT = 1                                                   000407
                   47 GAMMA1 = GAMMAS(NPT)                                      000412
                      M1 = WM(NPT)                                              000414
                      P1 = PPP(NPT)                                             000416
                      T1 = TTT(NPT)                                             000420
                      HS = HSUM(NPT)                                            000422
                      P21 = (2.*GAMMA1*MACH1(NPT)**2-GAMMA1+1.)/(GAMMA1+1.)     000424
                      T21 = P21*(2./MACH1(NPT)**2+GAMMA1-1.)/(GAMMA1+1.)        000436
                      IF((T1*T21).GT.2000..AND. EQL) T21 = .7*T21 + 600./T1     000453
                      MU12RT = AM1*U1(NPT)**2/(RBR*T1)                          000473
                      P21L=ALOG(P21)                                            000503
                      T21L=ALOG(T21)                                            000507
                      DO 100 I = 1,8                                            000520
                      TT=T21*T1                                                 000520
                      PP=P21*P1                                                 000523
                      IF (.NOT.EQL) GO TO 40                                    000526
                      CALL EQLBRM                                               000530
                      GO TO 50                                                  000532
                C  FROZEN                                                       000532
                   40 TLN = ALOG (TT)                                           000534
                      CALL HCALC                                                000537
                      HSUM(NPT) = HSUBO                                         000542
                      CPR(NPT) = CPR1                                           000544
                   50 RHO12 = M1*T21/(WM(NPT)*P21)                              000547
                      GG=RHO12*MU12RT                                           000556
                      G(1,1)=-GG*DLVPT(NPT)-P21                                 000564
                      G(1,2)=-GG*DLVTP(NPT)                                     000572
                      G(1,3)=P21-1.+MU12RT*(RHO12-1.)                           000576
                      GG = (U1(NPT)*RHO12)**2/RBR                               000605
                      G(2,1)=-GG*DLVPT(NPT)+TT*(DLVTP(NPT)-1.)/WM(NPT)          000613
                      G(2,2)=-GG*DLVTP(NPT)-TT*CPR(NPT)                         000626
                      G(2,3) = HSUM(NPT) - HS - U1(NPT)**2*(1.0 - RHO12**2)/(2.0*RBR)   000636
                      X(3)=G(1,1)*G(2,2)-G(1,2)*G(2,1)                          000652
                      X(1)=(G(1,3)*G(2,2)-G(2,3)*G(1,2))/X(3)                   000661
                      X(2)=(G(1,1)*G(2,3)-G(2,1)*G(1,3))/X(3)                   000671
                      AX = X(1)                                                 000701
                      AXX = X(2)                                                000703
                      IF(AX.LT.0.) AX = -AX                                     000705
                      IF (AXX.LT.0.) AXX = -AXX                                 000712
                      IF (AXX.GT.AX)  AX = AXX                                  000717
                      IF(AX.LT..00005)  GO TO 150                               000725
                      AX = AX/.4054652                                          000731
                      IF(AX.LE.1.)  GO TO 75                                    000734
                      X(1) = X(1)/AX                                            000737
                      X(2) = X(2)/AX                                            000743
                   75 P21L=P21L+X(1)                                            000750
                      T21L=T21L+X(2)                                            000753
                      P21=EXP(P21L)                                             000757
                  100 T21 = EXP(T21L)                                           000763
                      WRITE(JOUT,125) U1(NPT)                                   000771
                  125 FORMAT(25H0U1D1D NOT CONVERGE FOR U1=,F8.2,66H   ANSWERS PROBABLY NO   001001
                     1T RELIABLE, SOLUTION PROBABLY DOES NOT EXIST)             001001
                  150 RRHO(NPT) = 1./RHO12                                      001001
                      M2M1(NPT) = WM(NPT)/AM1                                   001004
                      PCP(NPT) = P21                                            001007
                      T2T1(NPT) = T21                                           001013
```

```
0044S    179*          IF (NPT .GE. IDEBUG .AND. IDEBUG .NE. 0) WRITE(JOUT,152) I,T21,P21                001013
0045S    180*      152 FORMAT(10HOITER NO.= ,I1,7X,7HT2/T1 =,F9.2,7X,7HP2/P1 =,F9.2 )                     001036
0046S    181*          UTWO(NPT) = U1(NPT)*RHO12                                                          001036
0047S    182*          U1U2(NPT) = U1(NPT)-UTWO(NPT)                                                      001042
0048S    183*          IF(.NOT.EQL)  GO TO 161                                                            001044
0049S    184*          DO 880 K=1,NS                                                                      001057
0050S    185*          IF(IUSE(K).LT.0)  GO TO 880                                                        001057
0051S    186*          IF(ENLN(K).GT.-87..AND.ENLN(K).LT.87.) EN(K,NPT) = EXP(ENLN(K))                    001061
0052S    187*      880 CONTINUE                                                                           001110
0053S    188*          GO TO 431                                                                          001110
0054S    189*      C  FROZEN                                                                              001110
0055S    190*      161 PPP(NPT) = PP                                                                      001112
0056S    191*          TTT(NPT) = TT                                                                      001114
0057S    192*          GAMMAS(NPT) = CPR(NPT)/(CPR(NPT) - 1.0/AMI)                                        001116
0058S    193*      431 ISV = 0                                                                            001125
0059S    194*          IF(NPT.LT.NSK)  ISV=NPT                                                            001125
0060S    195*          IF(NPT.EQ.1)  ISV=-1                                                               001133
0061S    196*          NPT = NPT+1                                                                        001140
0062S    197*          IF(EQL)  CALL SAVE                                                                 001143
0063S    198*          IF(NPT.LE.NSK)  GO TO 47                                                           001147
0064S    199*          NPT = NSK                                                                          001153
0065S    200*      C  OUTPUT--2ND CONDITION                                                               001153
0066S    201*          WRITE(JOUT,58)                                                                     001155
0067S    202*       58 FORMAT (16HOSHOCKED GAS (2) )                                                      001162
0068S    203*          FMT(4) = TWO                                                                       001162
0069S    204*          WRITE(JOUT,FMT) FU2,FVEL,(UTWO(J),J = 1,NPT)                                       001164
0070S    205*          CALL OUT2                                                                          001204
0071S    206*          WRITE(JOUT,68)                                                                     001206
0072S    207*       68 FORMAT (26HOINCIDENT SHOCK PARAMETERS  )                                           001216
0073S    208*          FMT(4) = THRLE                                                                     001216
0074S    209*          WRITE(JOUT,FMT) FPP,FB,FB,(PCP(J), J = 1,NPT)                                      001220
0075S    210*          WRITE(JOUT,FMT) FTT,FB,FB,(T2T1(J), J = 1,NPT)                                     001235
0076S    211*          FMT(4) = FOUR                                                                      001252
0077S    212*          WRITE(JOUT,FMT) FMM,FB,FB,(M2M1(J), J = 1,NPT)                                     001254
0078S    213*          WRITE(JOUT,FMT) FRA,FRB,FB,(RRHO(J), J = 1,NPT)                                    001271
0079S    214*          FMT(4) = TWO                                                                       001306
0080S    215*          WRITE(JOUT,FMT) FV21,FV22,FV23,(U1U2(J), J = 1,NPT)                                001310
0081S    216*          CALL OUT3                                                                          001325
0082S    217*          INCOLD = .FALSE.                                                                   001327
0083S    218*          IF(INCOFZ.AND.EQL)  GO TO 17                                                       001330
0084S    219*          IF(IOF.LT.NOF)  GO TO 21                                                           001333
0085S    220*          TP = .FALSE.                                                                       001341
0086S    221*          DO 999 K = 1,NHEAC                                                                 001345
0087S    222*      999 RTEMP(K) = T(I)                                                                    001345
0088S    223*          RETURN                                                                             001347
0089S    224*          END                                                                                001400
END FOR
```

```
$FOR,S LEWIS.THERMP,LEWIS.THERMP
H.A  ES -10/25/79-17:40:27 (8,)


    SUBROUTINE THERMP     ENTRY POINT 000376


    STORAGE USED: CODE(1) 000400; DATA(0) 000111; BLANK COMMON(2) 000000

     COMMON BLOCKS:

     0003    CONSTS 000006
     0004    POINTS 000335
     0005    MISC   001264
     0006    INDX   000041
     0007    OUPT   000073
     0010    CCC    000003


    EXTERNAL REFERENCES (BLOCK, NAME)

     0011    NEWOF
     0012    ECC,RM
     0013    OUT1
     0014    OUT2
     0015    OUT3
     0016    SAVE
     0017    NERR05
     0020    MIO,1
     0021    MIO19
     0022    NERR36


    STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

     0000    000017 10F      0000    000023 11F      0000    000031 12F      0001    000022 124G     0001    000044 131G
     0000    000037 20F      0000    000043 21F      0001    000220 217G     0000    000052 22F      0001    000245 233G
     0000    000004 5F       0001    000061 800L     0001    000111 860L     0001    000146 861L     0001    000173 862L
     0000    000060 863F     0001    000251 864L     0000    000066 868F     0001    000323 870L     0001    000352 871L
     0001    000006 95L      0005    000570 AM       0005    000624 AM1      0005    000741 ANUM     0003    000000 ATMN
     0005    000004 ATOM     0005    000502 B0       0005    000521 B0P      0006    000036 CALCH    0006    000001 CONVG
     0004    000032 CPR      0005    000625 CPR1     0005    000564 CPSUM    0005    000604 DATA     0010    000002 DEMAND
     0005    001167 DENS     0004    000064 DLVPT    0004    000047 DLVTP    0005    001263 ENLSAV   0005    000000 ENN
     0005    001261 ENNL     0005    001262 ENSAVE   0005    001073 ENTM     0005    000566 EQRAT    0007    000002 FA
     0007    000003 FAP      0005    001112 FAZ      0007 R  000005 FB       0007    000006 FC       0007    000007 FCP
     0007    000012 FCST     0007    000014 FCV      0007    000015 FG       0007    000017 FGE      0007    000020 FGV
     0007    000021 FH       0007    000023 FI       0007    000025 FIV      0007    000027 FM       0007 R  000031 FMT
     0007    000050 FN       0007    000052 FOUR     0005    001150 FOX      0007    000053 FP       0007    000054 FS
     0007    000056 FSV      0007    000057 FT       0007    000061 FTK      0000 R  000000 FUA      0000 R  000001 FUB
     0007    000063 FV       0007    000065 FVEL     0007    000001 F13      0007    000000 F9X      0004    000101 GAMMAS
     0005    000001 GMET     0010    000000 GRAPH    0006 L  000003 HP       0005    000572 HPP      0005 R  000567 HSUBO
     0004    000000 HSUM     0000 I  000003 I        0006    000030 IC       0006 I  000000 IDEBUG    0006    000015 IMAT
     0000    000072 INJP6    0000 I  000002 IOF      0006    000023 IONS     0006 I  000021 IP       0006    000037 IOSAVE
     0006    000016 IQ1      0006 I  000005 ISV      0006 I  000034 IT       0006    000026 JLIQ     0010 I  000001 JOUT
     0006    000025 JSOL     0006    000031 JSI      0006    000014 KMAT     0005    000463 LLMT     0006    000040 LSAVE
     0006    000006 MOLFS    0005    000626 NAME     0006    000024 NC       0006    000022 NEWR     0006    000035 NFZ
```

```
0004   000012 NLM        0006 I 000017 NOF        0006   000020 NOMIT      0006 I 000007 NP         0006 I 000011 NPT
0006   000027 NREAC      0006   000013 NS         0006 I 000010 NT         0005 R 000565 OF         0007 R 000067 ONE
0005 R 001227 OXF        0004 R 000116 P          0003   000002 PATM       0005   001054 PECWT      0005 R 000563 PP
0004   000217 PPP        0003 R 000003 RBAR       0003   000004 RBR        0005   000574 RH         0005   001206 RHOP
0005   001207 RMW        0005   001131 RTEMP      0003   000005 RVR        0006   000033 SHOCK      0004   000251 SONVEL
0006 L 000004 SP         0004   000015 SSUM       0005   000001 SUMN       0005   000003 SO         0004 R 000150 T
0005   000562 TMIGH      0007   000070 THREE      0005   001226 TLN        0005   000560 TLOW       0005   000557 TM
0005   000561 TMID       0004   000320 TOTN       0006 L 000002 TP         0005 R 000002 TT         0004   000266 TTT
0007 R 000071 TWO        0004 R 000202 V          0004 R 000303 VLM        0005   000576 VMIN       0006 L 000032 VOL
0005   000600 VPLS       0004   000234 WM         0005   000602 WP         0007   000072 ZERO
```

```
00101      1*            SUBROUTINE THERMP                                                                  000000
00101      2*      C                                                                          MOLIU001    000000
00103      3*            COMMON /CONSTS/ ATMN,GMET,PATM,RBAR,RBR,RVR                        /CONSTS/    000000
00104      4*            COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)                    000000
00104      5*           1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)               000000
00104      6*           2 ,VLM(13),TOTN(13)                                                             000000
00105      7*            COMMON /MISC/ ENN,SUMN,TI,SO,ATOM(3,101),LLMT(15),BO(15),          /MISC/      000000
00105      8*           1              BOP(15,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,    /MISC/      000000
00105      9*           2              HSUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),    /MISC/      000000
00105     10*           3              DATA(16),AM1,CPR1,NAME(15,5),ANUM(15,5),PECWT(15),  /MISC/      000000
00105     11*           4              ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),RHOP,   /MISC/      000000
00105     12*           5              RMW(15),TLN,OXF(26),ENNL,ENSAVE,ENLSAV              /MISC/      000000
00106     13*            COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,NLM,NS,    /INDX/      000000
00106     14*           1              KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,IONS,VC,JSOL,JLIQ,  /INDX/      000000
00106     15*           2              NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH,IQSAVE,LSAVE    /INDX/      000000
00107     16*            COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),   /OUPT/      000000
00107     17*           1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/      000000
00107     18*           2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,  /OUPT/      000000
00107     19*           3              TWO,ZERO                                            /OUPT/      000000
00107     20*      C                                                                                    000000
00110     21*               COMMON /CCC/ GRAPH,JOUT,DEMAND                                            000000
00110     22*      C                                                                                    000000
00111     23*            DATA FUA/6HU CAL//,FUB/6HGRAM  /                                             000000
00114     24*            LOGICAL HP,SP,TP,VOL                                                         000000
00114     25*      C                                                                                    000000
00115     26*            IF (T(1) .LE. 0.0)  T(1) = 3800.0                                            000000
00117     27*            IOF = 0                                                                      000004
00120     28*         95 IOF = IOF+1                                                                  000006
00121     29*            OF = OXF(IOF)                                                                000011
00122     30*            CALL NEWOF                                                                   000013
00122     31*      C     SET ASSIGNED P OR VOLUME                                                     000013
00123     32*            DO 871 IP = 1,NP                                                             000015
00126     33*            PP = P(IP)                                                                   000035
00127     34*            VLM(NPT) = P(IP)                                                             000037
00127     35*      C     SET ASSIGNED T                                                    MOLIU016   000037
00130     36*            DO 871 IT = 1,NT                                                             000044
00133     37*            TT = T(IT)                                                        MOLIU017   000044
00134     38*            CALL EQLBRM                                                       MOLIU025   000046
00135     39*            IF (TT .GT. 0.0)  GO TO 800                                                  000050
00137     40*            IF (NPT .EQ. 0)  RETURN                                                      000053
00141     41*       800  ISV = 0                                                                      000061
00142     42*            IF (IP .EQ. NP .AND. IT .EQ. NT .OR. TT .LE. 0.0)  GO TO 860                 000061
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00144      430           ISV = NPT                                                                    000104
00145      440           IF(NPT.NE.13)  GO TO 870                                    MOLI0030         000104
00147      450       860 WRITE(JOUT,5)                                                                000111
00151      460         5 FORMAT(1H1,41X,48HTHERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNEDMOLI0032   000115
00151      470          1)                                                                           000115
00152      480           IF(.NOT.VOL)  GO TO 861                                                    000115
00154      490           IF (HP)  WRITE(JOUT,10)                                                    000117
00157      500        10 FORMAT(1HO,62X,7H VOLUME /)                                                000126
00160      510           IF (TP)  WRITE(JOUT,11)                                                    000126
00163      520        11 FORMAT(1HO,54X,22HTEMPERATURE AND VOLUME/)                                 000135
00164      530           IF (SP)  WRITE(JOUT,12)                                                    000135
00167      540        12 FORMAT(1HO,56X,18HENTROPY AND VOLUME/)                                     000144
00170      550           GO TO 862                                                                  000144
00171      560       861 IF(HP)  WRITE(JOUT,20)                                                     000146
00174      570        20 FORMAT(1HO,62X,10H PRESSURES  /)                                           000154
00175      580           IF(TP)  WRITE(JOUT,21)                                                     000154
00200      590        21 FORMAT(1HO,53X,24HTEMPERATURE AND PRESSURE/)                               000163
00201      600           IF(SP)  WRITE(JOUT,22)                                                     000163
00204      610        22 FORMAT(1HO,55X,20HENTROPY AND PRESSURE/)                                   000173
00205      620       862 CALL OUT1                                                                  000173
00206      630           WRITE(JOUT,863)                                                            000174
00210      640       863 FORMAT (25HOTHERMODYNAMIC PROPERTIES//)                                    000207
00211      650           IF(.NOT.VOL)  GO TO 864                                                    000207
00213      660           FMT(3) = ONE                                                               000211
00214      670           IF (.NOT. HP)  GO TO 864                                                   000213
00216      680           DO 63 I=1,NPT                                                              000220
00221      690           FMT(I+2) = TWO                                                             000220
00222      700           IF (I .EQ. 13)  FMT(15) = 5HF9.2)                                          000222
00224      710       63  V(I) = RBAR*HSUBU                                                         000227
00226      720           WRITE(JOUT,FMT) FUA,FUB,FB,(V(I), I = 1,NPT)                               000233
00237      730       864 CALL OUT2                                                                  000251
00240      740           CALL OUT3                                                                  000252
00241      750           IF (ISV .EQ. 0 .AND. IOF .EQ. NOF)  RETURN                                 000254
00243      760           IF(IDEBUG.GT.13)  IDEBUG=IDEBUG-13                                         000271
00245      770           WRITE(JOUT,868)                                                            000300
00247      780       868 FORMAT(1H1)                                                                000305
00250      790           IF(NI.EQ.1.AND.NP.EQ.1)  GO TO 95                                          000305
00252      800           NPT = 0                                                                    000321
00253      810       870 NPT = NPT + 1                                           MOLI0037         000323
00254      820           IF(.NOT.TP)  T(I)=TT                                                       000325
00256      830           IF(IP.EQ.1.AND.IT.EQ.1)  ISV=-ISV                            12-22         000331
00260      840           IF(NI.EQ.1)  GO TO 871                                       12-22         000342
00262      850           IF(IT.EQ.NT)  ISV=0                                                        000345
00264      860       871 CALL SAVE                                                                  000352
00267      870           GO TO 95                                                                   000357
00270      880           END                                                         MOLI0045         000405
END OF
```

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@FOR,S LEWIS.VARFMT,LEWIS.VARFMT
M.A.E.S -10/25/79-17:40:34 (7,)


   SUBROUTINE VARFMT    ENTRY POINT 000115


   STORAGE USED: CODE(1) 000124; DATA(0) 000023; BLANK COMMON(2) 000000

    COMMON BLOCKS:

    0003   OUPT    000073


   EXTERNAL REFERENCES (BLOCK, NAME)

    0004   NERR3$


   STORAGE ASSIGNMENT  (BLOCK, TYPE, RELATIVE LOCATION, NAME)

    0001   000006 I14G      0001   000046 40L       0001   000100 45L       0003   000002 FA        0003   000003 FAP
    0001   000005 FB        0003   000006 FC        0003   000007 FCP       0003   000012 FCST      0003   000014 FCV
    0001 R 000000 FFOUR     0003   000015 FG        0003   000017 FGE       0003   000020 FGV       0003   000021 FH
    0003   000023 FI        0003   000025 FIV       0003   000027 FM        0003 R 000031 FMT       0003   000050 FN
    0000 R 000001 FONE      0003 R 000052 FOUR      0003   000053 FP        0003   000054 FS        0003   000056 FSV
    0001   000057 FT        0000 R 000002 FTHREE    0003   000061 FTK       0000 R 000003 FTWO      0003   000063 FV
    0003   000065 FVEL      0000 R 000004 FZERO     0003   000001 F13       0003   000000 F9X       0000 I 000005 I
    0000   000012 INJP$     0003 R 000067 ONE       0003 R 000070 THREE     0003 R 000071 TWO       0003 R 000072 ZERO


C-83


0001      1*            SUBROUTINE VARFMT(V,NPT)                                                    000006
0001      2*      C                                                                                 000006
0003      3*            COMMON /OUPT/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),     /OUPT/  000006
0013      4*           1              FGE,FGV,FH(2),FI(2),FIV(2),FM(2),FMT(15),FN(2),FOUR, /OUPT/  000006
0013      5*           2              FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,   /OUPT/  000006
0013      6*           3              TWO,ZERO                                             /OUPT/  000006
0013      7*      C                                                                                 000006
0014      8*            DATA FFOUR/5HF9.4)/,FONE/5HF9.1)/,FTHREE/5HF9.3)/,FTWO/5HF9.2)/,          000006
0014      9*           1     FZERO/5HF9.0)/                                                       000006
0012     10*            DIMENSION V(1)                                                            000006
0012     11*      C                                                                                 000006
0015     12*            DO 45 I = 1,NPT                                                           000006
0016     13*            IF (I .GE. 13)  GO TO 40                                                  000006
0020     14*            FMT(I*2) = FOUR                                                           000012
0023     15*            IF (V(I) .GE. 10.0)  FMT(I*2) = THREE                                     000014
0025     16*            IF (V(I) .GE. 100.0)  FMT(I*2) = TWO                                      000022
0027     17*            IF (V(I) .GE. 1.0E4)  FMT(I*2) = ONE                                      000030
0031     18*            IF (V(I) .GE. 1.0E6)  FMT(I*2) = ZERO                                     000036
0032     19*            GO TO 45                                                                  000044
0032     20*       40   FMT(15) = FFOUR                                                           000046
0043     21*            IF (V(I) .GE. 10.0)  FMT(15) = FTHREE                                     000047
0045     22*            IF (V(I) .GE. 100.0)  FMT(15) = FTWO                                      000055
0047     23*            IF (V(I) .GE. 1.0E4)  FMT(15) = FONE                                      000063
```

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00141     24*           IF (V(I) .GE. 1.0E6)  FMT(15) = FZERO                    000071
00143     25*       45  CONTINUE                                                 000102
00145     26*           RETURN                                                   000102
00146     27*           END                                                      000123
END FOR

~BKPT PRINT$
```

1234567890123456789012345678901234567990123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890**SEQ NO. 04

* * * * * * UNIVAC 1100 TIME/SHARING EXEC ACCOUNT NUMBER * 1HPD013K0000 VER. CR 33R3HOST1 SITE * HOST 1 * * * * * *

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