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Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications

II. Users Manual and Program Description

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Chapter 1

Introduction

This is the second part of a two-part report describing the NASA Lewis Research Center's computer program CEA (Chemical Equilibrium with Applications). The program is used to obtain chemical equilibrium compositions of complex mixtures with applications to several types of problems. Part I (Gordon and McBride, 1994) states the various assumptions on which the calculations are based and analyzes the appropriate equations and mathematical methods for their solution. The equations describe the conditions for chemical equilibrium and for applications such as rocket performance, shocks, and detonations. The thermodynamic and thermal transport property data bases are also briefly described.

This second part is a users manual. Chapter 2 presents details for preparing input files. The format for input differs considerably from that used in earlier versions of the CEA program (Gordon and McBride, 1976; McBride et al., 1994). The output tables for various types of problems and options are described in chapter 3. Chapter 4 presents the overall modular organization of the program with information on how to make modifications. Chapter 5 presents information on the function of each subroutine. Error messages and their significance are discussed in chapter 6. Chapter 7 gives a number of examples that illustrate various types of problems handled by CEA and cover many of the options available in both input and output.

Seven appendixes are also included. Appendixes A to D give information on the thermodynamic data used in CEA. Appendix A gives the format for the thermodynamic data file *thermo.inp*, and appendix B lists species names contained therein. This file contains data in the form of least-squares coefficients for reactants as well as for products. Some of the reactant data are itemized in appendix C; references for these data appear in appendix D. Appendix E presents the format for thermal transport property data. Appendix F contains some information on common variables used in or generated by the equilibrium module discussed in section 4.6. Finally, appendix G lists the tabular output for the example problems discussed in chapter 7. The mathematical symbols used in this report are defined in Gordon and McBride (1994).

The CEA program consists of the following five files: the source program (*cea.for*), thermodynamic data (*thermo.inp*), thermal transport properties (*trans.inp*), sample problems (*cea.inp*), and *readme.txt*. After the *cea.for* file has been compiled, the unprocessed thermodynamic and transport property data should be processed once (see section 2.8). These processed data (in binary form) are stored in *thermo.lib* and *trans.lib*, where they remain available for future use in running problems. Additional information on the *thermo.inp* and *trans.inp* files is given in section 2.8 and appendixes A to E.

The CEA program was written in ANSI standard FORTRAN 77. CEA should work on any system with sufficient storage. There are approximately 6300 lines in the source code, which uses 225 kilobytes of memory. The compiled program takes 975 kilobytes. Input data bases *thermo.inp* and *trans.inp* use approximately 850 and 32 kilobytes, respectively; the binary forms *thermo.lib* and *trans.lib* take approximately 425 and 20 kilobytes, respectively. These storage requirements for the program and the data files may be easily adjusted as discussed in the following chapters.

Chapter 2

Description of Program Input

The CEA program requires two types of input. One type consists of files of thermodynamic data (*thermo.inp*) and thermal transport property data (*trans.inp*), which are common to all problems. These two files accompany the CEA program. The second type is input for the specific problem to be solved and is prepared by the user. The problem input consists of seven categories of input datasets. These seven datasets are in a general free-form format that was not used in previous versions of the CEA program (e.g., Gordon and McBride, 1976, or McBride et al., 1994). Most of the material in this chapter describes the general rules (see section 2.1) as well as details for preparing input datasets (see sections 2.2 to 2.7).

Thermo.inp and *trans.inp* are not in the free-form format because the data were generated by other programs (e.g., McBride and Gordon, 1992). Section 2.8 gives some information on processing these files before running specific problems. Because these files contain unprocessed thermodynamic and thermal transport data, we recommend that you first preprocess these files with the CEA program, which will store the data in binary form in two libraries called *thermo.lib* and *trans.lib* (see section 2.8). The CEA program will then use these processed libraries for all future runs. The prefixes *thermo* and *trans* in the input data files could have been any other names; they were selected to be consistent with the prefixes automatically assigned by CEA to the library files.

2.1 General Rules

The general rules for preparing input pertain to file names, keywords, types of variables, and delimiters.

2.1.1 File Names

All input files must be named with an arbitrary prefix and the suffix *.inp* (i.e., (*input prefix*)*.inp*). Output files for listing are automatically given the same prefix as the input file and the suffix *.out*. As an option, additional output files of columns of numbers can be obtained for plotting purposes. These files will also be given the same prefix and the suffix *.plt*.

2.1.2 Datasets

All useful program input is divided into sets of records called datasets. The first record of each dataset starts with a keyword. Records that start with the symbols "#" and "!" or totally blank records will be considered comments (i.e., they will be printed but not used).

2.1.3 Keywords

The keywords must be

1. The first nonblank characters in a record
2. All lower-case letters
3. A word that starts with one of the following sets of three or four letters: **prob, reac, only, omit, inse, outp, end, ther**, and **tran**. Additional characters may be used in the keywords but will be ignored by the program (e.g., **problem** is equivalent to **prob**). The last two keywords must begin records that precede formatted data bases. The first seven keywords precede data in CEA's free form.

2.1.4 Mandatory Keywords

There are three mandatory keywords for every problem. These words, with a brief description of any associated data, are as follows:

Keyword	Data
prob	Problem type and associated input (see section 2.4)
reac	Reactant names and associated input (see section 2.3)
end	No data. Keyword signals the end of the problem.

2.1.5 Optional Keywords

There are four optional keywords for every problem. Three are always followed by product species names typed exactly as used in the coefficients data base (see appendix B). The keywords are as follows:

Keyword	Data
only	Set of names of species that are the only ones to be considered in the problem
omit	Set of names of species that are to be omitted as possible products
inse	Set of names of condensed species to be tried (inserted) with gaseous species for initial equilibrium iterations
outp	Nonstandard options for output

2.1.6 Types of Variables

There are three types of variables, each limited to 15 characters. Additional characters will be ignored. The variables are as follows:

Type	Characteristics

Literal	First character is alphabetic.
	
	All initial characters are lower case, with three exceptions which follow:
	
	Chemical element symbols start with upper-case letters; the second letter may be either upper or lower case.
	
	Reactant names may start with either upper- or lower-case letters.
	
	Case (problem) identification may be either upper- or lower-case letters or numbers (see section 2.4.1).
	
	Sometimes the program checks for embedded lower-case character strings as well as initial character strings. For example, the symbol for pressure is p and the embedded string indicates the units.
	
	Examples:
	
	`p,bars`
	
	`p(bars)`
	
	`pressure:bars`

Numeric	Any legimate integer, decimal, or floating-point number
Species names	The set of characters used with the coefficient data bases to identify the species. These names never have embedded blanks, tabs, or equal signs because these characters are delimiters.

2.1.7 Delimiters

There are several delimiters for separating variables. These delimiters, which follow the variable, are as follows:

Delimiter	Variables separated
One or more blanks or tabs	Any variables (literals, numerics, or species names).
Equal sign	Literals (may be used in combination with blanks and tabs)
Comma	Numerics (may be used in combination with blanks and tabs)

Example:

```
problem   tp   p,atm=1,  2,3,   t= 3000 2000 1000,500
```

(Note that `p,atm` is one literal variable; commas separate only numeric variables.)

2.2 Specific Free-Form Variables for CEA Datasets

As discussed in the general rules, CEA input consists of datasets and comments. Comments start with either "#" or "!". Datasets start with keywords. Datasets in the free-form format that are headed by the keywords **reac**, **prob**, **end**, **only**, **omit**, **inse**, and **outp** are discussed here. (Note that when defining keywords and literals in the following sections, only the abbreviated character strings checked by the program are listed.)

Free-form datasets have the following order:

1. If the thermodynamic and transport data bases have not been processed, any free-form input must follow these data.

2. Datasets may be in any order, except for the **end** dataset, which must be the last record for any problem.

3. Variables or species names within a dataset may be in any order, with one exception in the **reac** dataset (see section 2.3.1). Also, any numerics associated with a literal variable must follow the literal.

2.3 Dataset reac

The **reac** dataset includes names and parameters for the reactants. It replaces the fixed-format REACTANT records of previous versions of the CEA program (e.g., Gordon and McBride, 1976, or McBride et al., 1994). The details for preparing a **reac** dataset are given in the following subsections.

Chemical species (products as well as reactants) are identified in two forms in the CEA program. One form may be a name or a conventional formula of the species (without

subscripts), such as `H2O` for water, `CH4` for methane, or `Air` for air. This form is discussed in section 2.3.2. The other form for identifying a species is referred to as the "exploded" form or formula and is discussed in section 2.3.6. Both forms are required in the CEA program and both forms are given in the thermodynamic data file, *thermo.lib*. The exploded formula may be specified directly in the **reac** dataset or obtained from *thermo.lib* if it contains the species. Some comparisons of these two ways are given in section 2.3.8.

Most types of problems require a value for the enthalpy (or internal energy) of the reactant mixture at some specified temperature. Energies are discussed in section 2.3.5; and temperatures, in section 2.3.4. As in the case for exploded formulas, enthalpies (or internal energies) may be specified in the **reac** dataset or optionally obtained from *thermo.lib*. Some comparisons of these two options for specifying energy are given in section 2.3.8.

2.3.1 Identification and Order

Each reactant and its parameters are identified by one of three sets of initial characters: `fu`, `ox`, and `na`. Each of these literal variables must precede the reactant name. All associated parameters follow the reactant name in any order. This information will be printed in the final tables. Summarizing, the reactant identifiers are

Initial characters	Data
`fu`	Fuel name followed by associated data
`ox`	Oxidant name followed by associated data
`na`	Name and data of reactant not identified as a fuel or oxidant. When `name` is used in any particular dataset, all reactants must use the `name` label.

Examples:

```
reac fuel Jet-A(L) ...
     oxid Air ...

reac name H2 ...   name O2 ...   name Ar ...
```

(Note that the ellipses represent additional input not shown here.)

2.3.2 Names of Reactants

Restrictions on names of reactants are as follows:

1. As many as 15 characters will be stored. The names must not contain any embedded blanks, tabs, or equal signs, since they are delimiters (see section 2.1.7). Upper-case letters are acceptable. The first character must not be a "+", "-", ".", or number.

2. Section 2.3.8 presents some examples using the option for obtaining the exploded chemical formula and the enthalpy (or internal energy) from *thermo.lib*. When this option is used, the input name must match exactly the name used in *thermo.inp*. These names are given in appendix B. (Note that the list in appendix B is current as of the date of publication of this report but is often added to.) For example, `Jet-A(L)` and `Air`

used in an example in section 2.3.1 are exactly the names required to identify these species (including upper- and lower-case letters). By contrast, names such as `jet-A(l)` and `air` are incorrect.

2.3.3 Relative Amount of Reactant

Amounts of oxidants are given relative to total oxidant, and amounts of fuels are given relative to total fuel. If reactants are not specified as fuels or oxidants, the amounts of reactants are relative to total reactant. All values must follow a literal with one of the initial characters `m` or `w` defined here:

Initial character	Data
m	Amount given in moles. In a particular dataset, if any reactant amount is given in moles, the other reactants must be given in moles as well.
w	Amount given in weight fraction or weight percent. Values for fuels are relative to total fuel. Similarly, values for oxidants are relative to total oxidant. If these values are not normalized, they will be normalized by the program.

Examples:

```
reac name O2 moles=.5, …   name H2 moles=1, …

reactant fuel CH4 wt%=30 …
         fuel C6H6 wt%=70 …
         oxid Air wt%=100 …
```

2.3.4 Reactant Temperature

For combustion problems (`hp`, `uv`, or rocket (`ro` or `rkt`)) a temperature must be specified for each reactant whose enthalpy or internal energy value is taken from the product or reactant thermodynamic data files. The temperature value follows a literal that starts with `t`. Units are indicated by one of the following embedded characters:

Embedded character	Temperature unit
k	Kelvin (default unit if not specified)
r	Rankine
c	Celsius
f	Fahrenheit

Example:

```
reac fuel ...   t,f=212 ...
     oxidant ...   t,r=672 ...
     fuel= ...   t,k=373, ...
```

2.3.5 Assigned Enthalpy or Internal Energy

For a number of problems (`hp`, `uv`, or rocket (`ro` or `rkt`), detonation (`det`), or shock (`sh`)), a value of enthalpy or internal energy must be assigned for each reactant whose value is not taken from *thermo.lib*. The symbols used to specify enthalpy or internal energy and the unit of energy are as follows:

Initial character	Value
h	Assigned enthalpy
u	Assigned internal energy

Embedded characters	Enthalpy or internal energy unit
c	Calories per mole
kc	Kilocalories per mole
j	Joules per mole (default unit if not otherwise specified)
kj	Kilojoules per mole

Examples:

```
reac fuel AA ...   h,cal/mol=123.    t,k=445 ...
     fuel BB ...   h,j/mol=-9996.3    t,r=100 ...
     oxid XX ...   h,kj/mol=556    t,r=1000 ...
```

Some additional examples are given in section 2.3.8.

2.3.6 Exploded Chemical Formula

For each reactant the CEA program requires the atomic symbols and their corresponding relative numbers (stoichiometric coefficients). This information must be part of the user's input when the thermodynamic data are not obtained from *thermo.lib*. The requirements for the exploded formula are as follows:

1. Atomic symbols must start with an upper-case letter. A second letter may be either upper or lower case.

2. Relative numbers may be either integers or fractions.

3. The exploded formula is required to be in the **reac** dataset for two situations:

   a. When the reactant name is not in *thermo.lib*

   b. When an enthalpy or an internal energy is given with the reactant input (see section 2.3.8)

   Examples (note that spaces are used to separate atomic symbols and numbers):

```
reac name Water-vapor H 2 O 1 …
     name Species-X Al 6 Si 4 O 9 …
     name Species-Y C 1 H 1.0769 …

reac oxid Air N 1.56168 O .419590 Ar .009365 C
     .000319 …
```

Some additional examples given in section 2.3.8 compare the options of specifying the exploded formula in the **reac** dataset or obtaining it from *thermo.lib*.

2.3.7 Density of Reactant

Calculating the density of the total reactant is an option. It will be calculated according to equations (9.12) and (9.13) in Gordon and McBride (1994) only if a density is given for each reactant in the current **prob** dataset. (Note that this information is not stored in the thermodynamic data library.) Each value follows a variable starting with the letters `rho`, with possible embedded characters to indicate units as follows:

Embedded characters	Density units
`kg`	Kilograms per cubic meter
`g`	Grams per cubic centimeter (default unit if `kg` is not specified)

Example:

```
reac fuel=B2H6(L)  rho,g/cc= .4371 …
```

2.3.8 Option To Use *thermo.lib*

The exploded chemical formula and either the enthalpy or internal energy for each reactant may be specified in the **reac** dataset or may be taken from *thermo.lib*. If either the exploded chemical formula or a required enthalpy (or internal energy) or both are missing for a reactant in **reac**, CEA will try to find the information in the library by using the reactant name. If a search for a species in *thermo.lib* is successful, the exploded formula and energy data for that species from the library will override any data that might be in the **reac** dataset.

Example (`tp` problem that does not require an enthalpy):

```
reac ox=O2 wt%=30
```

Since `O2` is in *thermo.lib*, the exploded formula will be taken from there.

Examples (all for an hp problem that requires an enthalpy for each reactant):

```
reac  ox O2  wt%=30
```

gives error message; a temperature must be specified.

```
reac  ox O2  wt%=30  t,k=300
```

obtains exploded formula and enthalpy (ENERGY/R=6.53777 K) from *thermo.lib*.

```
reac  ox=O2  wt%=30  t,k=300  h,j/mol=55
```

obtains exploded formula and enthalpy (ENERGY/R=6.53777 K) from *thermo.lib*. This is equivalent to 54.3584 J/mol. The value of h,j/mol = 55 in the **reac** dataset is overridden because the exploded formula for O_2 was not given.

```
reac  oxid O2  wt%=30  O 2  t,k=300  h,j/mol=55
```

uses data exactly as specified in the above **reac** dataset and does not take any information for this reactant from *thermo.lib*. Specifying a temperature is optional in this example.

```
reac  ox O2  wt%=30  O 3  t,k=300
```

overrides the exploded formula (given intentionally incorrect as O 3 in the above **reac** dataset) and obtains the correct exploded formula O 2 and ENERGY/R=6.53777 K from *thermo.lib*.

```
reac  ox O2(L)  wt%=30  t,k=88
```

selects the one enthalpy value in *thermo.lib* for O2(L) that corresponds to a temperature of 90.17 K, inasmuch as 88 K is within 10 K of the one *thermo.lib* temperature value of 90.17 K (see section 5.24).

```
reac  ox=O2(L)  wt%=30  t,k=78
```

gives a fatal error message, inasmuch as 78 K is more than 10 K from the *thermo.lib* value of 90.17 K (see section 5.24).

Giving the exploded formula and enthalpy, as illustrated in the fourth example above, is required when the reactant is not contained in *thermo.lib*. Otherwise, unless there is some special reason not to do so, we prefer to use the simple method of obtaining the reactant information from *thermo.lib*, as illustrated in the second example above. In chapter 7, which gives examples of a number of problems, most of the examples use this simple method.

2.4 Dataset `prob`

The dataset **`prob`** includes all the input parameters associated with any problem with the exception of reactant information discussed previously. Some of these parameters are required and some are optional.

2.4.1 Case Identification

Case identification is an optional literal or numeric variable that follows the word `case`. The case identification will be printed on the final tables. As mentioned in section 2.1.6 the case identification may start with a number or either an upper- or lower-case letter.

Examples:

```
case=150

case=example2

case  Example 2
```

(The last example is unacceptable because blanks are not allowed in literal variables.)

2.4.2 Problem Type

For every problem one and only one problem type must be specified. The initial characters for various types of problems are as follows:

Initial characters	Type of problem
`tp or pt`	Assigned-temperature and -pressure problem
`hp or ph`	Assigned-enthalpy and -pressure problem
`sp or ps`	Assigned-entropy and -pressure problem
`tv or vt`	Assigned-temperature and -volume (or density) problem
`uv or vu`	Assigned-internal-energy and -volume (or density) problem
`sv or vs`	Assigned-entropy and -volume (or density) problem
`ro or rkt`	Rocket problem
`sh`	Shock problem
`det`	Chapman-Jouguet detonation problem

2.4.3 Fuel-Oxidant Mixture Values

If the reactant amounts are not completely specified in the **reac** dataset, 1 to 26 numerical values may follow the following initial characters:

Initial characters	Values
%f	Percent fuel by weight
f/o or f/a	Fuel-to-oxidant weight ratios
o/f	Oxidant-to-fuel weight ratios
phi	Equivalence ratios in terms of fuel-to-oxidant weight ratios (eq. (9.19) in Gordon and McBride, 1994)
r	Chemical equivalence ratios in terms of valences (eq. (9.18) in Gordon and McBride, 1994)

Examples:

```
r,eq.ratio= .9, 1, 1.1, 1.5, ...
%fuel 40 50 60 ...
```

2.4.4 Option To Include Ionized Species

The parameter `ions` instructs the CEA program to consider ionized species as possible products.

Example:

```
problem hp  ions  case=20 ...
```

2.4.5 Options for Rocket Problems

The following options are available for `rocket` performance problems:

Initial characters	Option
`fac`	Assumes a finite-area combustion chamber, `fac`. If the area is not given, the CEA program will default to the infinite-area combustor assumption, `iac`.
`eq`	Assumes equilibrium composition during expansion.
`fr or fz`	Assumes frozen composition during expansion (not available with fac option).
`nfr or nfz`	Is followed by integer which is the column number for freezing composition. Default is 1 (the combustion point).
`dbg or deb`	Prints intermediate output for the fac chamber and throat iteration procedure.

Examples:

```
! Calculate rocket performance parameters assuming
! both equilibrium compositions during
! expansion and compositions frozen at the chamber
! composition.
!
  problem  rocket equilibrium frozen ...

prob rkt fac dbg ...
```

2.4.6 Options for Shock Problems

The following options are available for shock problems:

Initials characters	Option
`inc`	Calculate incident shock parameters.
`ref`	Calculate reflected shock parameters.
`eq`	Assume equilibrium compositions.
`fr or fz`	Assume frozen compositions.
`dbg or deb`	Print intermediate output for shock iteration procedure.

Examples:

```
# Calculate incident shock parameters assuming
# frozen compositions.
#
  prob  shock  inc  frz ...

problem shock  incident  frozen  equil reflected ...
```

2.4.7 Temperature Schedule

Assigned values of temperature are required for `tp` or `tv` problems and for initial values for the `det` problem. An assigned combustion temperature is optional for an `iac` rocket problem. From 1 to 26 numerical values may be assigned after the variable starting with `t`, with one of the following embedded characters to indicate units:

Embedded character	Temperature unit
k	Kelvin (the default unit if units are not specified)
r	Rankine
c	Celsius
f	Fahrenheit

Examples:

```
t,k= 3000,2000,1000 ...

t(r) = 2500 2000 ...

prob  tp  t(r)=2500,2000 500 ...

problem  detonation  t =298.15 500, ...
```

2.4.8 Pressure Schedule

A schedule of 1 to 26 numerical values for pressure is required for the following types of problems: `tp`, `hp`, `sp`, `ro` or `rkt`, `sh`, and `det`. These values of pressure follow the variable starting with `p`, with one of the following embedded character strings for units:

Embedded characters	Pressure units
bar	Bars (default unit)
atm	Atmospheres
psi	Pounds per square inch absolute
mmh	Millimeters of mercury

Examples:

```
prob  tp p,bar=1,10,50 ...

problem  rocket p(psia) 1000 500 ...
```

2.4.9 Specific Volume Schedule

A schedule of 1 to 26 numerical values of volume is required for the following types of problems: `tv`, `uv`, or `sv`. This schedule follows the variable starting with `v`, with one of the following embedded character strings for units:

Embedded characters	Volume units
`kg`	Cubic meters per kilogram
`g`	Cubic centimeters per gram (default unit if `kg` is not specified)

Examples:

```
problem  tv  v,cc/g= 9.e+05 8.e+05, 7.e+07, ...

problem  tv  v,m**3/kg=900,8.e+03, 7.e+04 ...
```

2.4.10 Density Schedule

A schedule of densities may be specified instead of specific volume for `tv`, `uv`, or `sv` problems (see section 2.4.9). This schedule consists of 1 to 26 numerical values that follow the variable starting with `rho`, with one of the following embedded character strings for units:

Embedded characters	Density units
`kg`	Kilograms per cubic meter
`g`	Grams per cubic centimeter (default unit if `kg` is not specified)

Examples:

```
problem tv rho,g/cc=9.e-05, 8.e-06, 7.e-07 ...

problem  tv  rho-kg/m**3= .09,8.e-03,7.e-04 ...
```

2.4.11 Assigned Enthalpy

Rocket or `hp` problems require enthalpies to be assigned. Enthalpies of individual reactants may be assigned in the **`reac`** dataset (see section 2.3.5), or enthalpies for the entire reactant mixture may be assigned in the **`prob`** dataset. In the latter case, enthalpies must be in

units of *h/R* [(g-mole)(K)/(g of mixture)]. This value will override any enthalpies that may be given in the **reac** dataset.

Example:

```
prob hp h/r=2345 ...
```

2.4.12 Assigned Internal Energy

The uv type of problem requires internal energies to be assigned for the mixture. These energies may be assigned in the **reac** dataset (see section 2.3.5), or internal energies for the entire reactant mixture may be assigned in the **prob** dataset. In the latter case, internal energies must be in units of *u/R* [(g-mole)(K)/(g of mixture)]. This value will override any internal energies that may be given in the **reac** dataset.

Example:

```
prob uv  u/r=1.935 ...
```

2.4.13 Assigned Entropy

The sv and sp types of problems require an entropy of the reactant mixture to be assigned. These entropies must be in units of *s/R* [g-mole/(g of mixture)].

Example:

```
prob sp  s/r=1.363 ...
```

2.4.14 Assigned Values for Shock Problems

Initial Mach numbers (mach) or incident shock velocities (u1) may be assigned for shock problems. Velocities are in units of meters per second. The number of assigned values for either Mach number or velocity is limited to the number of columns in the output (generally, 13 or 7). In any one particular problem, either parameter may be assigned but not both.

For each of these velocities, there is a corresponding pair of assigned initial temperatures and pressures. If the schedules of temperatures and pressures are not the same length as the u1 (or mach1) schedule, the last value of the t or p schedule will be used to fill in the missing values. Refer to example 7 in appendix G (or the first example below). For this case, seven u1 values, no t schedule, and two pressures are given in the **prob** dataset. With no t schedule, the temperature given with the reactants is used throughout. The first pressure is used for the first u1 value, and the second pressure is used for the remaining values. If there had been a t schedule, these values would be paired one to one with the initial pressure and velocity schedules. Again, if the t schedule is too short, the last t value will be used to fill in any missing values.

Examples:

```
!  EXAMPLE 7: ...
problem case=7  p,mmhg=10,20,  shock u1=1000,1100,
1200,1250,1300,1350,1400,  incd froz eql ...
```

```
prob case 21  shock incd eql mach1 = 3, 4, 5,
     t1k=298,320,340, p1bar= .01,.02,.03
```

2.4.15 Assigned Values for Rocket Problems

A number of variables are involved in rocket (`ro` or `rkt`) problems. Some are required for all such problems; others are optional. Some comments on the requirements follow:

1. One or more chamber pressures must be assigned. The assignments for chamber pressure follow the rules for pressure discussed in section 2.4.8.

2. Assigning chamber temperature is an option, and the rules for its assignment follow those for temperature discussed in section 2.4.7. (Note that, generally, temperature is not assigned for rocket problems but is determined from the enthalpies of the reactants.)

3. Exit conditions may be assigned either in terms of ratios of chamber pressure to exit pressure or exit area to throat area (see `pi`...`p`, `sub`, and `sup` in the table below).

4. For the `fac` option, an assignment must be made for either the contraction ratio (see `ac` below) or the ratio of the mass flow rate to the chamber area (see `mdot` below).

The initial characters and a brief description of the rocket variables follow:

Initial characters	Associated numerical values
p	Chamber pressure (see section 2.4.8)
pi...p	Ratio of chamber pressure to exit pressure (P_{inf}/P_e or P_{inj}/P_e), not assignable for chamber and throat (1 to 22 values). (Note that the second p in pi...p is embedded. For example, pip, pi/p, pinj/pe, etc.)
sub	Subsonic area ratios (1 to 13 values)
sup	Supersonic area ratios (1 to 13 values)
mdot or ma	For fac option, ratio of mass flow rate to chamber area, $(kg/s)/m^2$
ac	For fac option, contraction ratio (ratio of finite chamber area to throat area (A_c/A_t))
nfz or nfr	Option for freezing composition at the throat (nfz=2) or at a supersonic exit condition (nfz>2). The output table has equilibrium properties through point nfz and frozen thereafter. If nfz>2, only NCOL – nfz additional exit points are allowed (where NCOL is the number of columns in the output set in the FORTRAN PARAMETER statement, usually 7 or 13).
tcest	Initial chamber temperature estimate in units of kelvin. The default value is 3800 K. (Setting this variable may be necessary only when a condensed species has been inserted in an **inse** dataset and 3800 K is outside its temperature range.)
t	Assigned chamber temperature, an option (see section 2.4.7)

Examples:

```
prob  rocket pi/pe=3,10,30,300, p,psia=3000, froz
      tcest=1100 …

prob  rocket p,bar=50, subsonic,ae/at=5,
      supersonic,ae/at=10,20,100, nfz=2
      equilibrium frozen

problem  rocket fac  p,atm=50, ac/at=1.58,
         supar=25,50,75, pi/pe=10,100, …
```

2.5 Dataset outp

Tables of calculated results are discussed in chapter 3. The **outp** dataset contains several variables that permit some options in these tables. The variables `cal`, `short`, `deb` (or `dbg`), `massf`, and `plot` involve only the output. However, the variables `trac` and `tran` (or `trn`) involve some aspects of the calculation procedure as well. Examples are given in sections 2.5.2 and 2.5.8.

2.5.1 cal

The default unit for energy in the table output is joules. The variable `cal` calls for the output energy unit to be calories.

2.5.2 deb (or dbg)

The variable `deb` permits the printing of intermediate output, which is useful in debugging the iteration process for obtaining the equilibrium composition. The points for which this information is desired can be specified by listing the column numbers.

Examples:

```
outp  cal deb=5

output deb=1,4,6
```

For each iteration the data printed include matrix arrays for obtaining corrections to species compositions, current compositions, and corrections to current compositions. This information is printed for each iteration until either equilibrium or the maximum number of iterations permitted by the program is reached.

2.5.3 massf

Until recently, the CEA program permitted equilibrium product compositions in final output tables to be expressed only in terms of mole fractions. The `massf` option in the **outp** dataset now specifies that compositions in the final tables are to be given in mass fractions.

2.5.4 plot

The variable `plot` is to be followed by a list of properties and/or species names whose values are to be stored in the (*input prefix*).*plt* file in columnar rather than horizontal form. The columns of numerical data in E-format are stored in the order requested. No alphabetic information is stored in this file. The numerical values are in the same units as in the file (*input prefix*).*out*. Allowance is made for eight columns of mixture properties, including mole or mass fractions, with a maximum of 100 values in each column. If more data are required, more runs can be made. For properties, the initial letters and possible embedded characters are listed following `plot`. For mole or mass fractions (equilibrium only), the full name of each species must be used. (See appendix B for exact names to be used.) Note that the `plot` dump is not currently set up for shock problems. The following variables may be listed:

1. Thermodynamic properties—all problems except shock problems

Initial characters	Property
p	Pressure
t	Temperature
rho	Density
h	Enthalpy
u	Internal energy
g	Gibbs energy
s	Entropy
m	Molecular weight ($1/n$) (eq. (2.3a) in Gordon and McBride, 1994)
mw	Molecular weight (eq. (2.4a) in Gordon and McBride, 1994)
cp	Specific heat
gam	Gamma(s)
son	Sonic velocity

2. Thermal transport properties

Initial characters	Property
vis	Viscosity
cond	Equilibrium thermal conductivity from table of equilibrium properties
cond...fz	Thermal conductivity from rocket output tables assuming frozen composition during expansion. (Note that fz may be embedded anywhere after initial cond.)
pran	Equilibrium Prandtl number from table of equilibrium properties
pran...fz	Frozen Prandtl number from rocket output tables assuming frozen composition during expansion. (Note that fz may be embedded anywhere after initial pran.)

3. Rocket performance parameters—rocket problems only. The following codes are for data from the equilibrium tables. In order to get data from the frozen tables, an `fz` must be embedded in the word after the letters listed. Frozen compositions are the same as the compositions at the equilibrium freezing point and are therefore not dumped. When rocket output tables are more than one page long, the combustion and throat values are repeated for convenience on pages past the first. However, these repeated values are omitted in the (*input prefix*).*plt* file.

Initial characters	Property
`pip`	Pressure ratio, P_{inj}/P_e for `fac` problems and P_{inf}/P_e for `iac` problems
`pi/p`	Same as `pip`
`mach`	Mach number
`ae`	Area ratio, A_e/A_t
`cf`	Coefficient of thrust, C_F
`ivac`	Vacuum specific impulse, I_{vac}
`isp`	Specific impulse, I_{sp}

4. Chapman-Jouguet detonation parameters—detonation problems only. The following properties are for unburned gas and all require an embedded `1` after the initial letters:

Initial characters	Property
`son...1`	Sonic velocity
`gam...1`	Gamma
`h...1`	Enthalpy
`t...1`	Temperature
`p...1`	Pressure

The following strings may be embedded

Embedded characters	Property
`vel`	Detonation velocity (e.g., `detvel`)
`mach`	Mach number

2.5.5 short

The variable short permits printing only the input file, error messages, and final tables. Other information, such as atom ratios and a list of species being considered during the calculations, is suppressed.

2.5.6 trac

The option trac instructs the CEA program to print compositions of species with mole or mass fractions greater than or equal to the assigned trace value. When this option is used, the criteria for equilibrium composition convergence are tighter to ensure accuracy of the trace species. With this option, mole or mass fractions are printed in E -format.

2.5.7 tran

The option tran (or trn) instructs the CEA program to calculate thermal transport properties and add them to the output tables.

2.5.8 Examples of outp Datasets

Some examples of **outp** datasets that use the information discussed in the previous sections are as follows:

```
output  trace=1.e-10, calories transport short

outp debugcols=1,3

output  transport  plot=p t CO2 vis cond condfz

output trace=1.e-15  plot pi/p  h ivac N2   Ar cpfz
       gamfz

outp plot=t1  h1  sonic1 t h  detvel mach.number
     sonicvel
```

2.6 Options Involving Species To Be Considered

The **only**, **omit**, and **inse** datasets control which species are to be considered by the CEA program either in the current problem or in the current equilibrium composition iteration. If no **only** or **omit** datasets are included in the input for the current problem, all gaseous species in the product thermodynamic data file for the current chemical system will be considered as possible products. (See section 2.6.3 for information on consideration of condensed species.) All three datasets must contain species names exactly as given in the thermodynamic data file with no embedded blanks, tabs, or equal signs. A current list of these species names, which were extracted from *thermo.inp*, is given in appendix B. This list is continually updated.

2.6.1 Dataset `only`

The dataset **only** permits the user to list only those species names from the product thermodynamic data file, *thermo.lib*, that are to be considered in the current problem. Names must be exactly as given in the data file (appendix B) with no embedded blanks, tabs, or equal signs.

Example:

```
only Ar CO CO2 H2 H2O HNO HO2 NH NO  N2  O2  OH
```

2.6.2 Dataset `omit`

The dataset **omit** specifies which product species are to be omitted from consideration for the current problem. Species names must be exactly as given in the product thermodynamic data file, *thermo.lib* (appendix B), with no embedded blanks, tabs, or equal signs.

Example:

```
omit  C8H17,n-octyl C8H18,isooctane C8H18,n-octane
      C9H19,n-nonyl
```

2.6.3 Dataset `inse`

The dataset **inse** specifies which condensed species are to be included as possible products for the first point in the schedule of points for the current problem. Species names must be exactly as given in the product thermodynamic data file, *thermo.lib* (appendix B). This dataset is usually optional but occasionally may be required to obtain convergence.

Example:

```
insert  BeO(L)
```

2.7 Dataset `end`

There are no variables in dataset **end**. The keyword signals the end of input for a particular problem.

2.8 Thermodynamic and Thermal Transport Property Data Bases

Inputs for thermodynamic and thermal transport properties are exceptions to the free form. Generally, they are processed once before running particular problems, and the processed data are automatically saved for further use. The format for representing the thermodynamic data is given in appendix A, and the names of species in the *thermo.inp* file (see below) are given in appendix B. The format for thermal transport property data is given in appendix E. The following keywords start the text on the single records that precede these data bases:

Keyword	Data in succeeding records
ther	Unprocessed (formatted) thermodynamic data. This input file is called *thermo.inp*. CEA processes the data from *thermo.inp* and then automatically stores the processed (unformatted) data in a file named *thermo.lib* (see sections 4.3 and 5.24). After *thermo.inp* has been processed, it need not be processed again. However, if the user desires to make changes to the *thermo.inp* file, the new file must be processed. These changes might include adding, deleting, or updating species data or creating special sets of thermodynamic data for special purposes.
tran	Unprocessed (formatted) thermal transport property data. This input file is called *trans.inp*. CEA processes the data from this file and then automatically stores the processed (unformatted) data in a file named *trans.lib* (see sections 4.3 and 5.25). The file *trans.lib* is optional and is required only if thermal transport properties of the reaction mixture are desired. After `tran` has been called once, it need not be called again.

Chapter 3

Description of Program Output

The program prints five kinds of output: input data used to specify the problem, tables of results, output files for plotting purposes, information concerning iteration procedures, and other intermediate output. The latter three types of output are optional. Examples of problems that generate various types of data are given in chapter 7. The actual tabular outputs for these problems are given in appendix G.

3.1 Input Data

Input data are described in chapter 2. The general procedure used in the CEA program is to list the free-form input data as they are read in and before they are processed by the program. The purpose is to show, as clearly as possible, what is actually on the input records. All problems list the following input data:

1. Comments
2. The **prob** dataset
3. The **reac** dataset
4. The **outp** dataset (if present)
5. The **only** or **omit** dataset (if present)
6. The **inse** dataset (if present)
7. The **end** dataset

3.2 Intermediate Input Data

A number of items of intermediate input information are printed after the input datasets. This intermediate information is often useful for debugging, such as verifying that input data have been correctly interpreted by the CEA program. Printing this intermediate information is optional, however, and may be suppressed by using the option `short` in the **outp** dataset. Intermediate data that are related to input are discussed in the following subsections.

3.2.1 True/False Options

The listing of true/false options contains three lines of information regarding a number of program parameters that have been set "true" or "false" depending on the input data. The first line starts with the word OPTIONS:. The default value of all parameters is "false" with the exception of SIUNIT=T and TRACE=0.00000. The parameters include

1. Specifying the type of problem (TP, HP, SP, TV, UV, SV, DETN, SHOCK, or RKT), one of which has been set to "true"
2. In shock problems, specifying whether incident shocks (INCD=T) and/or reflected shocks are to be considered (REFL=T)
3. In rocket problems, specifying whether performance is to be calculated based on equilibrium composition during expansion (EQL=T) and/or frozen composition during expansion (FROZ=T)
4. Specifying whether ionized species are to be considered (IONS=T)
5. Specifying that energy unit is to be in calories in final tables (SIUNIT=F)
6. Specifying that intermediate information is to be printed during the iteration procedure for `fac` rocket problems (DEBUGF=T)
7. Specifying that intermediate information on shock iteration procedures is to be printed (SHKDBG=T)
8. Specifying that intermediate information on detonation iteration procedures is to be printed (DETDBG=T)
9. Specifying that thermal transport properties are to be calculated and printed in final tables (TRNSPT=T)
10. Specifying the value for the `trace` parameter for consideration of minor species. (The default value, TRACE=0.00000, instructs the program to print compositions in fixed format only for those species with mole fractions greater than 0.000005.)

3.2.2 Schedules of Assigned Values

These lines list the schedules of parameter values that were read in with the input, such as schedules of temperatures and pressures. For rocket problems, a list of assigned values of area ratios and/or pressure ratios is printed. For shock problems, a list of assigned Mach numbers or incident velocities is printed. For detonation problems, a list of initial temperatures and pressures is printed.

3.2.3 Reactant Information

The reactant information contained in the **`reac`** dataset is listed in columns to simplify checking the data, if necessary. Some of this information is repeated in the final output tables.

3.2.4 Species Being Considered

This set of species is preceded by the heading SPECIES BEING CONSIDERED IN THIS SYSTEM (CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES). The species listed are all those in *thermo.lib* that subroutine SEARCH has found to be contained in the current problem's chemical system. Each species in the list is preceded by some identification, such as J12/65. The J (or j) refers to JANAF data (Chase, 1985). The number refers to the month and the year in which the data were published or calculated (12/65 is December 1965). Other identification codes are discussed in McBride et al. (1993). Lower case codes indicate that data have been revised since McBride et al. (1993). These data were fitted with seven coefficients for C_p^o rather than five. If the original data are different, the identification code will be different.

3.2.5 Species With Thermal Transport Properties

If the option `tran` is included in the **`outp`** dataset, a list of species is printed for which thermal transport property data are contained in the *trans.lib* file. Also printed are those pairs of species for which binary interaction data are contained in the *trans.lib* file.

3.2.6 Enthalpies and Relative Atoms per Kilogram

After the list of chemical species is a listing of the enthalpies or internal energies of the total fuel and oxidant and the total reactant. These values are obtained, respectively, from the following equations in Gordon and McBride (1994): equation (9.6) or (9.8) multiplied by T and equation (9.7) or (9.9) multiplied by T. After this is a list of the kilogram-atom per kilogram of each element in the total fuel and oxidant (eq. (9.1)) and in the total reactant (eq. (9.5)).

3.3 Tables of Results

The final output of the program is in the form of tables that are designed to be self-explanatory. Although each problem has its own kind of table, all the tables have many features in common. These features are

1. Heading
2. Case identification
3. Reactant data
4. Proportion of oxidant to fuel
5. Density of reactant mixture if available
6. Thermodynamic mixture properties and derivatives
7. Thermal transport mixture properties (if `tran` is specified in the **`outp`** dataset)
8. Equilibrium composition (mole fractions or mass fractions)

3.3.1 Thermodynamic Mixture Properties

The following thermodynamic mixture properties and derivatives are printed for all problems: P, T, ρ, h, s, M $(1/n)$, $(\partial \ln V/\partial \ln T)_P$, $(\partial \ln V/\partial \ln P)_T$, c_P, γ_s, and a. The molecular weight MW is also printed when condensed products are present. Two sets of units are currently available for these properties. The default set is the SI set of units. This set is also obtained when `siunit` is specified in the **`outp`** dataset. The second set is a mixed set of units with energy in calories, temperature in kelvin, pressure in atmospheres, and velocity in meters per second. This set is obtained when `cal` is specified in the **`outp`** dataset.

3.3.2 Thermal Transport Mixture Properties

Thermal transport properties of the equilibrium mixture are optionally calculated and printed if the **`outp`** dataset contains the word `tran`. These properties are viscosity and two sets of values for specific heat, thermal conductivity, and Prandtl number. The two sets are based on the assumption of an equilibrium reaction contribution or no reaction contribution (frozen composition). As pointed out in section 5.2.3 of Gordon and McBride (1994), the equilibrium contribution to specific heat is obtained by different methods for the value given in section 3.3.1 and here. For mixtures consisting of gaseous products only, the two values will agree in most cases to all figures given.

3.3.3 Rocket Performance Parameters

In addition to the properties discussed in sections 3.3.1 ar d 3.3.2, the rocket problem (`rkt` or `ro`) lists the following rocket performance data: P_{inf}/P_e (for the `iac` model) or P_{inj}/P_e (for the `fac` model), Mach number, A_e/a_t, c^*, C_F, I_{vac}, and I_{sp}. For the `fac` model, the parameters P_{inj}/P_{inf} and either $\dot{m}/A_c$ or A_c/A_t are also listed. These parameters are discussed in chapter 6 in Gordon and McBride (1994).

3.3.4 Shock Parameters

In addition to the properties discussed in sections 3.3.1 and 3.3.2, the shock problem lists data discussed in chapter 7 of Gordon and McBride (1994). For incident shock waves, the parameters listed are M, u_1, u_2, P_2/P_1, T_2/T_1, M_2/M_1, ρ_2/ρ_1, and v_2. For reflected shock waves, the parameters are u_5, P_5/P_2, T_5/T_2, M_5/M_2, ρ_5/ρ_2, and u_5+v_2.

3.3.5 Chapman-Jouguet Detonation Parameters

In addition to the properties discussed in sections 3.3.1 and 3.3.2, this problem lists the following properties: P/P_1, T/T_1, M/M_1, ρ/ρ_1, Mach number, and detonation velocity. These parameters are discussed in chapter 8 of Gordon and McBride (1994).

3.4 Intermediate Output Data

The option of printing intermediate output (`deb` or `dbg` in the **`outp`** dataset) is provided primarily as a means of obtaining additional information for debugging. There is usually no point in using this option when the program is working well. We have used this option in the past for the following reasons:

1. To find programming errors

2. To study the iteration process and rate of convergence

3. To verify that thermodynamic data have been properly prepared

4. To study the test for inclusion of condensed species

3.4.1 Number of Iterations

The output discussed in this section is automatically printed for all problems (except shock problems) unless `short` is included in the **`outp`** dataset (see section 2.5.5). Following the data discussed in section 3.2.6 is a line containing the terms POINT, ITN, and T and the chemical symbols of the elements for the problem (for example 3 the elements are N, O, Ar, C, and H). The numbers under this heading are printed out after any current estimate converges during the course of the iteration process. The numbers under POINT refer to the columns of data in the final tables. (One exception to this, for the `fac` rocket problem, is discussed at the end of this section.) ITN gives the number of iterations required to converge to equilibrium composition for the current estimate; T is the final temperature for the current estimate. The numbers under the chemical symbols are values of π_i (see section 2.3.1 of Gordon and McBride, 1994). In general there is only one line for each point unless there has been an addition, deletion, or switching of phases of a condensed species (see discussion of example 5, section 7.3).

For rocket and detonation problems, more than one line may be printed for conditions other than a change in condensed species. For a rocket problem, these conditions are for the throat and for an assigned area ratio, where a line is printed out for each estimate of pressure ratio during the iteration process. For example, the four lines for point 6 of example 8, appendix G, which is for an assigned area ratio, show that four separate convergences were required to find the correct pressure ratio for the assigned area ratio. For each of points 7 to 9 two convergences were required. For the throat, additional information is given for pressure ratio and temperature estimates. For a detonation problem, a line is printed for each set of temperature and pressure estimates.

As mentioned earlier in this section, the `fac` rocket problem is an exception to the statement that numbers under the word POINT refer to the columns of data in the final output tables. Solving for the end of combustion chamber and throat conditions in the `fac` problem involves an iteration loop that temporarily includes a point labeled 2 and corresponds to an infinite-area combustor (see section 6.4 of Gordon and McBride, 1994). When this iteration loop is completed, the message END OF COMBUSTOR ITERATION is printed. The data with index 4 (end of combustion chamber) are transferred to index 2 and appear in column 2 in the output tables. Index 3 refers to throat conditions, as usual for the `fac` problem. The next point in the schedule of exit points is assigned as point 4 and corresponds to column 4 in the output tables as usual (see example 9, section 7.6.2).

3.4.2 Iteration Matrices and Compositions

An option is provided to list intermediate output concerning the iteration process for obtaining equilibrium compositions and temperatures. The intermediate data will be listed for all points specified by the parameter `debug` in the **`outp`** dataset as illustrated in example 14, section 7.10 and appendix G. The option `debug=5` given in the **`outp`** dataset instructs the program to list intermediate output for point 5.

After the first line, which gives the iteration number, is the iteration matrix corresponding to table 2.1 or 2.2 in Gordon and McBride (1994). The next line contains the words SOLUTION VECTOR and is followed by a line containing the chemical names of the current components. This line is followed by a line containing the solution vector to the matrix. The next line gives the current values of some parameters, that is, T, n (ENN), ln n (ENNL), P (PP), ln(P/n) (LN P/N), and the control factor λ (AMBDA). The next group of

lines contains information on the individual species used in setting up the preceding matrix and the values of corrections to compositions. Even though listed under the heading DEL LN NJ, these corrections are $\Delta \ln n_j$ only for gases but are Δn_j for condensed species. The corrections for gases are obtained from the matrix solution and equation (2.18) (for assigned-pressure problems) or equation (2.40) (for assigned-volume or -density problems) from Gordon and McBride (1994). In addition to these corrections the information on the individual species includes the chemical name or formula, n_j, ln n_j, dimensionless enthalpy (H0j/RT≡H_j^o/RT), dimensionless entropy (S0j/R≡S_j^o/R), dimensionless standard-state Gibbs energy (G0j/RT≡μ_j^o/RT), and dimensionless Gibbs energy (Gj/RT≡μ_j/RT). Following this is additional information pertaining to testing for condensed species, which is discussed in the next section.

3.4.3 Condensed-Phases Test

The test for condensed phases is made after every convergence for equilibrium compositions. Details of this convergence test are listed with other intermediate output as part of the debug option discussed in the previous section. After the data for the last iteration, information concerning each condensed species is given. This information consists of the name, the temperature interval for which thermodynamic data exist, and the current number of moles of the condensed species. For those species whose temperature interval bands the current value of temperature, the quantity given by equation (3.7) in Gordon and McBride (1994) (divided by the molecular weight of the species) is calculated and listed with the notation [(G0j – SUM(Aij*PIi)]/M. After all condensed species have been tested, only that species with the largest negative value as shown by MAX NEG DELTA G is included as a possible reaction species, and the iteration procedure is restarted. Dividing the quantity G0j – SUM(Aij*PIi) by molecular weight usually improves the chances of selecting an appropriate condensed species. The condensed-phases test is illustrated in example 14, section 7.10.

3.4.4 Derivative Matrices

The two derivative matrices (tables 2.3 and 2.4 in Gordon and McBride, 1994) and their solutions are also given for the fifth point of example 14, section 7.10. These derivative matrices are set up after the composition converges. The derivative matrix for derivatives with respect to temperature follows the notation T DERIV MATRIX and is followed by the notation SOLUTION VECTOR and a line containing the solution to the previous set of equations. The derivative matrix for derivatives with respect to pressure follows the notation P DERIV MATRIX and again is followed by the notation SOLUTION VECTOR and a line containing the solution to this matrix. Then several lines of output summarize the results for the point. The printed variables are labeled POINT, P, T, H/R, S/R, M, CP/R, DLVPT, DLVTP, GAMMA(S), and V. The corresponding FORTRAN symbols, defined in appendix F, are Npt, Ppp, Ttt, Hsum, Ssum, Wm, Cpr, Dlvpt, Dlvtp, Gammas, and Vlm, respectively.)

Chapter 4

Modular Form and Modification of Program

To facilitate adding or deleting applications of the program, CEA was organized into eight modules. These modules are concerned with general input, preprocessing of thermodynamic and thermal transport property data, additional input processing, four applications, equilibrium calculations, thermal transport property calculations, and output. The general flow of these modules and associated routines is given in figure 4.1.

A subroutine tree diagram is given in figure 4.2. From this diagram, as well as from figure 4.1, it is clear that, for example, the rocket application could be eliminated by omitting subroutines ROCKET, RKTOUT, and FROZEN and by omitting the statement that calls ROCKET in the main program.

This chapter gives the general purpose of each module. Some details of the individual routines are given in chapter 5.

4.1 Main Program and BLOCKDATA Module

Some details of the main program are described in section 5.1. Among other things, the main program contains all the OPEN and CLOSE statements and interactively calls for the standard input file. It also calls for the routines in two modules:

1. The general input module for processing input (see section 4.2)
2. The applications module for solving various types of problems (see section 4.4)

Flow returns to the main program after the completion of a problem or when a fatal error has occurred.

BLOCKDATA (see section 5.2) is loaded with the program and contains data, such as atomic weights, that remain constant for all problems.

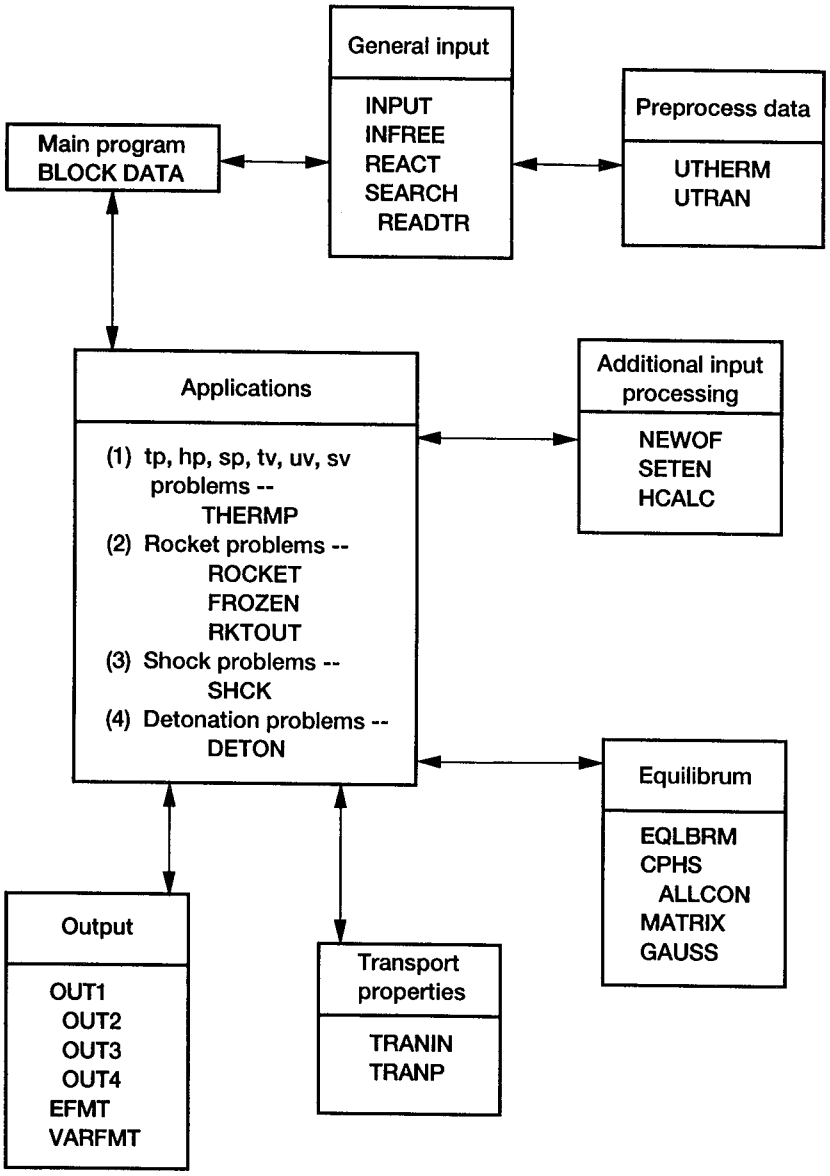

Figure 4.1.—Program modules.

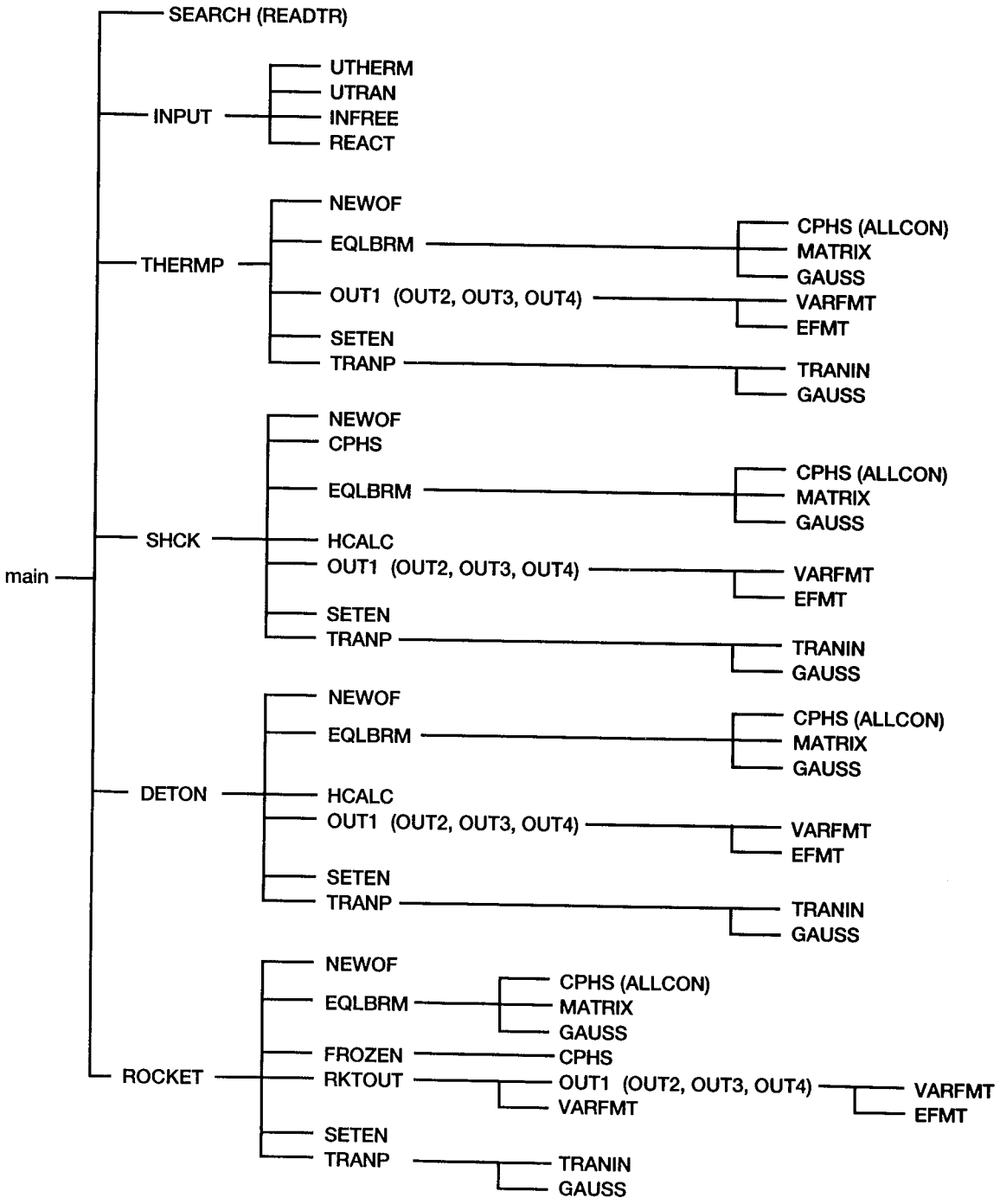

Figure 4.2.—Subroutine tree diagram.

4.2 General Input Module

The general input module contains four subroutines and an entry. The four subroutines and entry are INPUT, SEARCH, entry READTR, INFREE, and REACT. The first three are called from the main program to accomplish the following:

1. INPUT—to read and process input
2. SEARCH—to select the appropriate thermodynamic data for the current problem
3. READTR—to select the appropriate thermal transport property data for the current problem (if transport property calculations have been requested)

Subroutine INFREE is called by INPUT to convert the free-form input data to character and numerical variables. Subroutine REACT is called to process the reactants data. INPUT also calls UTHERM and UTRAN (described in the next section).

4.3 Data-Preprocessing Module

The data-preprocessing module consists of subroutine UTHERM to preprocess thermodynamic data and subroutine UTRAN to preprocess thermal transport property data. Subroutine INPUT calls these routines when it encounters the keywords `ther` and `tran`, respectively. UTHERM reads the formatted data from the *thermo.inp* file, processes the data, and stores the results in unformatted form in the *thermo.lib* file. Similarly, UTRAN reads the *trans.inp* file and stores the processed unformatted data in *trans.lib*. For any particular problem these libraries are searched for the appropriate data for the chemical system of the problem.

These routines have no other connection to the rest of the CEA program. They could be removed and run as separate programs simply for the purpose of preprocessing the thermodynamic and thermal transport property libraries.

4.4 Applications Module

The applications module contains the six subroutines THERMP, ROCKET, SHCK, DETON, FROZEN, and RKTOUT. The first four subroutines are called from the main program according to the type of problem specified in the **`prob`** dataset. The appropriate subroutine controls the flow of the program until the problem is completed, after which control is returned to the main program. These subroutines do the calculations unique to the problem type. They all call other subroutines in the four modules discussed in sections 4.5 to 4.8 and shown in figure 4.1. For rocket problems only, the other two routines are called from ROCKET (FROZEN for calculating rocket properties based on frozen composition and RKTOUT for printing output unique to rocket problems).

4.5 Additional Input-Processing Module

The application subroutines discussed in the previous section call the three subroutines in this input-processing module to accomplish the following purposes:

1. NEWOF—to adjust the initial variables that vary with assigned fuel-oxidant ratios. These variables include values of b_i^o, ρ_0, r, and either u_0'/R or h_0/R for each oxidant-to-fuel ratio. (The variables are defined in Gordon and McBride, 1994.)
2. SETEN—to obtain initial estimates for composition and temperature for a current point from a previously calculated point
3. HCALC—to calculate thermodynamic properties of the reactant mixture for shock and detonation problems only. Enthalpy is always calculated, but specific heat and entropy are calculated only if thermodynamic coefficients are available for the reactants.

4.6 Equilibrium Module

The equilibrium module calculates compositions and thermodynamic properties for a particular point Npt. The module is controlled by subroutine EQLBRM, which calls three subroutines and one entry:

1. CPHS—to calculate thermodynamic functions of the individual gaseous species with entry ALLCON for calculating thermodynamic functions of the individual condensed species
2. MATRIX—to set up the matrices as shown in tables 2.1 to 2.4 of Gordon and McBride (1994)
3. GAUSS—to solve the sets of equations represented by the matrices

Appendix F gives two tables of program variable definitions:

1. Table F1.—COMMON variables that must be initialized prior to entering the equilibrium module
2. Table F2.—COMMON variables that are calculated by the equilibrium module

4.7 Transport Properties Module

The transport properties module consists of two subroutines, TRANIN and TRANP, which are used only if the thermal transport option `tran` appears in the **`outp`** dataset. TRANIN is called from one of the applications routines for each point Npt after either the equilibrium or frozen thermodynamic properties of the mixture have been calculated. It selects the most abundant gases, reads in any data for these species from input/output unit

IOSCH, and estimates any missing data. It then calls TRANP to calculate the thermal transport properties of the mixture.

4.8 Output Module

The output module consists of the three subroutines, VARFMT, EFMT, and OUT1, with three entries, OUT2, OUT3, and OUT4. OUT1 lists data given in the **reac** dataset as well as o/f, %F, r, and ρ_0. OUT2 lists the properties $P, T, \rho, h, s, (\partial \ln V/\partial \ln P)_T$, $(\partial \ln V/\partial \ln T)_p$, c_p, γ_s, and a. (The variables are defined in Gordon and McBride, 1994.) OUT3 lists equilibrium mole or mass fractions of the reaction species. OUT4 lists the transport mixture properties η, λ, c_p, and Prandtl number.

Subroutine VARFMT is called from OUT1, OUT2, and OUT3, and subroutine EFMT is called from OUT2 and OUT3. VARFMT adjusts the number of decimal places in a variable format according to the size of the numbers. EFMT sets up a special E-format for printing density ρ and mole or mass fractions.

4.9 Modifications

Many users have modified various versions of the CEA program to meet their particular needs. These changes might include modifying one or more individual subroutines; adding or deleting an entire application; changing dimensions, such as for the number of species or the number of points permitted in a problem; and adding or deleting species to the thermodynamic data file, *thermo.inp*, or the thermal transport property data file, *trans.inp*.

4.9.1 PARAMETER Statements

Some changes concerning dimensions or assignment of input/output units are facilitated by the use of PARAMETER statements. The variables in these statements are defined as follows:

Parameter	Variable for which maximum number is set
MAXNGC	Species that can be considered in any problem. For condensed species, each temperature interval of a species counts as a separate species.
MAXNG	Gaseous products that can be considered in any problem
MAXNC	Condensed-species temperature intervals that can be considered in any problem. The number of intervals may be considerably greater than the number of condensed species.
MAXTR	Gaseous products that can be considered in any problem in thermal transport property calculations
MAXEL	Elements that can be considered in any problem
MAXMAT	Rows permitted in the composition iteration matrix
MAXR	Reactants permitted in a **reac** dataset
NCOL	Columns of data that can be printed on a page

The numbers to which these parameters are set depends to a large extent on the nature of the problems to which the CEA program is applied. Currently, for the large-scale computer version of CEA, we are using slightly larger numbers than the largest number required in any of many problems that we have run with the program. These numbers for most present-day computers and for smaller capacity computers are as follows:

Parameter	Computer	
	Large scale	Small scale
MAXNGC	600	300
MAXNG	400	200
MAXNC	300	200
MAXTR	50	40
MAXEL	20	15
MAXMAT	50	40
MAXR	24	24
NCOL	13	7 or 8

The names and current assigned values of input/output units in the parameter statements are as follows:

Input/output unit	Current value	File type	Contents
IOSCH	13	Unformatted	Scratch file for processing thermodynamic and thermal transport property data
IOTHM	14	Unformatted	*thermo.lib* (thermodynamic property data)
IOPLT	15	Formatted	(*input prefix*).*plt* file of numerical parameters dumped for plotting purposes
IOTRN	18	Unformatted	*trans.lib* (thermal transport property data)

4.9.2 Changing Number of Possible Reaction Products

The parameters involved with increasing or decreasing the number of possible products are MAXNGC, MAXNC, and MAXNG. We have found that the numbers set for these parameters for the small-scale version (see previous section) accommodate most problems. However, depending on the user's requirements, these numbers may be reduced considerably more, if so desired. Inasmuch as a single gaseous species requires more than 100 storages, reducing MAXNG by 300 saves more than 30 000 storages.

4.9.3 Eliminating an Application

Any application module may be removed simply by removing the statement calling the controlling subroutine (THERMP, ROCKET, SHCK, or DETON) and then removing the subroutine (or subroutines) in the application module. The calling statements are near the end of the main program.

4.9.4 Adding an Application

An application may be added by means of the following steps:

1. Giving the new type of problem a logical name
2. Revising subroutine INPUT to include all new input variables
3. Programming an applications module (see section 4.4)
4. Calling the module in the main program when the problem name variable is "true" after the input data have been processed in INPUT

Chapter 5
Routines

The CEA program consists of a main program, BLOCKDATA, 24 subroutines, and 5 entries. The function of each of these is described in this chapter. Most of the program variables mentioned in these sections are in labeled COMMON.

5.1 Main Program

Generally, the main program performs the following functions:

1. It uses the OPEN and CLOSE statements to define all input/output (I/O) unit numbers and corresponding files for the entire program. The standard input file uses I/O unit 5. All input data files are required to have the suffix *.inp*. The standard output file uses I/O unit 6 and has the suffix *.out* added to the input file prefix. Four other input/output units are used with numbers defined in PARAMETER statements. See section 4.9.1 for a description of these files.

2. It uses some interactive statements to read input files and to define output files.

3. It calls subroutine INPUT to read and process data from the input file through an **end** dataset or the end-of-file.

4. It calls subroutine SEARCH to read and store thermodynamic data from *thermo.lib* appropriate to the current chemical system processed in the input.

5. It calls entry READTR in subroutine SEARCH if the option `tran` is included in the **outp** dataset. Thermal transport data are read in READTR from input/output unit IOTRN, and data selected for the current chemical system are stored on input/output unit IOSCH.

6. It sets the initial composition estimates as follows:

   a. Enn—total number of moles per gram of mixture=0.1

   b. En(j,1)—number of moles of species j per gram of mixture

      =0.1/Ng for gases (where Ng is the number of gases)

      =0 for condensed species

7. It inserts any condensed species for consideration that appears in an **inse** dataset.

8. It calls either THERMP, ROCKET, SHCK, or DETON according to the problem type found in the **prob** dataset.

5.2 BLOCKDATA

BLOCKDATA contains the following types of data:

1. Fundamental constants (Cohen, 1987)

2. Data for the chemical elements

3. Initial setup for the variable format array Fmt

The chemical symbols for the elements are stored in the Symbol array; the atomic weights (Anon., 1995), in the Atmwt array; and the valences, in the Valnce array.

The variable format Fmt is used to adjust the number of decimal places in the output variables according to the sizes of the numbers. The format is also used to print a label and from 1 to NCOL associated numbers. NCOL is set by a PARAMETER statement to be the number of columns of output (generally, 7 or 13 depending on the paper width). The labels contain 15 characters.

5.3 Subroutine CPHS

5.3.1 General

Subroutine CPHS is called from subroutines SHCK and EQLBRM. For an assigned temperature Tt, it calculates thermodynamic properties of individual species by using equations (4.9) to (4.11) from Gordon and McBride (1994). These dimensionless properties are for heat capacity, enthalpy, and entropy, respectively. For gaseous species, subroutine CPHS uses one of three sets of coefficients: Coef(j,i,1) for the temperature interval Tg(1) to Tg(2); Coef(j,i,2) for the interval Tg(2) to Tg(3); and Coef(j,i,3) for the interval Tg(3) to Tg(4). The index j (j=1,Ng) refers to the jth gaseous species among the Ng gaseous species being considered in the current chemical system, and the index i (i=1,9) refers to the ith coefficient. At present the four Tg temperatures in the CEA program are 200, 1000, 6000, and 20 000 K. The calculated properties are stored in the COMMON arrays Cp, H0, and S, respectively.

5.3.2 Entry ALLCON

Subroutine CPHS has an entry ALLCON that calculates the properties of condensed-phase species. ALLCON is called from subroutine EQLBRM. ALLCON calculates thermodynamic properties of all condensed-phase species by using equations (4.9) to (4.11) from Gordon and McBride (1994). Properties are calculated for the current temperature Tt by using the coefficients stored in the Cft(jj,i) array (see section 5.18). The index i is for the ith coefficient, and jj is for the temperature interval (jj=1,MAXNC). The temperature intervals are stored in the Temp(2,jj) array. The calculated properties for molar heat capacity,

enthalpy, and entropy are dimensionless and stored in COMMON arrays Cp, H0, and S, respectively.

5.4 Subroutine DETON

Subroutine DETON does the calculations required to obtain Chapman-Jouguet detonation properties as described in chapter 8 of Gordon and McBride (1994). Detonation calculations are limited to gaseous reactants. When initial temperatures are given in the **prob** dataset, subroutine HCALC is called to get the thermodynamic properties of the initial mixture. If the reactant is not found in *thermo.lib*, an error message will be printed. When there is only one initial temperature, it may be specified in either the **prob** or **reac** dataset. In the latter case, if the enthalpy corresponding to the initial temperature is known, it may be included in the **reac** dataset. We usually prefer to specify the initial temperature or temperatures in the **prob** dataset unless the reactant species is not included in *thermo.lib*.

5.5 Subroutine EFMT

Subroutine EFMT (E-format) is called from entries OUT2 and OUT3. It writes statements in a special exponent form. This form is similar to the standard FORTRAN E-format, but the letter E and some of the spaces have been removed for compactness. It is used to write density and mole or mass fractions with the `trace` option.

5.6 Subroutine EQLBRM

Subroutine EQLBRM is the executive routine for calculating equilibrium compositions and mixture properties for point (output column) Npt. It is called from one of the application routines THERMP, SHCK, DETON, or ROCKET. Subroutine EQLBRM, in turn, calls subroutines CPHS, MATRIX, and GAUSS. Before calling EQLBRM, several variables will have already been set, such as the type of problem, the assigned or initial estimated values of the thermodynamic states for the problem, and initial estimates of composition. The COMMON variables that need to be set before entering EQLBRM are tabulated in appendix F (table F.1).

The iteration procedures used in subroutine EQLBRM are described in chapters 2 and 3 of Gordon and McBride (1994). The COMMON variables that are set in EQLBRM for output purposes are given in appendix F (table F.2).

5.7 Subroutine FROZEN

Subroutine FROZEN is called from ROCKET to calculate the temperature and thermodynamic properties for the following assigned theoretical rocket performance conditions:

1. Composition frozen at either combustion (Nfz=1), throat (Nfz=2), or any downstream point (Nfz>2)

2. An assigned exit pressure (Pp)

3. An assigned entropy equal to the entropy at combustion conditions (Ssum(1))

The iteration procedure used for obtaining the exit temperature is discussed in section 6.5 of Gordon and McBride (1994).

If a temperature is reached that is 50 K below the range of a condensed combustion species (Temp(1,j) to Temp(2,j)), calculations are stopped. Then, Tt is set to zero and control is returned to ROCKET where a message is printed and data for all preceding points are listed.

5.8 Subroutine GAUSS

Subroutine GAUSS is called from subroutine EQLBRM to solve the set of simultaneous linear iteration equations constructed by subroutine MATRIX. It is also called from subroutine TRANP to solve the simultaneous linear equations needed to obtain the mixture thermal transport properties. The simultaneous equations are solved by using a modified pivot technique to perform a Gauss reduction. In this modified pivot technique, only rows are interchanged. The row to be used for eliminating a variable is selected on the basis that the largest of its elements, after division by the leading element, must be smaller than the largest elements of the other rows after division by their leading elements.

The solution vector is stored in X(k). In the event of a singularity, Msing is set equal to the number of the first singular row. Msing is tested later in subroutine EQLBRM. In addition, Imat (which is equal to the number of rows) is set equal to Imat – 1.

5.9 Subroutine HCALC

Subroutine HCALC calculates thermodynamic properties for gaseous reactants in shock and detonation problems. It is called from subroutines SHCK and DETON only when there is a `t` schedule in the **`prob`** dataset. If the reactants are species that are included in the first part of *thermo.lib* (containing data for products), the thermodynamic coefficients will have already been stored in the common variable Coef(j,i,k), and these coefficients will be used to obtain the required thermodynamic properties. If the coefficients are in the last part of *thermo.lib* (reserved for reactants only), *thermo.lib* will be searched for the appropriate coefficients. If found, they will be stored at the end of the data already stored in the Coef array. The first index in this array indicates the species number. For the reactants these numbers are stored in the Jray array for future use. Subroutine HCALC also calculates the properties of the reactant mixture. The mixture properties h_0/R, c_0/R, and s_0/R (eqs. (9.7), (9.21), and (9.22), respectively, in Gordon and McBride, 1994) are stored in Hsub0, Cpmix, and Ssum(Npt), respectively, for the current temperature Tt.

5.10 Subroutine INFREE

Subroutine INFREE is called from subroutine INPUT. It reads, writes, and analyzes input for a complete dataset. As many as 132 characters are read and sorted for each record. The record is just printed without further analysis if the characters are all blanks and tabs or if the first nonblank or nontab character is a "#" or an "!". Character strings are formed by concatenating the characters between one or more special characters defined to be delimiters (see section 2.1.7). These strings are stored in the call-vector character array Cin. Variables starting with a "+", a "-", or an integer are assumed to be numeric. Other Cin variables are assumed to be literal.

Delimiters can be any consecutive combination of blanks and tabs. Other delimiters are an equal sign following a literal variable and a comma following a numerical variable. Numerical variables are converted to double-precision variables and stored in the Dpin array. The variables in the call vector are defined as follows:

Variable	Description
Code	Cin(1) assumed to be the keyword
Readok	Logical variable that is set to "false" when either there is an error in reading a record or a keyword is not found
Cin	Character strings between delimiters. As many as 15 characters are stored. Additional characters are ignored.
Ncin	Number of variables stored in Cin
Lcin	Integer array giving information about corresponding variable in Cin as follows: 1. If Cin(i) is literal, Lcin(i) gives the number of characters with a negative sign. 2. If Cin(i) is numeric, Lcin(i) gives the index of the previous literal.
Dpin	Array with numerics in Cin converted to double precision
Ndp	Integer giving the number of double-precision numbers in Dpin

5.11 Subroutine INPUT

Subroutine INPUT calls subroutine INFREE, which deciphers the characters in the free-form input. (See subroutine INFREE, section 5.10, for definitions of the call-vector variables.) It then checks for keywords. The data corresponding to the keywords are processed and stored as follows:

1. For the keywords **only**, **inse**, and **omit**, species names are stored in the COMMON variables `Prod`, `Ensert`, and `Omit`, respectively.

2. For the keywords **outp**, **reac**, and **prob**, the dataset information stored by subroutine INFREE in the Cin, Lcin, and Dpin arrays is examined, and the required COMMON data are stored.

3. For the keyword **reac**, subroutine REACT is called for further processing the **reac** data.

4. For the keyword **prob**, the literals that do not have associated numerical data are sorted and stored first. The numerical data are then analyzed and stored.

5. For the keywords **thermo** and **tran**, subroutines UTHERM and UTRAN are called, respectively, to process and convert the thermodynamic and thermal transport data to unformatted form.

6. For the keyword **outp**, if plotting parameters are listed, the input/output unit IOPLT is opened, and numerical data corresponding to the parameters are dumped as a (formatted) text file to input/output unit IOPLT. The file contains no alphanumeric information. Data that are generally listed horizontally in the standard output are listed vertically in this file. This file is named with the same prefix as the standard input but with the suffix *.plt*.

7. For the keyword **end**, after some additional processing, control is transferred to the main program.

5.12 Subroutine MATRIX

Subroutine MATRIX is called from subroutine EQLBRM to set up an appropriate matrix corresponding to one of tables 2.1 to 2.4 in Gordon and McBride (1994). These matrices are set up for the following purposes:

1. The matrix in table 2.1 corresponds to the iteration equations for determining equilibrium compositions for the following assigned-pressure problems:

   a. `tp` (assigned temperature and pressure) (`Tp=.TRUE., Vol=.FALSE.`)

   b. `hp` (assigned enthalpy and pressure) (`Hp=.TRUE., Vol=.FALSE.`)

   c. `sp` (assigned entropy and pressure) (`Sp=.TRUE., Vol=.FALSE.`)

   The logical variable Convg is "false" for these three problems.

2. The matrix in table 2.2 corresponds to the iteration equations for determining equilibrium compositions for the following assigned-volume (or -density) problems:

   a. `tv` (assigned temperature and volume or density) (`Tp=.TRUE., Vol=.TRUE.`)

   b. `uv` (assigned internal energy and volume or density) (`Hp=.TRUE., Vol=.TRUE.`)

   c. `sv` (assigned entropy and volume or density) (`Sp=.TRUE., Vol=.TRUE.`).

   These matrices are initially set up like those in table 2.1, and then, where necessary, elements of the matrices are corrected to match table 2.2. The logical variable Convg is false for these three problems.

3. The matrix in table 2.3 corresponds to the equations for calculating derivatives with respect to the logarithm of temperature at constant pressure. The logical variables are set

the same as for the matrices of tables 2.1 and 2.2 except for setting Convg=.TRUE. and Pderiv=.FALSE.

4. Similarly, the matrix in table 2.4 corresponds to the equations for calculating derivatives with respect to the logarithm of pressure at constant temperature. The logical variables are set the same as for table 2.3 except for Pderiv=.TRUE.

The elements in the matrices (G(i,j)) are generally summations of properties of product species. The matrix is cleared and then filled by two DO loops—one for gases (j=1,Ng) and one for condensed species (k=1,Npr). The appropriate contribution of each species is summed into the matrix elements.

5.13 Subroutine NEWOF

Subroutine NEWOF combines the properties of total oxidant and total fuel (calculated either in subroutine REACT or subroutine HCALC) for a particular oxidant-to-fuel ratio to give properties for the total reactant. NEWOF is called from either THERMP, ROCKET, SHCK, or DETON for each mixture ratio that was set in subroutine INPUT (Oxf array). The total reactant properties are calculated by using equations (9.5) to (9.22) from Gordon and McBride (1994). Values of $b_i^{(2)}$, $b_i^{(1)}$, and b_i^o (eqs. (9.1) and (9.5)) are printed for all problems. For problems with an assigned pressure, values are printed out for $h^{(2)}/R$, $h^{(1)}/R$, and h_0/R (eqs. (9.6) and (9.7) multiplied by T). For problems with an assigned volume or density, values are printed out for $(u')^{(2)}/R$, $(u')^{(1)}/R$, and u_0'/R (eqs. (9.8) and (9.9) multiplied by T). The initial value of the Size variable discussed in section 3.2 of Gordon and McBride (1994) is set in NEWOF. Adjusting Size for the value of Bratio is also done in this routine.

5.14 Subroutine OUT1

Subroutine OUT1 and entries OUT2, OUT3, and OUT4 write statements in the final output tables that are common to all problems. They are called from subroutines THERMP, ROCKET, DETON, and SHCK. Subroutine OUT1 writes the following information:

1. Case name or number
2. Reactant names and properties
3. Mixture values (oxidant-to-fuel ratio, percent fuel, and the two equivalence ratios defined in equations (9.18) and (9.19) of Gordon and McBride, 1994)
4. Reactant densities (if values are included in the input)

5.14.1 Entry OUT2

Entry OUT2 writes the final tables of the thermodynamic mixture properties and stores any requested plot data in the Pltout array. These variables and their corresponding labels are printed horizontally across the page with a variable format. Some format adjustments are made by calling subroutines VARFMT and EFMT. The maximum number of

columns of data on a page will vary depending on how the NCOL parameter is set in the PARAMETER statements. For wider paper, NCOL=13 works well. For 8 1/2x11-in. paper NCOL=7 works well.

The data that are dumped into the Pltout array are in the same units as the labeled listed data. They are listed vertically, however, rather than horizontally and there is no alphabetic output. The columnar data are in the same order as requested in the **outp** dataset. The Pltout array is dimensioned for eight parameters, each with 100 values. Mole or mass fractions may also be dumped into Pltout (see section 5.14.2).

5.14.2 Entry OUT3

Entry OUT3 writes product species names and equilibrium mole or mass fractions for the final tables. If any product names are listed for plotting, their mole or mass fractions will be dumped into the Pltout array in columns rather than in the horizontal form shown in the tables. All species are listed that have mole or mass fractions for at least some of the assigned conditions which are either greater than 5×10^{-6} or greater than the `trace` value if `trace` is given in the **outp** dataset. Unless the `short` output option has been specified, the names of the species with mole or mass fractions less than this amount for all assigned conditions will be listed at the end of the table. With the `trace` option, subroutine EFMT is called for printing mole or mass fractions in an E-format in order to retain more figures.

5.14.3 Entry OUT4

Entry OUT4 writes the values of thermal transport mixture properties in the final tables and also stores any of these properties that are requested for plotting purposes. The comments in the last paragraphs of sections 5.14.1 and 5.14.2 pertaining to number of columns and dumping for plotting purposes apply to transport properties as well.

5.15 Subroutine REACT

Subroutine REACT is called from subroutine INPUT to further process reactant data. Subroutine REACT does the following for each reactant:

1. Searches the *thermo.lib* file for a species with the same name as the reactant if one of the following is true:

   a. The exploded formula is missing.

   b. An assigned enthalpy value is missing for a rocket or `hp` problem.

   c. An assigned internal energy value is missing for a `uv` problem.

   For the case where *thermo.lib* has data for only one temperature (usually a transition point or 298.15 K), the temperature given in the input must be within 10 K of the *thermo.lib* value. Otherwise, the program will print a fatal error message. Some examples are given in section 2.3.8.

2. Calculates the enthalpy or internal energy from the coefficients in *thermo.lib* for (1b) or (1c) above.

3. For each new chemical element for the current problem, obtains the following data from BLOCKDATA (section 5.2) and stores them in their corresponding arrays: chemical

symbol in Elmt, atomic weight in Atwt, and valences in temporary storage. These valances are then used to calculate plus-and-minus valances for both total fuel and total oxidant that are stored in Vpls and Vmin (see eqs. (9.14) and (9.15) in Gordon and McBride, 1994).

4. Calculates the molecular weights of total oxidant $M^{(1)}$ and total fuel $M^{(2)}$ and stores values in the Am array (see eq. (9.10) in Gordon and McBride, 1994).

5. Determines if the reactant is labeled `oxid`, `fu`, or `na`. Reactants labeled `na` and `fu` are treated alike during further processing. Program variables relating to oxidants or fuels are indexed 1 for oxidants and 2 for fuels.

6. Adds the reactant contribution to the total oxidant or total fuel properties (see chapter 9 of Gordon and McBride, 1994).

If there are several reactants labeled `fu` or `na`, their properties are combined into properties of a total fuel by using the relative proportion of each fuel given in the **`reac`** dataset. Labeled oxidant species are also combined. These total fuel and oxidant values are later combined with oxidant-to-fuel ratio values in subroutine NEWOF to obtain total reactant properties. Equation (9.12) in Gordon and McBride (1994) gives the density of total oxidant $\rho^{(1)}$ (Rh(1)) and total fuel $\rho^{(2)}$ (Rh(2)). If any one of the densities used in equation (9.12) is zero, Rh(1)=Rh(2)=0.

5.16 Subroutine RKTOUT

Subroutine RKTOUT is called from ROCKET. It is the control program for writing the final output tables for rocket problems. It calculates various rocket performance parameters from previously calculated and stored thermodynamic mixture properties. It also stores any requested plot data involving rocket performance in the Pltout array. It calls subroutine OUT1 and entries OUT2 and OUT3 to write output common to all problems. The rocket parameters are printed with the variable format Fmt described in section 5.2.

5.17 Subroutine ROCKET

Subroutine ROCKET is the control program for rocket performance calculations described in chapter 6 of Gordon and McBride (1994). It is called from the main program if the problem type `rkt` or `ro` is included in the **`prob`** dataset. Subroutine ROCKET selects the appropriate iteration scheme for the assigned combustion chamber model `fac` or `iac`. It obtains the required thermodynamic properties for equilibrium performance by calling subroutine EQLBRM. For frozen performance, subroutine ROCKET calls subroutine FROZEN to obtain the required thermodynamic properties. It calls subroutine TRANP to obtain thermal transport properties if `trn` or `tran` has been included in the **`outp`** dataset.

The assignment of parameters for various points in the rocket problem is handled by various loops. An outer loop calls NEWOF for each new value of oxidant-to-fuel ratio. Another loop assigns chamber pressures. Within this loop are other loops for assigned exit conditions. For the exit conditions, assigned pressure ratios, if any, are processed first; then, assigned subsonic area ratios, if any; and finally, assigned supersonic area ratios, if any.

Subroutine RKTOUT is called for preparing output tables when either a page is filled (Npt=NCOL) or all exit points have been calculated for equilibrium compositions first and then for frozen compositions.

5.18 Subroutine SEARCH and Entry READTR

Subroutine SEARCH is called from the main program to search the *thermo.lib* file for thermodynamic data of possible products appropriate for the current chemical system. Data for all these species will be stored for consideration except for two situations:

1. When an **only** dataset specifies the species to be considered
2. When an **omit** dataset specifies the species to be omitted

For those selected species, the names are stored in the Prod(j) array, where j is the species index; the stoichiometric coefficients (index i) are stored in the A(i,j) array; and the thermodynamic coefficients (index i) are stored in the Coef(j,i,k) array for gases (where k is the temperature interval index) and in the Cft(j,i) array for condensed species. Since gases precede condensed species in *thermo.lib*, their names come first in the Prod(j) array. These names have a limit of 15 characters. The data for reactants only, which appear in *thermo.lib* after the data for all the products, are not stored in subroutine SEARCH but are stored in subroutine REACT. For condensed species, the name (including the phase), as well as the thermodynamic coefficients, is stored for each temperature interval. The total number of these stored condensed species names or temperature intervals is Nc. Therefore, the total number of stored names Ngc, including gases and condensed species, is Ngc=Ng + Nc. (Ngc is also the total number of gaseous species and condensed-phase temperature intervals.) Since the maximum values of Ng and Nc are MAXNG and MAXNC, respectively, the thermodynamic coefficients are dimensioned Coef(MAXNG,9,3) and Cft(MAXNC,9). If the `short` option is not used, the names in the Prod array are listed along with the date code stored with the data in *thermo.lib*.

If `tran` has been included as an option in the **outp** dataset, entry READTR is called from the main program to read thermal transport properties from *trans.lib* (stored on input/output unit IOTRN). Data for species with the same names as contained in the thermodynamic property data (Prod(j)) are stored in a scratch file IOSCH (I/O unit 13) for use in calculating mixture properties. Additional processing of thermal transport properties is discussed in section 5.22.

5.19 Subroutine SETEN

Subroutine SETEN is called from an application subroutine such as THERMP, SHCK, DETON, or ROCKET. It has several functions, all of which are concerned with saving some information from a completed calculation for subsequent use in later calculations. The primary purpose is to have reasonably good initial composition estimates for new points.

These estimates for the next point Npt come from either the point just completed Isv or some other previous point. The flow of the routine is directed by Isv as follows:

1. Isv positive—transfers compositions for the point just completed for use as initial estimates for the next point (transfer En(j,Isv) to En(j,Npt))
2. Isv negative—makes Isv positive and saves values of Enln(j) for gases and En(j,Isv) for condensed phases in Sln(j), Enn in Ensave, Ennl in Enlsav, Ttt(Isv) in tsave, and Lsave in lsav. (These values are saved because they are to be used as initial estimates for some future point and they may be overwritten in the meantime.) Values in En(j,Isv) are transferred to En(j,Npt). If the Isv point has two included condensed phases of the species, the indices for these species will be Jliq (for the higher temperature phase) and Jsol (for

the lower temperature phase). For this situation, En(Jliq,Isv) is combined with En(Jsol,Isv) and En(Jliq,Isv) is excluded. This procedure usually helps in obtaining convergence for the next point and other future points that start with the saved estimates.

3. Isv zero—uses the data previously saved (as discussed in (2) above) as initial estimates for the current point.

5.20 Subroutine SHCK

Subroutine SHCK is the application module for shock problems. It is called from the main program and calls the following subroutines: NEWOF, CPHS, EQLBRM, HCALC, OUT1, OUT2, OUT3, OUT4, SETEN, and TRANP. When initial temperatures are given in the **prob** dataset, subroutine HCALC is called to get the thermodynamic properties of the initial mixture. It calculates the shock parameters discussed in chapter 7 of Gordon and McBride (1994). For every assigned mixture, subroutine SHCK calculates properties for as many as NCOL assigned initial velocities or Mach numbers. NCOL is the number of columns in the output listing—generally, 7 or 8 for 8 1/2×11-in. paper and 13 for wider computer paper. Depending on the input options specified in the **prob** dataset, it calculates incident shock conditions based on equilibrium compositions after shock and/or based on compositions frozen at initial conditions. It also calculates, on the basis of specified options, frozen and/or equilibrium reflected shock conditions relative to the equilibrium and/or frozen incident shock conditions.

5.21 Subroutine THERMP

Subroutine THERMP is called from the main program to execute `tp`, `hp`, `sp`, `tv`, `uv`, and `sv` problems. Since EQLBRM calculates equilibrium compositions and mixture properties for one point at a time (see sections 2.3 and 2.4 of Gordon and McBride, 1994), THERMP sets up the necessary parameters for each point. This involves all combinations of oxidant-to-fuel ratios for all problems; assigned pressures for `tp`, `hp`, and `sp` problems; assigned volumes (or densities) for `tv`, `uv`, or `sv` problems; and either the estimated or assigned temperatures for all problems.

These parameters are assigned by means of three nested DO loops. The outermost loop is the Nof array of oxidant-to-fuel ratios. For each of these ratios, subroutine NEWOF is called to obtain the reactant mixture properties. The next loop is for the Np assigned pressures or volumes. Finally, the innermost loop is for temperature. For `tp` and `tv` problems, there are Nt assigned temperatures. For `hp`, `sp`, `uv`, and `sv` problems, Nt=1 and the initial temperature estimate for the first point is 3800 K. Succeeding initial estimates for new points are taken from the results of previous points. Subroutine EQLBRM is called in the temperature loop. Following the EQLBRM call, subroutine TRANP is called to calculate thermal transport properties if the `tran` option was included in the **outp** dataset. The initial estimate routine SETEN and the output routines OUT1, OUT2, OUT3, and OUT4 are called at appropriate times.

5.22 Subroutine TRANIN

Subroutine TRANIN is called from subroutine TRANP for each point to perform the preliminary steps for calculating thermal transport properties of the current mixture.

TRANIN first determines which species have the largest mole fractions. It next reads in the properties for these largest individual species and binary interactions containing these species from input/output unit IOSCH, estimates missing data, and eliminates species unimportant for transport property calculations. Subroutine TRANP then solves the necessary equations to obtain the thermal transport mixture properties.

Some processing accomplished in TRANIN is as follows:

1. For shock problems with the frozen composition option, mole fractions of the reactants are calculated and their thermal transport data are stored.

2. The En array is searched for atomic gases and species whose mole fraction is greater than 1×10^{-11}. The indices of the selected species are stored in the Ind array, with indices for the atomic gases stored first, followed by indices of other species stored generally in order of largest species first. A maximum of MAXTR species is allowed, where the number for MAXTR is set in a PARAMETER statement.

3. Mole fractions are recalculated by using only the compositions of the selected species.

4. Stoichiometric coefficients from the A array are copied into the Stc array in order to express them as a set of chemical reaction equations as required in equation (5.10) of Gordon and McBride (1994).

5. Thermal transport properties from input/output unit IOSCH are read in for the selected set of species. IOSCH is a scratch unit with properties for species appropriate to the current chemical system. IOSCH was written in entry READTR (subroutine SEARCH).

6. Estimates for thermal transport properties are made for those selected species for which no data exist in IOSCH. For neutral species, the estimating formula is

$$\overline{\Omega}_{jj}^{(2,2)} = \ln\left(\frac{50M_j^{4.6}}{T^{1.4}}\right)$$

This formula is a slightly modified version of equation (39) of Svehla (1973). It is used in equation (7c) in Svehla (1973) to obtain viscosity. For ionized species or ion-neutral pairs, estimating formulas were taken from Gupta et al. (1990).

5.23 Subroutine TRANP

Subroutine TRANP calculates mixture thermal transport properties as described in Gordon and McBride (1994). It is called only if the term `tran` has been included in the **`outp`** dataset in the standard input file. In that case, it is called for every point from one of the application routines, namely DETON, ROCKET, SHCK, or THERMP. Subroutine TRANIN is called to read in or estimate thermal transport property data for pure species or pairs of species. The reaction contribution to thermal conductivity and heat capacity involves solving sets of simultaneous linear equations. The matrix elements for these equations are calculated in subroutine TRANP, and subroutine GAUSS is called to solve the equations.

5.24 Subroutine UTHERM

Subroutine UTHERM is called from subroutine INPUT after the keyword **thermo** is read. UTHERM reads thermodynamic data from *thermo.inp*, which is a formatted (text) standard input file (i.e., input/output unit 5). For the most part, the data are in the form of least-squares coefficients as discussed in section 4.2 of Gordon and McBride (1994).

Data are stacked in *thermo.inp* in the following order:

1. Keyword **thermo**
2. Temperature intervals for the gaseous species
3. Sets of data for the gaseous product species
4. Sets of data for the condensed product species
5. END PRODUCTS record
6. Data for reactants only

The format for these data is given in appendix A. When subroutine INPUT reads the keyword **thermo** in the main program, it calls subroutine UTHERM to process the thermodynamic data that follow and to store them for further use in unformatted form in the *thermo.lib* file (input/output unit IOTHM). Input/output unit IOSCH is a scratch unit that is used in connection with the processing of the thermodynamic data. UTHERM sorts and counts the number of species sets. The sorting process stores all gaseous species ahead of all condensed species. The total number of gaseous species is stored in Ng, and the total number of condensed-phase temperature intervals is stored in Nc. (Note that each condensed-phase temperature interval is counted as a separate species.) The index Ngc contains the sum of the other two indices (i.e., Ngc=Ng + Nc). The current CEA program allows for three temperature intervals for gaseous species and a variable number of intervals for condensed phases. The standard set of gaseous species data that accompanies the CEA program is divided into the following three temperature intervals: 200 to 1000 K, 1000 to 6000 K, and 6000 to 20 000 K. However, most gaseous products exist in negligible amounts above 6000 K, and therefore no thermodynamic data are provided for the highest temperature interval for most of the species. During the iteration process, to obtain equilibrium compositions in the highest temperature interval, it may be necessary to have the missing thermodynamic data, at least temporarily, in order to obtain convergence. Subroutine UTHERM estimates these missing data by means of a straight line for C_p. The equation for the straight line is generated from the values of C_p at 6000 and 20 000 K, using the classical value at infinity for the value at 20 000 K.

The data for reactants are stored after the data for gaseous or condensed products. For some reactants, thermodynamic data (in the form of coefficients) are given over a temperature range. For other reactants, only one assigned enthalpy value is given at some specified temperature (usually 298.15 K or some transition temperature). For example, for O2(L), only one enthalpy value is given (at the boiling point of 90.17 K).

Any set of thermodynamic data needs to be read in and processed only once. If changes are made to the data, by adding, removing or changing data for various species, the new set will need to be read in. (However, data for one or more species may also be omitted from consideration during any particular run without reading in a new dataset by the use of the **omit** and **only** input datasets.)

5.25 Subroutine UTRAN

Thermal transport property data (viscosity and thermal conductivity) are read as formatted data from standard input (i.e., input/output unit 5). The data are in the form of least-squares coefficients as discussed in chapter 5 of Gordon and McBride (1994). Subroutine UTRAN processes these data and stores them for further use in unformatted form in the *trans.lib* file (input/output unit IOTRN). Input/output unit IOSCH is a scratch unit that is also used in processing the transport property data. Subsequently, in entry READTR (subroutine SEARCH), transport data for the current chemical system under consideration are stored in input/output unit IOSCH.

5.26 Subroutine VARFMT

Subroutine VARFMT (variable format) is called from entry OUT2 and subroutine RKTOUT. It adjusts the number of decimal places printed in F-format in the variable format Fmt according to the size of the number. It is used for P_{inf}/P_e or P_{inj}/P_e, P, and A_e/A_t. The variable format is described in section 5.2.

Chapter 6

Error Messages

This chapter contains a list of error messages and warnings and some discussion concerning them. The messages are grouped in alphabetical order within each subroutine in which they appear. The name of the subroutine is given in parentheses at the end of each message.

6.1 DETON Message

CONSERVATION EQNS WERE NOT SATISFIED IN 8 ITERATIONS (DETON)

Fatal error. Conservation equations for the detonation problem usually converge in three or four iterations. The program limits the number of iterations to eight, although we have never run a problem that required this many iterations. Therefore, we have not yet seen this message printed. If the message were to be printed, the program would skip to the next problem.

6.2 EQLBRM Messages

CALCULATIONS STOPPED AFTER POINT (number) (EQLBRM)

If a fatal error occurs in subroutine EQLBRM, this message will be printed, output tables for any completed points will be printed, and control will be returned to the main program, which continues with the next problem, if any.

(Number of) CONVERGENCES FAILED TO ESTABLISH SET OF CONDENSED SPECIES (EQLBRM)

Fatal error. The CEA program will attempt to obtain the correct set of condensed species up to 3 x Nlm times, where Nlm is the number of chemical elements in the system. If the program is unsuccessful after this number of attempts, this message will be printed as well as the previous message.

DERIVATIVE MATRIX SINGULAR (EQLBRM)

If singularities occur in the matrix solutions, they generally occur first in the iteration matrices and the program does not get as far as the derivative matrices. However, it is possible for the iteration matrix to just barely avoid being singular and for the derivative matrix to be

singular. When this occurs, this message is printed, Dlvpt is set equal to –1, Dlvtp is set equal to 1 (see appendix F for definitions), and the program continues.

DID NOT CONVERGE ON ELECTRON BALANCE (EQLBRM)

Fatal error. As discussed in section 3.7 of Gordon and McBride (1994), a special iteration procedure is used for ions. For all problems tried, this procedure has been successful in meeting the convergence criterion for ions. In the event convergence is not reached, this message is printed as well as the first EQLBRM message.

(Number of) ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS FOR THE POINT (Number) (EQLBRM)

Fatal error. The maximum number of iterations permitted to obtain convergence is either 50 + Ns/2 if `trace` is included in the **`outp`** dataset or 50 otherwise. Generally, convergence is obtained in considerably fewer iterations. The number 50 + Ns/2 was somewhat arbitrarily selected to indicate that, if convergence has not been reached by that number, the problem probably will not converge at all. This situation occurs rarely. When it occurs, this message is printed, as well as the first EQLBRM message. If the cause of nonconvergence is not obvious from the output, it may be helpful to rerun the problem with intermediate output. An examination of this output often pinpoints the source of the difficulty.

LOW TEMPERATURE IMPLIES A CONDENSED SPECIES SHOULD HAVE BEEN INSERTED. RESTART WITH `insert` DATASET (EQLBRM).

Fatal error. This message can occur only for an `hp` or `uv` problem. It occurs only when the omission of an important condensed reaction product causes the program to seek a combustion temperature that is unrealistically low ($T < 100$ K). When this occurs, the message is printed as well as the first EQLBRM message.

REINSERTION OF (name of species) LIKELY TO CAUSE SINGULARITY (EQLBRM)

Fatal error. In the process of inserting and removing condensed species, the program may attempt to insert a condensed species that it had just removed during the previous iteration cycle. To prevent a possible infinite cycle, this message is printed as well as the first EQLBRM message.

SINGULAR MATRIX, ITERATION (number) VARIABLE (number) (EQLBRM)

This message is printed whenever a singularity occurs during the matrix solution. As discussed in section 3.6 of Gordon and McBride (1994), several procedures are used in special singularity situations to obtain convergence. If none of the special techniques resolve the problem, the first EQLBRM message is also printed.

THE TEMPERATURE = (degrees K) IS OUT OF RANGE FOR POINT (number) (EQLBRM)

Except for the shock problem, this message is printed whenever the converged temperature for the indicated point is outside the temperature range read in on the second record of the *thermo.inp* file. This temperature range, which at present is 200 to 20 000 K, is the one over which some of the gas-phase thermodynamic data have been fitted. Generally,

the thermodynamic data can be extrapolated a short distance without much loss in accuracy. However, to prevent large errors due to extrapolation, the current temperature Tt is not permitted to be less than a factor of 1.5 below the lowest temperature in the range or more than a factor of 1.25 above the highest temperature in the range. If temperature is outside these limits, then after the above message has been printed, the first EQLBRM message is also printed.

TRY REMOVING CONDENSED SPECIES (EQLBRM)

As discussed in section 3.6 of Gordon and McBride (1994), several techniques are tried to obtain convergence after a singularity has occurred. This message is printed under the following circumstances: a singularity has occurred, the technique of adding small quantities of species to resolve the singularity has failed, and at least one condensed species is among the species currently being considered in the calculations. The CEA program then removes the first condensed species in the current array and makes another attempt at convergence.

WARNING! POINT (number of point) USES A REDUCED SET OF COMPONENTS. SPECIES CONTAINING THE ELIMINATED COMPONENT ARE OMITTED. IT MAY BE NECESSARY TO RERUN WITH INSERTED CONDENSED SPECIES CONTAINING COMPONENT (name of eliminated component) (EQLBRM)

After a component has been eliminated, it may be impossible to test for the possible presence of other condensed species containing the eliminated component. For this situation, as suggested by the message, it may be desirable to rerun with an insert of the condensed species to be considered.

WARNING!! RESULTS MAY BE WRONG FOR POINT (number) DUE TO LOW MOLE FRACTION OF GASES (value of molar gas fraction) (EQLBRM)

As discussed in section 2.2 of Gordon and McBride (1994), the equation of state for gases is assumed to be correct even when small amounts of condensed species (up to several percent by weight) are present. When the mole fraction of gases is less than 0.0001, the program prints this warning message and continues.

6.3 FROZEN Message

FROZEN DID NOT CONVERGE IN 8 ITERATIONS (FROZEN)

Rocket calculations based on frozen composition during expansion generally require from one to four iterations to reach convergence for each assigned point. We have not yet encountered a problem that required eight iterations. This error message was included primarily as a precaution to avoid infinite cycling of the iteration loop in the event of a machine error. The CEA program continues after printing this message.

6.4 HCALC Messages

COEFFICIENTS FOR (name of reactant) ARE NOT AVAILABLE (HCALC)

Fatal error. Reactant has thermodynamic data for only one temperature. Since shock and detonation problems permit more than one temperature in the temperature schedule, thermodynamic coefficients are needed to calculate thermodynamic properties. Control is returned to the main program, which continues with the next problem, if any.

REACTANT (name of species) NOT FOUND IN *thermo.lib* (HCALC)

Fatal error. Reactant was not found in the thermodynamic library, *thermo.lib*. Check for possible errors in reactant name. If the data are not in the library, the problem may still be run if all necessary information is given in the **reac** dataset. Control is returned to the main program, which continues with the next problem, if any.

REACTANTS MUST BE GASEOUS FOR THIS PROBLEM (HCALC)

Fatal error. Subroutine HCALC is used only for those detonation and shock problems for which reactants must be gaseous. Control is returned to the main program, which continues with the next problem, if any.

6.5 INFREE Messages

FATAL ERROR IN INPUT FORMAT (INFREE)

The CEA program was unable to decipher the line of input preceding this message. If it occurs, control is returned to the main program, which terminates further calculations.

WARNING!! UNACCEPTABLE NUMBER (value of number) (INFREE)

An illegal numerical variable was found. Possibly alphabetical characters were mixed with numbers. The variable is ignored and the program continues.

6.6 INPUT Messages

ERROR IN REACTANTS DATASET (INPUT)

Fatal error. This error, which is described in the printed message preceding this one in the listing, occurred when the CEA program was trying to process data in subroutine REACT. The following error message is also printed. Control is returned to the main program, which continues with the next problem, if any.

FATAL ERROR IN DATASET (INPUT)

Fatal error. This error is described in the printed message preceding this one in the listing.

MOLES AND WEIGHT PERCENTS SHOULD NOT BE MIXED (INPUT)

Fatal error. For each problem, reactant amounts should be given in terms of either all moles (all number of moles, all mole fractions, or all mole percents) or all weights (all weight fractions or all weight percents), but not in both moles and weights. The second INPUT error message is also printed, and control is returned to the main program, which continues with the next problem, if any.

REACTANT AMOUNT MISSING (INPUT)

Fatal error. The amount of a reactant (moles or weight) is missing. The second INPUT error message is also printed, and control is returned to the main program, which continues with the next problem, if any.

REACTANT TEMPERATURE MISSING (INPUT)

Fatal error. A numerical value is not given following a literal that starts with the letter `t` in the **`reac`** dataset. The second INPUT error message is also printed, and control is returned to the main program, which continues with the next problem, if any.

TYPE OF PROBLEM NOT SPECIFIED (INPUT)

Fatal error. The variable indicating the type of problem in the **`prob`** dataset was not recognized by the CEA program. The second INPUT error message is also printed, and control is returned to the main program, which continues with the next problem, if any.

UNABLE TO PROCESS EQUIVALENCE RATIO = (number) (INPUT)

Fatal error. The program is unable to convert equivalence ratio to oxidant-to-fuel ratio. Possibly, an oxidant is not labeled as an oxidant or a fuel is not labeled as a fuel. The second INPUT error message is also printed, and control is returned to the main program, which continues with the next problem, if any.

WARNING!! A KEYWORD IS MISSING (INPUT)

Program continues.

WARNING!! DID NOT RECOGNIZE (name of variable) (INPUT)

A literal variable in the dataset just processed was not recognized by the CEA program. The program ignores this variable and continues.

WARNING!! LITERAL EXPECTED FOR (name of variable) (INPUT)

A number was found instead of the literal that was expected for this variable in the **reac** dataset. This value is ignored and the program continues.

WARNING!! (atomic symbol) NOT RECOGNIZED (INPUT)

The program was unable to decipher the exploded chemical formula in the **reac** dataset. The species is ignored and the program continues.

6.7 REACT Messages

AMOUNT MISSING FOR REACTANT NO. (reactant number) (REACT)

Fatal error. The amount of reactant in the **reac** dataset is missing. Control is returned to the main program, which continues with the next problem, if any.

DATA FOR (name of reactant) NOT FOUND IN *thermo.lib* (REACT)

Fatal error. The CEA program was not able to match the name given in the **reac** dataset with a name from *thermo.lib*. If the exploded chemical formula of a reactant is not included in the dataset or if a required enthalpy or internal energy value is missing, the thermodynamic library *thermo.lib* will be searched for data for that reactant. The error message is printed if the search is unsuccessful. Control is returned to the main program, which continues with the next problem, if any.

(symbol of chemical element) NOT FOUND IN BLOCKDATA (REACT)

Fatal error. The symbol for a chemical element in the exploded formula of a reactant in the **reac** dataset was not found in BLOCKDATA. Control is returned to the main program, which continues with the next problem, if any.

T= (value of temperature) K MORE THAN 10 K FROM (value of temperature) FOR (name of species) (REACT)

Fatal error. For reactants in *thermo.lib*, where there is an assigned enthalpy and corresponding temperature but no thermodynamic coefficients, the temperature given in the **reac** dataset must be within 10 K of the temperature in *thermo.lib*. Control is returned to the main program, which continues with the next problem, if any.

WARNING!! AMOUNT MISSING FOR REACTANT (reactant number). PROGRAM SETS WEIGHT PERCENT = 100. (REACT)

If the problem contains only one fuel, or one oxidant, or one reactant in the **reac** dataset and the amount was not given, the CEA program will automatically set the amount to be 100% and continue.

6.8 ROCKET Messages

FATAL ERROR!! EITHER mdot/a or ac/at MISSING FOR THE fac PROBLEM (ROCKET)

The `fac` option for rocket performance calculations requires either the mass flow rate per unit chamber area $\dot{m}/A$ or the contraction area ratio A_c/A_t to be assigned in the **prob** dataset. If neither one is assigned, this message is printed and the program goes on to the next problem.

INPUT VALUE OF mdot/a = (value of $\dot{m}/A$) IS TOO LARGE. GIVES CONTRACTION RATIO ESTIMATE LESS THAN 1 (ROCKET)

Fatal error. In the rocket finite-area-combustor model `fac`, an option is provided to assign $\dot{m}/A$. If this assigned value gives a contraction ratio less than 1, the error message is printed and control is returned to the main program, which continues with the next problem, if any.

WARNING!! AREA RATIO CALCULATION CANNOT BE DONE BECAUSE GAMMAs CALCULATION IMPOSSIBLE (ROCKET)

The iteration procedure for obtaining a pressure ratio corresponding to an assigned area ratio requires a value of γ_s as well as some other parameters (eq. (6.23) of Gordon and McBride, 1994). If a value of γ_s cannot be calculated for this point, the error message is printed and the CEA program proceeds to the next point. The problem can be rerun using estimated pressure ratios to obtain area ratios at or near the desired value.

WARNING!! ASSIGNED pi/pe = (value of assigned P_t/P_e) IS NOT PERMITTED TO BE LESS THAN Pinj/Pc = (value of P_{inj}/P_c). POINT OMITTED (ROCKET)

In a rocket finite-area-combustor model `fac` it is not possible for an assigned input value of `pi/pc` to be less than P_{inj}/P_c (the ratio of pressures at the beginning and end of the combustion chamber). If such a value is assigned in the input, this error message is printed, the point is omitted, and the program continues with the next assigned point.

WARNING!! ASSIGNED subae/at = (value of assigned A_e/A_t) IS NOT PERMITTED TO BE GREATER THAN ac/at = (value of A_c/A_t). POINT OMITTED (ROCKET)

In a rocket finite-area-combustor model `fac`, it is physically impossible for a subsonic area ratio to be greater than the contraction ratio. The CEA program omits this incorrectly assigned area ratio and continues.

WARNING!! CALCULATIONS WERE STOPPED BECAUSE NEXT POINT IS MORE THAN 50 K BELOW THE TEMPERATURE RANGE OF A CONDENSED SPECIES (ROCKET)

For frozen composition, calculations a temperature was calculated to be more than 50 K below the temperature range of an included condensed species. Output tables are printed for all previous points and the program continues.

WARNING!! DID NOT CONVERGE FOR AREA RATIO = (value of area ratio) (ROCKET)

The CEA program permits a maximum of 10 iterations to converge to the pressure ratio corresponding to the assigned area ratio. The usual number of iterations required is 1 to 5. The only time the number of iterations has exceeded 10, in our experience, has been for an assigned area ratio very close to 1, such as $1.0 < A_e/A_t < 1.0001$. The reason is that the converged throat conditions do not correspond exactly to an area ratio of 1 (see eq. (6.16) of Gordon and McBride, 1994). If the number of iterations exceeds 10, the point is omitted and the program continues with the next assigned point.

WARNING!! DIFFICULTY IN LOCATING THROAT (ROCKET)

The test for convergence for throat conditions is given in equation (6.16) of Gordon and McBride (1994). If this test is not passed in 23 iterations, this warning message is printed and the program continues with the next point.

WARNING!! DISCONTINUITY AT THE THROAT (ROCKET)

Under some unusual circumstances involving condensed species in the region of the throat, a special technique is used to obtain throat conditions. This technique involves a discontinuous velocity of sound at the throat. Details are given in Gordon (1970).

WARNING!! FOR FROZEN PERFORMANCE, POINTS WERE OMITTED WHERE THE ASSIGNED PRESSURE RATIOS WERE LESS THAN THE VALUE AT POINT `nfz` = (value of `nfz`) (ROCKET)

Pressure ratios may be assigned only downstream of the pressure ratio where freezing is assigned to occur. Pressure ratios not meeting this requirement are omitted, and the calculations continue.

WARNING!! FOR FROZEN PERFORMANCE, POINTS WERE OMITTED WHERE THE ASSIGNED SUPERSONIC AREA RATIOS WERE LESS THAN THE VALUE AT POINT `nfz` = (value of `nfz`) (ROCKET)

Area ratios may be assigned only downstream of the area ratio where freezing occurs. Area ratios not meeting this requirement are omitted, and the calculations continue.

WARNING!! FOR FROZEN PERFORMANCE, SUBSONIC AREA RATIOS WERE OMITTED SINCE `nfz` IS GREATER THAN 1 (ROCKET)

Area ratios may be assigned only downstream of the area ratio where freezing is assigned to occur. Inasmuch as in this problem freezing is assigned to occur at `nfz` > 1 (the throat or some supersonic point), all subsonic area ratios are omitted and the calculations continue.

WARNING!! FREEZING IS NOT ALLOWED AT A SUBSONIC PRESSURE RATIO FOR `nfz` GREATER THAN 1. FROZEN PERFORMANCE CALCULATIONS WERE OMITTED (ROCKET)

For `nfz` > 1, throat conditions will be based on equilibrium compositions. For this situation, it is therefore not permitted to assign freezing to occur at a subsonic pressure ratio. Frozen performance is omitted and the program continues.

WARNING!! `nfz` NOT ALLOWED TO BE > 2 IF THE TOTAL NUMBER OF POINTS IS > (number) (ROCKET)

The CEA program permits freezing at a point greater than 2 if there is only one page of the equilibrium output table. The reason is that a second page wipes out the information from the first page except for the combustion and throat columns. This message is printed when the total number of assigned pressure ratios and area ratios (both subsonic and supersonic) is greater than NCOL (the number of columns in the output listing) minus 2 (the number of columns for combustion and throat). In this situation, frozen performance is omitted and the program continues.

6.9 SEARCH Messages

INSUFFICIENT STORAGE FOR (number of) SPECIES (SEARCH)

Fatal error. This statement shows that for the chemical system under consideration, the program found more possible species in *thermo.lib* than can be accommodated by storages reserved for the thermodynamic data in labeled COMMON /THERM/. This excess number of species is given in this error message. When this situation occurs, the names of the possible species are printed, and control is returned to the main program, which continues with the next problem, if any.

This situation can be resolved in two ways. First, the program can be recompiled with MAXNGC in the parameter statements increased to accommodate the excess species (see section 4.9.1). Secondly, an **`omit`** dataset can be used to eliminate the required number of excess species.

WARNING!! (name of species) MISSING IN *thermo.lib* FILE (SEARCH)

The species name was listed in the dataset **`only`**, but the species was not found in *thermo.lib*. The species is ignored and the program continues.

6.10 SHCK Messages

WARNING!! ONLY (NCOL) `u1` OR `mach1` VALUES ALLOWED (SHCK)

The number of assigned values of `u1` or `mach1` in dataset **`prob`** exceeded the maximum allowed. This maximum is NCOL (number of columns), which is set in a PARAMETER statement. `NCOL` is usually 7 or 13 depending on the width of the paper used for printing output. The excess points are ignored and the program continues.

WARNING!! NO CONVERGENCE FOR u1 = (value of u_1). ANSWERS NOT RELIABLE, SOLUTION MAY NOT EXIST (SHCK)

This message usually occurs when the assigned values of u_1, T_1, and P_1 do not have a solution. For example, for example 7 in section 7.5, no solution exists for values of shock u_1 less than approximately 1095 m/s using the current set of thermodynamic data. The message will therefore be printed for this problem for these low values, and the program continues.

WARNING!! TEMPERATURE = (value) IS OUT OF EXTENDED RANGE FOR POINT (value) (SHCK)

Fatal error. This message is printed whenever a converged temperature for a shock problem is higher than the highest T in the temperature range times 1.25 or if the assigned temperature `t1` is less than the lowest T in the range divided by 1.5. The program prints all the converged values up to this point and continues with the next problem, if any.

6.11 TRANIN Message

WARNING!! MAXIMUM ALLOWED NO. OF SPECIES (number) WAS USED IN TRANSPORT PROPERTY CALCULATIONS FOR POINT (number of point) (TRANIN)

The number of gaseous species used in the thermal transport properties calculations was cut off at the maximum number MAXTR set in a PARAMETER statement. The omitted species are the ones with the smallest mole fractions.

6.12 UTHERM Message

ERROR IN PROCESSING *thermo.inp* AT OR NEAR (name of species) (UTHERM)

Fatal error. An error occurred in reading or processing the *thermo.inp* file. After the message is printed, the program terminates.

6.13 UTRAN Message

ERROR IN PROCESSING *trans.inp* (UTRAN) (name of 1 or 2 species)

Fatal error. An error occurred in reading or processing the *trans.inp* file. After the message is printed, the program terminates.

Chapter 7

Example Problems

Fourteen example problems are given to illustrate some features of the program. The output for these problems is given in appendix G. Inasmuch as the thermodynamic and thermal transport data are updated periodically, the answers given for these examples may change somewhat from time to time. In the **prob** datasets the case designations were chosen to match the example numbers. Examples 1 and 14 are assigned-temperature and assigned-pressure problems, `tp`; example 2 is an assigned-temperature and assigned-volume (or assigned density) problem, `tv`; three are combustion problems (examples 3 and 5 are for combustion at constant pressure, `hp`, and example 4 is for combustion at constant volume, `uv`); example 6 is a detonation problem, `det`; example 7 is a shock problem, `sh`; and six (examples 8 to 13) are rocket problems, `ro` or `rkt`. These problems were run with NCOL set to 8 (see section 4.9.1).

It would not be practical to illustrate every possible variation of options permitted by the program. However, the example problems were selected to illustrate many of the possible variations and in particular those variations that we feel might often be used. Included in the features illustrated are the following:

1. Specifying proportions of various reactants
    a. Relative weights of reactants
        i. Complete information in **reac** dataset: example 5
        ii. Information in **reac** and **prob** datasets: examples 2 to 4, 6, 8 to 10, 12, and 13
    b. Relative moles of reactants
        i. Complete information in **reac** dataset: examples 7, 11, and 14
        ii. Information in **reac** and **prob** datasets: example 1
    c. Type of information provided in **prob** dataset (in addition to that given in **reac** dataset):
        i. o/f: examples 3, 4, 8 to 10, and 12
        ii. Chemical equivalence ratio r: examples 1 and 6
        iii. Fuel-air equivalence ratio ϕ: example 2
        iv. Percent fuel by weight, %fuel: example 13

2. Exploded formula

    a. Obtained directly from *thermo.lib*: 1 to 4, 5 (partly), and 6 to 13

    b. Specified in **reac** dataset: 5 (partly) and 14

3. Specifying enthalpies or internal energies

    a. In **reac** dataset: example 5 (partly)

    b. In **prob** dataset: example 4

    c. Automatically calculated by program from data in *thermo.lib*: examples 3, 5 (partly), and 6 to 13

    d. Not needed: examples 1, 2, and 14

4. Pressure units

    a. atm: examples 1 and 14

    b. psia: examples 5 and 11 to 13

    c. mm Hg: example 7

    d. bar: examples 3, 6, and 8 to 10

    e. Not required: examples 2 and 4

5. **inse**: example 13

6. **omit**: examples 3 to 5

7. **only**: examples 1 and 2

8. **trace** (composition in floating-point format): examples 3, 4, and 13

9. Considering ions: example 11

10. Propellant density: example 12

11. Output units

    a. In SI units: examples 3, 4, 7 to 12, and 14

    b. Not in SI units: examples 1, 2, 5, 6, and 13

12. Output composition units

    a. Mass fractions: example 12

    b. Mole fractions: all examples except 12

13. Transport properties included: examples 2, 6, and 11

14. Dump for plotting: example 12

15. Special thermodynamic derivatives: example 13

16. Two definitions of molecular weight: examples 5, 13, and 14 (discussed in section 7.10)

17. Internal thermodynamic consistency: examples 1 to 4

The following discussion of the 14 example cases includes the features outlined above plus some additional features of the program.

7.1 Examples 1 and 2

Examples 1 and 2 are used, among other things, to demonstrate internal consistency in the CEA program for assigned-temperature and assigned-pressure problems, `tp`; and assigned-temperature and assigned-volume problems, `tv`. The same reactants are used in the two examples, and part of the output from example 1 is used as input for example 2.

7.1.1 Example 1

Example 1 is an example of a `tp` problem. Properties will be calculated for all combinations of temperatures and pressures specified. In this example, two temperatures (3000 and 2000 K) and three pressures (1, 0.1, and 0.01 atm) are specified, for a total of six combinations. Each of these six combinations will be run for two equivalence ratios (r=1 and 1.5). The exploded formulas for the fuel (`H2`) and oxidant (`Air`) are obtained automatically from *thermo.lib* (see section 2.3.8). Enthalpies of the reactants are not needed for a `tp` problem.

7.1.2 Example 2

Example 2 is an example of an assigned-temperature and assigned-volume (or -density) problem, `tv`. As previously stated, examples 1 and 2 are used to demonstrate internal consistency in the CEA program for `tp` and `tv` problems. The combustion mixture densities taken from example 1 output for the equivalence ratio of 1 and for 3000 K were used as part of the input for example 2. It may be seen in the output of example 2 that the pressures of 1, 0.1, and 0.01 atm, used as input in example 1, are reproduced exactly. The equivalence ratio was specified here in terms of ϕ rather than r as in example 1. For stoichiometric conditions, the two definitions give equal values (see discussion in chapter 9 of Gordon and McBride, 1994).

Example 2 also includes thermal transport properties (`tran` in the **`outp`** dataset). As discussed in section 5.2.3 of Gordon and McBride (1994), the specific heat for thermal transport property calculations $c_{p,\text{equil}}$ is calculated by a different method from the more general specific heat $c_{p,\text{eq}}$. When no condensed species are present, the two methods should give the same numerical values of specific heat, except possibly for rounding errors. This agreement, which occurs here as well as in examples 6 and 11, confirms the accuracy of the calculations.

7.2 Examples 3 and 4

Examples 3 and 4 illustrate, among other things, internal consistency in combustion problems (example 3 for combustion at constant pressure, `hp`; and example 4 for combustion at constant volume, `uv`). The same propellants are used in the two examples, and part of the output of example 3 is used as input for example 4.

7.2.1 Example 3

Example 3 is an example of a combustion problem at constant pressure, `hp`. Three pressures were selected: 1, 10, and 100 bars. Reactant enthalpies and exploded formulas for all reactants in this problem will be obtained automatically from *thermo.lib*. Note that the fuel and oxidant do not have to be at the same initial temperature. In this problem, the air is preheated to 700 K. The results of the enthalpy calculation for the oxidants may be seen in reactants data in the output.

This example also illustrates the option of listing compositions whose amounts are smaller than those listed in the fixed-point output (i.e., smaller than 0.000005). This is accomplished by using the `trace` option in the **`outp`** dataset. In this example, `trace=1.E-15`.

Some of the output of this case will be used as input for example 4.

7.2.2 Example 4

Example 4 illustrates combustion at constant volume (or density), `uv`. This type of problem generally requires as input the internal energies of the reactants at some initial temperature as well as the assigned volume (or density). In this case, we are using as input the density and internal energy of the combustion mixture resulting from the first point of example 3. The reason for this selection is to verify the internal consistency and accuracy of the calculation procedures. Verification will be accomplished if the same combustion temperature and pressure are obtained as in example 3. From example 3, the value for density is 14.428 kg/m^3. The input for internal energy is required to be in the form of u/R, where u is internal energy and R is the universal gas constant in consistent units. From example 3, output u=–375.27 kJ/kg is obtained. This gives u/R=–375.27/8.31451=–45.1343 (kg-mol)(K)/kg. As expected, the resulting combustion temperature of 2419.33 K and combustion pressure of 100 bars match those of example 3 exactly.

7.3 Example 5

Example 5 is for a typical solid propellant. The relative amounts of reactants are given in weight percents. Unless an **`inse`** dataset is present, the CEA program initially considers only gaseous combustion products. An initial combustion temperature of 2223.217 K was reached in 15 iterations. This information may be seen in the output under the heading POINT ITN. The program then checks for the possibility that condensed species should have been considered. In this example, it determined that the solid phase Al_2O_3(a) should be added. (The solid phase exists below the melting point of 2327 K.) With Al_2O_3 (a) added, the temperature converged in seven iterations to 2800.188 K. The program now checks for the appropriate phase and determines that the phase at this temperature is liquid and makes the appropriate switch. This may be seen by the message PHASE CHANGE, REPLACE AL2O3(a) WITH AL2O3(L). The next convergence took just two iterations and gave a final combustion temperature of 2724.464 K.

Had the keyword **inse** followed by AL2O3(L) been used in the input, convergence would have been reached in 15 iterations rather than 24 iterations needed with no **inse** being used. However, the use of **inse** often implies some prior knowledge of which condensed species or phases exist. If one is starting a new problem, it may be better to just let the program figure this out rather than inserting a possibly incorrect condensed species that the program must then remove. The **inse** option may be used only for the first point. After the first point the insertions and removals of condensed phases are all handled automatically by the program.

In some situations, however, the keyword **inse** is required, as in a combustion problem when temperature is driven down too low without the appropriate condensed species present. When this happens, an error message will be printed.

7.4 Example 6

Example 6 is an example of a detonation problem, `det`. Calculations will be made for all combinations of pressures and temperatures specified. In this example, two pressures (1 and 20 bars) and two temperatures (298.15 and 500 K) have been scheduled. When temperatures are specified in the **prob** dataset, enthalpies for the `det` problem are calculated automatically by the program for the assigned temperatures. For this situation, this implies that only those gaseous species whose thermodynamic data are in the *thermo.lib* file (such as H_2 and O_2 in this example) may be considered as possible reactants. This example also includes thermal transport property calculations (see discussion in section 7.1.2).

7.5 Example 7

Example 7 is an example of a shock problem, `sh`. The input permits a schedule of either velocities `u1` or Mach numbers `mach1`, but not both in the same input dataset. For this example, a set of velocities was assigned. Only the incident shock conditions were calculated. To obtain reflected shock conditions, the **prob** dataset would have required `refleq` for reflected shocks based on equilibrium incident conditions and/or `reflfr` for reflected shocks based on frozen incident conditions. The message that starts with WARNING!! NO CONVERGENCE FOR `u1=1000.0` usually indicates that no solution exists for the assigned condition.

7.6 Examples 8, 9, and 10

Examples 8 to 10 illustrate some similarities and differences in rocket performance calculations for the two models of an infinite-area combustor, `iac`, and a finite-area combustor, `fac`. All three examples are for the same propellant, chamber pressure, o/f ratio, pressure ratios, and area ratios. Example 8 is for the `iac` assumption. Inasmuch as the default is for the `iac` assumption, this information is not required in the **prob** dataset. Examples 9 and 10, by contrast, are for the `fac` assumption, and this needs to be specified in the **prob** dataset. A subsonic area ratio of 1.58 (`subar=1.58`) was assigned in order to compare the results with those obtained when using the same assigned value of A_c/A_t (the contraction ratio assigned for examples 9 and 10). The outputs for examples 8 to 10 will be compared in the discussion of examples 9 and 10.

7.6.1 Example 8

Example 8 illustrates a typical rocket performance problem based on the model of an infinite-area combustor, `iac`. Note that there are nine output points (columns): the chamber, the throat, three pressure ratios, one subsonic area ratio, and three supersonic area ratios. Since NCOL (number of columns or points) was set to 8 in the program, output for the last supersonic area ratio was printed on the second page along with the chamber and throat, which are repeated for convenience.

7.6.2 Example 9

Examples 9 and 10 are for the `fac` model. Two options are permitted with this model. The first option, assigning the contraction ratio A_c/A_t (`acat`) is illustrated in example 9. The second option, assigning the mass flow rate per unit area $\dot{m}/A_c$ (`ma`) is illustrated in example 10. The results of example 9 for an assigned value of A_c/A_t=1.58 were used to calculate a value of $\dot{m}/A_c$=1333.9. This value was used as input in example 10 in order to verify the consistency of the results.

7.6.3 Example 10

As mentioned in the previous section, example 10 is identical to example 9 except for using a value of $\dot{m}/A_c$ instead of A_c/A_t as input. The input value of `ma`=1333.9 for example 10 was calculated from the results of example 9. As expected, the value of A_c/A_t=1.5800 calculated in example 10 matches the example 9 input value of 1.58. This result confirms the accuracy and consistency of the calculations and iteration procedures.

As pointed out in Gordon (1988), the calculated values of specific impulse for the `fac` and `iac` rocket models are extremely close for the same assigned area ratios. For example, at an area ratio of 75, the `iac` rocket model in example 8 gives a specific impulse of 4399.7 m/s, which compares closely with 4399.0 m/s obtained for the `fac` model of examples 9 and 10. The difference is only 0.02%.

7.7 Example 11

Example 11 illustrates including ions as possible combustion species (the option `ions` is part of the **`prob`** dataset). At the high combustion temperature of 5686 K, about 1.5% of the species are the result of ionization. This example also shows that it is possible to assign a schedule of points for expansion in a rocket that includes a mixture of pressure ratios, subsonic area ratios, and supersonic area ratios. Note in the output that two area ratios are assigned the value of 10. Their corresponding Mach numbers indicate which is subsonic and which is supersonic. Example 11 also includes thermal transport property calculations (see discussion in section 7.1.2).

7.8 Example 12

Example 12 is another example of rocket performance. Several options are illustrated in this example: the `nfz` option for freezing composition, the calculation of reactant density, the option of obtaining compositions as mass fractions rather than mole fractions, and the `plot` option for obtaining an output dump for plotting purposes. By setting `nfz`=2, frozen composition rocket performance calculations are based on compositions frozen at the second point. By including densities of all individual reactants (`rho` in the **`reac`** dataset), the program will calculate the reactant mixture density. By including `massf` in the **`outp`** dataset, compositions are given as mass fractions. By including `plot` in the **`outp`** dataset, a dump of values for the parameters following `plot` is generated in the file (*input suffix*)*.plt.* (see section 2.5.4).

7.9 Example 13

Example 13 illustrates some unusual values of thermodynamic derivatives that occur when two condensed phases are present simultaneously. The appropriate equation for $\gamma_{S,T}$, which is needed to calculate velocity of sound under these conditions, is equation (3.9) in Gordon and McBride (1994). As may be seen in the output of example 13 for the second and third points, $\gamma_{S,T}$ equals 0.9979 and 0.9974, respectively. This topic is covered more completely in Gordon (1970).

7.10 Example 14

Example 14 was chosen for three reasons. The first was to check out the size of the error caused by assuming zero volume of condensed species in the equation of state (eq. (2.1a) in section 2.2 of Gordon and McBride, 1994). The second was to look at an example of the two definitions of molecular weight given as equations (2.3b) and (2.4a) in Gordon and McBride (1994). The third reason was to illustrate `debug` output (see section 3.4 for further discussion). The reactants are hydrogen and oxygen. This example is a `tp` problem where the pressure (0.05 atm), the schedule of temperatures (1000, 500, 350, 305, 304.3, 304.2, 304, and 300 K), and the relative number of moles of hydrogen to oxygen were chosen to produce a large calculated mole fraction of liquid water for some conditions.

For T=304 K the mole fraction of liquid water is 0.24681. Using the density 0.99539 g/cm^3 at this temperature (Lide, 1992–1993), the volume of water in 1 mole of mixture is calculated to be 4.5 cm^3, in contrast to 375 900 cm^3 for the gases. Therefore, even though the mole fraction of the condensed species is about 25%, the relative volume of the condensed phase is only 0.001%. Thus, in this example, the assumption of negligible volume for condensed species that is incorporated into the equation of state (eqs. (2.1a) and (2.1b) in Gordon and McBride, 1994) is valid for most practical purposes. For other problems with higher pressures than in this case, the relative volume of the condensed species will be generally be greater than here but less than 0.1%.

For those problems with combustion products containing condensed phases, two values of molecular weight are given in the output (see final table in example 14, appendix G). These values are based on definitions given in section 2.2 of Gordon and McBride (1994). Note that in the present example the product compositions remain constant if all phases of water are combined. It is therefore to be expected that the molecular weights of the mixture would be the same for all points. This is indeed the case for the molecular weight MW, where the value for all points is 19.287. However, the molecular weight M increases for those points with increasing amounts of liquid water, consistent with the assumptions incorporated in the equation of state (eq. (2.1) in Gordon and McBride, 1994). The molecular weight M is obtained by means of equations (2.3a) or (2.3b), MW is given by equation (2.4a), and the relationship between M and MW is given by equation (2.4b) in Gordon and McBride (1994). For the T=304 K point equation (2.4b) gives MW=25.607×0.75319=19.287, which matches exactly the molecular weight of 19.287 given in the table.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, January 28, 1996.

Appendix A

Format for Thermodynamic Data

The library of thermodynamic data contains data for both reaction products and reactants. All reaction products and some reactants are in the nine-constant functional form discussed in section 4.2 of Gordon and McBride (1994). The format for these data is given here. Thermodynamic data are provided with the program on a separate file, *thermo.inp*. Sections 2.8 and 5.24 discuss the processing of the *thermo.inp* data and the storing of the processed data in *thermo.lib* for subsequent use in the CEA program. Names of species contained in *thermo.inp* are listed in appendix B.

The general format is given in table A1. This format is applicable for all gaseous species and for those condensed species whose data extend over a temperature range. For those condensed species with data given at only one temperature, the format is somewhat different. On record 2, instead of the last number being a heat of formation, it is an assigned enthalpy. (Note that if the temperature is 298.15 K, the heat of formation and the assigned enthalpy are equivalent.) The first number in record 2 (number of temperature intervals) is always zero. On record 3, only one number is given, the temperature of the assigned enthalpy on record 2. Two examples are given. Example A1, for chlorine gas, illustrates the general format. Example A2, for liquid acetylene, illustrates the format for a condensed species with data given at only one temperature. The general equations for dimensionless heat capacity, enthalpy, and entropy (eqs. (4.6) to (4.8) from Gordon and McBride, 1994) are repeated for convenience.

TABLE A.1.—GENERAL FORMAT FOR NINE-CONSTANT FUNCTIONAL FORM

Record	Constants	Format	Columns
1	Species name or formula	A24	1–24
	Comments (data source)	A56	25–80
2	Number of T intervals	I2	2
	Optional identification code	A6	4–9
	Chemical formulas, symbols, and numbers	5(A2,F6.2)	11–50
	Zero for gas and nonzero for condensed phases	I1	52
	Molecular weight	F13.5	53–65
	Heat of formation at 298.15 K, J/mol	F13.5	66–80
3	Temperature range	2F10.3	2–21
	Number of coefficients for C_p°/R	I1	23
	T exponents in empirical equation for C_p°/R	8F5.1	24–63
	$\{H^\circ(298.15) - H^\circ(0)\}$, J/mol	F15.3	66–80
4	First five coefficients for C_p°/R	5D16.8	1–80
5	Last three coefficients for C_p°/R	3D16.8	1–48
	Integration constants b_1 and b_2	2D16.8	49–80
----	Repeat 3, 4, and 5 for each interval	----------	---------

Example A.1:

```
CL2             Chlorine gas. TPIS 1989, v1, pt2, p88.
 2 tpis89 CL  2.00    0.00    0.00    0.00    0.00 0     70.90540          0.000
   200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9181.110
 3.46281724D+04 -5.54712949D+02  6.20759103D+00 -2.98963673D-03  3.17303416D-06
-1.79363467D-09  4.26005863D-13  0.00000000D+00  1.53407075D+03 -9.43835303D+00
  1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           9181.110
 6.09256675D+06 -1.94962688D+04  2.85453491D+01 -1.44996828D-02  4.46388943D-06
-6.35852403D-10  3.32735931D-14  0.00000000D+00  1.21211722D+05 -1.69077832D+02
```

Empirical equations for example A.1:

Heat capacity: $\frac{C_p^o}{R} = a_1T^{-2} + a_2T^{-1} + a_3 + a_4T + a_5T^2 + a_6T^3 + a_7T^4$

Enthalpy: $\frac{H^o(T)}{RT} = -a_1T^{-2} + a_2T^{-1}\ln T + a_3 + a_4\frac{T}{2} + a_5\frac{T^2}{3} + a_6\frac{T^3}{4} + a_7\frac{T^4}{5} + \frac{b_1}{T}$

Entropy: $\frac{S^o(T)}{R} = -a_1\frac{T^{-2}}{2} - a_2T^{-1} + a_3\ln T + a_4T + a_5\frac{T^2}{2} + a_6\frac{T^3}{3} + a_7\frac{T^4}{4} + b_2$

Example A.2:

```
C2H2(L),acetyle   Acetylene. JANAF Prop.Ser.E,1/67. TRC a-3000,10/86.
 0 1 3/95 C   2.00H   2.00    0.00    0.00    0.00 1     26.03788     207599.000
   192.35
```

Appendix B

Names of Species in Thermodynamic Data File (*thermo.inp*)

The *thermo.inp* file is arranged with data for the products listed first, followed by data for the reactants. Among the products, all gas-phase species data are listed first, followed by condensed-phase species data (liquid and/or solid). The names of gas-phase products are listed in table B.1; the names of condensed-phase products are listed in table B.2. No subscripts are used and no phase is indicated for the gas phase. That is, O2 in *thermo.inp* is gas-phase oxygen, O_2(g), and O2(L) is liquid-phase oxygen, O_2(l). An upper case "L" is used to designate the liquid phase to avoid confusion between the lower case "l" and the number "1." Most of the reactant species are cryogenic fuels or oxidants. Reactant names are listed in table B.3. Species that may be considered as either products or reactants (such as H_2(g), CH_4(g), or O_2(g) and listed as H2, CH4, and O2) are generally included with the products. Occasionally, additional information is added after the chemical formula for clarification. For example, two names start with C4H10(L). One is followed by *n*-butan to indicate normal butane; the other is followed by isobuta to indicate isobutane. (A maximum of 15 characters is allowed for a name.)

As discussed in section 2.3.2, in order for the CEA program to use the data in *thermo.inp* for reactants, the names used in the **reac** dataset must match the names in the *thermo.inp* file exactly. The search for a reactant name starts at the beginning of the file, first with gaseous products, then with condensed products, and finally with reactants.

A complete documentation of references for the thermodynamic data selected for products was not available at the time of publication of this report. Some of the references are given in McBride et al. (1993). Data for the reactants are given in tables C.1 and C.2. (References for the data in table C.1 are given in table D.1.) At the time of publication of this report, the approximate number of species in the *thermo.inp* file was 1340 reaction products and 60 reactants. However, data for species are constantly being added to the file, so that the data and the total number of species keep changing.

TABLE B.1.—NAMES OF GAS-PHASE PRODUCTS IN *thermo.inp*

e-	B-	BeF2	CF3Br
AL	BCL	BeH	CF3CL
AL+	BCL+	BeH+	CF4
AL-	BCLF	BeH2	CH
ALBO2	BCL2	BeI	CH+
ALBr	BCL2+	BeI2	CHBr3
ALBr3	BCL2-	BeN	CHCL
ALC	BCL3	BEO	CHCLBr2
ALCL	BF	BeOH	CHCL2
ALCL+	BF2	BeOH+	CHCL2Br
ALCLF	BF2+	BeO2H2	CHCL3
ALCLF+	BF2-	BeS	CHF
ALCLF2	BF3	Be2O	CHFBr2
ALCL2	BH	Be2OF2	CHFCL
ALCL2+	BHF2	Be2O2	CHFCLBr
ALCL2-	BH2	Be3O3	CHFCL2
ALCL2F	BH3	Be4O4	CHF2
ALCL3	BN	Be5O5	CHF2Br
ALF	BO	Be6O6	CHF2CL
ALF+	BOCL	Br	CHF3
ALF2	BOF	BrCL	CH2
ALF2+	BOF2	BrF	CH2Br2
ALF2-	BO2	BrF3	CH2CL
ALF2O	BO2-	BrF5	CH2CLBr
ALF2O-	BS	BrO	CH2CL2
ALF3	B2	Br2	CH2F
ALF4-	B2H6	C	CH2FBr
ALH	B2O	C+	CH2FCl
ALI	B2O2	C-	CH2F2
ALI3	B2O3	CBr	CH3
ALN	B3O3CL3	CBr2	CH3Br
ALO	B3O3F3	CBr3	CH3CL
ALO+	B3O3H3	CBr4	CH3F
ALO-	Ba	CCL	CH2OH
ALOCL	BaBr	CCLBr3	CH3O
ALOF	BaBr2	CCL2	CH4
ALOH	BaCL	CCL2Br2	CH3OH
ALOH+	BaCL2	CCL3	CI
ALOH-	BaF	CCL3Br	CN
ALO2	BaF+	CCL4	CN+
ALO2-	BaF2	CF	CN-
ALO2H	BaOH	CF+	CNN
ALS	BaOH+	CFBr3	CO
AL2	BaO2H2	CFCL	CO+
AL2Br6	BaS	CFCLBr2	COCL
AL2CL6	Be	CFCL2	COCL2
AL2F6	Be+	CFCL2Br	COF
AL2I6	Be++	CFCL3	COFCL
AL2O	BeBO2	CF2	COF2
AL2O+	BeBr	CF2+	COHCL
AL2O2	BeBr2	CF2Br2	COHF
AL2O2+	BeCL	CF2CL	COS
Ar	BeCL+	CF2CLBr	CO2
Ar+	BeCLF	CF2CL2	CO2+
B	BeCL2	CF3	COOH
B+	BeF	CF3+	CP

TABLE B.1.—Continued.

CS	C3H5,allyl	C7H15,n-heptyl	Cs2CL2
CS2	C3H6,propylene	C7H16,2-methylh	Cs2F2
C2	C3H6,cyclo-	C7H16,n-heptane	Cs2O
C2+	C3H6O,propyle-o	C8H8,styrene	Cs2O2H2
C2-	C3H7,n-propyl	C8H10,ethylbenz	Cs2SO4
C2CL	C3H7,i-propyl	C8H16,1-octene	Cu
C2CL2	C3H8	C8H17,n-octyl	Cu+
C2CL3	C3H8O,1propanol	C8H18,n-octane	CuCL
C2CL4	C3H8O,2propanol	C8H18,isooctane	CuF
C2CL6	C3O2	C9H19,n-nonyl	CuF2
C2F	C4	C10H8,naphthale	CuO
C2FCL	C4H2	C10H21,n-decyl	Cu2
C2FCL3	C4H4,1,3-cyclo-	C12H9,o-bipheny	Cu3CL3
C2F2	C4H6,butadiene	C12D9,o-bipheny	D
C2F2CL2	C4H6,1-butyne	C12H10,biphenyl	D+
C2F3	C4H6,2-butyne	C12D10,biphenyl	D-
C2F3CL	C4H6,cyclo-	Ca	DBr
C2F4	C4H8,1-butene	Ca+	DCL
C2F6	C4H8,cis2-buten	CaBr	DF
C2H	C4H8,tr2-butene	CaBr2	DOCL
C2HCL	C4H8,isobutene	CaCL	DO2
C2HCL3	C4H8,cyclo-	CaCL2	DO2-
C2HF	(CH3COOH)2	CaF	D2
C2HFCL2	C4H9,n-butyl	CaF2	D2+
C2HF2CL	C4H9,i-butyl	CaI	D2-
C2HF3	C4H9,s-butyl	CaI2	D2O
CHCO,ketyl	C4H9,t-butyl	CaO	D2O2
C2H2,vinylidene	C4H10,isobutane	CaOH	D2S
C2H2,acetylene	C4H10,n-butane	CaOH+	F
C2H2CL2	C4N2	CaO2H2	F+
C2H2FCL	C5	CaS	F-
C2H2F2	C5H6,1,3cyclo-	Ca2	FCN
CH2CO,ketene	C5H8,cyclo-	CL	FO
C2H3,vinyl	C5H10,1-pentene	CL+	FO2
C2H3CL	C5H10,cyclo-	CL-	F2
C2H3F	C5H11,pentyl	CLCN	F2O
CH3CN	C5H11,t-pentyl	CLF	FS2F,fluorodisu
CH3CO,acetyl	C5H12,n-pentane	CLF3	Fe
C2H4	C5H12,i-pentane	CLF5	Fe+
C2H4O,ethylen-o	CH3C(CH3)2CH3	CLO	Fe-
CH3CHO,ethanal	C6H2	CLO2	FeC5O5
CH3COOH	C6H5,phenyl	CL2	FeCL
C2H5	C6D5,phenyl	CL2O	FeCL2
C2H6	C6H5O,phenoxy	Cr	FeCL3
CH3N2CH3	C6H6	CrN	FeO
C2H5OH	C6D6	CrO	Fe(OH)2
CH3OCH3	C6H5OH,phenol	CrO2	Fe2CL4
CCN	C6H10,cyclo-	CrO3	Fe2CL6
CNC	C6H12,1-hexene	Cs	GeBr
C2N2	C6H12,cyclo-	Cs+	GeBr2
C2O	C6H13,n-hexyl	CsCL	GeBr3
C3	C6H14,n-hexane	CsF	GeBr4
C3H3,propargyl	C7H7,benzyl	CsO	GeCL
C3H4,allene	C7H8	CsOH	GeCL2
C3H4,propyne	C7H8O,cresol-mx	CsOH+	GeCL3
C3H4,cyclo-	C7H14,1-heptene	Cs2	GeCL4

TABLE B.1.—Continued.

GeF	H3F3	Li2SO4	NO2-
GeF2	H3O+	Li3CL3	NO2CL
GeF3	(HCOOH)2	Li3F3	NO2F
GeF4	H4F4	Mg	NO3
GeI	H5F5	Mg+	NO3-
GeO	H6F6	MgBr	NO3F
GeO2	H7F7	MgBr2	N2
GeS	He	MgCL	N2+
GeS2	He+	MgCL+	N2-
Ge2	Hg	MgCLF	NCN
H	HgBr2	MgCL2	cis-N2D2
H+	I	MgF	N2F2
H-	IF5	MgF+	N2F4
HALO	IF7	MgF2	N2H2
HBO	I2	MgF2+	NH2NO2
HBO+	K	MgH	N2H4
HBO-	K+	MgI	N2O
HBO2	KBO2	MgI2	N2O+
HBS	KCN	MgN	N2O3
HBS+	KCL	MgO	N2O4
HBr	KF	MgOH	N2O5
HCN	KF2-	MgOH+	N3
HCO	KH	MgO2H2	N3H
HCO+	KO	MgS	Na
HCCN	KO-	Mg2	Na+
HCL	KOH	Mg2F4	NaALF4
HD	KOH+	MoO3	NaBO2
HD+	K2	Mo2O6	NaBr
HD-	K2C2N2	Mo3O9	NaCN
HDO	K2CL2	Mo4O12	NaCL
HDO2	K2F2	Mo5O15	NaF
HF	K2O2H2	N	NaF2-
HI	K2SO4	N+	NaH
HNC	Kr	N-	NaI
HNCO	Kr+	NCO	NaO
HNO	Li	ND	NaO-
HNO2	Li+	ND2	NaOH
HNO3	LiALF4	ND3	NaOH+
HOCL	LiBO2	NF	Na2
HOF	LiCL	NF2	Na2C2N2
HO2	LiF	NF3	Na2CL2
HO2-	LiFO	NH	Na2F2
HPO	LiF2-	NH+	Na2O
HSO3F	LiH	NHF	Na2O2H2
H2	LiN	NHF2	Na2SO4
H2+	LiO	NH2	Nb
H2-	LiO-	NH2F	NbO
HCHO,formaldehy	LiOH	NH3	NbO2
HCOOH	LiOH+	NH2OH	Ne
H2F2	LiON	NH4+	Ne+
H2O	Li2	NO	Ni
H2O+	Li2CL2	NO+	NiCL
H2O2	Li2F2	NOCL	NiCL2
H2S	Li2O	NOF	NiO
H2SO4	Li2O2	NOF3	NiS
H3B3O6	Li2O2H2	NO2	O

TABLE B.1.—Concluded.

O+	PbBr	SO2F2	Si2
O-	PbBr2	SO3	Si2C
OD	PbBr3	S2	Si2N
OD-	PbBr4	S2-	Si3
OH	PbCL+	S2F2,thiothiony	SnBr3
OH+	PbCL2	S2O	SnBr4
OH-	PbCL2+	S3	SnCL2
O2	PbCL3	S4	SnCL3
O2+	PbCL4	S5	SnCL4
O2-	PbF	S6	SnF2
O3	PbF2	S7	SnF3
P	PbF3	S8	SnF4
P+	PbF4	Si	SnO2
PCL	PbI	Si+	SnS2
PCL2	PbI2	SiBr	Sr
PCL2-	PbI3	SiBr2	SrBr
PCL3	PbI4	SiBr3	SrCL
PCL5	PbO	SiBr4	SrCL2
PF	PbO2	SiC	SrF
PF+	PbS	SiC2	SrF+
PF-	PbS2	SiC4H12	SrF2
PFCL	Pb2	SiCL	SrI2
PFCL-	S	SiCL2	SrO
PFCL2	S+	SiCL3	SrOH
PFCL4	S-	SiCL4	SrOH+
PF2	SCL	SiF	SrO2H2
PF2-	SCL2	SiFCL	SrS
PF2CL	SCL2+	SiF2	Ta
PF2CL3	SD	SiF3	Ta+
PF3	SF	SiF4	TaO
PF3CL2	SF+	SiH	TaO2
PF4CL	SF-	SiH+	Ti
PF5	SF2	SiHBr3	Ti+
PH	SF2+	SiHCL	Ti-
PH2	SF2-	SiHCL3	TiCL
PH2-	SF3	SiHF	TiCL2
PH3	SF3+	SiHF3	TiCL3
PN	SF3-	SiHI3	TiCL4
PO	SF4	SiH2	TiO
PO-	SF4+	SiH2Br2	TiOCL
POCL3	SF4-	SiH2CL2	TiOCL2
POFCL2	SF5	SiH2F2	TiO2
POF2CL	SF5+	SiH2I2	V
POF3	SF5-	SiH3	VCL4
PO2	SF6	SiH3Br	VN
PO2-	SF6-	SiH3CL	VO
PS	SH	SiH3F	VO2
P2	SH-	SiH3I	Xe
P2O3	SN	SiH4	Xe+
P2O4	SO	SiI	Zn
P2O5	SO-	SiI2	Zn+
P3	SOF2	SiN	Zn-
P4	SO2	SiO	Zr
P4O6	SO2-	SiO2	ZrN
P4O10	SO2CLF	SiS	ZrO
Pb	SO2CL2	SiS2	ZrO2

TABLE B.2.—NAMES OF CONDENSED-PHASE PRODUCTS IN *thermo.inp*

Ag(cr)	BeS(s)	CuO(s)	KO2(s)
Ag(L)	Be2C(s)	CuO2H2(s)	K2CO3(s)
AL(cr)	Be2C(L)	CuSO4(s)	K2CO3(L)
AL(L)	Br2(cr)	Cu2O(s)	K2O(s)
ALBr3(s)	Br2(L)	Cu2O(L)	K2O2(s)
ALBr3(L)	C(gr)	Cu2O5S(s)	K2S(1)
ALCL3(s)	Ca(a)	Fe(a)	K2S(2)
ALCL3(L)	Ca(b)	Fe(a)	K2S(3)
ALF3(a)	Ca(L)	Fe(c)	K2S(L)
ALF3(b)	CaBr2(s)	Fe(d)	K2SO4(a)
ALF3(L)	CaBr2(L)	Fe(L)	K2SO4(b)
ALI3(s)	CaCO3(caL)	FeC5O5(L)	K2SO4(L)
ALI3(L)	CaCL2(s)	FeCL2(s)	Li(cr)
ALN(s)	CaCL2(L)	FeCL2(L)	Li(L)
AL2O3(a)	CaF2(a)	FeCL3(s)	LiALO2(s)
AL2O3(L)	CaF2(b)	FeCL3(L)	LiALO2(L)
AL2SiO5(an)	CaF2(L)	FeO(s)	LiCL(s)
AL6Si2O13(s)	CaO(s)	FeO(L)	LiCL(L)
B(b)	CaO(L)	Fe(OH)2(s)	LiF(s)
B(L)	CaO2H2(s)	Fe(OH)3(s)	LiF(L)
BN(s)	CaS(s)	FeS(a)	LiH(s)
B2O3(L)	CaSO4(s)	FeS(b)	LiH(L)
B3O3H3(cr)	Cd(cr)	FeS(c)	LiOH(s)
Ba(cr)	Cd(L)	FeS(L)	LiOH(L)
Ba(L)	Co(a)	FeSO4(s)	Li2O(s)
BaBr2(s)	Co(b)	FeS2(s)	Li2O(L)
BaBr2(L)	Co(b)	Fe2O3(s)	Li2SO4(a)
BaCL2(a)	Co(L)	Fe2S3O12(s)	Li2SO4(b)
BaCL2(b)	Cr(cr)	Fe3O4(s)	Li2SO4(L)
BaCL2(L)	Cr(cr)	Ge(cr)	Li3N(s)
BaF2(a)	Cr(cr)	Ge(L)	Mg(cr)
BaF2(b,c)	Cr(L)	H2O(s)	Mg(L)
BaF2(L)	CrN(s)	H2O(L)	MgAL2O4(s)
BaO(s)	Cr2N(s)	H2SO4(L)	MgAL2O4(L)
BaO(L)	Cr2O3(s)	Hg(cr)	MgBr2(s)
BaO2H2(s)	Cr2O3(L)	Hg(L)	MgBr2(L)
BaO2H2(L)	Cs(cr)	HgBr2(s)	MgCO3(s)
BaS(s)	Cs(L)	HgBr2(L)	MgCL2(s)
Be(a)	CsCL(a)	HgO(s)	MgCL2(L)
Be(b)	CsCL(b)	I2(cr)	MgF2(s)
Be(L)	CsCL(L)	I2(L)	MgF2(L)
BeAL2O4(s)	CsF(s)	K(cr)	MgI2(s)
BeAL2O4(L)	CsF(L)	K(L)	MgI2(L)
BeBr2(s)	CsOH(a)	KCN(s)	MgO(s)
BeCL2(s)	CsOH(b)	KCN(L)	MgO(L)
BeCL2(L)	CsOH(c)	KCL(s)	MgO2H2(s)
BeF2(Lqz)	CsOH(L)	KCL(L)	MgS(s)
BeF2(hqz)	Cs2SO4(II)	KF(s)	MgSO4(s)
BeF2(L)	Cs2SO4(I)	KF(L)	MgSO4(L)
BeI2(s)	Cs2SO4(L)	KHF2(a)	MgSiO3(I)
BeI2(L)	Cu(cr)	KHF2(b)	MgSiO3(II)
BeO(a)	Cu(L)	KHF2(L)	MgSiO3(III)
BeO(b)	CuF(s)	KOH(a)	MgSiO3(L)
BeO(L)	CuF2(s)	KOH(b)	MgTiO3(s)
BeO2H2(b)	CuF2(L)	KOH(L)	MgTiO3(L)

TABLE B.2.—Concluded.

MgTi2O5(s)	NbO(s)	SiO2(b-qz)	Ti(b)
MgTi2O5(L)	NbO(L)	SiO2(b-crt)	Ti(L)
Mg2SiO4(s)	NbO2(I)	SiO2(L)	TiC(s)
Mg2SiO4(L)	NbO2(II)	SiS(cr)	TiC(L)
Mg2TiO4(s)	NbO2(III)	SiS(L)	TiCL2(s)
Mg2TiO4(L)	NbO2(L)	SiS2(cr)	TiCL3(s)
Mn(a)	Nb2O5(s)	SiS2(L)	TiCL4(L)
Mn(b)	Nb2O5(L)	Si2N2O(s)	TiN(s)
Mn(c)	Ni(cr)	Si3N4(cr)	TiN(L)
Mn(d)	Ni(cr)	Sn(cr)	TiO(a)
Mn(L)	Ni(L)	Sn(L)	TiO(b)
Mo(cr)	NiS(b)	SnBr2(s)	TiO(L)
Mo(L)	NiS(a)	SnBr2(L)	TiO2(ru)
NH4CL(a)	NiS(L)	SnBr4(s)	TiO2(L)
NH4CL(b)	NiS2(s)	SnBr4(L)	Ti2O3(a)
NH4F(cr)	NiS2(L)	SnCL2(s)	Ti2O3(b)
NH4F(L)	Ni3S2(I)	SnCL2(L)	Ti2O3(L)
Na(cr)	Ni3S2(II)	SnCL4(L)	Ti3O5(a)
Na(L)	Ni3S2(L)	SnCL4(L)	Ti3O5(b)
NaALO2(a)	Ni3S4(s)	SnF2(s)	Ti3O5(L)
NaALO2(b)	P(cr)	SnF2(L)	Ti4O7(s)
NaBr(s)	P(L)	SnI2(s)	Ti4O7(L)
NaBr(L)	P4O10(cr)	SnI2(L)	U(a)
NaCN(s)	P4O10(L)	SnI4(s)	U(b)
NaCN(L)	Pb(cr)	SnI4(L)	U(c)
NaCL(s)	Pb(L)	SnO(s)	U(L)
NaCL(L)	PbBr2(s)	SnO(L)	V(cr)
NaF(s)	PbBr2(L)	SnO2(s)	V(L)
NaF(L)	PbCL2(s)	SnO2(L)	VCL2(s)
NaI(s)	PbCL2(L)	SnS(rh)	VCL3(s)
NaI(L)	PbF2(II)	SnS(cu)	VCL4(L)
NaOH(a)	PbF2(I)	SnS(L)	VN(s)
NaOH(L)	PbF2(L)	SnS2(s)	VO(s)
NaO2(s)	PbI2(s)	Sr(a)	VO(L)
Na2CO3(I)	PbI2(L)	Sr(b)	V2O3(s)
Na2CO3(II)	PbO(II-r)	Sr(L)	V2O3(L)
Na2CO3(L)	PbO(I-y)	SrCL2(a)	V2O4(I)
Na2O(c)	PbO(L)	SrCL2(b)	V2O4(II)
Na2O(a)	PbO2(s)	SrCL2(L)	V2O4(L)
Na2O(L)	PbS(s)	SrF2(s)	V2O5(s)
Na2O2(a)	PbS(L)	SrF2(L)	V2O5(L)
Na2O2(b)	Pb2O3(s)	SrO(s)	W(cr)
Na2S(1)	Pb3O4(s)	SrO(L)	W(L)
Na2S(2)	Rb(cr)	SrO2H2(s)	Zn(cr)
Na2S(L)	Rb(L)	SrO2H2(L)	Zn(L)
Na2SO4(V)	S(cr1)	SrS(s)	ZnSO4(a)
Na2SO4(IV)	S(cr2)	Ta(cr)	ZnSO4(a)
Na2SO4(I)	S(L)	Ta(L)	ZnSO4(b)
Na2SO4(L)	SCL2(L)	TaC(s)	Zr(a)
Na3ALF6(a)	S2CL2(L)	TaC(L)	Zr(b)
Na3ALF6(b)	Si(cr)	Ta2O5(s)	Zr(L)
Na3ALF6(L)	Si(L)	Ta2O5(L)	ZrN(s)
Na5AL3F14(s)	SiC(b)	Th(a)	ZrN(L)
Na5AL3F14(L)	SiC(b)	Th(b)	ZrO2(a)
Nb(cr)	SiC(L)	Th(L)	ZrO2(b)
Nb(L)	SiO2(a-qz)	Ti(a)	ZrO2(L)

TABLE B.3.—NAMES OF REACTANTS IN *thermo.inp*

```
Air
B2H6(L)
B5H9(L)
(CH2)x(s)
CH3NO2(L)
CH4(L)
CH3OH(L)
CH6N2(L)
C2H2(L),acetyle
CH3CN(L)
C2H4(L)
C2H4O(L),ethyle
C2H6(L)
C2H5OH(L)
C2H8N2(L),UDMH
C2N2(L)
C3H6(L),propyle
C3H7NO3(L)
C3H8(L)
C4H8(L),1-buten
C4H10(L),n-buta
C4H10(L),isobut
C5H12(L),n-pent
C6H6(L)
C6H5NH2(L)
C6H14(L),n-hexa
C7H8(L)
C7H16(L),n-hept
C8H18(L),n-octa
C8H18(L),isooct
Jet-A(g)
Jet-A(L)
CLF3(L)
CLO3F
CLO3F(L)
CL2(L)
F2(L)
F2O(L)
JP-4
JP-5
HNO3(L)
IRFNA
H2(L)
H2O2(L)
LiCLO4(s)
NF3(L)
NH3(L)
NH4CLO4(I)
NH4CLO4(II)
NH4NO3(IV)
NH4NO3(III)
NH4NO3(II)
NH4NO3(I)
NH4NO3(L)
N2(L)
N2H4(L)
N2O4(L)
O2(L)
O3(L)
```

Appendix C

Thermodynamic and Density Data for Reactants

Thermodynamic and density data for the reactants are given in tables C.1 and C.2. Some reactants are in the condensed phase; others are in the gaseous phase. Density data are given only for the condensed phase. For those reactants whose normal boiling points are below 298.15 K, the following energy data in kilojoules per mole are given are given in table C.1:

1. Heat of formation of the gaseous phase at 298.15 K, $\Delta H_{298.15} = H_{298.15}$
2. Sensible heat of the ideal state of the gas from 298.15 K to the boiling point, $H_{298.15} - H_{bp}$
3. Difference in enthalpy between ideal and real states of the gas at the normal boiling point, $H_{bp} - H_{bp,re}$
4. Heat of vaporization at the normal boiling point $\Delta H_{vap} = H_{bp,re} - H(c)_{bp}$

The assigned enthalpy of the condensed phase at the normal boiling point is calculated from these data by means of the formula

$$H(c)_{bp} = H(g)_{298.15} - (H_{298.15} - H_{bp}) - (H_{bp} - H_{bp,re}) - \Delta H_{vap}$$

(Note that in the thermodynamic enthalpy base in *thermo.lib*, the assigned value of enthalpy at 298.15 K ($H_{298.15}$) is equal to the heat of formation at 298.15 K (i.e., $H_{298.15} = \Delta H_{298.15}$; see eq. (4.2) in Gordon and McBride, 1994). For those species for which the quantity ($H_{bp} - H_{bp,re}$) was unknown, it was taken as zero inasmuch as it is a relatively small quantity (say, 0.1 to 0.5 kJ/mol). A blank in the temperature column indicates that the temperature is 298.15 K and not a boiling point. References for the data in table C.1 are given in table D.1 in appendix D. Table C.2 gives the data and references for reactants in the format of the *thermo.inp* file (see table A.1). For some reactants, only one enthalpy value is given.; for others, thermodynamic coefficients for heat capacity, enthalpy, and entropy are given for one or more temperature intervals. Reactant species names used in **reac** datasets should match those in tables B.1 to B.3.

TABLE C.1.—THERMODYNAMIC AND DENSITY DATA FOR REACTANTS

Species	Phase	Boiling point, K	Assigned enthalpy, kJ/mol	$H_{298.15} - H_{bp}$, kJ/mol	$H_{bp} - H_{bp,re}$, kJ/mol	ΔH_{vap}, kJ/mol	Density, g/cm^3
Acetonitrile, C_2H_3N	L	----------	31.38	--------	--------	--------	0.7793
Acetylene, C_2H_2	g	----------	228.2	4.187	0.172	16.242	----------
	L	192.35	207.599	--------	--------	--------	.729
Air[a]	g	----------	-.126	--------	--------	--------	----------
Ammonia, NH_3	g	----------	-45.940	2.042	.222	23.351	----------
	L	239.72	-71.555	--------	--------	--------	.6821
Ammonium perchlorate, NH_4ClO_4	I	----------	-295.767	--------	--------	--------	1.95
Ammonium nitrate, NH_4NO_3	IV	----------	-365.6	--------	--------	--------	1.725
Aniline, $C_6H_5NH_2$	L	----------	31.5	--------	--------	--------	1.02173
Benzene, C_6H_6	L	----------	49.08	--------	-------	--------	.87366
Beryllium, Be	s	----------	0	--------	--------	--------	1.85
n-Butane, C_4H_{10}	g	----------	-125.79	2.434	--------	22.44	----------
	L	272.638	-150.664	--------	--------	--------	.06012
i-Butane, C_4H_{10}	g	----------	-134.99	3.374	--------	21.30	----------
	L	261.361	-159.664	--------	--------	--------	.5941
1-Butene, C_4H_8	g	----------	-.54	2.563	--------	22.07	----------
	L	266.92	-25.173	--------	--------	--------	.6254
Chlorine, Cl_2	g	----------	0	1.968	.172	20.410	----------
	L	239.12	-22.550	--------	--------	--------	1.559
Chlorine trifluoride, ClF_3	g	----------	-164.6	.842	.414	27.53	----------
	L	284.89	-193.386	--------	--------	--------	1.850
Cyanogen, C_2N_2	g	----------	309.100	2.561	--------	23.33	----------
	L	252.05	283.209	--------	--------	--------	.9577
Diborane, B_2H_6	g	----------	36.6	5.695	.197	14.263	----------
	L	180.59	16.445	--------	--------	--------	.4371
Ethane, C_2H_6	g	----------	-83.852	5.267	--------	14.70	----------
	L	184.559	-103.819	--------	--------	--------	.5465
Ethanol, C_2H_5OH	L	----------	-277.51	--------	--------	--------	.78509
Ethylene, C_2H_4	g	----------	52.50	4.865	.163	13.527	----------
	L	169.42	33.945	--------	--------	--------	.5690
Ethylene oxide, C_2H_4O	g	----------	-52.635	.676	--------	25.53	----------
	L	283.65	-78.841	--------	--------	--------	.8824
Ethylene polymer, $(CH_2)_x$	s	----------	-25.6	--------	--------	--------	.935
Fluorine, F_2	g	----------	0	6.353	.078	6.66	----------
	L	85.02	-13.091	--------	--------	--------	1.5021
n-Heptane, C_7H_{16}	L	----------	-224.35	--------	--------	--------	.67950
n-Hexane, C_6H_{14}	L	----------	-198.66	--------	--------	--------	.65484
Hydrazine, N_2H_4	L	----------	50.38	--------	--------	--------	1.0040
Hydrogen, H_2	g	----------	0	8.043	.070	.899	----------
	L	20.27	-9.012	--------	--------	--------	.0709
Hydrogen peroxide, H_2O_2	L	----------	-187.78	--------	--------	--------	1.4425
IRFNA[b]	L	----------	-270.496	--------	--------	--------	1.478
Jet-A, $C_{12}H_{23}$[c]	L	----------	-303.403	--------	--------	--------	.818

a. Air is based on the following molar percents: N_2=78.084, O_2=20.9476, Ar=0.9365, CO_2, 0.0319 (Gordon, 1982). The empirical formula for 1 mole of air is $N_{1.56168}O_{.41959}Ar_{.009365}C_{.000319}$.

b. Inhibited red fuming nitric acid based on the following weight percents: HNO_3(L)=83.5, N_2O_4(L)=14, H_2O(L)=2, HF(g)=0.5. (This gives the following empirical formula defined as 1 mole: $H_{1.57216}N_{1.62945}O_{4.69505}F_{.02499}$.)

c. Typical jet fuel having the following properties: empirical formula defined as 1 mole is $C_{12}H_{23}$ (equivalent to H/C weight ratio of 0.16084); heat of combustion, 18 500 Btu/lb.

TABLE C.1.—Concluded.

Species	Phase	Boiling point, K	Assigned enthalpy, kJ/mol	$H_{298.15} - H_{bp}$, kJ/mol	$H_{bp} - H_{bp,re}$, kJ/mol	ΔH_{vap}, kJ/mol	Density, g/cm^3
JP–4, RP–1[d]	L	----------	–22.723	--------	--------	--------	0.773
JP–5, ASTMA1[e]	L	----------	–22.183	--------	--------	--------	.807
Lithium, Li	s	----------	0	--------	--------	--------	.534
	L	[f]453.69	7.187	--------	--------	--------	.512
Lithium perchlorate, $LiClO_4$	s	----------	–380.7	--------	--------	--------	2.428
Methane, CH_4	g	----------	–74.6	6.318	0.126	8.189	----------
	L	111.643	–89.233	--------	--------	--------	.4211
Methanol, CH_3OH	L	----------	–238.91	--------	--------	--------	.78664
Monomethyl hydrazine, CH_6N_2	L	----------	54.2	--------	--------	--------	.874
Nitric acid, HNO_3	g	----------	–133.913	--------	--------	39.1	----------
	L	----------	–173.013	--------	--------	--------	1.5037
Nitrogen, N_2	g	----------	0	6.427	.103	5.577	----------
	L	77.352	–12.107	--------	--------	--------	.8081
Nitrogen tetroxide, N_2O_4	g	----------	11.111	--------	--------	28.66	----------
	L	----------	–17.549	--------	--------	--------	1.431
Nitrogen trifluoride, NF_3	g	----------	–131.7	6.960	.142	11.585	----------
	L	144.09	–150.387	--------	--------	--------	1.537
Nitromethane, CH_3NO_2	L	----------	–113.1	--------	--------	--------	1.1286
n-Octane, C_8H_{18}	L	----------	–250.26	--------	--------	--------	.69854
i-Octane, C_8H_{18}	L	----------	–259.16	--------	--------	--------	.68784
Oxygen, O_2	g	----------	0	6.065	.094	6.820	----------
	L	90.17	–12.979	--------	--------	--------	1.149
Oxygen difluoride, OF_2	g	----------	24.5	6.608	.130	11.09	----------
	L	128.40	6.672	--------	--------	--------	1.518
Ozone, O_3	g	----------	141.8	4.964	.113	14.196	----------
	L	161.85	122.527	--------	--------	--------	1.449
Pentaborane, B_5H_9	L	----------	42.84	--------	--------	--------	.6183
n-Pentane, C_5H_{12}	L	----------	–173.49	--------	--------	--------	.6213
Perchloryl fluoride, $ClFO_3$	g	----------	–23.8	4.306	---------	19.33	----------
	L	226.40	–47.436	--------	--------	--------	1.392
Propane, C_3H_8	g	----------	–104.68	4.508	--------	19.04	----------
	L	231.076	–128.228	--------	--------	--------	.5810
Propylene, C_3H_6	g	----------	20.00	4.284	--------	18.42	----------
	L	225.46	–2.704	--------	--------	--------	.6093
Propyl nitrate, $C_3H_7NO_3$	L	----------	–214.5	--------	--------	--------	1.0538
Toluene, C_7H_8	L	----------	12.18	--------	--------	--------	.86220
Unsymmetrical dimethyl hydrazine (UDMH), $C_2H_8N_2$	L	----------	48.9	--------	--------	--------	.7914

d. Typical jet fuel having the following properties: H/C weight ratio, 0.163; heat of combustion, 18 640 Btu/lb (giving the following empirical formula defined as 1 mole: $C_1H_{1.9423}$).

e. Typical jet fuel having the following properties: H/C weight ratio, 0.161; heat of combustion, 18 600 Btu/lb (giving the following empirical formula defined as 1 mole: $C_1H_{1.9185}$).

f. Melting point for Li.

TABLE C.2.—REACTANT THERMODYNAMIC DATA IN *thermo.inp* FORMAT

```
Air             Mole%:N2 78.084,O2 20.9476,Ar .9365,CO2 .0319.NASA TP1906 1982
 2 1 9/95 N 1.5617O .41959AR.00937C .00032  .00000 0   28.9651785       -125.530
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8649.264
  1.00995016D+04 -1.96827561D+02  5.00915511D+00 -5.76101373D-03  1.06685993D-05
 -7.94029797D-09  2.18523191D-12  0.00000000D+00 -1.76796731D+02 -3.92150098D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8649.264
  2.41521443D+05 -1.25787460D+03  5.14455867D+00 -2.13854179D-04  7.06522784D-08
 -1.07148349D-11  6.57780015D-16  0.00000000D+00  6.46226319D+03 -8.14740866D+00
B2H6(L)         Diborane. JANAF Prop.Ser.E,1/67. TPIS v.III,1981.
 0 1 4/95 B   2.00H   6.00    0.00    0.00    0.00 1     27.66964      16445.000
    180.59
B5H9(L)         Pentaborane. JANAF June 1963 p300.
 0 j 6/63 B   5.00H   9.00    0.00    0.00    0.00 1     63.12646      42840.000
    298.15
(CH2)x(s)       Ethylene polymer. Est.from paraffin HC series,TRC p-2500,4/88.
 0 1 4/95 C   1.00H   2.00    0.00    0.00    0.00 1     14.02688      -25600.000
    298.15
CH3NO2(L)       Nitromethane. TRC p-9520,12/91.
 0 x12/91 C   1.00H   3.00N   1.00O   2.00    0.00 1     61.04036     -113100.000
    298.15
CH4(L)          Methane. TRC m-1350,10/93. JANAF Prop.Ser.E,1/67.
 0 1 4/95 C   1.00H   4.00    0.00    0.00    0.00 1     16.04276      -89233.000
    111.643
CH3OH(L)        Methanol. TRC p-5000,12/87; tc,uc,vc-5031-3,12/84.
 1 x12/84 C   1.00H   4.00O   1.00    0.00    0.00 1     32.04216     -238910.000
    175.610   390.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          18995.000
 -1.30200518D+06  3.16698523D+04 -3.03124315D+02  1.60223163D+00 -4.59450874D-03
  6.99018037D-06 -4.20739019D-09  0.00000000D+00 -1.65616865D+05  1.51434714D+03
CH6N2(L)        Monomethyl Hydrazine. TRC p-9220,12/93.
 0 x12/93 C   1.00H   6.00N   2.00    0.00    0.00 1     46.07212      54200.000
    298.15
C2H2(L),acetyle  Acetylene. Dens:JANAF Prop.Ser.E,1/67. B.P.:TRC a-3000,10/86.
 0 1 3/95 C   2.00H   2.00    0.00    0.00    0.00 1     26.03788      207599.000
    192.35
CH3CN(L)        Ethanenitrile (Acetonitrile). JPCRD v11,Sup.2,1982.
 0 1 3/95 C   2.00H   3.00N   1.00    0.00    0.00 1     41.05256      31380.
    298.15
C2H4(L)         Ethylene. TRC m-2600,10/93.
 0 1 4/95 C   2.00H   4.00    0.00    0.00    0.00 1     28.05376      33945.000
    169.42
C2H4O(L),ethyle  Ethylene oxide (Oxirane). TRC m-6150,6/94.
 0 1 4/95 C   2.00H   4.00O   1.00    0.00    0.00 1     44.05316      -78841.000
    283.65
C2H6(L)         Ethane. TRC m-1350, 10/93.
 0 1 4/95 C   2.00H   6.00    0.00    0.00    0.00 1     30.06964     -103819.000
    184.559
C2H5OH(L)       TRC p-5000,12/31/87; tc,uc,vc-5031-3,12/31/84.
 1 x12/84 C   2.00H   6.00O   1.00    0.00    0.00 1     46.06904     -277510.000
    159.000   390.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24082.000
  4.50111594D+05 -1.02082899D+04  1.01426678D+02 -3.87467261D-01  7.12139261D-04
 -1.85707145D-07 -2.03762257D-10  0.00000000D+00  7.44855790D+03 -5.04425552D+02
C2H8N2(L),UDMH  Unsymmetrical Dimethyl Hydrazine. TRC p9220,12/93.
 0 1 4/95 C   2.00H   8.00N   2.00    0.00    0.00 1     60.099        48900.000
    298.15
C2N2(L)         Cyanogen. Hdbk C&P Ed.73,1992-3.
 0 1 3/95 C   2.00N   2.00    0.00    0.00    0.00 1     52.03548      283209.000
    252.05
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TABLE C.2.—Continued.

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C3H6(L),propyle   Propylene. TRC m2600,10/93.
 0 1 4/95 C   3.00H   6.00    0.00    0.00    0.00 1     42.08064      -2704.000
    225.46
C3H7NO3(L)        Propyl Nitrate. Pedley,Naylor,Kirby,1986,p178.
 0 1 4/95 C   3.00H   7.00N   1.000   3.00    0.00 1    105.09352     -214500.000
    298.15
C3H8(L)           Propane. TRC m1350,10/93.
 0 1 4/95 C   3.00H   8.00    0.00    0.00    0.00 1     44.09652     -128228.000
    231.076
C4H8(L),1-buten   1-Butene. TRC m-2600,10/93. p-2600,4/88.
 0 1 3/95 C   4.00H    8.0    0.00    0.00    0.00 1     56.10752      -25173.000
    266.92
C4H10(L),n-buta   n-Butane. TRC m-1350,10/93.
 0 1 3/95 C   4.00H   10.0    0.00    0.00    0.00 1     58.12340     -150664.000
    272.638
C4H10(L),isobut   Isobutane(2-methyl propane). TRC m-1350,10/93.
 0 1 3/95 C   4.00H   10.0    0.00    0.00    0.00 1     58.12340     -159664.000
    261.361
C5H12(L),n-pent   n-Pentane. TRC p-1350,4/85.
 0 1 4/85 C   5.00H   12.0    0.00    0.00    0.00 1     72.15028     -173490.000
    298.15
C6H6(L)           Benzene. TRC tc,uc,vc-3201,10/31/86; p-3200,4/30/83.
 1 x10/86 C   6.00H   6.00    0.00    0.00    0.00 1     78.11364       49080.000
    278.680   500.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         30110.000
 -2.56013710D+06  4.13674588D+04 -2.12297357D+02  3.72357902D-01  7.56106887D-04
 -3.07721509D-06  2.78750625D-09  0.00000000D+00 -1.93546778D+05  1.23184575D+03
C6H5NH2(L)        Aniline. TRC p9370 6/30/90. TRC tc,uc,vc-9370 12/31/88
 1 x12/88 C   6.00H   7.00N   1.00    0.00    0.00 1     93.12832       31500.000
    267.130   460.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         34020.000
  6.26773441D+07 -8.94751040D+05  5.06761571D+03 -1.40216320D+01  1.89963591D-02
 -9.31666484D-06 -1.23822249D-09  0.00000000D+00  4.27541061D+06 -2.80777408D+04
C6H14(L),n-hexa   n-hexane. TRC p,tc,uc,vc-1440-1,4/85.
 1 x 4/85 C   6.00H  14.00    0.00    0.00    0.00 1     86.17716      -198660.000
    177.860   300.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         46920.000
  7.73091716D+06 -2.25189247D+05  2.71990284D+03 -1.69986707D+01  5.91239759D-02
 -1.07540944D-04  8.03043709D-08  0.00000000D+00  8.81946638D+05 -1.29413841D+04
C7H8(L)           TRC tc,uc,vc-3200-1,10/31/86; p-3200,4/30/83.
 1 x10/86 C   7.00H   8.00    0.00    0.00    0.00 1     92.14052       12180.000
    178.150   500.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         33470.000
 -3.71356003D+06  7.77255072D+04 -6.31228799D+02  2.72439986D+00 -6.10355386D-03
  7.02244524D-06 -3.11372750D-09  0.00000000D+00 -3.45212505D+05  3.26599001D+03
C7H16(L),n-hept   TRC m-1460,4/93; tc,uc,vc-1460,10/31/75.
 1 x10/75 C   7.00H  16.00    0.00    0.00    0.00 1    100.20404      -224350.000
    182.580   380.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         52640.000
  1.76003600D+06 -3.74960173D+04  3.96325980D+02 -2.11792498D+00  6.82851971D-03
 -1.13190177D-05  7.73709883D-09  0.00000000D+00  1.26916032D+05 -1.92178419D+03
C8H18(L),n-octa   TRC tables tc,uc,vc-1491-2. Hf298: p-1010,Oct.31,1984.
 1 x10/76 C   8.00H  18.00    0.00    0.00    0.00 1    114.23092      -250260.000
    216.370   310.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         61490.000
 -2.32282501D+07  4.84653545D+05 -4.08481823D+03  1.82081928D+01 -4.46566290D-02
  5.81410134D-05 -3.14960334D-08  0.00000000D+00 -2.16627048D+06  2.09165973D+04
C8H18(L),isooct   TRC tables tc,uc,vc-1491-2. Hf298: p-1490,Oct.31,1982.
 1 x10/76 C   8.00H  18.00    0.00    0.00    0.00 1    114.23092      -259160.000
    165.790   380.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         50190.000
  4.78104766D+06 -1.12691138D+05  1.09652177D+03 -5.34411704D+00  1.46003724D-02
 -2.02871999D-05  1.13340043D-08  0.00000000D+00  4.43284874D+05 -5.45790515D+03
CLF3(L)           JANAF Prop.SerD,3/66. TRC k-140,12/73.
 0 1 3/95 CL  1.00F   3.00    0.00    0.00    0.00 1     92.44791      -193386.000
    284.89
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TABLE C.2.—Continued.

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CLO3F             Perchloryl Fluoride. JPCRD v22 sup2,1982. JANAF 3/61.
 2 l 5/95 CL  1.00O   3.00F   1.00    0.00    0.00 0    102.44930     -23800.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13298.823
  4.46087770D+04 -5.89208408D+02  3.55871337D+00  2.80962019D-02 -3.61092477D-05
  2.27336016D-08 -5.71680272D-12  0.00000000D+00 -1.38879811D+03  4.59151362D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         13298.823
 -3.91041344D+05 -1.19325902D+03  1.38866330D+01 -3.54168398D-04  7.82659835D-08
 -8.97991688D-12  4.16469843D-16  0.00000000D+00 -1.27485199D+03 -5.10649344D+01
CLO3F(L)          Perchloryl Fluoride. Hdbk C&P,ED.73,1992-3.
 0 l 4/95 CL  1.00O   3.00F   1.00    0.00    0.00 1    102.44930     -47436.000
    226.40
CL2(L)            Chlorine. HdbkC&P Ed.73,1992-3. JANAF Prop.Ser.E,1/67
 0 l 4/95 CL  2.00    0.00    0.00    0.00    0.00 1     70.90540     -22550.000
    239.12
F2(L)             Fluorine. Hdbk C&P Ed.73 1992-3. JANAF Prop.Ser.D,3/66.
 0 l 4/95 F   2.00    0.00    0.00    0.00    0.00 1     37.99681     -13091.000
     85.02
F2O(L)            Oxygen Difluoride.Hdbk C&P Ed.73,1992-3.JANAF Prop.Ser.E,1/67.
 0 l 4/95 F   2.00O   1.00    0.00    0.00    0.00 1     53.99621       6672.000
    128.40
HNO3(L)           Nitric Acid. Hdbk C&P Ed.73,1992-3,p6-102.
 0 l 4/95 H   1.00N   1.00O   3.00    0.00    0.00 1     63.01288     -173013.000
    298.15
H2(L)             Hydrogen. JANAF Prop.Ser.D,3/66.
 0 jp3/66 H   2.00    0.00    0.00    0.00    0.00 1      2.01588       -9012.000
     20.27
H2O2(L)           Hydrogen Peroxide Liquid.TPIS,1989.
 1 tpis89 H   2.00O   2.00    0.00    0.00    0.00 1     34.01468     -187780.000
    272.740  6000.000 1  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0         22949.000
  1.07438683D+01  0.00000000D+00  0.00000000D+00  0.00000000D+00  0.00000000D+00
  0.00000000D+00  0.00000000D+00  0.00000000D+00 -2.57878985D+04 -4.80322129D+01
IRFNA             Wt%: HNO3(L) 83.5; N2O4(L) 14.; H2O(L) 2.; HF(g) .5.
 0 l 4/95 H 1.5722N 1.6294O 4.6950F .02499          1     100.        -270496.000
    298.15
JP-4              Also RP-1. NASA RP-1311, Part II, 1996. Hcomb = 18640.BTU/#
 0 l 5/95 C   1.00H 1.9423                          1     13.96872     -22723.000
    298.15
JP-5              Also ASTMA1. NASA RP-1311, Part II, 1996. Hcomb = 18600.BTU/#
 0 l 5/95 C   1.00H 1.9185                          1     13.94473     -22183.000
    298.15
Jet-A(L)          NASA TM-101475,1988. Hcomb=18500 BTU/#:NASA CR-72951,1971.
 1 l 2/96 C  12.00H  23.00    0.00    0.00    0.00 1    167.31462     -303403.000
    220.000   550.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-4.218467340D+05-5.576234840D+03 1.522094335D+02-8.610096140D-01 3.071640926D-03
-4.702766120D-06 2.743009309D-09 0.000000000D+00-3.238535350D+04-6.780954740D+02
Jet-A(g)          NASA TM-101475,1988. NASA CR-72951,1971.
 2 l 2/96 C  12.00H  23.00    0.00    0.00    0.00 0    167.31462     -249657.000
    273.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
-6.068699280D+05 8.328264220D+03-4.312323550D+01 2.572391032D-01-2.629316827D-04
 1.644989491D-07-4.645336690D-11 0.000000000D+00-7.606965040D+04 2.794307229D+02
   1000.000  5000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0             0.000
 1.541871660D+07-7.433869020D+04 1.468645380D+02-1.297042936D-02 2.159140196D-06
-1.887183642D-10 6.604559540D-15 0.000000000D+00 3.996323340D+05-9.266674660D+02
LiCLO4(s)         Lithium Perchlorate. JANAF, March, 1964.
 0 j 3/64 LI  1.00CL  1.00O   4.00    0.00    0.00 1    106.3913      -380700.000
    298.15
NF3(L)            Nitrogen trifluoride. JANAF Prop.Ser.E,1/67.
 0 l 3/95 N   1.00F   3.00    0.00    0.00    0.00 1    71.001950     -150387.000
    144.09
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TABLE C.2.—Concluded.

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NH3(L)              Ammonia. TRC m-500,6/56,B.P.a-500,12/63. JANAF Prop.Ser.E,1/67
 0 1 3/95 N   1.00H    3.00     0.00     0.00     0.00 1      17.03056     -71555.000
    239.72
NH4CLO4(I)          Ammonium Perchlorate. JANAF Dec.1962.
 1 j12/62 N   1.00H    4.00CL   1.00O    4.00     0.00 1     117.48880     -295767.000
    100.000   513.150 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          25238.000
 -3.07534557D+03 -2.13650594D+02  1.02158307D+01  1.65946375D-02  1.66526642D-05
 -2.30609605D-08  1.54365732D-11  0.00000000D+00 -3.82576726D+04 -4.23025427D+01
NH4CLO4(II)         Ammonium Perchlorate. JANAF Dec.1962.
 1 j12/62 N   1.00H    4.00CL   1.00O    4.00     0.00 2     117.48880     -295767.000
    513.150  1500.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          25238.000
  4.29699948D+07 -3.17841780D+05  9.59143755D+02 -1.43988137D+00  1.22267365D-03
 -5.21540162D-07  8.80361276D-11  0.00000000D+00  1.68744630D+06 -5.88947816D+03
NH4NO3(IV)          Ammonium Nitrate Rhombic Crystal(IV). TPIS,1989.
 2 tpis89 N   2.00H    4.00O    3.00     0.00     0.00 1      80.04344     -365600.000
    256.200   298.150 6 -2.0 -1.0  0.0  1.0  2.0  3.0  0.0  0.0          23662.000
 -1.62667900D+07  2.61460339D+05 -1.68004630D+03  5.44897154D+00 -8.58784985D-03
  5.34327778D-06  0.00000000D+00  0.00000000D+00 -1.26419517D+06  9.08569617D+03
    298.150   305.380 2  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0          23662.000
  5.86564933D+00  3.64302887D-02  0.00000000D+00  0.00000000D+00  0.00000000D+00
  0.00000000D+00  0.00000000D+00  0.00000000D+00 -4.73393723D+04 -2.61436244D+01
NH4NO3(III)         Ammonium Nitrate Rhombic Crystal(III). TPIS,1989.
 1 tpis89 N   2.00H    4.00O    3.00     0.00     0.00 3      80.04344     -365600.000
    305.380   357.250 2  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0          23662.000
  7.23313821D+00  2.33327039D-02  0.00000000D+00  0.00000000D+00  0.00000000D+00
  0.00000000D+00  0.00000000D+00  0.00000000D+00 -4.69417938D+04 -2.92985169D+01
NH4NO3(II)          Ammonium Nitrate Tetragonal Crystal(II). TPIS,1989.
 1 tpis89 N   2.00H    4.00O    3.00     0.00     0.00 4      80.04344     -365600.000
    357.250   399.000 3  0.0  1.0  3.0  0.0  0.0  0.0  0.0  0.0          23662.000
  6.02320522D+01 -1.76799354D-01  4.52882972D-07  0.00000000D+00  0.00000000D+00
  0.00000000D+00  0.00000000D+00  0.00000000D+00 -5.47863351D+04 -2.75780621D+02
NH4NO3(I)           Ammonium Nitrate Cubic Crystal(I). TPIS,1989.
 1 tpis89 N   2.00H    4.00O    3.00     0.00     0.00 5      80.04344     -365600.000
    399.000   442.850 2  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0          23662.000
  1.29532588D+01  1.56353171D-02  0.00000000D+00  0.00000000D+00  0.00000000D+00
  0.00000000D+00  0.00000000D+00  0.00000000D+00 -4.78370128D+04 -5.84851082D+01
NH4NO3(L)           Ammonium Nitrate Liquid. TPIS,1989.
 1 tpis89 N   2.00H    4.00O    3.00     0.00     0.00 6      80.04344     -365600.000
    442.850  6000.000 1  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0          23662.000
  1.93637388D+01  0.00000000D+00  0.00000000D+00  0.00000000D+00  0.00000000D+00
  0.00000000D+00  0.00000000D+00  0.00000000D+00 -4.84379330D+04 -8.90300528D+01
N2(L)               Nitrogen. TRC k-460,6/60, m-470,6/56. JANAF Prop.Ser.D,3/66.
 0 1 4/95 N   2.00     0.00     0.00     0.00     0.00 1      28.01348     -12107.000
     77.352
N2H4(L)             Hydrazine. Hf298: TPIS89. Props: JANAF 12/65.
 1 j12/65 N   2.00H    4.00     0.00     0.00     0.00 1      32.04524      50380.000
    100.000   800.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
  2.08096574D+04 -7.41816770D+02  1.91656919D+01 -4.53933014D-02  1.34202426D-04
 -1.47087394D-07  6.05628828D-11  0.00000000D+00  5.73540821D+03 -8.82021397D+01
N2O4(L)             Dinitrogen tetroxide. Hvap: JANAF Prop.Ser.C,4/65.
 0 1 4/95 N   2.00O    4.00     0.00     0.00     0.00 1      92.01108     -17549.000
    298.15
O2(L)               Oxygen. Hvap: TRC m-10,12/63. JANAF Prop.Ser.D,3/66.
 0 1 4/95 O   2.00     0.00     0.00     0.00     0.00 1      31.99880     -12979.000
     90.17
O3(L)               Ozone. Hvap: TRC m-10,12/63. JANAF Prop.Ser.E,1/67.
 0 1 4/95 O   3.00     0.00     0.00     0.00     0.00 1      47.99820     122527.000
    161.85
```

Appendix D

References for Reactant Data in Table C.1

References given in this appendix correspond to the data in table C.1. The references, given at the end of this appendix, are indicated in table D.1 by the following brief codes:

Code	Abbreviated reference
AUTH	Authors
FAITH	Faith: NASA CR–72951
GRACIA	Gracia: NASA TM–101475
H1	Lide: Handbook of Chem. & Phys., 73rd Ed
H2	Weast: Handbook of Chem. & Phys., 65th Ed.
J	Chase: JANAF Thermochemical Table
JCS	Banks: J. Chem. Soc.
JPR	Stull: JANAF Thermo. Data (Propellants)
MARK	Mark: Encyclopedia of Polymer Science
PED	Pedley: Thermo. Data of Organic Compounds
RD1	Pamidimukkala: JPCRD, Vol. 11, No. 1
RDS2	Wagman: JPCRD, Vol. 11, Supp. 2
SP273	Gordon: NASA SP–273, Interim Revision
TP81	Gurvich: TPIS, Vol. 3, Pts. 1 & 2, 1981
TP82	Gurvich: TPIS, Vol. 4, Pts. 1 & 2, 1982
TP89:	Gurvich: TPIS, Vol. 1, Pts. 1 & 2, 1989
TP91:	Gurvich: TPIS, Vol. 2, Pts. 1 & 2, 1991
X	TRC Thermodynamic Tables

Page numbers follow all codes except AUTH and JPR. Following JPR is a series code, either A, B, C, D, or E (examples: X w–3040 refers to reference X, page w–3040; JPR E refers to reference JPR, series E). The data from TP81, TP82, TP89, and TP91 are often found in both parts 1 and 2 of these references. In this situation the page numbers refer to part 1 with a few exceptions.

TABLE D.1.—REFERENCES FOR REACTANT DATA IN TABLE C.1

Species	Phase	Boiling point, K	Assigned enthalpy, kJ/mol	$H_{298.15} - H_{bp}$, kJ/mol	$H_{bp} - H_{bp,re}$, kJ/mol	ΔH_{vap}, kJ/mol	Density, g/cm^3
Acetonitrile, C_2H_3N	L	----------	RDS2 2–103	--------	--------	----------	H1 15–43
Acetylene, C_2H_2	g	----------	X w–3040	AUTH	JPR E	JPR E	----------
	L	X a–3000	AUTH	--------	--------	----------	JPR E
Air	g	----------	AUTH	--------	--------	----------	----------
Ammonia, NH_3	g	----------	TP89 354	AUTH	JPR E	X m–500	----------
	L	X a–500	AUTH	--------	--------	----------	H2 B–365
Ammonium perchlorate, NH_4ClO_4	I	----------	J 747	--------	--------	----------	H1 4–38
Ammonium nitrate, NH_4NO_3	IV	----------	TP89 371	--------	--------	----------	H1 4–39
Aniline, $C_6H_5NH_2$	L	----------	X p–9370	--------	--------	----------	H1 3–37
Benzene, C_6H_6	L	----------	X p–3200	--------	--------	----------	X d–3200
Beryllium, Be	s	----------	ref. element	--------	--------	----------	H1 4–43
n-Butane, C_4H_{10}	g	----------	X w–1350	AUTH	--------	X m–1350	----------
	L	X m–1350	AUTH	--------	--------	----------	X d–1350
i-Butane, C_4H_{10}	g	----------	X w–1350	AUTH	--------	X m–1350	----------
	L	X m–1350	AUTH	--------	--------	----------	X d–1350
1-Butene, C_4H_8	g	----------	X w–2600	AUTH	--------	X m–2600	----------
	L	X m–2600	AUTH	--------	--------	----------	X d–2500
Chlorine, Cl_2	g	----------	ref. element	AUTH	JPR E	H1 6–101	----------
	L	X k–120	AUTH	--------	--------	----------	X d–120
Chlorine trifluoride, ClF_3	g	----------	TP89 194	AUTH	JPR D	H1 6–101	----------
	L	X a–140	AUTH	--------	--------	----------	JCS50 191
Cyanogen, C_2N_2	g	----------	TP91 225	AUTH	--------	H1 6–104	----------
	L	H1 6–104	AUTH	--------	--------	----------	H1 4–58
Diborane, B_2H_6	g	----------	TP81 35	AUTH	JPR E	JPR E	----------
	L	JPR E	AUTH	--------	--------	----------	JPR E
Ethane, C_2H_6	g	----------	RD1 85	AUTH	--------	X m–1350	----------
	L	X m–1350	AUTH	--------	--------	----------	X d–1350
Ethanol, C_2H_5OH	L	----------	X p–5000	--------	--------	----------	X a–5030
Ethylene, C_2H_4	g	----------	X w–2600	AUTH	JPR E	X m–2600	----------
	L	X m–2600	AUTH	--------	--------	----------	X d–2500
Ethylene oxide, C_2H_4O	g	----------	J 662	AUTH	--------	X m–6150	----------
	L	X m–6150	AUTH	--------	--------	----------	H1 3–243
Ethylene polymer, $(CH_2)_x$	s	----------	AUTH	--------	--------	----------	MARK
Fluorine, F_2	g	----------	ref. element	AUTH	JPR D	H1 6–102	----------
	L	H1 6–102	AUTH	--------	--------	----------	X d–90
n-Heptane, C_7H_{16}	L	----------	X p–1010	--------	--------	----------	X d–1460
n-Hexane, C_6H_{14}	L	----------	X p–1440	--------	--------	----------	X a–1010
Hydrazine, N_2H_4	L	----------	TP89 361	--------	--------	----------	X a–500
Hydrogen, H_2	g	----------	ref. element	JPR E	JPR E	JPR E	----------
	L	JPR E	AUTH	--------	--------	----------	JPR D

TABLE D.1—Continued.

Species	Phase	Boiling point, K	Assigned enthalpy, kJ/mol	$H_{298.15} - H_{bp}$, kJ/mol	$H_{bp} - H_{bp,re}$, kJ/mol	ΔH_{vap}, kJ/mol	Density, g/cm^3
Hydrogen peroxide, H_2O_2	L	----------	X p–30	--------	--------	----------	X d–30
IRFNA	L	----------	AUTH	--------	--------	----------	AUTH
Jet-A	L	----------	GRACIA	--------	--------	----------	FAITH
JP–4, RP–1	L	----------	AUTH	--------	--------	----------	SP273
JP–5, ASTMA1	L	----------	AUTH	--------	--------	----------	SP273
Lithium, Li	s	----------	ref. element	--------	--------	----------	H1 4–69
	L	TP82 286	TP82 286	--------	--------	----------	SP273
Lithium perchlorate, $LiClO_4$	s	----------	J 763	--------	--------	----------	H1 4–469
Methane, CH_4	g	----------	TP91 46	AUTH	JPR E	Xm–1350	----------
	L	X m–1010	AUTH	--------	--------	----------	X d–1010
Methanol, CH_3OH	L	----------	X p–5000	--------	--------	----------	X a–5030
Monomethyl hydrazine, CH_6N_2	L	----------	X p–9220	--------	--------	----------	H1 3–283
Nitric acid, HNO_3	g	----------	TP89 231	--------	--------	H1 6–102	----------
	L	----------	AUTH	--------	--------	----------	X a–510
Nitrogen, N_2	g	----------	ref. element	AUTH	JPR D	X m–470	----------
	L	X k–460	AUTH	--------	--------	----------	H1 4–79
Nitrogen tetroxide, N_2O_4	g	----------	TP89 212	--------	--------	JPR C	----------
	L	----------	AUTH	--------	--------	----------	JPR C
Nitrgen trifluoride, NF_3	g	----------	TP89 376	AUTH	JPR E	JPR E	----------
	L	X a–520	AUTH	--------	--------	----------	H1 4–79
Nitromethane, CH_3NO_2	L	----------	X p–9520	--------	--------	----------	H1 15–47
n-Octane, C_8H_{18}	L	----------	X p–1010	--------	--------	----------	X d–1490
i-Octane, C_8H_{18}	L	----------	X p–1490	--------	--------	----------	X d–1493
Oxygen, O_2	g	----------	ref. element	AUTH	JPR D	X m–10	----------
	L	X m–10	AUTH	--------	--------	----------	H1 4–80
Oxygen difluoride, OF_2	g	----------	TP89 162	AUTH	JPR E	H1 6–102	----------
	L	H1 6–102	AUTH	--------	--------	----------	X d–90
Ozone, O_3	g	----------	TP89 103	AUTH	JPR E	X m–10	----------
	L	X m–10	AUTH	--------	--------	----------	JPR E
Pentaborane, B_5H_9	L	----------	J 300	--------	--------	----------	JPR A
n-Pentane, C_5H_{12}	L	----------	X p–1350	--------	--------	----------	X a–1010
Perchloryl fluoride, $ClFO_3$	g	----------	RDS2 2–49	AUTH	--------	H1 6–101	----------
	L	H1 6–101	AUTH	--------	--------	----------	H1 4–53
Propane, C_3H_8	g	----------	X w–1350	AUTH	--------	X m–1350	----------
	L	X m–1350	AUTH	--------	--------	----------	X d–1350
Propylene, C_3H_6	g	----------	X w–2600	AUTH	--------	X m–2600	----------
	L	X m–2600	AUTH	--------	--------	----------	X d–2600
Propyl nitrate, $C_3H_7NO_3$	L	----------	PED 178	--------	--------	----------	H1 3–427
Toluene, C_7H_8	L	----------	X p–3200	--------	--------	----------	X a–3200
Unsymmetrical dimethyl hydrazine (UDMH), $C_2H_8N_2$	L	----------	X p–9220	--------	--------	----------	H1 3–283

TABLE D.1.—Concluded.

References:

AUTH: Calculated by the authors (assigned enthalpy either from the equation in appendix C or from heats of combustion for jet fuels; sensible heat from molecular data).

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TP82: Gurvich, L.V., et al., 1982, *Thermodynamic Properties of Individual Substances*, Vol. IV, Pts. 1–2, Nauka, Moscow, U.S.S.R

TP89: Gurvich, L.V., Veyts, I.V., and Alcock, C.B., 1989, *Thermodynamic Properties of Individual Substances*, Fourth Ed., Vol. 1, Pts. 1 & 2, Hemisphere Publishing Corp., Washington, DC.

TP91: Gurvich, L.V., Veyts, I.V., and Alcock, C.B., 1991, *Thermodynamic Properties of Individual Substances*, Fourth Ed., Vol. 1, Pts. 1 & 2, Hemisphere Publishing Corp., Washington, DC.

X: Anon., 1985–1986, *TRC Thermodynamic Tables, Nonhydrocarbons*; or *TRC Thermodynamic Tables, Hydrocarbons*. Thermodynamics Research Center, Texas A&M University, College Station, TX. (Looseleaf Tables.)

Appendix E

Format and List of Species With Thermal Transport Property Data

Most of the library of thermal transport property data in the form of least-squares coefficients (*trans.inp*) are taken from Svehla (1995). However, since the publication of his report, Mr. Svehla has revised some of the data (Svehla, 1996). At present, this library contains data for 65 reaction products and 42 binary interaction parameters. However, as data for species or interactions are added, revised, or deleted, these numbers may change. The format for the functional form used in *trans.inp* is given in table E.1. The current set of least-squares coefficients in *trans.inp* is given in table E.2. This set replaces the set given in table III of Svehla (1995). The last column in table E.2 indicates whether the coefficients were taken from Svehla (1995) or Svehla (1996). Chapter 1 and section 5.25 discuss processing the *trans.inp* data and storing the processed data in *trans.lib* for subsequent use in the CEA program.

TABLE E.1.—FORMAT FOR THERMAL TRANSPORT PROPERTY DATA

Records	Contents	Format	Columns
1[a]	Species name	A15	1–15
	Second species name if binary interaction (blank for pure species)	A15	17–31
	V if there are viscosity coefficients	A1	35
	Temperature intervals for viscosity (0, 1, 2, or 3)	I1	36
	C if there are thermal conductivity coefficients	A1	37
	Temperature intervals for thermal conductivity (0, 1, 2, or 3)	I1	38
	Comments (references, date, etc.)	A40	41–80
Any number from 1 to 6[b]	V if coefficients are for viscosity	A1	2
	C if coefficients are for thermal conductivity	A1	2
	First and last temperatures of temperature interval	2F9.2	3–20
	Four coefficients in equations below[c]	4E15.8	21–80

a. Header record for each pure species or binary interaction.

b. The number of records for each pure species or binary interaction equals the sum of the number of temperature intervals for both viscosity and thermal conductivity (sum of numbers in columns 36 and 38 of header record). Temperature intervals must be in increasing order. Viscosity or thermal conductivity order is immaterial. Any number of species is permitted between the first record (`tran`) and the last record (`end`).

c. The empirical equations follow (coefficients are different for each property):

$$\left.\begin{array}{ll} \text{Viscosity:} & \ln \eta \\ \text{Thermal conductivity:} & \ln \lambda \\ \text{Interaction parameter:} & \ln \eta_{(i,j)} \end{array}\right\} = A \ln T + \frac{B}{T} + \frac{C}{T^2} + D$$

TABLE E.2.—VISCOSITY AND THERMAL CONDUCTIVITY COEFFICIENTS IN *trans.inp*

trans.inp File						Ref.
transport property coefficients						
Ar			V3C3 BICH ET AL (1990)			
V 200.0	1000.0	0.61205763E 00	-0.67714354E 02	0.19040660E 03	0.21588272E 01	a
V 1000.0	5000.0	0.69357334E 00	0.70953943E 02	-0.28386007E 05	0.14856447E 01	a
V 5000.0	15000.0	0.76608935E+00	0.67867215E+03	-0.84991417E+06	0.77935167E+00	b
C 200.0	1000.0	0.60968928E 00	-0.70892249E 02	0.58420624E 03	0.19337152E 01	a
C 1000.0	5000.0	0.69075463E 00	0.62676058E 02	-0.25667413E 05	0.12664189E 01	a
C 5000.0	15000.0	0.76269502E+00	0.62341752E+03	-0.71899552E+06	0.56927918E+00	b
BCL3			V2C2 SVEHLA (1962)			
V 300.0	1000.0	0.52572590E 00	-0.27803504E 03	0.19159256E 05	-0.24373790E 01	a
V 1000.0	5000.0	0.62929553E 00	-0.60723560E 02	-0.37711618E 05	0.15615047E 01	a
C 300.0	1000.0	0.41518585E 00	-0.48149960E 03	0.30788060E 05	0.33168239E 01	a
C 1000.0	5000.0	0.61148589E 00	-0.18167042E 03	-0.20976969E 05	0.17127671E 01	a
BF3			V2C2 SVEHLA (1962,1994)			
V 300.0	1000.0	0.58778079E 00	-0.96213686E 02	-0.37660007E 03	0.21035273E 01	a
V 1000.0	5000.0	0.64430285E 00	0.73362845E 01	-0.23890605E 05	0.16330508E 01	a
C 300.0	1000.0	0.39288181E 00	-0.53781426E 03	0.39023491E 05	0.42287006E 01	a
C 1000.0	5000.0	0.60695214E 00	-0.19889031E 03	-0.23403767E 05	0.24734586E 01	a
Br2			V2C2 SVEHLA (1962,1994)			
V 300.0	1000.0	0.45241871E 00	-0.52542766E 03	0.61354230E 05	0.35322870E 01	a
V 1000.0	5000.0	0.60111079E 00	-0.22499274E 03	-0.14517179E 05	0.22805949E 01	a
C 300.0	1000.0	0.13579199E 00	-0.80137295E 03	0.83046621E 05	0.48052172E 01	a
C 1000.0	5000.0	0.13602376E 00	-0.21904601E 04	0.77769913E 06	0.54980508E 01	a
C			V2C2 BIOLSI (1982)			
V 1000.0	5000.0	0.80124735E+00	0.17261643E+03	-0.69940019E+05	0.88364870E-01	b
V 5000.0	15000.0	0.10344416E+01	0.31310924E+04	-0.45512020E+07	-0.23102402E+01	b
C 1000.0	5000.0	0.80224051E+00	0.17739617E+03	-0.72350849E+05	0.10329911E+01	b
C 5000.0	15000.0	0.10355137E+01	0.31489830E+04	-0.45854028E+07	-0.13676372E+01	b
C	O		V1C0 CAPITELLI & FICOCELLI (1973)			
V 4000.0	15000.0	0.12635466E+01	0.46866528E+04	-0.59789292E+07	-0.43066246E+01	b
CCLF3			V2C2 SVEHLA (1994)			
V 300.0	1000.0	0.57775962E 00	-0.11595656E 03	0.13894846E 04	0.20719367E 01	a
V 1000.0	5000.0	0.64278913E 00	0.18533422E 01	-0.25000775E 05	0.15313091E 01	a
C 300.0	1000.0	0.30701673E 00	-0.58621120E 03	0.37562739E 05	0.45977739E 01	a
C 1000.0	5000.0	0.59447897E 00	-0.25405493E 03	0.15214514E 05	0.23022470E 01	a
CCL2F2			V2C2 SVEHLA (1994)			
V 300.0	1000.0	0.55188576E 00	-0.18084616E 03	0.74399094E 04	0.22089157E 01	a
V 1000.0	5000.0	0.63820813E 00	-0.16395245E 02	-0.31624406E 05	0.14872353E 01	a
C 300.0	1000.0	0.37505967E 00	-0.45975338E 03	0.13246268E 05	0.38355232E 01	a
C 1000.0	5000.0	0.59226968E 00	-0.25988712E 03	0.21916978E 05	0.21265525E 01	a
CCL3F			V2C2 SVEHLA (1994)			
V 300.0	1000.0	0.52599241E 00	-0.27466441E 03	0.18699061E 05	0.23965367E 01	a
V 1000.0	5000.0	0.62963969E 00	-0.58775545E 02	-0.37421689E 05	0.15207986E 01	a
C 300.0	1000.0	0.25082525E 00	-0.69236016E 03	0.58465610E 05	0.46480202E 01	a
C 1000.0	5000.0	0.58847038E 00	-0.29613903E 03	0.29176214E 05	0.19487185E 01	a
CCL4			V2C2 SVEHLA (1994)			
V 300.0	1000.0	0.52914726E 00	-0.26173707E 03	0.16983586E 05	0.22508228E 01	a
V 1000.0	5000.0	0.63117223E 00	-0.50873987E 02	-0.37435436E 05	0.13896152E 01	a
C 300.0	1000.0	0.39796301E 00	-0.45970713E 03	0.25887539E 05	0.32182809E 01	a
C 1000.0	5000.0	0.60345477E 00	-0.22665258E 03	0.12105253E 05	0.15795218E 01	a
CF4			V2C2 BOUSHEHRI ET AL (1987) SVEHLA (1994)			
V 300.0	1000.0	0.62364242E 00	-0.15734540E 02	-0.11268526E 05	0.17826560E 01	a
V 1000.0	5000.0	0.52895824E 00	-0.34441290E 03	0.10572786E 06	0.26483931E 01	a
C 300.0	1000.0	0.29102001E 00	-0.62544847E 03	0.40137545E 05	0.50559989E 01	a
C 1000.0	5000.0	0.46958735E 00	-0.71864138E 03	0.17601542E 06	0.37798145E 01	a

TABLE E.2.—Continued.

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CHCLF2                                    V2C2  SVEHLA (1994)
 V  300.0   1000.0   0.55518512E 00-0.19151112E 03 0.92302454E 04 0.22465942E 01  a
 V 1000.0   5000.0   0.63832814E 00-0.18642363E 02-0.35632589E 05 0.15442566E 01  a
 C  300.0   1000.0   0.57111784E 00-0.40344356E 03 0.76841854E 04 0.26855196E 01  a
 C 1000.0   5000.0   0.57237181E 00-0.42144805E 03 0.17313314E 05 0.26852328E 01  a
CHCL2F                                    V2C2  SVEHLA (1994)
 V  300.0   1000.0   0.54261029E 00-0.23693132E 03 0.14722387E 05 0.22950603E 01  a
 V 1000.0   5000.0   0.63322050E 00-0.43091499E 02-0.36892355E 05 0.15269221E 01  a
 C  300.0   1000.0   0.64554399E 00-0.29614334E 03-0.34305973E 04 0.18524599E 01  a
 C 1000.0   5000.0   0.58133799E 00-0.38461009E 03 0.86999769E 04 0.23723154E 01  a
CHCL3                                     V2C2  SVEHLA (1962,1994)
 V  300.0   1000.0   0.52563815E 00-0.28025371E 03 0.19479241E 05 0.23475804E 01  a
 V 1000.0   5000.0   0.62913497E 00-0.61794789E 02-0.38001753E 05 0.14716717E 01  a
 C  300.0   1000.0   0.43704658E 00-0.53648192E 03 0.29187663E 05 0.32672103E 01  a
 C 1000.0   5000.0   0.55383193E 00-0.51059645E 03 0.74636570E 05 0.23891512E 01  a
CHF3                                      V2C2  SVEHLA (1994)
 V  300.0   1000.0   0.58092199E 00-0.11862927E 03 0.25039931E 04 0.20948315E 01  a
 V 1000.0   5000.0   0.64363521E 00-0.70920001E 00-0.25099472E 05 0.15713073E 01  a
 C  300.0   1000.0   0.73882642E 00-0.17058713E 03-0.32698111E 05 0.16126977E 01  a
 C 1000.0   5000.0   0.58787951E 00-0.35203256E 03-0.17448254E 05 0.28215977E 01  a
CH2CL2                                    V2C2  SVEHLA (1994)
 V  300.0   1000.0   0.57185884E 00-0.34599168E 03 0.32975791E 05 0.21786059E 01  a
 V 1000.0   5000.0   0.60922943E 00-0.18784625E 03-0.27411214E 05 0.18227006E 01  a
 C  300.0   1000.0   0.25979341E 00-0.10510041E 04 0.11078850E 06 0.51956543E 01  a
 C 1000.0   5000.0   0.48080771E 00-0.95120530E 03 0.17139452E 06 0.35085367E 01  a
CH3CL                                     V2C2  MONCHICK & MASON (1961)  SVEHLA (1994)
 V  300.0   1000.0   0.58181268E 00-0.30714376E 03 0.27516618E 05 0.20941516E 01  a
 V 1000.0   5000.0   0.61479454E 00-0.16327574E 03-0.27926072E 05 0.17778956E 01  a
 C  300.0   1000.0   0.43048390E 00-0.96586387E 03 0.91616260E 05 0.44424192E 01  a
 C 1000.0   5000.0   0.44418462E 00-0.11573896E 04 0.19422838E 06 0.44366915E 01  a
CH4                                       V2C2  BOUSHEHRI ET AL (1987)  SVEHLA (1994)
 V  200.0   1000.0   0.57643622E 00-0.93704079E 02 0.86992395E 03 0.17333347E 01  a
 V 1000.0   5000.0   0.66400044E 00 0.10860843E 02-0.76307841E 04 0.10323984E 01  a
 C  200.0   1000.0   0.10238177E 01-0.31092375E 03 0.32944309E 05 0.67787437E 00  a
 C 1000.0   5000.0   0.77485028E 00-0.40089627E 03-0.46551082E 05 0.25671481E 01  a
CH4              O2                       V2C0  SVEHLA (1994)
 V  300.0   1000.0   0.68971658E 00-0.82884483E 00-0.47557575E 04 0.11497470E 01  a
 V 1000.0   5000.0   0.69426262E 00-0.17685146E 02 0.59452784E 04 0.11244994E 01  a
CH3OH                                     V2C2  MONCHICK & MASON (1961)  SVEHLA (1994)
 V  300.0   1000.0   0.58408390E 00-0.30677174E 03 0.27569892E 05 0.19794348E 01  a
 V 1000.0   5000.0   0.61454903E 00-0.16540203E 03-0.27881995E 05 0.16830713E 01  a
 C  300.0   1000.0   0.33374512E 00-0.11617154E 04 0.10894211E 06 0.57684124E 01  a
 C 1000.0   5000.0   0.42733576E 00-0.12682528E 04 0.20900463E 06 0.51283860E 01  a
CO                                        V3C3  SVEHLA (1994)
 V  200.0   1000.0   0.62526577E 00-0.31779652E 02-0.16407983E 04 0.17454992E 01  a
 V 1000.0   5000.0   0.87395209E 00 0.56152222E 03-0.17394809E 06-0.39335958E 00  a
 V 5000.0  15000.0   0.88503551E+00 0.90902171E+03-0.73129061E+06-0.53503838E+00  b
 C  200.0   1000.0   0.85439436E+00 0.10573224E+03-0.12347848E+05 0.47793128E+00  b
 C 1000.0   5000.0   0.88407146E+00 0.13357293E+03-0.11429640E+05 0.24417019E+00  b
 C 5000.0  15000.0   0.24175411E+01 0.80462671E+04 0.31090740E+07-0.14516932E+02  b
CO              CO2                       V3C0  SVEHLA (1995)
 V  300.0   1000.0   0.68926185E 00-0.13796096E 01-0.46847568E 04 0.13060681E 01  b
 V 1000.0   5000.0   0.69417954E 00-0.18021840E 02 0.60950694E 04 0.12779603E 01  b
 V 5000.0  10000.0   0.61979004E+00-0.79830067E+03 0.11130858E+07 0.20233248E+01  b
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TABLE E.2.—Continued.

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CO                N2                  V3C0  SVEHLA (1994)
 V  200.0   1000.0   0.62526577E 00-0.31779652E 02-0.16407983E 04 0.17454992E 01   a
 V 1000.0   5000.0   0.87395209E 00 0.56152222E 03-0.17394809E 06-0.39335958E 00   a
 V 5000.0  15000.0   0.88503551E+00 0.90902171E+03-0.73129061E+06-0.53503838E+00   b
CO                O2                  V3C0  SVEHLA (1994)
 V  300.0   1000.0   0.70122551E 00 0.51717887E 01-0.14240838E 04 0.12895991E 01   a
 V 1000.0   5000.0   0.66744478E 00-0.86348036E 02 0.27445341E 05 0.15855986E 01   a
 V 5000.0  15000.0   0.21151565E+00-0.91881544E+04 0.18253525E+08 0.65600002E+01   b
COS                               V2C2  SVEHLA (1962)
 V  300.0   1000.0   0.52573161E 00-0.27668290E 03 0.18982511E 05 0.25359860E 01   a
 V 1000.0   5000.0   0.62947137E 00-0.59744762E 02-0.37616630E 05 0.16590382E 01   a
 C  300.0   1000.0   0.56172985E 00-0.42167958E 03 0.28198920E 05 0.26921796E 01   a
 C 1000.0   5000.0   0.65503267E 00-0.17103349E 03-0.50472397E 05 0.18756918E 01   a
CO2                               V3C3  BOUSHEHRI ET AL (1987)  SVEHLA (1994)
 V  200.0   1000.0   0.51137258E 00-0.22951321E 03 0.13710678E 05 0.27075538E 01   a
 V 1000.0   5000.0   0.63978285E 00-0.42637076E 02-0.15522605E 05 0.16628843E 01   a
 V 5000.0  10000.0   0.72150912E+00 0.75012895E+03-0.11825507E+07 0.85493645E+00   b
 C  200.0   1000.0   0.48056568E+00-0.50786720E+03 0.35088811E+05 0.36747794E+01   b
 C 1000.0   5000.0   0.69857277E+00-0.11830477E+03-0.50688859E+05 0.18650551E+01   b
 C 5000.0  10000.0   0.10518358E+01-0.42555944E+04 0.14288688E+08-0.88950473E+00   b
CO2               H2                  V3C0  SVEHLA (1994)
 V  300.0   1000.0   0.66101867E 00-0.40651732E 02-0.42877325E 04 0.74444661E 00   a
 V 1000.0   5000.0   0.70351908E 00 0.19946369E 02-0.13336698E 05 0.39931502E 00   a
 V 5000.0  10000.0   0.66401272E+00-0.33671205E+03 0.41670634E+06 0.78993145E+00   b
CO2               H2O                 V3C0  SVEHLA (1994)
 V  300.0   1000.0   0.56499100E 00-0.32219550E 03 0.26301733E 05 0.26351165E 01   a
 V 1000.0   5000.0   0.68455483E 00-0.33114757E 02-0.58456473E 05 0.16048763E 01   a
 V 5000.0  10000.0   0.70748069E+00 0.11586070E+03-0.22772841E+06 0.13865863E+01   b
CO2               N2                  V3C0  SVEHLA (1994)
 V  300.0   1000.0   0.68926185E 00-0.13796096E 01-0.46847568E 04 0.13060681E 01   a
 V 1000.0   5000.0   0.69417954E 00-0.18021840E 02 0.60950694E 04 0.12779603E 01   a
 V 5000.0  10000.0   0.61979004E+00-0.79830067E+03 0.11130858E+07 0.20233248E+01   b
CO2               O2                  V3C0  SVEHLA (1994)
 V  300.0   1000.0   0.55753165E 00-0.17140020E 03 0.72594450E 04 0.24603725E 01   a
 V 1000.0   5000.0   0.66011947E 00 0.25362441E 02-0.39828007E 05 0.16020458E 01   a
 V 5000.0  10000.0   0.66564107E+00 0.13062608E+03-0.27519463E+06 0.15433736E+01   b
CS2                               V2C2  SVEHLA (1962)
 V  300.0   1000.0   0.54573740E 00-0.36042852E 03 0.33177885E 05 0.23235206E 01   a
 V 1000.0   5000.0   0.61427787E 00-0.15337427E 03-0.36078656E 05 0.17122621E 01   a
 C  300.0   1000.0   0.52603181E 00-0.50780062E 03 0.41502601E 05 0.26684257E 01   a
 C 1000.0   5000.0   0.66331137E 00-0.15058989E 03-0.68462565E 05 0.14728865E 01   a
C2H2,acetylene                    V2C2  SVEHLA (1962,1994)
 V  300.0   1000.0   0.56299896E 00-0.15304865E 03 0.46019734E 04 0.18854528E 01   a
 V 1000.0   5000.0   0.64038318E 00-0.72360229E 01-0.29612277E 05 0.12393032E 01   a
 C  300.0   1000.0   0.84030505E 00-0.10051610E 03-0.26171483E 05 0.11926036E 01   a
 C 1000.0   5000.0   0.62672572E 00-0.58147342E 03 0.10751724E 06 0.30152260E 01   a
C2H4                              V2C2  BOUSHEHRI ET AL (1987)  SVEHLA (1994)
 V  200.0   1000.0   0.59136053E 00-0.14088938E 03 0.30012800E 04 0.17018932E 01   a
 V 1000.0   5000.0   0.66000894E 00 0.39114999E 02-0.52676489E 05 0.11033601E 01   a
 C  200.0   1000.0   0.24736650E 00-0.10589987E 04 0.89911568E 05 0.64456092E 01   a
 C 1000.0   5000.0   0.51616035E 00-0.92486351E 03 0.15723887E 06 0.43873845E 01   a
C2H6                              V2C2  BOUSHEHRI ET AL (1987)  SVEHLA (1994)
 V  200.0   1000.0   0.59089348E 00-0.13994405E 03 0.29868374E 04 0.15988866E 01   a
 V 1000.0   5000.0   0.66061323E 00 0.41062220E 02-0.52656212E 05 0.99191640E 00   a
 C  200.0   1000.0   0.70867490E 00-0.63016563E 03 0.50951026E 05 0.29508724E 01   a
 C 1000.0   5000.0   0.57947247E 00-0.64990228E 03-0.37806714E 04 0.39178395E 01   a
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TABLE E.2.—Continued.

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C2H5OH                                V2C2  SVEHLA (1994)
 V  300.0   1000.0   0.54586031E 00-0.31382676E 03 0.26089200E 05 0.21078504E 01  a
 V 1000.0   5000.0   0.61957901E 00-0.11935847E 03-0.34285357E 05 0.14645259E 01  a
 C  300.0   1000.0   0.22185435E 00-0.12251941E 04 0.11716632E 06 0.65571580E 01  a
 C 1000.0   5000.0   0.42915840E 00-0.12128199E 04 0.21462928E 06 0.50153152E 01  a
C2N2                                  V2C2  SVEHLA (1962)
 V  300.0   1000.0   0.52471007E 00-0.28839713E 03 0.20625913E 05 0.23625791E 01  a
 V 1000.0   5000.0   0.62832879E 00-0.66440897E 02-0.38542772E 05 0.14840188E 01  a
 C  300.0   1000.0   0.76361743E 00-0.24078764E 03 0.11152243E 05 0.13726624E 01  a
 C 1000.0   5000.0   0.66495585E 00-0.19733792E 03-0.59902201E 05 0.20817971E 01  a
CL2                                   V2C2  SVEHLA (1994)
 V  300.0   1000.0   0.53516134E 00-0.23624735E 03 0.13738454E 05 0.24970463E 01  a
 V 1000.0   5000.0   0.63348430E 00-0.38786240E 02-0.35830615E 05 0.16699633E 01  a
 C  300.0   1000.0   0.34156262E 00-0.46059166E 03 0.34712872E 05 0.37412367E 01  a
 C 1000.0   5000.0   0.87392526E 00 0.19876120E 03-0.28784264E 05-0.53204988E 00  a
D2                                    V2C2  SVEHLA (1994)
 V  200.0   1000.0   0.74566381E 00 0.43611949E 02-0.32396252E 04 0.48064872E 00  a
 V 1000.0   5000.0   0.96835229E 00 0.68241861E 03-0.21129775E 06-0.14883773E 01  a
 C  200.0   1000.0   0.11180891E 01 0.29771761E 03-0.23323095E 05 0.94208300E-01  a
 C 1000.0   5000.0   0.10670411E 01 0.49811245E 03-0.14904299E 06 0.37216028E 00  a
D2O                                   V2C2  MATSUNAGA & NAGASHIMA(1983) SVEHLA(1994)
 V  300.0   1000.0   0.51773336E 00-0.66413680E 03 0.82973607E 05 0.29575078E 01  a
 V 1000.0   5000.0   0.58703537E 00-0.55101540E 03 0.61063786E 05 0.23875750E 01  a
 C  300.0   1000.0   0.74656939E 00-0.10592831E 04 0.17838377E 06 0.26602773E 01  a
 C 1000.0   5000.0   0.50642285E 00-0.16925317E 04 0.37493403E 06 0.47558493E 01  a
e-                                    V1C1  MASON ET AL (1967)
 V 2000.0   5000.0   0.59319174E 01 0.56594215E 04-0.22576125E 07-0.53458874E 02  a
 C 2000.0   5000.0   0.59320964E 01 0.56601476E 04-0.22577332E 07-0.42512600E 02  a
e-              H                     V2C0  CAPITELLI ET AL (1976)
 V 2000.0   8000.0   0.12996657E+01 0.29049200E+04-0.19315880E+07-0.96081497E+01  b
 V 8000.0  15000.0   0.13439163E+01 0.62981265E+04-0.14088393E+08-0.10240040E+02  b
e-              H2                    V2C0  CAPITELLI ET AL (1976)
 V 1000.0   8000.0   0.13682927E+01 0.70665102E+04-0.56748561E+07-0.10480386E+02  b
 V 8000.0  15000.0   0.20875514E+01 0.27345700E+05-0.63775336E+08-0.18571585E+02  b
e-              N                     V2C0  CAPITELLI & DEVOTO (1973)
 V 5000.0  10000.0   0.14373966E+01 0.18230345E+05-0.27492090E+08-0.96279246E+01  b
 V10000.0  15000.0   0.22566004E+01 0.48916050E+05-0.13996043E+09-0.19116958E+02  b
e-              NO                    V2C0  GUPTA ET AL (1990)
 V 2000.0   6000.0   0.61252493E+00 0.46768585E+04-0.30292080E+07-0.30467956E+01  b
 V 6000.0  15000.0  -0.31058569E+01-0.69841116E+05 0.15359384E+09 0.37370344E+02  b
e-              N2                    V2C0  CAPITELLI & DEVOTO (1973)
 V 5000.0  10000.0   0.22167522E+01 0.22078280E+05-0.26142843E+08-0.18975334E+02  b
 V10000.0  15000.0   0.14276153E+01 0.81306835E+04 0.41382925E+07-0.10615166E+02  b
e-              O                     V2C0  GUPTA ET AL (1990)
 V 2000.0   6000.0  -0.36876460E+00-0.19261587E+04 0.72235159E+06 0.82699294E+01  b
 V 6000.0  15000.0   0.12858415E+00 0.88173340E+04-0.22555849E+08 0.27992711E+01  b
e-              O2                    V2C0  GUPTA ET AL (1990)
 V 2000.0   6000.0  -0.12686144E+01-0.64961158E+04 0.37615998E+07 0.15676996E+02  b
 V 6000.0  15000.0   0.44642126E+01 0.65553833E+05-0.10919736E+09-0.43066392E+02  b
F2                                    V2C2  SVEHLA (1962,1994)
 V  200.0   1000.0   0.61198519E 00-0.39647960E 02-0.17294474E 04 0.21237710E 01  a
 V 1000.0   5000.0   0.64406091E 00-0.58273377E 00-0.52243255E 04 0.18666294E 01  a
 C  200.0   1000.0   0.46767823E 00-0.26624115E 03 0.18169657E 05 0.36165585E 01  a
 C 1000.0   5000.0  -0.19981248E 00-0.25129092E 04 0.80775379E 06 0.96845049E 01  a
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TABLE E.2.—Continued.

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H                                        V2C2  VANDERSLICE ET AL (1962)
 V 1000.0   5000.0   0.74226149E+00-0.40132865E+03 0.18554165E+06 0.46741844E-01  b
 V 5000.0  15000.0   0.87486623E+00-0.25022902E+04 0.70955048E+07-0.93888455E+00  b
 C 1000.0   5000.0   0.74166119E+00-0.40487203E+03 0.18775642E+06 0.34843121E+01  b
 C 5000.0  15000.0   0.87447639E+00-0.25089452E+04 0.71081294E+07 0.24970991E+01  b
H                H+                      V2C0  CAPITELLI ET AL (1976)
 V 2000.0   8000.0   0.65497943E+00 0.43620326E+03-0.20032290E+06-0.15933989E+01  b
 V 8000.0  15000.0   0.35775595E+00-0.56298406E+04 0.14552701E+08 0.16055465E+01  b
H                H2                      V2C0  TANG & WEI (1974)  SVEHLA (1994)
 V 1000.0   5000.0   0.91735768E+00 0.22052887E+03-0.57464994E+05-0.93741490E+00  b
 V 5000.0  15000.0   0.94056210E+00-0.17266834E+02 0.82707957E+06-0.11228741E+01  b
H                Li                      V2C0  KRUPENIE ET AL (1963)
 V 1000.0   5000.0   0.88870800E+00 0.25460216E+03-0.71635951E+05-0.24355021E+01  b
 V 5000.0  10000.0   0.96451195E+00 0.78151762E+03-0.44137515E+06-0.31717326E+01  b
H                N                       V2C0  STALLCOP ET AL (1992b)
 V 1000.0   6000.0   0.75455738E+00-0.15697085E+03 0.97258456E+05-0.48331565E-01  b
 V 6000.0  16000.0   0.15653364E+01 0.87404680E+04-0.12001036E+08-0.82485581E+01  b
H                N2                      V2C0  STALLCOP ET AL (1992b)
 V  600.0   3000.0   0.10228384E+01 0.53349114E+03-0.11365313E+06-0.23880331E+01  b
 V 3000.0  10000.0   0.13275932E+01 0.14701554E+04-0.14725296E+06-0.51365002E+01  b
H                O                       V2C0  KRUPENIE ET AL (1963)
 V 1000.0   5000.0   0.85479480E+00 0.18680077E+03-0.46790687E+05-0.11272657E+01  b
 V 5000.0  10000.0   0.88515794E+00 0.64127280E+02 0.63943230E+06-0.13887887E+01  b
HBr                                      V2C2  ZELEZNIK & SVEHLA (1970)  SVEHLA (1994)
 V  300.0   1000.0   0.54286515E 00-0.32909036E 03 0.28143861E 05 0.29266732E 01  a
 V 1000.0   5000.0   0.61904039E 00-0.12370443E 03-0.36461217E 05 0.22596924E 01  a
 C  300.0   1000.0   0.91269760E 00-0.15456150E 03 0.21177636E 05-0.43914664E 00  a
 C 1000.0   5000.0   0.63722827E 00-0.35434488E 03-0.16663585E 05 0.17013527E 01  a
HCN                                      V2C2  ZELEZNIK & SVEHLA (1970)  SVEHLA (1994)
 V  300.0   1000.0   0.94863717E 00-0.14891490E 03 0.15258721E 05-0.72592817E 00  a
 V 1000.0   5000.0   0.57370725E 00-0.85239973E 03 0.17953641E 06 0.24032031E 01  a
 C  300.0   1000.0   0.11749061E 01-0.19100307E 03 0.15714065E 05-0.13488014E 01  a
 C 1000.0   5000.0   0.50543688E 00-0.13891056E 04 0.28003144E 06 0.42095130E 01  a
HCL                                      V2C2  SVEHLA (1994)
 V  300.0   1000.0   0.54302009E 00-0.27882979E 03 0.20927618E 05 0.25895500E 01  a
 V 1000.0   5000.0   0.62673906E 00-0.81516979E 02-0.35869154E 05 0.18707238E 01  a
 C  300.0   1000.0   0.90670645E 00-0.13561693E 03 0.18563886E 05 0.60312859E-01  a
 C 1000.0   5000.0   0.62521138E 00-0.43742347E 03 0.28720932E 05 0.22964614E 01  a
HF                                       V2C2  SVEHLA (1994)
 V  300.0   1000.0   0.81674828E 00-0.23635428E 03 0.22759084E 05 0.70625888E 00  a
 V 1000.0   5000.0   0.58742532E 00-0.55543347E 03 0.67637899E 05 0.25645661E 01  a
 C  300.0   1000.0   0.12590294E 01 0.11896441E 01-0.47558763E 03-0.19367617E 01  a
 C 1000.0   5000.0   0.51518587E 00-0.14932469E 04 0.37482086E 06 0.43206676E 01  a
HF              H6F6                     V2C0  SVEHLA (1994)
 V  300.0   1000.0   0.52633473E 00-0.32896634E 03 0.26842682E 05 0.22132195E 01  a
 V 1000.0   5000.0   0.62213454E 00-0.10239431E 03-0.38543254E 05 0.13902717E 01  a
HI                                       V2C2  SVEHLA (1962)
 V  300.0   1000.0   0.53718504E 00-0.22504609E 03 0.12416876E 05 0.27888146E 01  a
 V 1000.0   5000.0   0.63448421E 00-0.33714923E 02-0.34599137E 05 0.19723806E 01  a
 C  300.0   1000.0   0.83653272E 00-0.10434645E 03 0.90075923E 04-0.38982280E 00  a
 C 1000.0   5000.0   0.65866010E 00-0.18846822E 03-0.37866478E 05 0.96987360E 00  a
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TABLE E.2.—Continued.

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H2                                          V3C3  ASSAEL ET AL (1986)  SVEHLA (1994)
 V  200.0   1000.0   0.74553182E 00 0.43555109E 02-0.32579340E 04 0.13556243E 00  a
 V 1000.0   5000.0   0.96730605E 00 0.67931897E 03-0.21025179E 06-0.18251697E 01  a
 V 5000.0  15000.0   0.10126129E+01 0.14973739E+04-0.14428484E+07-0.23254928E+01  b
 C  200.0   1000.0   0.10059461E+01 0.27951262E+03-0.29792018E+05 0.11996252E+01  b
 C 1000.0   5000.0   0.10582450E+01 0.24875372E+03 0.11736907E+05 0.82758695E+00  b
 C 5000.0  15000.0  -0.22364420E+00-0.69650442E+04-0.77771313E+05 0.13189369E+02  b
H2                H2O                       V3C0  SVEHLA (1964)
 V  300.0   1000.0   0.60085490E 00-0.67691161E 02-0.21319326E 04 0.14199776E 01  a
 V 1000.0   5000.0   0.64550551E 00 0.10165601E 02-0.18735061E 05 0.10502885E 01  a
 V 5000.0  10000.0   0.66153255E+00 0.22389456E+03-0.37073622E+06 0.88511419E+00  b
H2                N2                        V3C0  SVEHLA (1994)
 V  300.0   1000.0   0.66038264E 00 0.35574798E 01-0.95778014E 03 0.70536614E 00  a
 V 1000.0   5000.0   0.62938039E 00-0.69072207E 02 0.19855881E 05 0.97133819E 00  a
 V 5000.0   8000.0  -0.77818660E-01-0.82764842E+04 0.11699769E+08 0.81689807E+01  b
H2                O2                        V3C0  SVEHLA (1994)
 V  300.0   1000.0   0.69018087E 00-0.23876092E 00-0.48432502E 04 0.66856355E 00  a
 V 1000.0   5000.0   0.69427291E 00-0.17583177E 02 0.58748504E 04 0.64692305E 00  a
 V 5000.0  10000.0   0.62089983E+00-0.78264233E+03 0.10864044E+07 0.13816401E+01  b
H2O                                         V3C3  SENGERS & WATSON (1986)  SVEHLA (1994)
 V  373.2   1073.2   0.50019557E+00-0.69712796E+03 0.88163892E+05 0.30836508E+01  b
 V 1073.2   5000.0   0.58988538E+00-0.53769814E+03 0.54263513E+05 0.23386375E+01  b
 V 5000.0  15000.0   0.64330087E+00-0.95668913E+02-0.37742283E+06 0.18125190E+01  b
 C  373.2   1073.2   0.10966389E+01-0.55513429E+03 0.10623408E+06-0.24664550E+00  b
 C 1073.2   5000.0   0.39367933E+00-0.22524226E+04 0.61217458E+06 0.58011317E+01  b
 C 5000.0  15000.0  -0.41858737E+00-0.14096649E+05 0.19179190E+08 0.14345613E+02  b
H2O               N2                        V3C0  SVEHLA (1994)
 V  300.0   1000.0   0.57304553E 00-0.14853813E 03 0.39029324E 04 0.23462780E 01  a
 V 1000.0   5000.0   0.64243064E 00 0.25018380E 01-0.36924430E 05 0.17567700E 01  a
 V 5000.0  10000.0   0.64420052E+00 0.10592615E+01-0.34300588E+05 0.17418827E+01  b
H2O               O2                        V3C0  SVEHLA (1994)
 V  300.0   1000.0   0.64727375E 00-0.42110733E 01-0.45255490E 04 0.16510807E 01  a
 V 1000.0   5000.0   0.65299406E 00-0.17723412E 02 0.50906530E 04 0.16154623E 01  a
 V 5000.0  10000.0   0.60614671E+00-0.45218012E+03 0.56149352E+06 0.20791053E+01  b
H2S                                         V2C2  ZELEZNIK & SVEHLA (1970)  SVEHLA (1994)
 V  300.0   1000.0   0.54078516E 00-0.30304377E 03 0.24073168E 05 0.24952022E 01  a
 V 1000.0   5000.0   0.62320319E 00-0.98355396E 02-0.37061803E 05 0.17823252E 01  a
 C  300.0   1000.0   0.99442135E 00-0.19849376E 03 0.18380943E 05-0.19947763E 00  a
 C 1000.0   5000.0   0.60597875E 00-0.56357581E 03 0.67027311E 04 0.28605490E 01  a
H6F6                                        V2C2  SVEHLA (1994)
 V  300.0   1000.0   0.59712969E 00-0.36775006E 03 0.38256100E 05 0.15811495E 01  a
 V 1000.0   5000.0   0.60263706E 00-0.23619918E 03-0.24765049E 05 0.14745761E 01  a
 C  300.0   1000.0   0.82019209E 00-0.29783007E 03 0.17372752E 05 0.94706680E 00  a
 C 1000.0   5000.0   0.53249125E 00-0.75921725E 03 0.10421649E 06 0.33089772E 01  a
He                                          V3C3  BICH ET AL (1990)
 V  200.0   1000.0   0.75015944E 00 0.35763243E 02-0.22121291E 04 0.92126352E 00  a
 V 1000.0   5000.0   0.83394166E 00 0.22082656E 03-0.52852591E 05 0.20809361E 00  a
 V 5000.0  15000.0   0.86316349E+00 0.96205176E+03-0.12498705E+07-0.14115714E+00  b
 C  200.0   1000.0   0.75007833E 00 0.36577987E 02-0.23636600E 04 0.29766475E 01  a
 C 1000.0   5000.0   0.83319259E 00 0.22157417E 03-0.53304530E 05 0.22684592E 01  a
 C 5000.0  15000.0   0.85920953E+00 0.89873206E+03-0.11069262E+07 0.19535742E+01  b
He                N2                        V3C0  SVEHLA (1994)
 V  300.0   1000.0   0.70332377E 00 0.77412205E 01-0.17715400E 04 0.11440787E 01  b
 V 1000.0   5000.0   0.66785742E 00-0.84659628E 02 0.26695708E 05 0.14530051E 01  b
 V 5000.0  15000.0   0.16804077E+01 0.15615203E+05-0.28112833E+08-0.91877596E+01  b
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TABLE E.2.—Continued.

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I2                                  V2C2  SVEHLA (1962)
 V  300.0   1000.0   0.54929498E 00-0.36186119E 03 0.33655931E 05 0.26154108E 01  a
 V 1000.0   5000.0   0.61338027E 00-0.15938416E 03-0.35539572E 05 0.20394438E 01  a
 C  300.0   1000.0   0.29817264E 00-0.62470054E 03 0.63289228E 05 0.30234067E 01  a
 C 1000.0   5000.0  -0.15544742E 00-0.28843448E 04 0.96629457E 06 0.75135419E 01  a
Kr                                  V3C3  BICH ET AL (1990)
 V  200.0   1000.0   0.58597795E 00-0.12924832E 03 0.47495759E 04 0.25793650E 01  a
 V 1000.0   5000.0   0.68985845E 00 0.56296306E 02-0.36082600E 05 0.17170715E 01  a
 V 5000.0  15000.0   0.76582939E+00 0.68610377E+03-0.82537190E+06 0.97565128E+00  b
 C  200.0   1000.0   0.58008139E 00-0.13792556E 03 0.60771460E 04 0.16420039E 01  a
 C 1000.0   5000.0   0.68859431E 00 0.51765647E 02-0.34512131E 05 0.74332130E 00  a
 C 5000.0  15000.0   0.76365443E+00 0.65175847E+03-0.73589800E+06 0.12112126E-01  b
Li                                  V2C2  HOLLAND ET AL (1986)
 V 1000.0   3000.0   0.11808900E+01 0.10427008E+04-0.42642819E+06-0.40060038E+01  b
 V 3000.0  10000.0   0.13061758E+01 0.10446775E+04 0.13439272E+06-0.50720601E+01  b
 C 1000.0   3000.0   0.11802957E+01 0.10408710E+04-0.42655445E+06-0.24982084E+01  b
 C 3000.0  10000.0   0.13086032E+01 0.10695497E+04 0.10781083E+06-0.35944181E+01  b
N                                   V2C2  LEVIN ET AL (1990)
 V 1000.0   5000.0   0.83724737E+00 0.43997150E+03-0.17450753E+06 0.10365689E+00  b
 V 5000.0  15000.0   0.89986588E+00 0.14112801E+04-0.18200478E+07-0.55811716E+00  b
 C 1000.0   5000.0   0.83771661E+00 0.44243270E+03-0.17578446E+06 0.89942915E+00  b
 C 5000.0  15000.0   0.90001710E+00 0.14141175E+04-0.18262403E+07 0.24048513E+00  b
N              N+                   V2C0  STALLCOP ET AL (1991)
 V 1000.0   5000.0   0.81904143E+00-0.59239089E+02 0.21722555E+05-0.14759287E+00  b
 V 5000.0  15000.0   0.14065434E+01 0.52447258E+04-0.58944155E+07-0.59756079E+01  b
N              NO                   V2C0  CUBLEY & MASON (1975)
 V 1000.0   5000.0   0.79891098E+00 0.16929386E+03-0.49068896E+05 0.47986716E+00  b
 V 5000.0  15000.0   0.85695322E+00 0.70223546E+03-0.65589491E+06-0.96805084E-01  b
N              N2                   V2C0  CUBLEY & MASON (1975)
 V 1000.0   5000.0   0.84730498E+00 0.22158858E+03-0.65003723E+05 0.51991532E-01  b
 V 5000.0  15000.0   0.92821273E+00 0.97122155E+03-0.92773923E+06-0.75253261E+00  b
N               O                   V2C0  LEVIN ET AL (1990)
 V 1000.0   5000.0   0.70857405E+00-0.14025530E+03 0.76739975E+05 0.13001914E+01  b
 V 5000.0  15000.0   0.98622236E+00 0.23653200E+04-0.27165945E+07-0.14539746E+01  b
N              O+                   V2C0  PARTRIDGE ET AL (1991)
 V 1000.0   5000.0   0.71806621E+00-0.22692123E+03 0.63051343E+03 0.88739853E+00  b
 V 5000.0  15000.0   0.12913413E+01 0.49522731E+04-0.57814165E+07-0.47998532E+01  b
N              O2                   V2C0  CUBLEY & MASON (1975)
 V 1000.0   5000.0   0.76538325E+00 0.13624746E+03-0.39083438E+05 0.80110069E+00  b
 V 5000.0  15000.0   0.81011289E+00 0.54373468E+03-0.49868094E+06 0.35701613E+00  b
N+              O                   V2C0  PARTRIDGE ET AL (1991)
 V 1000.0   5000.0   0.11462863E+01 0.12410378E+04-0.56794094E+06-0.29071183E+01  b
 V 5000.0  15000.0   0.10155522E+01-0.32731184E+03 0.17187573E+07-0.15714289E+01  b
NH3                                 V2C2  ZELEZNIK & SVEHLA (1970)  SVEHLA (1994)
 V  200.0   1000.0   0.56652403E 00-0.36718083E 03 0.31663844E 05 0.22647443E 01  a
 V 1000.0   5000.0   0.59761003E 00-0.28027339E 03 0.37532457E 04 0.19910129E 01  a
 C  200.0   1000.0   0.17498387E 01 0.29195254E 03-0.33033738E 05-0.50944985E 01  a
 C 1000.0   5000.0   0.64477673E 00-0.91294723E 03 0.16890182E 05 0.36939751E 01  a
NO                                  V3C3  BOUSHEHRI ET AL (1987)  SVEHLA (1994)
 V  200.0   1000.0   0.60262029E 00-0.62017783E 02-0.13954524E 03 0.20268332E 01  a
 V 1000.0   5000.0   0.78009050E 00 0.30486891E 03-0.94847722E 05 0.52873381E 00  a
 V 5000.0  15000.0   0.80580582E+00 0.62427878E+03-0.57879210E+06 0.26516450E+00  b
 C  200.0   1000.0   0.95028758E+00 0.76667058E+02-0.99894764E+04-0.62776717E-02  b
 C 1000.0   5000.0   0.86215238E+00 0.44568223E+03-0.23856466E+06 0.46209876E+00  b
 C 5000.0  15000.0  -0.10377865E+01-0.34486864E+05 0.67451187E+08 0.20928749E+02  b
```

TABLE E.2.—Continued.

NO	O	V2C0 CUBLEY & MASON (1975)	
V 1000.0	5000.0	0.75990752E+00 0.13133851E+03-0.37679635E+05 0.87807540E+00	b
V 5000.0	15000.0	0.80259080E+00 0.51991196E+03-0.47557226E+06 0.45433467E+00	b
NOCL		V2C2 SVEHLA (1994)	
V 300.0	1000.0	0.60503640E 00-0.30599542E 03 0.28616290E 05 0.20637208E 01	a
V 1000.0	5000.0	0.60958727E 00-0.19972327E 03-0.22243863E 05 0.19768724E 01	a
C 300.0	1000.0	0.52036442E 00-0.53758642E 03 0.52600561E 05 0.29380096E 01	a
C 1000.0	5000.0	0.92835992E 00 0.13511240E 03-0.79751817E 05-0.42066992E 00	a
NO2		V2C2 SVEHLA (1966)	
V 300.0	1000.0	0.57379100E 00-0.12636034E 03 0.21566823E 04 0.22287492E 01	a
V 1000.0	5000.0	0.64239645E 00 0.60012144E 00-0.27020876E 05 0.16570566E 01	a
C 300.0	1000.0	0.48574998E 00-0.50702110E 03 0.46605820E 05 0.36444556E 01	a
C 1000.0	5000.0	0.97660465E 00 0.72760751E 03-0.32527989E 06-0.60899123E 00	a
N2		V3C3 BOUSHEHRI ET AL (1987) SVEHLA (1994)	
V 200.0	1000.0	0.62526577E 00-0.31779652E 02-0.16407983E 04 0.17454992E 01	a
V 1000.0	5000.0	0.87395209E 00 0.56152222E 03-0.17394809E 06-0.39335958E 00	a
V 5000.0	15000.0	0.88503551E+00 0.90902171E+03-0.73129061E+06-0.53503838E+00	b
C 200.0	1000.0	0.85439436E+00 0.10573224E+03-0.12347848E+05 0.47793128E+00	b
C 1000.0	5000.0	0.88407146E+00 0.13357293E+03-0.11429640E+05 0.24417019E+00	b
C 5000.0	15000.0	0.24176185E+01 0.80477749E+04 0.31055802E+07-0.14517761E+02	b
N2	O	V2C0 CUBLEY & MASON (1975)	
V 1000.0	5000.0	0.79176378E+00 0.16226176E+03-0.47001647E+05 0.58989646E+00	b
V 5000.0	15000.0	0.84676036E+00 0.66685159E+03-0.62101896E+06 0.43522696E-01	b
N2	O2	V3C0 SVEHLA (1994)	
V 300.0	1000.0	0.70122551E 00 0.51717887E 01-0.14240838E 04 0.12895991E 01	a
V 1000.0	5000.0	0.66744478E 00-0.86348036E 02 0.27445341E 05 0.15855986E 01	a
V 5000.0	15000.0	0.21151565E+00-0.91881544E+04 0.18253525E+08 0.65600002E+01	b
N2O		V2C2 BOUSHEHRI ET AL(1987) URIBE ET AL(1990)	
V 200.0	1000.0	0.58959112E 00-0.15565178E 03 0.37630431E 04 0.21223853E 01	a
V 1000.0	5000.0	0.64571469E 00-0.88806585E 01-0.41560559E 05 0.16332498E 01	a
C 200.0	1000.0	0.65165376E 00-0.34373058E 03 0.15090399E 05 0.24242359E 01	a
C 1000.0	5000.0	0.64720604E 00-0.78680195E 02-0.11965729E 06 0.23246569E 01	a
N2O4		V2C2 SVEHLA (1966)	
V 300.0	1000.0	0.52508683E 00-0.28652689E 03 0.20354406E 05 0.25287873E 01	a
V 1000.0	5000.0	0.62841605E 00-0.65798081E 02-0.38345315E 05 0.16529852E 01	a
C 300.0	1000.0	0.33364942E 00-0.68702644E 03 0.52625318E 05 0.47685793E 01	a
C 1000.0	5000.0	0.59441359E 00-0.26239268E 03-0.29309960E 05 0.26245858E 01	a
Na		V2C2 HOLLAND & BIOLSI (1987)	
V 500.0	2000.0	0.91803855E+00 0.22790517E+03-0.63721828E+05-0.12813410E+01	b
V 2000.0	10000.0	0.11882599E+01 0.48628768E+03 0.21833835E+06-0.35349734E+01	b
C 500.0	2000.0	0.91834808E+00 0.22837346E+03-0.63906051E+05-0.97901956E+00	b
C 2000.0	10000.0	0.11900946E+01 0.49842922E+03 0.20953120E+06-0.32479254E+01	b
Ne		V3C3 BICH ET AL (1990)	
V 200.0	1000.0	0.68398511E 00 0.18732366E 02-0.23663189E 04 0.18284755E 01	a
V 1000.0	5000.0	0.72333495E 00 0.10420872E 03-0.25429545E 05 0.14942434E 01	a
V 5000.0	15000.0	0.77549350E+00 0.59414850E+03-0.69670786E+06 0.97885712E+00	b
C 200.0	1000.0	0.68509965E 00 0.19794924E 02-0.24525539E 04 0.22586136E 01	a
C 1000.0	5000.0	0.72278122E 00 0.10528290E 03-0.26355706E 05 0.19367337E 01	a
C 5000.0	15000.0	0.77589413E+00 0.61283778E+03-0.74015705E+06 0.14114011E+01	b
O		V2C2 LEVIN ET AL (1990)	
V 1000.0	5000.0	0.77269241E+00 0.83842977E+02-0.58502098E+05 0.85100827E+00	b
V 5000.0	15000.0	0.87669586E+00 0.10158420E+04-0.10884566E+07-0.18001077E+00	b
C 1000.0	5000.0	0.77271664E+00 0.83989100E+02-0.58580966E+05 0.15179900E+01	b
C 5000.0	15000.0	0.87676666E+00 0.10170744E+04-0.10906690E+07 0.48644232E+00	b

TABLE E.2.—Concluded.

```
O                O+                  V2C0  STALLCOP ET AL (1991)
 V 1000.0   5000.0   0.96270522E+00 0.57916036E+03-0.28549938E+06-0.12297154E+01  b
 V 5000.0  15000.0   0.99113919E+00-0.80815595E+02 0.17198651E+07-0.14201124E+01  b
O                O2                  V2C0  CUBLEY & MASON (1975)
 V 1000.0   5000.0   0.73493993E+00 0.10911663E+03-0.31057767E+05 0.10998186E+01  b
 V 5000.0  15000.0   0.76924754E+00 0.42004937E+03-0.37954441E+06 0.75936688E+00  b
OH                                   V2C2  SVEHLA (1994)
 V 1000.0   5000.0   0.59711536E+00-0.46100678E+03 0.37606286E+05 0.24041761E+01  b
 V 5000.0  15000.0   0.64287721E+00-0.18173747E+03-0.88543767E+05 0.19636057E+01  b
 C 1000.0   5000.0   0.68627561E+00-0.74033274E+03 0.27559033E+05 0.28308741E+01  b
 C 5000.0  15000.0  -0.47918112E+00-0.93769908E+04 0.70509952E+07 0.14203688E+02  b
O2                                   V3C3  BOUSHEHRI ET AL (1987)  SVEHLA (1994)
 V  200.0   1000.0   0.60916180E 00-0.52244847E 02-0.59974009E 03 0.20410801E 01  a
 V 1000.0   5000.0   0.72216486E 00 0.17550839E 03-0.57974816E 05 0.10901044E 01  a
 V 5000.0  15000.0   0.73981127E+00 0.39194906E+03-0.37833168E+06 0.90931780E+00  b
 C  200.0   1000.0   0.77229167E+00 0.68463210E+01-0.58933377E+04 0.12210365E+01  b
 C 1000.0   5000.0   0.90917351E+00 0.29124182E+03-0.79650171E+05 0.64851631E-01  b
 C 5000.0  15000.0  -0.11218262E+01-0.19286378E+05 0.23295011E+08 0.20342043E+02  b
SF6                                  V2C2  BOUSHEHRI ET AL (1987)  SVEHLA (1994)
 V  300.0   1000.0   0.49748474E 00-0.21864084E 03 0.14509989E 05 0.27631958E 01  a
 V 1000.0   5000.0   0.60769589E 00-0.14230978E 03 0.31449312E 05 0.19086137E 01  a
 C  300.0   1000.0   0.41857258E 00-0.19733612E 03-0.25661949E 05 0.34555207E 01  a
 C 1000.0   5000.0   0.60633905E 00 0.44458129E 02-0.52676509E 05 0.19436963E 01  a
SO2                                  V2C2  ZELEZNIK & SVEHLA (1970)  SVEHLA (1994)
 V  300.0   1000.0   0.53157084E 00-0.29589873E 03 0.21224840E 05 0.25975549E 01  a
 V 1000.0   5000.0   0.60783098E 00-0.19283581E 03 0.78232002E 04 0.19811072E 01  a
 C  300.0   1000.0   0.61476551E 00-0.56409295E 03 0.49580787E 05 0.23940064E 01  a
 C 1000.0   5000.0   0.53617558E 00-0.69413085E 03 0.75304908E 05 0.30412002E 01  a
SiCL4                                V2C2  SVEHLA (1994)
 V  300.0   1000.0   0.52724861E 00-0.26992512E 03 0.18062726E 05 0.22413435E 01  a
 V 1000.0   5000.0   0.63025696E 00-0.55616232E 02-0.37587506E 05 0.13711284E 01  a
 C  300.0   1000.0   0.48928637E 00-0.34031669E 03 0.15336652E 05 0.23608171E 01  a
 C 1000.0   5000.0   0.62189282E 00-0.14644974E 03-0.15293955E 05 0.12815679E 01  a
SiF4                                 V2C2  SVEHLA (1962,1994)
 V  300.0   1000.0   0.59609697E 00-0.79178529E 02-0.15915012E 04 0.19580540E 01  a
 V 1000.0   5000.0   0.64527457E 00 0.10348180E 02-0.21766101E 05 0.15489951E 01  a
 C  300.0   1000.0   0.44281914E 00-0.38082561E 03 0.16794039E 05 0.35456135E 01  a
 C 1000.0   5000.0   0.62544021E 00-0.11192686E 03-0.26345285E 05 0.20583524E 01  a
SiH4                                 V2C2  SVEHLA (1962)
 V  300.0   1000.0   0.57519423E 00-0.12326162E 03 0.18824028E 04 0.18761319E 01  a
 V 1000.0   5000.0   0.64257687E 00 0.12846016E 01-0.26699436E 05 0.13147047E 01  a
 C  300.0   1000.0   0.55408670E 00-0.64339630E 03 0.55747611E 05 0.37641386E 01  a
 C 1000.0   5000.0   0.56234379E 00-0.44931035E 03-0.37165926E 05 0.36059282E 01  a
UF6                                  V2C0  SVEHLA (1962)
 V  300.0   1000.0   0.56019928E 00-0.15978215E 03 0.52866529E 04 0.24249812E 01  a
 V 1000.0   5000.0   0.63981806E 00-0.95366264E 01-0.30026765E 05 0.17600620E 01  a
Xe                                   V3C3  BICH ET AL (1990)
 V  200.0   1000.0   0.57988418E 00-0.18806666E 03 0.10508723E 05 0.26502107E 01  a
 V 1000.0   5000.0   0.68506945E 00 0.47671749E 02-0.54767718E 05 0.17531546E 01  a
 V 5000.0  15000.0   0.75436414E+00 0.69100248E+03-0.75140593E+06 0.10621747E+01  b
 C  200.0   1000.0   0.57308328E 00-0.19991432E 03 0.12872027E 05 0.12718931E 01  a
 C 1000.0   5000.0   0.68319650E 00 0.40020092E 02-0.52038474E 05 0.33623407E 00  a
 C 5000.0  15000.0   0.75593640E+00 0.72923858E+03-0.82407834E+06-0.39025477E+00  b
end
```

a. Svehla, R.A., 1995, "Transport Coefficients for the NASA Lewis Chemical Equilibrium Program," NASA TM-4647.

b. Svehla, R.A., 1996, Private communication.

Appendix F

COMMON Variables Used in Equilibrium Module

This appendix contains two tables. Table F.1 is entitled "COMMON Variables That Must Be Initialized Before Entering Equilibrium Module". It gives the following information:

1. The name of the variable
2. Its dimension
3. The type of variable, such as R*8 or L*4
4. The COMMON label
5. The subroutine where the variable is set
6. Whether the variable can be reset within the module
7. Information describing the variable, such as its symbol and the equation number in Gordon and McBride (1994)

Table F.2, entitled "COMMON Variables Calculated by Equilibrium Module", gives information similar to that described above.

TABLE F.1.—COMMON VARIABLES THAT MUST BE INITIALIZED BEFORE ENTERING EQUILIBRIUM MODULE

Variable	Dimension	Type	COMMON label	Where set	Reset?	Description (symbols and equations from Gordon and McBride,1994)
A	MAXEL, MAXNGC	R*8	MISCR	SEARCH	Yes	a_{ij}, eq. (2.7a)
Atwt	MAXEL	R*8	MISCR	REACT SEARCH	Yes	Atomic weight of elements
B0	MAXEL	R*8	MISCR	NEWOF	Yes	b_i°, eq. (9.5)
B0p	MAXEL, 2	R*8	INPT	REACT	Yes	$b_i^{(k)}$, eq. (9.1)
Bratio	----------	R*4	INPT	NEWOF	No	Bratio is discussed in sec. 3.2.
Cft	MAXNC, 9	R*8	THERM	SEARCH	No	a_{ij}, eqs. (4.9) to (4.11) for condensed species and each temperature interval
Coef	MAXNG,9, 3	R*8	THERM	SEARCH	No	a_{ij}, eqs. (4.9) to (4.11) for gases and three temperature intervals
Debug	NCOL	L*4	MISCL	INPUT	No	If true, print intermediate output for output column number Npt.
Elmt	MAXEL	C*2	CDATA	REACT	Yes	Element chemical symbol
En	MAXNGC, NCOL	R*8	COMP	Main SETEN	Yes	n_i, eq. (2.2); second index is Npt
Enln	MAXNGC	R*8	COMP	Main SETEN	Yes	ln n_i
Enn	----------	R*8	COMP	Main SETEN	Yes	n, eq. (2.1a)
Ennl	----------	R*8	COMP	Main SETEN	Yes	ln n
Gonly	----------	L*4	MISCL	Main	Yes	If true, all product species are gaseous.
Hp	----------	L*4	MISCL	Main DETON INPUT ROCKET SHCK THERMP	No	If true, either enthalpy and pressure or internal energy and volume (or density) have been assigned.
Hsub0	----------	R*8	MISCR	DETON HCALC NEWOF INPUT SHCK	No	h_0/R, assigned specific enthalpy of mixture divided by universal gas constant, eq. (9.7)
Ifz	MAXNC	I*4	INDX	REACT SEARCH	No	Positive integer numbering condensed phases of a species starting with 1 and increasing with temperature ranges
Ions	----------	L*4	MISCL	INPUT	No	If true, ionic species are to be considered.
Jcm	MAXEL	I*4	TRNP	SEARCH	Yes	Indices of species currently used as components (usually monatomic gases)
Jcond	45	I*4	INDX	Main SETEN	Yes	Indices of condensed species currently being considered

TABLE F.1.—Continued.

Variable	Dimension	Type	COMMON label	Where set	Reset?	Description (symbols and equations from Gordon and McBride, 1994)
Jliq	----------	I*4	MISCI	NEWOF SETEN	Yes	Index of condensed species that is included simultaneously with another condensed phase of same species. Jsol is for the adjacent species; Jliq is for the higher temperature interval.
Jsol	----------	I*4	MISCI	NEWOF SETEN	Yes	See Jliq.
Jx	MAXEL	I*4	INDX	SEARCH	Yes	Indices of monatomic gases
Lsave	----------	I*4	MISCI	INPUT SETEN	Yes	0 when processing input; Nlm+1 in EQLBRM after convergence when ionic species are included as products, and Nlm when they are not
Mw	MAXNGC	R*8	THERM	HCALC SEARCH	No	Molecular weight of product species
Nc	----------	I*4	INDX	SEARCH	No	Number of temperature intervals for all possible condensed products for current problem
Ng	----------	I*4	INDX	SEARCH	Yes	Number of possible gaseous products for current problem
Ngc	----------	I*4	INDX	SEARCH	No	Ng+Nc
Ngpl	----------	I*4	INDX	SEARCH	No	Ng+1
Nlm	----------	I*4	INDX	Main REACT	Yes	Number of elements in current chemical system
Npr	----------	I*4	INDX	Main SEARCH	Yes	Number of condensed species currently being considered
Npt	----------	I*4	INDX	DETON NEWOF ROCKET SHCK THERMP	No	Index of column for data saved for output (1≤Npt≤NCOL)
Nspx	----------	I*4	INDX	SEARCH	No	Ngc plus number of monatomic gases without thermo data
Pp	----------	R*8	MISCR	DETON ROCKET SHCK THERMP	Yes	Assigned pressure in bars for current point
Prod	0:MAXNGC	C*15	CDATA	SEARCH	No	Species names
Rr	----------	R*8	MISCR	BLOCKDATA	No	Universal gas constant, 8314.51 J/(kg-mol)K
S0	----------	R*8	MISCR	INPUT ROCKET	No	s_0/R, assigned specific entropy of mixture divided by universal gas constant
Shock	----------	L*4	MISCL	INPUT	No	If true, shock problem.
Short	----------	L*4	MISCL	INPUT	No	If true, listed output is abbreviated.
Size	----------	R*8	MISCR	INPUT NEWOF	Yes	SIZE as discussed in sec. 3.2 of Gordon and McBride (1994)
Sp	----------	L*4	MISCL	INPUT ROCKET	No	If true, entropy and pressure (or volume) have been assigned.
Sumn	----------	R*8	COMP	Main SETEN	Yes	Value of summation in eq. (2.2)
Temp	2,MAXNC	R*8	THERM	SEARCH	No	Temperature ranges for thermodynamic properties of all condensed products

TABLE F.1.—Concluded.

Variable	Dimension	Type	COMMON label	Where set	Reset?	Description (symbols and equations from Gordon and McBride, 1994)
Tg	4	R*8	THERM	SEARCH	No	Temperature ranges for thermodynamic properties of gases
Tp	----------	L*4	MISCL	DETON INPUT ROCKET SHCK	No	If true, temperature and pressure (or volume) have been assigned.
Trace	----------	R*8	MISCR	INPUT SHCK	No	If Trace>0, print mole (or mass) fractions ≥ Trace in special E-format
Tt	----------	R*8	MISCR	DETON ROCKET SETEN SHCK THERMP	Yes	Current temperature in kelvin
Vol	----------	L*4	MISCL	INPUT	No	If true, volume has been assigned.
Vv	----------	R*8	MISCR	THERMP	No	Assigned specific volume times 10^{-5}, $(m^3/kg)10^{-5}$, eq. (2.1a)

TABLE F.2.—COMMON VARIABLES CALCULATED BY EQUILIBRIUM MODULE

Variable	Dimension	Type	COMMON label	Where set	Description (symbols and equations from Gordon and McBride, 1994)
Cp	MAXNGC	R*8	THERM	CPHS	Molar heat capacity for species divided by universal gas constant, eq. (4.9)
Cpr	NCOL	R*8	PRTOUT	EQLBRM	Specific heat of mixture divided by universal gas constant, eq. (2.59)
Dlvpt	NCOL	R*8	PRTOUT	EQLBRM	Derivative defined by eq. (2.51)
Dlvtp	NCOL	R*8	PRTOUT	EQLBRM	Derivative defined by eq. (2.50)
Gammas	NCOL	R*8	PRTOUT	EQLBRM	Isentropic exponent, eqs. (2.71)
H0	MAXNGC	R*8	THERM	CPHS	Molar standard-state enthalpy of species divided by universal gas constant, eq. (4.10)
Hsum	NCOL	R*8	PRTOUT	MATRIX	Specific enthalpy of mixture divided by universal gas constant, eq. (2.14)
Mu	MAXNGC	R*8	THERM	MATRIX	Molar Gibbs energy for each species
Ppp	NCOL	R*8	PRTOUT	EQLBRM	Static pressure in bars stored for output
S	MAXNGC	R*8	THERM	CPHS	Molar standard-state entropy of species divided by universal gas constant, eq. (4.11)
Ssum	NCOL	R*8	PRTOUT	EQLBRM	Specific entropy of mixture divided by universal gas constant, eq. (2.16)
Totn	NCOL	R*8	PRTOUT	EQLBRM	Totn(i)=sum of En(j,Npt) for all species, denominator of eq. (2.4a)
Ttt	NCOL	R*8	PRTOUT	EQLBRM	Temperature in kelvin stored for output
Vlm	NCOL	R*8	PRTOUT	EQLBRM	Specific volume times 10^{-5}, $(m^3/kg)10^{-5}$, eq. (2.1a)
Wm	NCOL	R*8	PRTOUT	EQLBRM	Molecular weight of mixture, eq. (2.3a)

Appendix G

Example Problems

This appendix presents the output for the example problems discussed in chapter 7.

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         NASA-LEWIS CHEMICAL EQUILIBRIUM PROGRAM CEA,  MARCH 1996
                  BY  BONNIE MCBRIDE AND SANFORD GORDON
       REFS: NASA RP-1311, PART I, 1994 AND NASA RP-1311, PART II, 1996

*******************************************************************************


!                                SAMPLE PROBLEMS


!  EXAMPLE 1:
!     (a)  Assigned-temperature-and-pressure problem (tp).
!     (b)  Reactants are H2 and Air.  Since "exploded" formulas are not given,
!          these formulas will be taken from the thermodynamic data library,
!          thermo.lib.
!     (c)  Calculations are for two equivalence ratios (r,eq.ratio =1,1.5).
!     (d)  Assigned pressures are 1, 0.1, and 0.01 atm (p(atm)=1,.1,.01).
!     (e)  Assigned temperatures are 3000 and 2000 K (t(k)=3000,2000).
!     (f)  'only' dataset is used to restrict possible products.
!     (g)  Energy units in the final tables are in calories (calories).

! 'problem' dataset:
   problem case=Example-1 tp  p(atm)=1,.1,.01,t(k)=3000,2000,
            r,eq.ratio=1,1.5
! 'reactants' dataset:
   reac
     fuel= H2  moles = 1.
     oxid= Air moles = 1.
! 'only' dataset:
   only  Ar    C   CO  CO2  H   H2   H2O  HNO   HO2   HNO2  HNO3  N   NH
      NO   N2   N2O3  O  O2  OH  O3
! 'output' dataset:
   output calories
! 'end' dataset
   end

OPTIONS: TP=T  HP=F  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=F  FROZ=F  EQL=F  IONS=F  SIUNIT=F  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

T,K =  3000.0000  2000.0000

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

P,BAR =     1.013250     0.101325     0.010132

   REACTANT            MOLES     (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
F: H2                1.000000   0.000000E+00      0.00  0.0000
         H  2.00000
O: Air               1.000000   0.000000E+00      0.00  0.0000
         N  1.56170  O  0.41959  AR 0.00937  C  0.00032
```

SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)

l 6/88	*Ar	l11/88	*C	tpis79	*CO
l 7/88	*CO2	l 6/94	*H	l12/89	HNO
tpis89	HNO2	l 4/90	HNO3	l 5/89	HO2
tpis78	*H2	l 8/89	H2O	l 6/88	*N
l11/89	*NH	tpis89	*NO	tpis78	*N2
l 4/90	N2O3	l 1/90	*O	tpis78	*OH
tpis89	*O2	l 5/90	O3		

O/F = 34.297046

	EFFECTIVE FUEL	EFFECTIVE OXIDANT	MIXTURE
ENTHALPY	h(2)/R	h(1)/R	h0/R
(KG-MOL)(K)/KG	0.00000000E+00	0.00000000E+00	0.00000000E+00
KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*H	0.99212255E+00	0.00000000E+00	0.28107807E-01
*N	0.00000000E+00	0.53915548E-01	0.52388068E-01
*O	0.00000000E+00	0.14485769E-01	0.14075373E-01
*Ar	0.00000000E+00	0.32348639E-03	0.31432170E-03
*C	0.00000000E+00	0.11047560E-04	0.10734572E-04

POINT	ITN	T	H	N	O	AR
		C				
1	13	3000.000	-11.767	-14.452	-17.112	-27.077
		-25.140				
2	6	2000.000	-12.631	-13.684	-17.810	-26.104
		-28.010				
3	5	3000.000	-12.811	-15.668	-18.090	-29.507
		-26.387				
4	7	2000.000	-13.414	-14.837	-18.560	-28.409
		-28.858				
5	6	3000.000	-14.310	-16.920	-19.495	-32.012
		-27.378				
6	8	2000.000	-14.202	-15.991	-19.318	-30.716
		-29.736				

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

TEMPERATURE AND PRESSURE

CASE = Example-1

	REACTANT	MOLES	ENERGY CAL/MOL	TEMP K
FUEL	H2	1.0000000	0.000	0.000
OXIDANT	Air	1.0000000	0.000	0.000

O/F= 34.29705 %FUEL= 2.833098 R,EQ.RATIO= 1.000000 PHI,EQ.RATIO= 1.000000

THERMODYNAMIC PROPERTIES

P, ATM	1.0000	1.0000	0.10000	0.10000	0.01000	0.01000
T, K	3000.00	2000.00	3000.00	2000.00	3000.00	2000.00
RHO, G/CC	9.1864-5	1.4990-4	8.0877-6	1.4957-5	6.6054-7	1.4878-6
H, CAL/G	658.91	-203.80	1367.61	-192.33	2655.92	-165.41
U, CAL/G	395.29	-365.35	1068.18	-354.25	2289.29	-328.19
G, CAL/G	-7973.51	-5290.34	-8615.20	-5662.69	-9379.92	-6036.36
S, CAL/(G)(K)	2.8775	2.5433	3.3276	2.7352	4.0119	2.9355
M, (1/n)	22.615	24.601	19.910	24.547	16.261	24.417
(dLV/dLP)t	-1.03437	-1.00062	-1.07935	-1.00143	-1.07486	-1.00352
(dLV/dLT)p	1.6948	1.0200	2.5468	1.0452	2.4145	1.1090
Cp, CAL/(G)(K)	1.6795	0.4539	3.4666	0.5187	3.7240	0.6801
GAMMAs	1.1311	1.2263	1.1203	1.2035	1.1318	1.1677
SON VEL,M/SEC	1117.0	910.4	1184.7	902.9	1317.6	891.8

MOLE FRACTIONS

*Ar	0.00711	0.00773	0.00626	0.00772	0.00511	0.00767
*CO	0.00017	0.00001	0.00018	0.00002	0.00017	0.00004
*CO2	0.00007	0.00025	0.00003	0.00024	0.00001	0.00022
*H	0.04069	0.00009	0.14315	0.00041	0.31984	0.00185
HO2	0.00001	0.00000	0.00001	0.00000	0.00000	0.00000
*H2	0.06708	0.00304	0.08301	0.00633	0.04144	0.01309
H2O	0.20936	0.34216	0.09741	0.33736	0.01193	0.32683
*N	0.00001	0.00000	0.00003	0.00000	0.00009	0.00000
*NO	0.01247	0.00049	0.01389	0.00073	0.00974	0.00108
*N2	0.58613	0.64416	0.51456	0.64261	0.42102	0.63903
*O	0.01560	0.00002	0.05864	0.00010	0.14381	0.00047
*OH	0.04205	0.00100	0.05562	0.00216	0.03048	0.00460
*O2	0.01925	0.00104	0.02721	0.00232	0.01637	0.00510

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	HNO	HNO2	HNO3	*NH
N2O3	O3			

O/F = 22.853060

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	0.00000000E+00	0.00000000E+00	0.00000000E+00
KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*H	0.99212255E+00	0.00000000E+00	0.41593093E-01
*N	0.00000000E+00	0.53915548E-01	0.51655228E-01
*O	0.00000000E+00	0.14485769E-01	0.13878477E-01
*Ar	0.00000000E+00	0.32348639E-03	0.30992476E-03
*C	0.00000000E+00	0.11047560E-04	0.10584410E-04

POINT	ITN	T	H	N	O	AR
		C				
1	5	3000.000	-11.376	-14.517	-17.824	-27.214
		-24.401				
2	6	2000.000	-10.689	-13.763	-21.840	-26.262
		-21.257				
3	5	3000.000	-12.569	-15.737	-18.424	-29.649
		-26.155				
4	7	2000.000	-11.843	-14.915	-21.838	-28.566
		-23.564				
5	6	3000.000	-14.102	-17.003	-19.691	-32.180
		-27.343				
6	8	2000.000	-13.001	-16.068	-21.831	-30.871
		-25.879				

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

TEMPERATURE AND PRESSURE

CASE = Example-1

	REACTANT	MOLES	ENERGY CAL/MOL	TEMP K
FUEL	H2	1.0000000	0.000	0.000
OXIDANT	Air	1.0000000	0.000	0.000

O/F= 22.85306 %FUEL= 4.192334 R,EQ.RATIO= 1.500000 PHI,EQ.RATIO= 1.500764

THERMODYNAMIC PROPERTIES

P, ATM	1.0000	1.0000	0.10000	0.10000	0.01000	0.01000
T, K	3000.00	2000.00	3000.00	2000.00	3000.00	2000.00
RHO, G/CC	8.1298-5	1.2975-4	7.1204-6	1.2964-5	5.6650-7	1.2930-6
H, CAL/G	712.66	-120.74	1545.93	-116.35	3217.90	-102.27
U, CAL/G	414.78	-307.39	1205.82	-303.16	2790.41	-289.56
G, CAL/G	-8817.98	-5830.59	-9543.81	-6260.51	-10423.3	-6691.09
S, CAL/(G)(K)	3.1769	2.8549	3.6966	3.0721	4.5471	3.2944
M, (1/n)	20.013	21.294	17.528	21.276	13.946	21.220
(dLV/dLP)t	-1.03292	-1.00019	-1.08636	-1.00060	-1.08730	-1.00194
(dLV/dLT)p	1.6619	1.0054	2.6809	1.0172	2.6458	1.0556
Cp, CAL/(G)(K)	1.8179	0.4667	4.2215	0.4987	4.9387	0.6036
GAMMAs	1.1337	1.2531	1.1194	1.2394	1.1295	1.2062
SON VEL,M/SEC	1188.7	989.2	1262.1	984.2	1421.4	972.2

MOLE FRACTIONS

*Ar	0.00620	0.00660	0.00543	0.00659	0.00432	0.00658
*CO	0.00018	0.00016	0.00017	0.00016	0.00014	0.00016
*CO2	0.00004	0.00007	0.00002	0.00007	0.00000	0.00007
*H	0.06014	0.00062	0.18240	0.00196	0.39382	0.00616
*H2	0.14653	0.14737	0.13477	0.14674	0.06283	0.14483
H2O	0.22436	0.29510	0.11320	0.29456	0.01486	0.29279
*N	0.00001	0.00000	0.00003	0.00000	0.00008	0.00000
*NO	0.00573	0.00001	0.00928	0.00003	0.00737	0.00008
*N2	0.51403	0.54996	0.44806	0.54950	0.35646	0.54803
*O	0.00765	0.00000	0.04197	0.00000	0.11820	0.00004
*OH	0.03049	0.00012	0.05073	0.00039	0.03085	0.00124
*O2	0.00463	0.00000	0.01394	0.00000	0.01106	0.00003

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	HNO	HNO2	HNO3	HO2
*NH	N2O3	O3		

```
!  EXAMPLE 2:
!      (a)  Assigned-temperature-and-volume (or density) problem (tv).
!      (b)  Reactants are the same as in example 1.
!      (c)  One temperature was taken from example 1 (t(k)=3000).
!      (d)  One mixture was taken from example 1 (phi,eq.ratio=1).
!           Note: For stoichiometric mixtures, phi = r = 1.
!      (e)  Densities (rho) were obtained from the results of example 1.
!           Composition and properties in examples 1 and 2 should match for
!           these input values.
!      (f)  'only' dataset is used to restrict possible products.
!      (g)  Transport properties are to be calculated (transport).

      reac   fuel=H2    wt%=100
             oxid Air   wt%=100
      prob  case=Example-2  phi,eq.ratio=1, tv  t(k)=3000
            rho,g/cc=9.1864d-05,8.0877d-06,6.6054d-07
      only  Ar C CO CO2 H H2 H2O HNO HO2 HNO2 HNO3 N NH NO N2 N2O3 O O2 OH  O3
      outp  transport calories
      end

OPTIONS: TP=T  HP=F  SP=F  TV=T  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=F  FROZ=F  EQL=F  IONS=F  SIUNIT=F  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=T

T,K =  3000.0000

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

SPECIFIC VOLUME,M**3/KG = 1.0885657E+01 1.2364455E+02 1.5139129E+03

   REACTANT           WT.FRAC    (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
F: H2                1.000000   0.000000E+00     0.00  0.0000
         H  2.00000
O: Air               1.000000   0.000000E+00     0.00  0.0000
         N  1.56170  O  0.41959  AR 0.00937  C  0.00032

      SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)

 l 6/88  *Ar              l11/88  *C               tpis79  *CO
 l 7/88  *CO2             l 6/94  *H               l12/89  HNO
 tpis89  HNO2             l 4/90  HNO3            l 5/89  HO2
 tpis78  *H2              l 8/89  H2O             l 6/88  *N
 l11/89  *NH              tpis89  *NO             tpis78  *N2
 l 4/90  N2O3             l 1/90  *O              tpis78  *OH
 tpis89  *O2              l 5/90  O3

SPECIES WITH TRANSPORT PROPERTIES

       PURE SPECIES
 Ar                C                 CO                CO2
 H                 H2
 H2O               N                 NO                N2
 O                 OH
 O2
```

BINARY INTERACTIONS

C	O
CO	CO2
CO	N2
CO	O2
CO2	H2
CO2	H2O
CO2	N2
CO2	O2
H	H2
H	N
H	N2
H	O
H2	H2O
H2	N2
H2	O2
H2O	N2
H2O	O2
N	NO
N	N2
N	O
N	O2
NO	O
N2	O
N2	O2
O	O2

O/F = 34.297046

	EFFECTIVE FUEL	EFFECTIVE OXIDANT	MIXTURE
INTERNAL ENERGY	u(2)/R	u(1)/R	u0/R
(KG-MOL)(K)/KG	0.00000000E+00	0.00000000E+00	0.00000000E+00
KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*H	0.99212255E+00	0.00000000E+00	0.28107807E-01
*N	0.00000000E+00	0.53915548E-01	0.52388068E-01
*O	0.00000000E+00	0.14485769E-01	0.14075373E-01
*Ar	0.00000000E+00	0.32348639E-03	0.31432170E-03
*C	0.00000000E+00	0.11047560E-04	0.10734572E-04

POINT	ITN	T	H	N	O	AR
		C				
1	13	3000.000	-11.767	-14.452	-17.112	-27.077
		-25.140				
2	5	3000.000	-12.811	-15.668	-18.090	-29.507
		-26.387				
3	5	3000.000	-14.310	-16.920	-19.495	-32.012
		-27.378				

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

TEMPERATURE AND VOLUME

CASE = Example-2

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	TEMP K
FUEL	H2	1.0000000	0.000	0.000
OXIDANT	Air	1.0000000	0.000	0.000

O/F= 34.29705 %FUEL= 2.833098 R,EQ.RATIO= 1.000000 PHI,EQ.RATIO= 1.000000

THERMODYNAMIC PROPERTIES

P, ATM	1.0000	0.10000	0.01000
T, K	3000.00	3000.00	3000.00
RHO, G/CC	9.1864-5	8.0877-6	6.6054-7
H, CAL/G	658.92	1367.61	2655.91
U, CAL/G	395.30	1068.18	2289.29
G, CAL/G	-7973.51	-8615.20	-9379.92
S, CAL/(G)(K)	2.8775	3.3276	4.0119
M, (1/n)	22.615	19.910	16.261
(dLV/dLP)t	-1.03437	-1.07935	-1.07486
(dLV/dLT)p	1.6948	2.5468	2.4145
Cp, CAL/(G)(K)	1.6795	3.4666	3.7240
GAMMAs	1.1311	1.1203	1.1318
SON VEL,M/SEC	1117.0	1184.7	1317.6

TRANSPORT PROPERTIES (GASES ONLY)
CONDUCTIVITY IN UNITS OF MILLICALORIES/(CM)(K)(SEC)

VISC,MILLIPOISE	0.93569	0.94006	0.94815

WITH EQUILIBRIUM REACTIONS

Cp, CAL/(G)(K)	1.6795	3.4666	3.7240
CONDUCTIVITY	4.4242	9.6933	8.8440
PRANDTL NUMBER	0.3552	0.3362	0.3992

WITH FROZEN REACTIONS

Cp, CAL/(G)(K)	0.4250	0.4283	0.4369
CONDUCTIVITY	0.6289	0.7269	0.8650
PRANDTL NUMBER	0.6324	0.5539	0.4789

MOLE FRACTIONS

*Ar	0.00711	0.00626	0.00511
*CO	0.00017	0.00018	0.00017
*CO2	0.00007	0.00003	0.00001
*H	0.04069	0.14315	0.31984
HO2	0.00001	0.00001	0.00000
*H2	0.06708	0.08301	0.04144
H2O	0.20936	0.09741	0.01193
*N	0.00001	0.00003	0.00009
*NO	0.01247	0.01389	0.00974
*N2	0.58613	0.51456	0.42102
*O	0.01560	0.05864	0.14381
*OH	0.04205	0.05562	0.03048
*O2	0.01925	0.02721	0.01637

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	HNO	HNO2	HNO3	*NH
N2O3	O3			

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

```
!  EXAMPLE 3:
!      (a)  Combustion or assigned-enthalpy-and-pressure problem (hp).
!      (b)  Fuels are 'C7H8(L)' and 'C8H18(L),n-octa' at 298.15 K. The oxidant is
!           air at 700 K.
!      (c)  Oxidant-to-fuel weight ratio is 17 (o/f =17).  Weight fractions are
!           fractions of fuel relative to total fuel and fractions of oxidant
!           relative to total oxidant.
!      (d)  Mixture enthalpy is calculated from reactant values given in
!           thermo.lib. This is because data for these species are given in
!           thermo.lib and the species names match exactly.
!      (e)  Many species are omitted from the product data base ('omit' dataset).
!           Note:  these species names must match those used in thermo.lib.
!      (f)  Assigned pressures are 100, 10, and 1 bar (p(bar)=100,10,1).
!      (g)  Mixture properties are to be printed in SI units (siunits).
!      (h)  Mole fractions > 1.e-15 are to be in e-format (trace=1.e-15).
!
reac
     oxid Air  wtfrac= 1   t(k)=700.0
     fuel C7H8(L)   wtfrac= .4   t(k)= 298.15
     fuel C8H18(L),n-octa   wtfrac= .6 t(k)= 298.15
prob   case=Example-3   hp  p(bar)=100,10,1, o/f = 17
output siunits  trace=1.e-15

omit CCN              CNC              C2N2             C2O
     C3H4,allene      C3H4,propyne     C3H4,cyclo-      C3
     C3H5,allyl       C3H6,propylene   C3H6,cyclo-      C3H3,propargyl
     C3H6O            C3H7,n-propyl    C3H7,i-propyl    Jet-A(g)
     C3O2             C4               C4H2             C3H8O,2propanol
     C4H4,1,3-cyclo-  C4H6,butadiene   C4H6,2-butyne    C3H8O,1propanol
     C4H8,tr2-butene  C4H8,isobutene   C4H8,cyclo-      C4H6,cyclo-
     (CH3COOH)2       C4H9,n-butyl     C4H9,i-butyl     C4H8,1-butene
     C4H9,s-butyl     C4H9,t-butyl     C4H10,isobutane  C4H8,cis2-buten
     C4H10,n-butane   C4N2             C5               C3H8
     C5H6,1,3cyclo-   C5H8,cyclo-      C5H10,1-pentene  C10H21,n-decyl
     C5H10,cyclo-     C5H11,pentyl     C5H11,t-pentyl   C12H10,biphenyl
     C5H12,n-pentane  C5H12,i-pentane  CH3C(CH3)2CH3    C12H9,o-bipheny
     C6H6             C6H5OH,phenol    C6H10,cyclo-     C6H2
     C6H12,1-hexene   C6H12,cyclo-     C6H13,n-hexyl    C6H5,phenyl
     C7H7,benzyl      C7H8             C7H8O,cresol-mx  C6H5O,phenoxy
     C7H14,1-heptene  C7H15,n-heptyl   C7H16,n-heptane  C10H8,azulene
     C8H8,styrene     C8H10,ethylbenz  C8H16,1-octene   C10H8,napthlene
     C8H17,n-octyl    C8H18,isooctane  C8H18,n-octane   C9H19,n-nonyl
     Jet-A(L)         C6H6(L)          H2O(s)           H2O(L)
end  End all input for example 3

OPTIONS: TP=F  HP=T  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=F  FROZ=F  EQL=F  IONS=F  SIUNIT=T  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

TRACE= 1.00E-15  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

P,BAR =   100.000000    10.000000     1.000000
```

REACTANT	WT.FRAC	(ENERGY/R),K	TEMP,K	DENSITY
EXPLODED FORMULA				
O: Air	1.000000	0.143092E+04	700.00	0.0000
N 3.56170 O 0.41959 AR 0.00937 C 0.00032				
F: C7H8(L)	0.400000	0.146491E+04	298.15	0.0000
C 7.00000 H 8.00000				
F: C8H18(L),n-octa	0.600000	-0.300992E+05	298.15	0.0000
C 8.00000 H 18.00000				

SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)

l 6/88	*Ar	l11/88	*C	tpis79	*CH
l11/89	CH2	l11/89	CH3	l12/92	CH2OH
l10/92	CH3O	l 8/88	CH4	l 8/88	CH3OH
tpis91	*CN	l12/89	CNN	tpis79	*CO
l 7/88	*CO2	tpis91	COOH	tpis91	*C2
l 1/91	C2H	l 6/89	CHCO,ketyl	l12/89	C2H2,vinylidene
l 1/91	C2H2,acetylene	l 5/90	CH2CO,ketene	l 2/92	C2H3,vinyl
l12/92	CH3CN	l 6/96	CH3CO,acetyl	l 1/91	C2H4
l 8/88	C2H4O,ethylen-o	l 8/88	CH3CHO,ethanal	l 8/88	CH3COOH
l12/92	C2H5	l 8/88	C2H6	l 8/88	CH3N2CH3
l 8/88	C2H5OH	l12/92	CH3OCH3	x10/93	C4H6,1-butyne
x 4/85	C6H14,n-hexane	x10/85	C7H16,2-methylh	l 8/93	C10H8,naphthale
l 6/94	*H	l 7/88	HCN	l12/89	HCO
tpis89	HCCN	l11/92	HNC	l 2/96	HNCO
l12/89	HNO	tpis89	HNO2	l 4/90	HNO3
l 5/89	HO2	tpis78	*H2	l 8/88	HCHO,formaldehy
l 8/88	HCOOH	l 8/89	H2O	l 2/93	H2O2
l 8/88	(HCOOH)2	l 6/88	*N	l 2/96	NCO
l11/89	*NH	l12/89	NH2	tpis89	NH3
tpis89	NH2OH	tpis89	*NO	l 7/88	NO2
j12/64	NO3	tpis78	*N2	l12/89	NCN
l 5/90	N2H2	tpis89	NH2NO2	l 5/90	N2H4
l 7/88	N2O	l 4/90	N2O3	tpis89	N2O4
l 4/90	N2O5	tpis89	N3	l 7/88	N3H
l 1/90	*O	tpis78	*OH	tpis89	*O2
l 5/90	O3	x 4/83	C(gr)	x 4/83	C(gr)
x 4/83	C(gr)				

O/F = 17.000000

	EFFECTIVE FUEL	EFFECTIVE OXIDANT	MIXTURE
ENTHALPY	h(2)/R	h(1)/R	h0/R
(KG-MOL)(K)/KG	-0.15173707E+03	0.49400444E+02	0.38226138E+02
KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*N	0.00000000E+00	0.53915548E-01	0.50920240E-01
*O	0.00000000E+00	0.14485769E-01	0.13681004E-01
*Ar	0.00000000E+00	0.32348639E-03	0.30551493E-03
*C	0.72408514E-01	0.11047560E-04	0.40331290E-02
*H	0.12927489E+00	0.00000000E+00	0.71819385E-02

POINT	ITN	T	N	O	AR	C
		H				
1	18	2419.334	-11.651	-14.247	-21.786	-21.401
		-11.891				
2	5	2391.604	-12.783	-15.355	-24.066	-21.672
		-12.538				
3	5	2340.157	-13.898	-16.426	-26.325	-22.191
		-13.247				

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = Example-3

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
OXIDANT	Air	1.0000000	11897.374	700.000
FUEL	C7H8(L)	0.4000000	12180.000	298.150
FUEL	C8H18(L),n-octa	0.6000000	-250259.981	298.150

O/F= 17.00000 %FUEL= 5.555556 R,EQ.RATIO= 0.852074 PHI,EQ.RATIO= 0.851848

THERMODYNAMIC PROPERTIES

P, BAR	100.00	10.000	1.0000
T, K	2419.33	2391.60	2340.16
RHO, KG/CU M	1.4428 1	1.4565 0	1.4827-1
H, KJ/KG	317.83	317.83	317.83
U, KJ/KG	-375.27	-368.76	-356.61
G, KJ/KG	-19443.2	-20795.8	-21891.3
S, KJ/(KG)(K)	8.1680	8.8282	9.4904
M, (1/n)	29.023	28.962	28.849
(dLV/dLP)t	-1.00067	-1.00157	-1.00322
(dLV/dLT)p	1.0186	1.0442	1.0914
Cp, KJ/(KG)(K)	1.6068	1.8127	2.2013
GAMMAs	1.2260	1.2064	1.1803
SON VEL,M/SEC	921.8	910.1	892.2

MOLE FRACTIONS			
*Ar	8.8668-3	8.8483-3	8.8139-3
*CN	5.454-14	9.975-14	1.106-13
*CO	1.6811-3	4.3275-3	9.2288-3
*CO2	1.1537-1	1.1248-1	1.0712-1
COOH	5.1792-8	2.3423-8	8.6875-9
*H	2.7692-5	1.2480-4	4.5990-4
HCN	9.662-12	1.081-11	7.934-12
HCO	7.579-10	9.191-10	7.862-10
HNC	1.024-12	1.107-12	7.601-13
HNCO	1.229 -9	5.144-10	1.646-10
HNO	4.2385-7	2.0929-7	9.1839-8
HNO2	1.8549-6	3.2796-7	5.7687-8
HNO3	1.133 -9	6.656-11	4.067-12
HO2	7.8127-6	4.1701-6	2.1216-6
*H2	2.5156-4	6.6471-4	1.4948-3
HCHO,formaldehy	1.723-11	1.172-11	5.625-12
HCOOH	6.485 -9	1.651 -9	3.455-10
H2O	1.0288-1	1.0154-1	9.9280-2
H2O2	1.0129-6	3.0297-7	8.6257-8
*N	1.1572-8	2.7706-8	5.1386-8
NCO	8.645-11	6.074-11	3.090-11
*NH	2.9542-9	3.9044-9	3.9370-9
NH2	1.721 -9	1.291 -9	7.472-10
NH3	3.909 -9	1.731 -9	6.186-10
NH2OH	1.027-11	1.461-12	1.702-13
*NO	6.7922-3	6.5768-3	6.1768-3
NO2	2.3525-5	7.5946-6	2.4942-6
NO3	1.932-10	1.962-11	2.015-12
*N2	7.3550-1	7.3408-1	7.3142-1
N2H2	5.207-13	1.210-13	2.129-14
NH2NO2	2.449-15	6.786-17	1.669-18
N2O	3.6532-6	1.1174-6	3.3132-7
N2O3	2.448-11	7.760-13	2.459-14
N2O4	3.110-15	3.306-17	3.704-19
N3	1.241-12	3.029-13	5.825-14
N3H	3.876-13	5.282-14	5.650-15
*O	1.5576-4	4.3417-4	1.0769-3
*OH	2.1257-3	3.4565-3	5.1814-3
*O2	2.6302-2	2.7452-2	2.9742-2
O3	1.2251-8	3.7798-9	1.1377-9

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 1.000000E-15 FOR ALL ASSIGNED CONDITIONS

*C	*CH	CH2	CH3	CH2OH
CH3O	CH4	CH3OH	CNN	*C2
C2H	CHCO,ketyl	C2H2,vinylidene	C2H2,acetylene	CH2CO,ketene
C2H3,vinyl	CH3CN	CH3CO,acetyl	C2H4	C2H4O,ethylen-o
CH3CHO,ethanal	CH3COOH	C2H5	C2H6	CH3N2CH3
C2H5OH	CH3OCH3	C4H6,1-butyne	C6H14,n-hexane	C7H16,2-methylh
C10H8,naphthale	HCCN	(HCOOH)2	NCN	N2H4
N2O5	C(gr)			

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

```
!  EXAMPLE 4:
!      (a)  Assigned-internal-energy-and-density problem (uv).
!      (b)  Fuel, oxidant, and oxidant-to-fuel weight ratio are the same as in
!           example 3.
!      (c)  Internal energy u was taken from col. 1 of the output of example 3.
!           However, input requires u/R, i.e., u = -375.27 kJ/kg and
!           u/R = -375.27/8.31451 = -45.1343 (kg-mol)(K)/kg  (u/r=-45.1343).
!      (d)  Units for density input are limited to g/cc and kg/m**3.  From
!           example 3 point 1, rho = 14.428 kg/m**3 (rho,kg/m**3=14.428).
!      (e)  Mixture properties are to be printed in SI units (default unit).
!      (f)  Mole fractions > 1.e-15 are to be in e-format (trace=1.e-15).
!      (g)  Note that since all parameters for this example are the same as
!           those used for col. 1 of example 3, assigning u and rho from
!           this column should yield the same pressure and temperature assigned
!           for that point in example 3.

 prob   case=Example-4, o/f=17   uv  u/r=-45.1343, rho,kg/m**3=14.428

output  trace=1.e-15

reac   oxid Air        wtfrac= 1    t(k)=700.0
       fuel C7H8(L)    wtfrac= .4   t(k)= 298.15
       fuel C8H18(L),n-octa wtfrac= .6 t(k)= 298.15

omit CCN  CNC  C2N2  C2O  C3H4,allene  C3H4,propyne  C3H4,cyclo-  C3
     C3H5,allyl      C3H6,propylene  C3H6,cyclo-     C3H3,propargyl
     C3H6O           C3H7,n-propyl   C3H7,i-propyl   Jet-A(g)
     C3O2            C4              C4H2            C3H8O,2propanol
     C4H4,1,3-cyclo- C4H6,butadiene  C4H6,2-butyne   C3H8O,1propanol
     C4H8,tr2-butene C4H8,isobutene  C4H8,cyclo-     C4H6,cyclo-
     (CH3COOH)2      C4H9,n-butyl    C4H9,i-butyl    C4H8,1-butene
     C4H9,s-butyl    C4H9,t-butyl    C4H10,isobutane C4H8,cis2-buten
     C4H10,n-butane  C4N2            C5              C3H8
     C5H6,1,3cyclo-  C5H8,cyclo-     C5H10,1-pentene C10H21,n-decyl
     C5H10,cyclo-    C5H11,pentyl    C5H11,t-pentyl  C12H10,biphenyl
     C5H12,n-pentane C5H12,i-pentane CH3C(CH3)2CH3   C12H9,o-bipheny
     C6H6            C6H5OH,phenol   C6H10,cyclo-    C6H2
     C6H12,1-hexene  C6H12,cyclo-    C6H13,n-hexyl   C6H5,phenyl
     C7H7,benzyl     C7H8            C7H8O,cresol-mx C6H5O,phenoxy
     C7H14,1-heptene C7H15,n-heptyl  C7H16,n-heptane C10H8,azulene
     C8H8,styrene    C8H10,ethylbenz C8H16,1-octene  C10H8,napthlene
     C8H17,n-octyl   C8H18,isooctane C8H18,n-octane  C9H19,n-nonyl
     C7H8(L)  C8H18(L),n-octa Jet-A(L)  C6H6(L)  H2O(s)  H2O(L)
 end

OPTIONS: TP=F  HP=T  SP=F  TV=F  UV=T  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=F  FROZ=F  EQL=F  IONS=F  SIUNIT=T  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

TRACE= 1.00E-15  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R=-4.513430E+01

SPECIFIC VOLUME,M**3/KG = 6.9309676E-02
```

```
   REACTANT          WT.FRAC    (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
O: Air              1.000000   0.730917E+03   700.00  0.0000
         N  1.56170  O  0.41959  AR 0.00937  C  0.00032
F: C7H8(L)          0.400000   0.146491E+04   298.15  0.0000
         C  7.00000  H  8.00000
F: C8H18(L),n-octa  0.600000  -0.300992E+05   298.15  0.0000
         C  8.00000  H 18.00000

      SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)

 l 6/88  *Ar              l11/88  *C              tpis79  *CH
 l11/89  CH2              l11/89  CH3             l12/92  CH2OH
 l10/92  CH3O             l 8/88  CH4             l 8/88  CH3OH
 tpis91  *CN              l12/89  CNN             tpis79  *CO
 l 7/88  *CO2             tpis91  COOH            tpis91  *C2
 l 1/91  C2H              l 6/89  CHCO,ketyl      l12/89  C2H2,vinylidene
 l 1/91  C2H2,acetylene   l 5/90  CH2CO,ketene    l 2/92  C2H3,vinyl
 l12/92  CH3CN            l 6/96  CH3CO,acetyl    l 1/91  C2H4
 l 8/88  C2H4O,ethylen-o  l 8/88  CH3CHO,ethanal  l 8/88  CH3COOH
 l12/92  C2H5             l 8/88  C2H6            l 8/88  CH3N2CH3
 l 8/88  C2H5OH           l12/92  CH3OCH3         x10/93  C4H6,1-butyne
 x 4/85  C6H14,n-hexane   x10/85  C7H16,2-methylh l 8/93  C10H8,naphthale
 l 6/94  *H               l 7/88  HCN             l12/89  HCO
 tpis89  HCCN             l11/92  HNC             l 2/96  HNCO
 l12/89  HNO              tpis89  HNO2            l 4/90  HNO3
 l 5/89  HO2              tpis78  *H2             l 8/88  HCHO,formaldehy
 l 8/88  HCOOH            l 8/89  H2O            l 2/93  H2O2
 l 8/88  (HCOOH)2         l 6/88  *N             l 2/96  NCO
 l11/89  *NH              l12/89  NH2            tpis89  NH3
 tpis89  NH2OH            tpis89  *NO            l 7/88  NO2
 j12/64  NO3              tpis78  *N2            l12/89  NCN
 l 5/90  N2H2             tpis89  NH2NO2         l 5/90  N2H4
 l 7/88  N2O              l 4/90  N2O3           tpis89  N2O4
 l 4/90  N2O5             tpis89  N3             l 7/88  N3H
 l 1/90  *O               tpis78  *OH            tpis89  *O2
 l 5/90  O3               x 4/83  C(gr)          x 4/83  C(gr)
 x 4/83  C(gr)

O/F =  17.000000

                      EFFECTIVE FUEL      EFFECTIVE OXIDANT        MIXTURE
INTERNAL ENERGY          u(2)/R              u(1)/R                  u0/R
(KG-MOL)(K)/KG      -0.15173707E+03     0.25233905E+02          -0.45134300E+02

KG-FORM.WT./KG          bi(2)               bi(1)                   b0i
 *N                 0.00000000E+00      0.53915548E-01          0.50920240E-01
 *O                 0.00000000E+00      0.14485769E-01          0.13681004E-01
 *Ar                0.00000000E+00      0.32348639E-03          0.30551493E-03
 *C                 0.72408514E-01      0.11047560E-04          0.40331290E-02
 *H                 0.12927489E+00      0.00000000E+00          0.71819385E-02
```

POINT	ITN	T	N	O	AR	C
		H				
1	16	2419.335	-11.651	-14.247	-21.786	-21.401
		-11.891				

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

VOLUME

CASE = Example-4,

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
OXIDANT	Air	1.0000000	6077.217	700.000
FUEL	C7H8(L)	0.4000000	12180.000	298.150
FUEL	C8H18(L),n-octa	0.6000000	-250259.981	298.150

O/F= 17.00000 %FUEL= 5.555556 R,EQ.RATIO= 0.852074 PHI,EQ.RATIO= 0.851848

THERMODYNAMIC PROPERTIES

P, BAR	100.00
T, K	2419.34
RHO, KG/CU M	1.4428 1
H, KJ/KG	317.83
U, KJ/KG	-375.27
G, KJ/KG	-19443.2
S, KJ/(KG)(K)	8.1680
M, (1/n)	29.023
(dLV/dLP)t	-1.00067
(dLV/dLT)p	1.0186
Cp, KJ/(KG)(K)	1.6068
GAMMAs	1.2260
SON VEL,M/SEC	921.8

MOLE FRACTIONS

*Ar	8.8668-3
*CN	5.454-14
*CO	1.6811-3
*CO2	1.1537-1
COOH	5.1793-8
*H	2.7692-5
HCN	9.662-12
HCO	7.579-10
HNC	1.024-12
HNCO	1.2290-9

HNO	4.2385-7
HNO2	1.8549-6
HNO3	1.1332-9
HO2	7.8128-6
*H2	2.5156-4
HCHO,formaldehy	1.723-11
HCOOH	6.4854-9
H2O	1.0288-1
H2O2	1.0130-6
*N	1.1572-8
NCO	8.645-11
*NH	2.9542-9
NH2	1.7208-9
NH3	3.9091-9
NH2OH	1.027-11
*NO	6.7922-3
NO2	2.3525-5
NO3	1.932-10
*N2	7.3550-1
N2H2	5.207-13
NH2NO2	2.450-15
N2O	3.6532-6
N2O3	2.448-11
N2O4	3.110-15
N3	1.241-12
N3H	3.876-13
*O	1.5576-4
*OH	2.1257-3
*O2	2.6302-2
O3	1.2251-8

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 1.000000E-15 FOR ALL ASSIGNED CONDITIONS

*C	*CH	CH2	CH3	CH2OH
CH3O	CH4	CH3OH	CNN	*C2
C2H	CHCO,ketyl	C2H2,vinylidene	C2H2,acetylene	CH2CO,ketene
C2H3,vinyl	CH3CN	CH3CO,acetyl	C2H4	C2H4O,ethylen-o
CH3CHO,ethanal	CH3COOH	C2H5	C2H6	CH3N2CH3
C2H5OH	CH3OCH3	C4H6,1-butyne	C6H14,n-hexane	C7H16,2-methylh
C10H8,naphthale	HCCN	(HCOOH)2	NCN	N2H4
N2O5	C(gr)			

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

```
!  EXAMPLE 5:
!      (a)  Combustion problem (hp) for solid propellant with 5 ingredients.
!      (b)  The assigned enthalpies and "exploded" formulas for four of the
!           components are to be taken from thermo.lib.  However, data for
!           'CHOS-Binder' are not available in thermo.lib and thus the "exploded"
!           formula and enthalpy are given in the 'reac' dataset.
!      (c)  The reactants are given in percent by weight (wt%=...).  The
!           propellant components are not designated as fuel and oxidant - they
!           are labelled with the 'name' alternative.  Weight fractions are
!           relative to the total reactant.
!      (d)  Five pressures are given in units of psia (p,psia=500,250,
!           125,50,5,).
!      (e)  As with examples 3 and 4, many species in thermo.lib are omitted
!           as possible products by means of an 'omit' dataset.
!      (f)  Energy units in the final tables are in calories (calories).

reac
   name NH4CLO4(I)    wt%= 72.06   t(k)=298.15
   name CHOS-Binder C 1 H 1.86955 O .031256 S .008415 wt%=18.58
                           h,cal=-2999.082 t(k)=298.15
   name AL(cr)   wt%= 9.    t(k)=298.15
   name MgO(s)   wt%= .2    t(k)=298.15
   name H2O(L)   wt%=.16    t(k)=298.15

prob     case=5, hp   p,psia=500,250,125,50,5,

outp   calories

omit COOH  C2 C2H CHCO,ketyl  C2H2,vinylidene  CH2CO,ketene  C2H3,vinyl
     CH3CO,acetyl  C2H4O,ethylen-o CH3CHO,ethanal  CH3COOH   (HCOOH)2
     C2H5             C2H6             CH3N2CH3         CH3OCH3
     C2H5OH           CCN              CNC              C2N2
     C2O              C3               C3H3,propargyl   C3H4,allene
     C3H4,propyne     C3H4,cyclo-      C3H5,allyl       C3H6,propylene
     C3H6,cyclo-      C3H6O            C3H7,n-propyl    C3H7,i-propyl
     C3H8             C3H8O,1propanol C3H8O,2propanol C3O2
     C4               C4H2             C4H4,1,3-cyclo- C4H6,butadiene
     C4H6,2-butyne    C4H6,cyclo-      C4H8,1-butene    C4H8,cis2-buten
     C4H8,tr2-butene C4H8,isobutene   C4H8,cyclo-      (CH3COOH)2
     C4H9,n-butyl     C4H9,i-butyl     C4H9,s-butyl     C4H9,t-butyl
     C4H10,isobutane C4H10,n-butane   C4N2             C5
     C5H6,1,3cyclo-   C5H8,cyclo-      C5H10,1-pentene C5H10,cyclo-
     C5H11,pentyl     C5H11,t-pentyl   C5H12,n-pentane C5H12,i-pentane
     CH3C(CH3)2CH3    C6H2             C6H5,phenyl      C6H5O,phenoxy
     C6H6             C6H5OH,phenol    C6H10,cyclo-     C6H12,1-hexene
     C6H12,cyclo-     C6H13,n-hexyl     C7H7,benzyl     C7H8
     C7H8O,cresol-mx C7H14,1-heptene C7H15,n-heptyl   C7H16,n-heptane
     C8H8,styrene     C8H10,ethylbenz C8H16,1-octene   C8H17,n-octyl
     C8H18,isooctane C8H18,n-octane   C9H19,n-nonyl    C10H8,naphthale
     C10H21,n-decyl   C12H9,o-bipheny C12H10,biphenyl Jet-A(g)
     HNCO    HNO  HNO2   HNO3   HCCN    HCHO,formaldehy  HCOOH
     NH      NH2  NH2OH  NCN    N2H2  NH2NO2   N2H4  H2O2
 (HCOOH)2   C6H6(L)  C7H8(L)  C8H18(L),n-octa  Jet-A(L)  H2O(s) H2O(L)
 end
```

```
OPTIONS: TP=F  HP=T  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=F  FROZ=F  EQL=F  IONS=F  SIUNIT=F  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

P,BAR =     34.473652     17.236826      8.618413      3.447365      0.344737

   REACTANT            WT.FRAC    (ENERGY/R),K   TEMP,K  DENSITY
      EXPLODED FORMULA
N: NH4CLO4(I)         0.720600  -0.355724E+05   298.15  0.0000
         N  1.00000  H  4.00000  CL 1.00000  O  4.00000
N: CHOS-Binder        0.185800  -0.150919E+04   298.15  0.0000
         C  1.00000  H  1.86955  O  0.03126  S  0.00841
N: AL(cr)             0.090000   0.496279E-05   298.15  0.0000
         AL 1.00000
N: MgO(s)             0.002000  -0.723139E+05   298.15  0.0000
         MG 1.00000  O  1.00000
N: H2O(L)             0.001600  -0.343773E+05   298.15  0.0000
         H  2.00000  O  1.00000

      SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)

j 6/83  *AL              J 6/63  ALC             J 9/79  ALCL
J 6/76  ALCL2            J 9/79  ALCL3           J 6/63  ALH
J12/79  ALN              J12/79  ALO             J 9/64  ALOCL
J12/67  ALOH             J12/79  ALO2            J12/68  ALO2H
j12/79  ALS              J 6/79  AL2             J 9/79  AL2CL6
J12/79  AL2O             J12/79  AL2O2           l11/88  *C
l11/95  CCL              l11/95  CCL2            x12/93  CCL3
tpis91  CCL4             tpis79  *CH             l11/95  CHCL
x12/93  CHCL2            l 6/95  CHCL3           l11/89  CH2
l 2/96  CH2CL            tpis91  CH2CL2          l11/89  CH3
tpis91  CH3CL            l12/92  CH2OH           l10/92  CH3O
l 8/88  CH4              l 8/88  CH3OH           tpis91  *CN
l12/89  CNN              tpis79  *CO             tpis91  COCL
tpis91  COCL2            tpis91  COHCL           l 6/95  COS
l 7/88  *CO2             l 7/95  CS              l 6/95  CS2
tpis91  C2CL             tpis91  C2CL2           tpis91  C2CL3
tpis91  C2CL4            tpis91  C2CL6           tpis91  C2HCL
tpis91  C2HCL3           l 1/91  C2H2,acetylene  tpis91  C2H2CL2
tpis91  C2H3CL           l12/92  CH3CN           l 1/91  C2H4
x10/93  C4H6,1-butyne    x 4/85  C6H14,n-hexane  x10/85  C7H16,2-methylh
J 6/82  CL               l 6/95  CLCN            tpis89  CLO
l 7/93  CLO2             tpis89  CL2             tpis89  CL2O
l 6/94  *H               J 3/64  HALO            l 7/88  HCN
l12/89  HCO              tpis89  HCL             l11/92  HNC
tpis89  HOCL             l 5/89  HO2             tpis78  *H2
l 8/89  H2O              tpis89  H2S             tpis89  H2SO4
J 9/83  Mg               J 3/66  MgCL            J12/69  MgCL2
J12/66  MgH              J 3/64  MgN             J12/74  MgO
J12/75  MgOH             J12/75  MgO2H2          J 9/77  MgS
J 9/83  Mg2              l 6/88  *N              l 2/96  NCO
tpis89  NH3              tpis89  *NO             l 5/95  NOCL
```

l 7/88	NO2	l 5/95	NO2CL	j12/64	NO3
tpis78	*N2	l 7/88	N2O	l 4/90	N2O3
tpis89	N2O4	l 4/90	N2O5	tpis89	N3
l 7/88	N3H	l 1/90	*O	tpis78	*OH
tpis89	*O2	l 5/90	O3	J 9/82	S
J 6/78	SCL	J 6/78	SCL2	tpis89	SH
tpis89	SN	tpis89	SO	tpis89	SO2
J 6/71	SO2CL2	tpis89	SO3	tpis89	S2
L 4/93	S2CL2	tpis89	S2O	tpis89	S3
tpis89	S4	tpis89	S5	tpis89	S6
tpis89	S7	tpis89	S8	coda89	AL(cr)
coda89	AL(L)	J 9/79	ALCL3(s)	J 9/79	ALCL3(L)
J 9/79	ALCL3(L)	J12/79	ALN(s)	J12/79	ALN(s)
coda89	AL2O3(a)	coda89	AL2O3(a)	coda89	AL2O3(a)
coda89	AL2O3(L)	x 4/83	C(gr)	x 4/83	C(gr)
x 4/83	C(gr)	J 9/77	H2SO4(L)	srd 93	Mg(cr)
srd 93	Mg(cr)	srd 93	Mg(L)	J12/79	MgAL2O4(s)
J12/79	MgAL2O4(s)	J12/79	MgAL2O4(L)	J12/66	MgCO3(s)
J12/65	MgCL2(s)	J12/65	MgCL2(L)	J12/65	MgCL2(L)
J12/74	MgO(s)	J12/74	MgO(s)	J12/74	MgO(L)
J12/75	MgO2H2(s)	J 9/77	MgS(s)	J 9/77	MgS(s)
L 7/76	MgSO4(s)	L 7/76	MgSO4(s)	L 7/76	MgSO4(L)
BAR 73	NH4CL(a)	BAR 73	NH4CL(b)	tpis89	S(cr1)
tpis89	S(cr2)	tpis89	S(L)	tpis89	S(L)
tpis89	S(L)	tpis89	S(L)	tpis89	S(L)
J 6/78	SCL2(L)	J 6/78	SCL2(L)	J 6/78	S2CL2(L)
J 6/78	S2CL2(L)				

O/F = 0.000000

	EFFECTIVE FUEL	EFFECTIVE OXIDANT	MIXTURE
ENTHALPY	h(2)/R	h(1)/R	h0/R
(KG-MOL)(K)/KG	-0.24393994E+03	0.00000000E+00	-0.24393994E+03
KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*N	0.61333506E-02	0.00000000E+00	0.61333506E-02
*H	0.48397025E-01	0.00000000E+00	0.48397025E-01
CL	0.61333506E-02	0.00000000E+00	0.61333506E-02
*O	0.25067832E-01	0.00000000E+00	0.25067832E-01
*C	0.12669356E-01	0.00000000E+00	0.12669356E-01
S	0.10661263E-03	0.00000000E+00	0.10661263E-03
*AL	0.33356140E-02	0.00000000E+00	0.33356140E-02
Mg	0.49622374E-04	0.00000000E+00	0.49622374E-04

POINT	ITN	T	N	H	CL	O
		C	S	AL	MG	
1	15	2223.217	-13.211	-8.721	-22.552	-21.610
		-10.257	-16.675	-13.362	-21.039	
ADD AL2O3(a)						
1	7	2800.188	-13.618	-9.082	-20.821	-19.613
		-11.789	-17.418	-18.816	-21.663	
PHASE CHANGE, REPLACE AL2O3(a) WITH AL2O3(L)						
1	2	2724.464	-13.567	-9.031	-20.870	-19.869
		-11.563	-17.289	-19.670	-21.824	
2	3	2708.020	-13.903	-9.369	-21.234	-19.927
		-12.208	-17.473	-19.750	-21.884	
3	3	2687.754	-14.237	-9.704	-21.603	-19.999
		-12.840	-17.703	-19.850	-21.967	
4	3	2654.796	-14.675	-10.143	-22.098	-20.119
		-13.657	-18.073	-20.018	-22.121	
5	4	2542.768	-15.754	-11.231	-23.383	-20.548
		-15.608	-19.236	-20.635	-22.836	

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED PRESSURES

CASE = 5

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	TEMP K
NAME	NH4CLO4(I)	0.7206000	-70690.009	298.150
NAME	CHOS-Binder	0.1858000	-2999.082	298.150
NAME	AL(cr)	0.0900000	0.000	298.150
NAME	MgO(s)	0.0020000	-143703.308	298.150
NAME	H2O(L)	0.0016000	-68315.026	298.150

O/F= 0.00000 %FUEL= 0.000000 R,EQ.RATIO= 1.947910 PHI,EQ.RATIO= 0.000000

THERMODYNAMIC PROPERTIES

P, ATM	34.023	17.011	8.5057	3.4023	0.34023
T, K	2724.46	2708.02	2687.75	2654.80	2542.77
RHO, G/CC	3.5209-3	1.7681-3	8.8885-4	3.5874-4	3.7034-5
H, CAL/G	-484.76	-484.76	-484.76	-484.76	-484.76
U, CAL/G	-718.77	-717.76	-716.50	-714.44	-707.24
G, CAL/G	-7370.89	-7490.69	-7598.71	-7721.56	-7925.43
S, CAL/(G)(K)	2.5275	2.5871	2.6468	2.7259	2.9262
M, (1/n)	23.136	23.096	23.048	22.970	22.712
MW, MOL WT	22.282	22.246	22.202	22.130	21.893
(dLV/dLP)t	-1.00263	-1.00342	-1.00438	-1.00590	-1.01098
(dLV/dLT)p	1.0518	1.0686	1.0892	1.1228	1.2412
Cp, CAL/(G)(K)	0.5744	0.6051	0.6435	0.7082	0.9512
GAMMAs	1.1945	1.1890	1.1828	1.1738	1.1504
SON VEL,M/SEC	1081.4	1076.6	1070.9	1062.1	1034.8

MOLE FRACTIONS

ALCL	0.00019	0.00024	0.00030	0.00037	0.00052
ALCL2	0.00014	0.00013	0.00011	0.00010	0.00005
ALCL3	0.00007	0.00005	0.00003	0.00002	0.00000
ALO	0.00000	0.00000	0.00000	0.00000	0.00001
ALOCL	0.00008	0.00010	0.00012	0.00015	0.00023
ALOH	0.00001	0.00002	0.00002	0.00003	0.00004
ALO2H	0.00002	0.00003	0.00003	0.00004	0.00006
*CO	0.26445	0.26396	0.26337	0.26238	0.25895
COS	0.00005	0.00004	0.00003	0.00002	0.00001
*CO2	0.01779	0.01783	0.01788	0.01797	0.01841
CL	0.00168	0.00222	0.00290	0.00401	0.00790
*H	0.00591	0.00785	0.01027	0.01427	0.02829
HCN	0.00001	0.00000	0.00000	0.00000	0.00000
HCO	0.00001	0.00000	0.00000	0.00000	0.00000
HCL	0.13214	0.13144	0.13055	0.12912	0.12434
*H2	0.32150	0.32075	0.31979	0.31813	0.31176
H2O	0.14659	0.14594	0.14516	0.14391	0.13984
H2S	0.00136	0.00113	0.00089	0.00060	0.00018
Mg	0.00002	0.00004	0.00007	0.00013	0.00044
MgCL	0.00003	0.00004	0.00005	0.00006	0.00008
MgCL2	0.00104	0.00101	0.00096	0.00088	0.00054
MgOH	0.00001	0.00001	0.00001	0.00002	0.00002
MgO2H2	0.00001	0.00000	0.00000	0.00000	0.00000
NH3	0.00001	0.00001	0.00000	0.00000	0.00000
*NO	0.00003	0.00003	0.00004	0.00005	0.00009
*N2	0.06831	0.06820	0.06806	0.06784	0.06710
*O	0.00001	0.00001	0.00002	0.00005	0.00016
*OH	0.00070	0.00092	0.00118	0.00157	0.00275
*O2	0.00000	0.00000	0.00000	0.00001	0.00003
S	0.00009	0.00013	0.00019	0.00027	0.00043
SH	0.00062	0.00069	0.00073	0.00071	0.00049
SO	0.00015	0.00023	0.00033	0.00048	0.00082
SO2	0.00006	0.00009	0.00013	0.00019	0.00036
S2	0.00002	0.00003	0.00004	0.00004	0.00002
AL2O3(L)	0.03691	0.03682	0.03672	0.03655	0.03606

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*AL	ALC	ALH	ALN	ALO2
ALS	AL2	AL2CL6	AL2O	AL2O2
*C	CCL	CCL2	CCL3	CCL4
*CH	CHCL	CHCL2	CHCL3	CH2
CH2CL	CH2CL2	CH3	CH3CL	CH2OH
CH3O	CH4	CH3OH	*CN	CNN

COCL	COCL2	COHCL	CS	CS2
C2CL	C2CL2	C2CL3	C2CL4	C2CL6
C2HCL	C2HCL3	C2H2,acetylene	C2H2CL2	C2H3CL
CH3CN	C2H4	C4H6,1-butyne	C6H14,n-hexane	C7H16,2-methylh
CLCN	CLO	CLO2	CL2	CL2O
HALO	HNC	HOCL	HO2	H2SO4
MgH	MgN	MgO	MgS	Mg2
*N	NCO	NOCL	NO2	NO2CL
NO3	N2O	N2O3	N2O4	N2O5
N3	N3H	O3	SCL	SCL2
SN	SO2CL2	SO3	S2CL2	S2O
S3	S4	S5	S6	S7
S8	AL(cr)	AL(L)	ALCL3(s)	ALCL3(L)
ALN(s)	AL2O3(a)	C(gr)	H2SO4(L)	Mg(cr)
Mg(L)	MgAL2O4(s)	MgAL2O4(L)	MgCO3(s)	MgCL2(s)
MgCL2(L)	MgO(s)	MgO(L)	MgO2H2(s)	MgS(s)
MgSO4(s)	MgSO4(L)	NH4CL(a)	NH4CL(b)	S(cr1)
S(cr2)	S(L)	SCL2(L)	S2CL2(L)	

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

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!  EXAMPLE 6:
!      (a)  Chapman-Jouguet detonation problem (detonation)
!      (b)  The reactants are H2 and O2 gases.  The mixture is
!           stoichiometric (r,e=1).
!      (c)  The unburned gases are at 298.15 and 500 K and pressures
!           1 bar and 30 bars (t,k=298.15,500, pbar=1,30)
!      (d)  Thermal transport properties are called for (transport).
!      (e)  Energy units in the final tables are in calories (calories).

reac  oxid O2  wt%=100       t(k)=298.15
      fuel H2  wt%=100.      t(k)=298.15

 prob  detonation   case=6  t=298.15,500, r,e=1, pbar=1,20

output  calories transport
end

OPTIONS: TP=F  HP=F  SP=F  TV=F  UV=F  SV=F  DETN=T  SHOCK=F  REFL=F  INCD=F
RKT=F  FROZ=F  EQL=F  IONS=F  SIUNIT=F  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=T

T,K =   298.1500   500.0000

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

P,BAR =     1.000000    20.000000

   REACTANT          WT.FRAC    (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
O: O2               1.000000  -0.988319E-06   298.15  0.0000
         O  2.00000
F: H2               1.000000  -0.489101E-05   298.15  0.0000
         H  2.00000

      SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)

 l 6/94  *H              l 5/89  HO2             tpis78  *H2
 l 8/89  H2O             l 2/93  H2O2            l 1/90  *O
 tpis78  *OH             tpis89  *O2            l 5/90  O3
 l 8/89  H2O(s)          l 8/89  H2O(L)
```

SPECIES WITH TRANSPORT PROPERTIES

PURE SPECIES

H	H2	H2O	O
OH	O2		

BINARY INTERACTIONS

H	H2
H	O
H2	H2O
H2	O2
H2O	O2
O	O2

O/F = 7.936683

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.24262412E-05	-0.30886113E-07	-0.29892238E-06
KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*O	0.00000000E+00	0.62502344E-01	0.55508435E-01
*H	0.99212255E+00	0.00000000E+00	0.11101687E+00

POINT	ITN	T	O	H
1	8	3609.250	-15.678	-10.324

POINT	ITN	T	O	H
1	3	3637.136	-15.600	-10.241

POINT	ITN	T	O	H
1	3	3680.926	-15.602	-10.237

POINT	ITN	T	O	H
1	2	3679.599	-15.602	-10.237
2	5	4147.454	-14.591	-9.159
2	3	4219.559	-14.489	-9.047
2	3	4292.394	-14.492	-9.042
2	2	4290.262	-14.492	-9.042
3	6	3727.581	-15.710	-10.339
3	3	3669.044	-15.808	-10.446
3	3	3606.911	-15.806	-10.454
3	2	3604.962	-15.806	-10.454
4	5	4336.573	-14.632	-9.177
4	3	4267.642	-14.689	-9.242
4	3	4216.603	-14.687	-9.247
4	2	4216.063	-14.687	-9.247

DETONATION PROPERTIES OF AN IDEAL REACTING GAS

CASE = 6

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	TEMP K
OXIDANT	O2	1.0000000	0.000	298.150
FUEL	H2	1.0000000	0.000	298.150

O/F= 7.93668 %FUEL= 11.189834 R,EQ.RATIO= 1.000000 PHI,EQ.RATIO= 1.000000

UNBURNED GAS				
P1, ATM	0.9869	19.7385	0.9869	19.7385
T1, K	298.15	298.15	500.00	500.00
H1, CAL/G	0.00	0.00	118.41	118.41
M1, (1/n)	12.010	12.010	12.010	12.010
GAMMA1	1.4016	1.4016	1.3858	1.3858
SON VEL1,M/SEC	537.9	537.9	692.6	692.6
BURNED GAS				
P, ATM	18.542	409.40	10.824	240.42
T, K	3679.60	4290.26	3604.96	4216.06
RHO, G/CC	8.9087-4	1.7754-2	5.2196-4	1.0421-2
H, CAL/G	677.36	752.70	758.96	837.29
U, CAL/G	173.32	194.25	256.74	278.61
G, CAL/G	-14642.7	-15416.7	-14599.2	-15431.0
S, CAL/(G)(K)	4.1635	3.7689	4.2603	3.8587
M, (1/n)	14.507	15.267	14.264	14.996
(dLV/dLP)t	-1.08257	-1.06066	-1.08950	-1.06761
(dLV/dLT)p	2.3666	1.8752	2.5062	1.9883
Cp, CAL/(G)(K)	3.9031	2.4578	4.3365	2.7278
GAMMAs	1.1287	1.1436	1.1265	1.1421
SON VEL,M/SEC	1542.8	1634.6	1538.5	1633.9

TRANSPORT PROPERTIES (GASES ONLY)
CONDUCTIVITY IN UNITS OF MILLICALORIES/(CM)(K)(SEC)

VISC,MILLIPOISE	1.1411	1.2744	1.1243	1.2591
WITH EQUILIBRIUM REACTIONS				
Cp, CAL/(G)(K)	3.9031	2.4578	4.3365	2.7278
CONDUCTIVITY	9.1690	5.9829	10.1413	6.6951
PRANDTL NUMBER	0.4857	0.5235	0.4808	0.5130
WITH FROZEN REACTIONS				
Cp, CAL/(G)(K)	0.7788	0.7939	0.7769	0.7923
CONDUCTIVITY	1.2925	1.4230	1.2844	1.4190
PRANDTL NUMBER	0.6876	0.7110	0.6800	0.7030

DETONATION PARAMETERS

P/P1	18.788	20.741	10.968	12.180
T/T1	12.341	14.390	7.210	8.432
M/M1	1.2079	1.2712	1.1877	1.2486
RHO/RHO1	1.8388	1.8322	1.8067	1.8037
DET MACH NUMBER	5.2744	5.5684	4.0135	4.2551
DET VEL,M/SEC	2836.9	2995.1	2779.7	2947.1

MOLE FRACTIONS

*H	0.08098	0.04765	0.09195	0.05702
HO2	0.00019	0.00069	0.00015	0.00058
*H2	0.16234	0.14401	0.16705	0.15222
H2O	0.53502	0.61304	0.51045	0.58216
H2O2	0.00002	0.00017	0.00001	0.00012
*O	0.03848	0.02411	0.04330	0.02868
*OH	0.13460	0.13210	0.13646	0.13826
*O2	0.04837	0.03823	0.05063	0.04096

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

O3 H2O(s) H2O(L)

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

```
!  EXAMPLE 7:
!       (a)  Shock tube problem (shock).
!       (b)  Reactants are H2, O2, and Ar gases at 300 K.  Note that for shock
!            problems reactants must be gaseous species in the thermodynamic
!            data base.  The program calculates properties of the
!            reactants at the temperature given (300 K) using the thermo.lib
!            coefficients.
!       (c)  Reactants are given in moles (moles = ...).
!       (d)  Initial gas pressures are 10 and 20 mm Hg (p,mmhg=10,20,)
!       (e)  Seven initial gas velocities are assigned (u1=1000,1100,1200,
!            1250,1300,1350,1400,).  Note units of u1 are always m/s.
!       (f)  Equilibrium calculations are to be performed for incident shock
!            conditions (incd  eql).
!       (g)  Frozen calculations are to be performed for incident shock
!            conditions (incd  froz).
!       (h)  No 'outp' dataset is given since the default values of the
!            the parameters have the desired  values (e.g. SI units).

reac    name= H2  moles= 0.050  t(k) 300.00
        name= O2  moles= 0.050  t(k) 300.00
        name= Ar  moles= 0.900  t(k) 300.00

problem  case=7 p,mmhg=10,20, shock u1=1000,1100,1200,1250,1300,1350,1400,
  incd froz  eql

end

OPTIONS: TP=F  HP=F  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=T  REFL=F  INCD=T
RKT=F  FROZ=T  EQL=T  IONS=F  SIUNIT=T  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

P,BAR =      0.013332      0.026664

   REACTANT            MOLES     (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
N: H2                0.050000    0.641758E+01   300.00  0.0000
         H  2.00000
N: O2                0.050000    0.653777E+01   300.00  0.0000
         O  2.00000
N: Ar                0.900000    0.462500E+01   300.00  0.0000
         AR 1.00000

     SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)

 l 6/88  *Ar              l 6/94  *H               l 5/89  HO2
 tpis78  *H2              l 8/89  H2O              l 2/93  H2O2
 l 1/90  *O               tpis78  *OH             tpis89  *O2
 l 5/90  O3               l 8/89  H2O(s)          l 8/89  H2O(L)
```

*** INPUT FOR SHOCK PROBLEMS ***

INCDEQ = T REFLEQ = F INCDFZ = T REFLFZ = F

U1 = 1.000000E+03 1.100000E+03 1.200000E+03 1.250000E+03 1.300000E+03
1.350000E+03 1.400000E+03

MACH1 = 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00

O/F = 0.000000

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	0.12774941E+00	0.00000000E+00	0.12774941E+00
KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*H	0.26557650E-02	0.00000000E+00	0.26557650E-02
*O	0.26557650E-02	0.00000000E+00	0.26557650E-02
*Ar	0.23901885E-01	0.00000000E+00	0.23901885E-01

SHOCK WAVE PARAMETERS ASSUMING
EQUILIBRIUM COMPOSITION FOR INCIDENT SHOCKED CONDITIONS

CASE = 7

REACTANT		MOLES	ENERGY KJ/KG-MOL	TEMP K
NAME	H2	0.0500000	53.359	300.000
NAME	O2	0.0500000	54.358	300.000
NAME	Ar	0.9000000	38.455	300.000

O/F= 0.00000 %FUEL= 0.000000 R,EQ.RATIO= 0.500000 PHI,EQ.RATIO= 0.000000

INITIAL GAS (1)							
MACH NUMBER1	3.0480	3.3528	3.6576	3.8100	3.9624	4.1148	4.2672
U1, M/SEC	1000.00	1100.00	1200.00	1250.00	1300.00	1350.00	1400.00
P, BAR	0.01333	0.02666	0.02666	0.02666	0.02666	0.02666	0.02666
T, K	300.00	300.00	300.00	300.00	300.00	300.00	300.00
RHO, KG/CU M	2.0126-2	4.0252-2	4.0252-2	4.0252-2	4.0252-2	4.0252-2	4.0252-2
H, KJ/KG	1.0622	1.0622	1.0622	1.0622	1.0622	1.0622	1.0622
U, KJ/KG	-65.182	-65.182	-65.182	-65.182	-65.182	-65.182	-65.182
G, KJ/KG	-1556.26	-1510.35	-1510.35	-1510.35	-1510.35	-1510.35	-1510.35
S, KJ/(KG)(K)	5.1911	5.0380	5.0380	5.0380	5.0380	5.0380	5.0380
M, (1/n)	37.654	37.654	37.654	37.654	37.654	37.654	37.654
Cp, KJ/(KG)(K)	0.5742	0.5742	0.5742	0.5742	0.5742	0.5742	0.5742
GAMMAs	1.6249	1.6249	1.6249	1.6249	1.6249	1.6249	1.6249
SON VEL,M/SEC	328.1	328.1	328.1	328.1	328.1	328.1	328.1

WARNING!! NO CONVERGENCE FOR u1= 1000.0
ANSWERS NOT RELIABLE, SOLUTION MAY NOT EXIST (SHCK)

SHOCKED GAS (2)--INCIDENT--EQUILIBRIUM							
U2, M/SEC	703.53	666.91	576.09	560.23	549.01	540.16	532.35
P, BAR	0.08449	0.21842	0.32803	0.37372	0.41964	0.46673	0.51561
T, K	1371.90	1528.10	1816.96	1932.22	2043.84	2152.73	2258.45
RHO, KG/CU M	2.8607-2	6.6391-2	8.3844-2	8.9812-2	9.5312-2	1.0060-1	1.0586-1
H, KJ/KG	292.39	383.68	555.13	625.39	695.35	766.43	839.37
U, KJ/KG	-2.9743	54.682	163.89	209.27	255.08	302.48	352.28
G, KJ/KG	-7331.22	-7891.77	-9312.23	-9886.05	-10444.2	-10990.3	-11520.9
S, KJ/(KG)(K)	5.5570	5.4155	5.4307	5.4401	5.4503	5.4613	5.4729
M, (1/n)	38.619	38.619	38.614	38.608	38.597	38.580	38.552
(dLV/dLP)t	-1.00000	-1.00000	-1.00005	-1.00010	-1.00021	-1.00040	-1.00072
(dLV/dLT)p	1.0001	1.0002	1.0018	1.0037	1.0070	1.0123	1.0207
Cp, KJ/(KG)(K)	0.5827	0.5869	0.6041	0.6187	0.6412	0.6747	0.7226
GAMMAs	1.5861	1.5798	1.5570	1.5397	1.5162	1.4857	1.4497
SON VEL,M/SEC	684.5	720.9	780.5	800.4	817.0	830.2	840.3
P2/P1	6.654	8.192	12.302	14.016	15.738	17.504	19.337
T2/T1	4.656	5.094	6.057	6.441	6.813	7.176	7.528
M2/M1	1.0256	1.0256	1.0255	1.0253	1.0251	1.0246	1.0238
RHO2/RHO1	1.4214	1.6494	2.0830	2.2312	2.3679	2.4993	2.6299
V2, M/SEC	296.47	433.09	623.91	689.77	750.99	809.84	867.65

MOLE FRACTIONS

*Ar	9.2307-1	9.2306-1	9.2294-1	9.2280-1	9.2255-1	9.2213-1	9.2146-1
*H	6.3878-9	7.1872-8	4.2701-6	1.5520-5	4.7038-5	1.2367-4	2.8725-4
HO2	5.7290-9	2.4000-8	1.4081-7	2.4561-7	3.9562-7	5.9860-7	8.5747-7
*H2	3.2023-7	1.8716-6	3.5078-5	8.8322-5	1.9485-4	3.8722-4	7.0178-4
H2O	5.1272-2	5.1248-2	5.1025-2	5.0780-2	5.0378-2	4.9752-2	4.8831-2
H2O2	2.311-10	9.754-10	4.623 -9	7.549 -9	1.149 -8	1.654 -8	2.266 -8
*O	3.3351-7	2.0203-6	3.9781-5	1.0183-4	2.2822-4	4.6110-4	8.5170-4
*OH	1.8151-5	6.1566-5	4.2535-4	7.8035-4	1.3111-3	2.0550-3	3.0302-3
*O2	2.5636-2	2.5625-2	2.5530-2	2.5435-2	2.5293-2	2.5094-2	2.4835-2

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-09 FOR ALL ASSIGNED CONDITIONS

O3 H2O(s) H2O(L)

SHOCK WAVE PARAMETERS ASSUMING
FROZEN COMPOSITION FOR INCIDENT SHOCKED CONDITI1ONS

CASE = 7

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
NAME	H2	0.0500000	53.359	300.000
NAME	O2	0.0500000	54.358	300.000
NAME	Ar	0.9000000	38.455	300.000

O/F= 0.00000 %FUEL= 0.000000 R,EQ.RATIO= 0.500000 PHI,EQ.RATIO= 0.000000

INITIAL GAS (1)							
MACH NUMBER1	3.0480	3.3528	3.6576	3.8100	3.9624	4.1148	4.2672
U1, M/SEC	1000.00	1100.00	1200.00	1250.00	1300.00	1350.00	1400.00
P, BAR	0.01333	0.02666	0.02666	0.02666	0.02666	0.02666	0.02666
T, K	300.00	300.00	300.00	300.00	300.00	300.00	300.00
RHO, KG/CU M	2.0126-2	4.0252-2	4.0252-2	4.0252-2	4.0252-2	4.0252-2	4.0252-2
H, KJ/KG	1.0622	1.0622	1.0622	1.0622	1.0622	1.0622	1.0622
U, KJ/KG	-65.182	-65.182	-65.182	-65.182	-65.182	-65.182	-65.182
G, KJ/KG	-1556.26	-1510.35	-1510.35	-1510.35	-1510.35	-1510.35	-1510.35
S, KJ/(KG)(K)	5.1911	5.0380	5.0380	5.0380	5.0380	5.0380	5.0380
M, (1/n)	37.654	37.654	37.654	37.654	37.654	37.654	37.654
Cp, KJ/(KG)(K)	0.5742	0.5742	0.5742	0.5742	0.5742	0.5742	0.5742
GAMMAs	1.6249	1.6249	1.6249	1.6249	1.6249	1.6249	1.6249
SON VEL,M/SEC	328.1	328.1	328.1	328.1	328.1	328.1	328.1
SHOCKED GAS (2)--INCIDENT--FROZEN							
U2, M/SEC	317.26	332.77	349.41	358.06	366.89	375.87	384.99
P, BAR	0.15074	0.36638	0.43752	0.47544	0.51494	0.55601	0.59865
T, K	1076.14	1247.03	1433.31	1532.25	1635.05	1741.69	1852.17
RHO, KG/CU M	6.3438-2	1.3305-1	1.3824-1	1.4052-1	1.4263-1	1.4457-1	1.4637-1
H, KJ/KG	450.75	550.72	660.02	718.21	778.76	841.67	906.95
U, KJ/KG	213.13	275.36	343.52	379.87	417.72	457.08	497.97
G, KJ/KG	-5354.24	-6039.09	-6975.05	-7475.96	-7998.88	-8543.88	-9111.04
S, KJ/(KG)(K)	5.3943	5.2844	5.3269	5.3478	5.3684	5.3888	5.4088
M, (1/n)	37.654	37.654	37.654	37.654	37.654	37.654	37.654
Cp, KJ/(KG)(K)	0.5841	0.5858	0.5876	0.5886	0.5895	0.5904	0.5913
GAMMAs	1.6078	1.6049	1.6019	1.6005	1.5989	1.5974	1.5960
SON VEL,M/SEC	618.1	664.8	712.0	735.9	759.8	783.8	807.9
P2/P1	11.307	13.740	16.408	17.831	19.312	20.852	22.451
T2/T1	3.587	4.157	4.778	5.108	5.450	5.806	6.174
M2/M1	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
RHO2/RHO1	3.1520	3.3056	3.4344	3.4911	3.5433	3.5917	3.6365
V2, M/SEC	682.74	767.23	850.59	891.94	933.11	974.13	1015.01

MOLE FRACTIONS

*H2	0.05000	0.05000	0.05000	0.05000	0.05000	0.05000	0.05000
*O2	0.05000	0.05000	0.05000	0.05000	0.05000	0.05000	0.05000
*Ar	0.90000	0.90000	0.90000	0.90000	0.90000	0.90000	0.90000

```
#  EXAMPLE 8:
#      (a)  Rocket problem with infinite-area combustor (rocket iac by default).
#      (b)  The fuel is H2(L) at 20.27 K; the oxidant is O2(L) at 90.17 K.
#           Both are in thermo.lib so that the enthalpies and "exploded" formulas
#           do not need to be given.
#      (c)  The oxidant-to-fuel ratio is 5.55157 (o/f=5.55157).
#      (d)  The chamber pressure is 53.3172 bars (p,bar=53.3172).
#      (e)  Calculations are with equilibrium chemistry only (equilibrium).
#      (f)  For exit points there are three pressure ratios (pi/p=10,100,1000),
#           one subsonic area ratio (subar=1.58), and three supersonic area
#           ratios (supar=25,50,75).

      problem  rocket  equilibrium  o/f=5.55157
case=8  p,bar=53.3172 subar=1.58,pi/p=10,100,1000,supar=25,50,75
      reactants
fuel = H2(L)   wt% 100.    t(k) 20.27
oxid = O2(L)   wt% 100.    t(k) 90.17
      output  siunits
      end

OPTIONS: TP=F  HP=F  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=T  FROZ=F  EQL=T  IONS=F  SIUNIT=T  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

Pc,BAR =     53.317200

Pc/P =     10.0000   100.0000  1000.0000

SUBSONIC AREA RATIOS =      1.5800

SUPERSONIC AREA RATIOS =     25.0000    50.0000    75.0000

NFZ=  1  Mdot/Ac= 0.000000E+00  Ac/At= 0.000000E+00

   REACTANT           WT.FRAC    (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
F: H2(L)             1.000000  -0.108389E+04    20.27  0.0000
         H  2.00000
O: O2(L)             1.000000  -0.156101E+04    90.17  0.0000
         O  2.00000
```

SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)

l 6/94	*H	l 5/89	HO2	tpis78	*H2
l 8/89	H2O	l 2/93	H2O2	l 1/90	*O
tpis78	*OH	tpis89	*O2	l 5/90	O3
l 8/89	H2O(s)	l 8/89	H2O(L)		

O/F = 5.551570

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.53767500E+03	-0.48783267E+02	-0.12340534E+03
KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*H	0.99212255E+00	0.00000000E+00	0.15143279E+00
*O	0.00000000E+00	0.62502344E-01	0.52962288E-01

POINT	ITN	T	H	O
1	9	3389.270	-9.266	-16.561
Pinf/Pt = 1.737856				
2	4	3190.532	-9.433	-16.968
Pinf/Pt = 1.739443				
2	2	3190.207	-9.434	-16.968
3	4	2568.396	-9.922	-18.802
4	4	1759.119	-10.454	-23.533
5	4	1115.280	-10.958	-32.668
6	3	3360.178	-9.291	-16.616
6	2	3354.650	-9.295	-16.627
6	2	3353.978	-9.296	-16.628
6	1	3353.970	-9.296	-16.628
7	5	1441.190	-10.682	-26.980
7	2	1467.038	-10.662	-26.641
8	3	1241.429	-10.845	-30.099
8	2	1218.630	-10.864	-30.523

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM

COMPOSITION DURING EXPANSION FROM INFINITE AREA COMBUSTOR

Pinj = 773.3 PSIA
CASE = 8

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
FUEL	H2(L)	1.0000000	-9012.000	20.270
OXIDANT	O2(L)	1.0000000	-12979.000	90.170

O/F= 5.55157 %FUEL= 15.263517 R,EQ.RATIO= 1.429629 PHI,EQ.RATIO= 1.429628

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
Pinf/P	1.0000	1.7394	10.000	100.00	1000.00	1.1020	260.57	655.41
P, BAR	53.317	30.652	5.3317	0.53317	0.05332	48.381	0.20462	0.08135
T, K	3389.27	3190.21	2568.40	1759.12	1115.28	3353.97	1467.04	1218.63
RHO, KG/CU M	2.4071 0	1.4848 0	3.2770-1	4.8139-2	7.5938-3	2.2113 0	2.2155-2	1.0604-2
H, KJ/KG	-1026.05	-2210.09	-5432.07	-8564.25	-10623.5	-1239.91	-9535.06	-10313.3
U, KJ/KG	-3241.04	-4274.40	-7059.06	-9671.81	-11325.7	-3427.81	-10458.6	-11080.5
G, KJ/KG	-64259.7	-61729.8	-53350.7	-41384.1	-31431.3	-63814.9	-36905.6	-33049.3
S, KJ/(KG)(K)	18.6570	18.6570	18.6570	18.6570	18.6570	18.6570	18.6570	18.6570
M, (1/n)	12.723	12.849	13.125	13.206	13.207	12.746	13.207	13.207
(dLV/dLP)t	-1.01996	-1.01459	-1.00317	-1.00005	-1.00000	-1.01897	-1.00000	-1.00000
(dLV/dLT)p	1.3627	1.2808	1.0739	1.0017	1.0000	1.3482	1.0001	1.0000
Cp, KJ/(KG)(K)	8.2837	7.4299	4.8447	3.4332	2.9621	8.1390	3.2226	3.0413
GAMMAs	1.1449	1.1472	1.1732	1.2254	1.2699	1.1451	1.2429	1.2610
SON VEL,M/SEC	1592.4	1538.9	1381.6	1165.0	944.3	1582.8	1071.4	983.6
MACH NUMBER	0.000	1.000	2.149	3.333	4.640	0.413	3.850	4.382
PERFORMANCE PARAMETERS								
Ae/At		1.0000	2.3489	12.225	68.680	1.5800	25.000	50.000
CSTAR, M/SEC		2333.4	2333.4	2333.4	2333.4	2333.4	2333.4	2333.4
CF		0.6595	1.2722	1.6640	1.8776	0.2803	1.7679	1.8470
Ivac, M/SEC		2880.3	3516.6	4168.1	4541.5	3999.5	4349.2	4487.8
Isp, M/SEC		1538.9	2968.5	3882.8	4381.2	654.0	4125.3	4309.8
MOLE FRACTIONS								
*H	0.03390	0.02683	0.00797	0.00019	0.00000	0.03265	0.00001	0.00000
HO2	0.00002	0.00001	0.00000	0.00000	0.00000	0.00001	0.00000	0.00000
*H2	0.29410	0.29373	0.29695	0.30040	0.30052	0.29398	0.30051	0.30052
H2O	0.63643	0.65440	0.69081	0.69938	0.69948	0.63976	0.69948	0.69948
H2O2	0.00001	0.00000	0.00000	0.00000	0.00000	0.00001	0.00000	0.00000
*O	0.00214	0.00124	0.00007	0.00000	0.00000	0.00196	0.00000	0.00000
*OH	0.03162	0.02271	0.00413	0.00003	0.00000	0.02998	0.00000	0.00000
*O2	0.00179	0.00108	0.00007	0.00000	0.00000	0.00165	0.00000	0.00000

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

O3 H2O(s) H2O(L)

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

3	3	1067.058	-11.004	-33.815
3	2	1087.734	-10.984	-33.311

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM
COMPOSITION DURING EXPANSION FROM INFINITE AREA COMBUSTOR

Pinj = 773.3 PSIA
CASE = 8

REACTANT		WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
FUEL	H2(L)	1.0000000	-9012.000	20.270
OXIDANT	O2(L)	1.0000000	-12979.000	90.170

O/F= 5.55157 %FUEL= 15.263517 R,EQ.RATIO= 1.429629 PHI,EQ.RATIO= 1.429628

	CHAMBER	THROAT	EXIT
Pinf/P	1.0000	1.7394	1124.40
P, BAR	53.317	30.652	0.04742
T, K	3389.27	3190.21	1087.73
RHO, KG/CU M	2.4071 0	1.4848 0	6.9247-3
H, KJ/KG	-1026.05	-2210.09	-10704.9
U, KJ/KG	-3241.04	-4274.40	-11389.6
G, KJ/KG	-64259.7	-61729.8	-30998.7
S, KJ/(KG)(K)	18.6570	18.6570	18.6570
M, (1/n)	12.723	12.849	13.207
(dLV/dLP)t	-1.01996	-1.01459	-1.00000
(dLV/dLT)p	1.3627	1.2808	1.0000
Cp, KJ/(KG)(K)	8.2837	7.4299	2.9409
GAMMAs	1.1449	1.1472	1.2724
SON VEL,M/SEC	1592.4	1538.9	933.4
MACH NUMBER	0.000	1.000	4.714

PERFORMANCE PARAMETERS

Ae/At	1.0000	75.000
CSTAR, M/SEC	2333.4	2333.4
CF	0.6595	1.8856
Ivac, M/SEC	2880.3	4555.4
Isp, M/SEC	1538.9	4399.7

MOLE FRACTIONS

*H	0.03390	0.02683	0.00000
HO2	0.00002	0.00001	0.00000
*H2	0.29410	0.29373	0.30052
H2O	0.63643	0.65440	0.69948
H2O2	0.00001	0.00000	0.00000
*O	0.00214	0.00124	0.00000
*OH	0.03162	0.02271	0.00000
*O2	0.00179	0.00108	0.00000

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

O3 H2O(s) H2O(L)

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

```
#  EXAMPLE 9:
#      (a)  Rocket problem with a finite-area combustor (rocket  fac).
#      (b)  Contraction ratio of 1.58 (acat=1.58) is assigned.
#      (c)  Fuel, oxidant, and the remaining parameters are the same as in
#           example 8.

reac  fuel = H2(L)  wt%=100.  t,k= 20.27
      oxid = O2(L)  wt%=100.  t,k= 90.17
problem  o/f=5.55157 case=9  rocket  fac  p,bar=53.3172 acat=1.58
         pi/p=10,100,1000, supar=25,50,75
output  siunits
end

OPTIONS: TP=F  HP=F  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=T  FROZ=F  EQL=T  IONS=F  SIUNIT=T  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

Pc,BAR =     53.317200

Pc/P =     10.0000   100.0000  1000.0000

SUBSONIC AREA RATIOS =

SUPERSONIC AREA RATIOS =     25.0000     50.0000     75.0000

NFZ=  1  Mdot/Ac= 0.000000E+00  Ac/At= 1.580000E+00

   REACTANT           WT.FRAC    (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
F: H2(L)             1.000000  -0.108389E+04    20.27  0.0000
         H  2.00000
O: O2(L)             1.000000  -0.156101E+04    90.17  0.0000
         O  2.00000

      SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)

 l 6/94  *H              l 5/89  HO2             tpis78  *H2
 l 8/89  H2O             l 2/93  H2O2            l 1/90  *O
 tpis78  *OH             tpis89  *O2            l 5/90  O3
 l 8/89  H2O(s)          l 8/89  H2O(L)

O/F =    5.551570

                        EFFECTIVE FUEL      EFFECTIVE OXIDANT        MIXTURE
ENTHALPY                    h(2)/R              h(1)/R                 h0/R
(KG-MOL)(K)/KG         -0.53767500E+03     -0.48783267E+02     -0.12340534E+03

KG-FORM.WT./KG              bi(2)               bi(1)                  b0i
 *H                     0.99212255E+00      0.00000000E+00      0.15143279E+00
 *O                     0.00000000E+00      0.62502344E-01      0.52962288E-01
```

POINT	ITN	T	H	O
1	9	3389.270	-9.266	-16.561
2	3	3381.326	-9.303	-16.578
Pinf/Pt = 1.737476				
3	4	3184.432	-9.471	-16.983
Pinf/Pt = 1.739009				
3	2	3184.121	-9.471	-16.984
4	3	3352.506	-9.328	-16.634
4	2	3347.029	-9.332	-16.644
4	2	3346.363	-9.333	-16.645
4	1	3346.355	-9.333	-16.645
2	1	3381.345	-9.303	-16.578
Pinf/Pt = 1.737477				
3	4	3184.446	-9.471	-16.983
Pinf/Pt = 1.739010				
3	2	3184.135	-9.471	-16.984
4	3	3352.524	-9.327	-16.634
4	2	3347.047	-9.332	-16.644
4	2	3346.381	-9.333	-16.645
4	1	3346.373	-9.333	-16.645
END OF CHAMBER ITERATIONS				
4	5	2596.353	-9.941	-18.697
5	4	1786.498	-10.478	-23.297
6	4	1135.439	-10.981	-32.218
7	5	1442.273	-10.724	-26.966
7	2	1468.448	-10.704	-26.623
8	3	1242.967	-10.885	-30.071
8	2	1219.873	-10.905	-30.499

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM

COMPOSITION DURING EXPANSION FROM FINITE AREA COMBUSTOR

Pinj = 773.3 PSIA
Ac/At = 1.5800 Pinj/Pinf = 1.084780
CASE = 9

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
FUEL	H2(L)	1.0000000	-9012.000	20.270
OXIDANT	O2(L)	1.0000000	-12979.000	90.170

O/F= 5.55157 %FUEL= 15.263517 R,EQ.RATIO= 1.429629 PHI,EQ.RATIO= 1.429628

	INJECTOR	COMB END	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT
Pinj/P	1.0000	1.1954	1.8864	10.000	100.00	1000.00	282.15	709.71
P, BAR	53.317	44.602	28.263	5.3317	0.53317	0.05332	0.18897	0.07513
T, K	3389.27	3346.37	3184.14	2596.35	1786.50	1135.44	1468.45	1219.87
RHO, KG/CU M	2.4071 0	2.0416 0	1.3709 0	3.2390-1	4.7400-2	7.4589-3	2.0441-2	9.7824-3
H, KJ/KG	-1026.05	-1239.49	-2207.90	-5294.68	-8469.93	-10563.7	-9530.50	-10309.5
U, KJ/KG	-3241.04	-3424.10	-4269.63	-6940.78	-9594.77	-11278.5	-10455.0	-11077.5
G, KJ/KG	-64259.7	-63850.8	-61783.7	-53873.0	-41895.7	-31808.0	-37005.5	-33133.6
S, KJ/(KG)(K)	18.6570	18.7102	18.7102	18.7102	18.7102	18.7102	18.7102	18.7102
M, (1/n)	12.723	12.736	12.841	13.114	13.205	13.207	13.207	13.207
(dLV/dLP)t	-1.01996	-1.01940	-1.01495	-1.00361	-1.00007	-1.00000	-1.00000	-1.00000
(dLV/dLT)p	1.3627	1.3567	1.2882	1.0834	1.0022	1.0000	1.0001	1.0000
Cp, KJ/(KG)(K)	8.2837	8.2508	7.5303	4.9862	3.4569	2.9777	3.2237	3.0422
GAMMAs	1.1449	1.1445	1.1465	1.1705	1.2238	1.2681	1.2428	1.2609
SON VEL,M/SEC	1592.4	1581.2	1537.4	1388.1	1173.3	952.1	1071.9	984.0
MACH NUMBER	0.000	0.413	1.000	2.105	3.289	4.587	3.848	4.379

PERFORMANCE PARAMETERS

Ae/At	1.5800	1.0000	2.2270	11.524	64.695	25.000	50.000
CSTAR, M/SEC	2332.1	2332.1	2332.1	2332.1	2332.1	2332.1	2332.1
CF	0.2802	0.6593	1.2529	1.6545	1.8728	1.7685	1.8477
Ivac, M/SEC	3997.0	2878.5	3485.2	4150.0	4531.2	4348.3	4487.2
Isp, M/SEC	653.4	1537.4	2921.9	3858.5	4367.5	4124.2	4308.9

MOLE FRACTIONS

*H	0.03390	0.03336	0.02747	0.00893	0.00024	0.00000	0.00002	0.00000
HO2	0.00002	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000
*H2	0.29410	0.29384	0.29358	0.29659	0.30037	0.30052	0.30051	0.30052
H2O	0.63643	0.63858	0.65337	0.68952	0.69935	0.69948	0.69948	0.69948
H2O2	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
*O	0.00214	0.00204	0.00130	0.00009	0.00000	0.00000	0.00000	0.00000
*OH	0.03162	0.03045	0.02314	0.00477	0.00004	0.00000	0.00000	0.00000
*O2	0.00179	0.00172	0.00113	0.00009	0.00000	0.00000	0.00000	0.00000

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

O3 H2O(s) H2O(L)

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

4	3	1067.940	-11.046	-33.793
4	2	1088.883	-11.025	-33.283

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM
COMPOSITION DURING EXPANSION FROM FINITE AREA COMBUSTOR

Pinj = 773.3 PSIA
Ac/At = 1.5800 Pinj/Pinf = 1.084780
CASE = 9

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
FUEL	H2(L)	1.0000000	-9012.000	20.270
OXIDANT	O2(L)	1.0000000	-12979.000	90.170

O/F= 5.55157 %FUEL= 15.263517 R,EQ.RATIO= 1.429629 PHI,EQ.RATIO= 1.429628

	INJECTOR	COMB END	THROAT	EXIT
Pinj/P	1.0000	1.1954	1.8864	1217.53
P, BAR	53.317	44.602	28.263	0.04379
T, K	3389.27	3346.37	3184.14	1088.88
RHO, KG/CU M	2.4071 0	2.0416 0	1.3709 0	6.3882-3
H, KJ/KG	-1026.05	-1239.49	-2207.90	-10701.5
U, KJ/KG	-3241.04	-3424.10	-4269.63	-11387.0
G, KJ/KG	-64259.7	-63850.8	-61783.7	-31074.7
S, KJ/(KG)(K)	18.6570	18.7102	18.7102	18.7102
M, (1/n)	12.723	12.736	12.841	13.207
(dLV/dLP)t	-1.01996	-1.01940	-1.01495	-1.00000
(dLV/dLT)p	1.3627	1.3567	1.2882	1.0000
Cp, KJ/(KG)(K)	8.2837	8.2508	7.5303	2.9418
GAMMAs	1.1449	1.1445	1.1465	1.2723
SON VEL,M/SEC	1592.4	1581.2	1537.4	933.9
MACH NUMBER	0.000	0.413	1.000	4.710

PERFORMANCE PARAMETERS

Ae/At	1.5800	1.0000	75.000
CSTAR, M/SEC	2332.1	2332.1	2332.1
CF	0.2802	0.6593	1.8863
Ivac, M/SEC	3997.0	2878.5	4554.8
Isp, M/SEC	653.4	1537.4	4399.0

MOLE FRACTIONS

*H	0.03390	0.03336	0.02747	0.00000
HO2	0.00002	0.00001	0.00001	0.00000
*H2	0.29410	0.29384	0.29358	0.30052
H2O	0.63643	0.63858	0.65337	0.69948
H2O2	0.00001	0.00001	0.00000	0.00000
*O	0.00214	0.00204	0.00130	0.00000
*OH	0.03162	0.03045	0.02314	0.00000
*O2	0.00179	0.00172	0.00113	0.00000

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

O3 H2O(s) H2O(L)

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

```
#  EXAMPLE 10:
#     (a)  Rocket problem with a finite-area combustor (rocket fac).
#     (b)  A ratio of mass flow rate to chamber area of 1333.9 (ma=1333.9)
#          is assigned.  This value was calculated from the results
#          of example 9 where a contraction ratio of 1.58 was assigned.
#     (c)  Fuel, oxidant, and the remaining parameters are the same as in
#          examples 8 and 9.

reac  fuel = H2(L)  t,k= 20.27
      oxid = O2(L)  t,k= 90.17
problem  o/f=5.55157 case=10  rocket  fac  p,bar=53.3172 ma=1333.9
         pi/p=10,100,1000, sup-ae/at=25,50,75
output  short
end

WARNING!!  AMOUNT MISSING FOR REACTANT  1.
PROGRAM SETS WEIGHT PERCENT = 100. (REACT)

WARNING!!  AMOUNT MISSING FOR REACTANT  2.
PROGRAM SETS WEIGHT PERCENT = 100. (REACT)
```

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM
COMPOSITION DURING EXPANSION FROM FINITE AREA COMBUSTOR

Pinj = 773.3 PSIA
MDOT/Ac = 1333.500 (KG/S)/M**2 Pinj/Pinf = 1.084780
CASE = 10

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
FUEL	H2(L)	1.0000000	-9012.000	20.270
OXIDANT	O2(L)	1.0000000	-12979.000	90.170

O/F= 5.55157 %FUEL= 15.263517 R,EQ.RATIO= 1.429629 PHI,EQ.RATIO= 1.429628

	INJECTOR	COMB END	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT
Pinj/P	1.0000	1.1954	1.8864	10.000	100.00	1000.00	282.15	709.71
P, BAR	53.317	44.602	28.263	5.3317	0.53317	0.05332	0.18897	0.07513
T, K	3389.27	3346.37	3184.14	2596.35	1786.50	1135.44	1468.45	1219.87
RHO, KG/CU M	2.4071 0	2.0417 0	1.3709 0	3.2390-1	4.7400-2	7.4589-3	2.0441-2	9.7824-3
H, KJ/KG	-1026.05	-1239.48	-2207.90	-5294.68	-8469.93	-10563.7	-9530.50	-10309.5
U, KJ/KG	-3241.04	-3424.09	-4269.63	-6940.78	-9594.77	-11278.5	-10455.0	-11077.5
G, KJ/KG	-64259.7	-63850.8	-61783.7	-53873.0	-41895.7	-31808.0	-37005.5	-33133.6
S, KJ/(KG)(K)	18.6570	18.7102	18.7102	18.7102	18.7102	18.7102	18.7102	18.7102
M, (1/n)	12.723	12.736	12.841	13.114	13.205	13.207	13.207	13.207
(dLV/dLP)t	-1.01996	-1.01940	-1.01495	-1.00361	-1.00007	-1.00000	-1.00000	-1.00000
(dLV/dLT)p	1.3627	1.3567	1.2882	1.0834	1.0022	1.0000	1.0001	1.0000
Cp, KJ/(KG)(K)	8.2837	8.2508	7.5303	4.9862	3.4569	2.9777	3.2237	3.0422
GAMMAs	1.1449	1.1445	1.1465	1.1705	1.2238	1.2681	1.2428	1.2609
SON VEL,M/SEC	1592.4	1581.2	1537.4	1388.1	1173.3	952.1	1071.9	984.0
MACH NUMBER	0.000	0.413	1.000	2.105	3.289	4.587	3.848	4.379
PERFORMANCE PARAMETERS								
Ae/At		1.5800	1.0000	2.2270	11.524	64.695	25.000	50.000
CSTAR, M/SEC		2332.1	2332.1	2332.1	2332.1	2332.1	2332.1	2332.1
CF		0.2802	0.6593	1.2529	1.6545	1.8728	1.7685	1.8477
Ivac, M/SEC		3997.1	2878.5	3485.2	4150.0	4531.2	4348.3	4487.2
Isp, M/SEC		653.3	1537.4	2921.9	3858.5	4367.5	4124.2	4308.9
MOLE FRACTIONS								
*H	0.03390	0.03336	0.02747	0.00893	0.00024	0.00000	0.00002	0.00000
HO2	0.00002	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000
*H2	0.29410	0.29384	0.29358	0.29659	0.30037	0.30052	0.30051	0.30052
H2O	0.63643	0.63858	0.65337	0.68952	0.69935	0.69948	0.69948	0.69948
H2O2	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
*O	0.00214	0.00204	0.00130	0.00009	0.00000	0.00000	0.00000	0.00000
*OH	0.03162	0.03045	0.02314	0.00477	0.00004	0.00000	0.00000	0.00000
*O2	0.00179	0.00172	0.00113	0.00009	0.00000	0.00000	0.00000	0.00000

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

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

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM
COMPOSITION DURING EXPANSION FROM FINITE AREA COMBUSTOR

Pinj = 773.3 PSIA
MDOT/Ac = 1333.900 (KG/S)/M**2 Pinj/Pinf = 1.084780
CASE = 10

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
FUEL	H2(L)	1.0000000	-9012.000	20.270
OXIDANT	O2(L)	1.0000000	-12979.000	90.170

O/F= 5.55157 %FUEL= 15.263517 R,EQ.RATIO= 1.429629 PHI,EQ.RATIO= 1.429628

	INJECTOR	COMB END	THROAT	EXIT
Pinj/P	1.0000	1.1954	1.8864	1217.53
P, BAR	53.317	44.602	28.263	0.04379
T, K	3389.27	3346.37	3184.14	1088.88
RHO, KG/CU M	2.4071 0	2.0417 0	1.3709 0	6.3882-3
H, KJ/KG	-1026.05	-1239.48	-2207.90	-10701.5
U, KJ/KG	-3241.04	-3424.09	-4269.63	-11387.0
G, KJ/KG	-64259.7	-63850.8	-61783.7	-31074.7
S, KJ/(KG)(K)	18.6570	18.7102	18.7102	18.7102
M, (1/n)	12.723	12.736	12.841	13.207
(dLV/dLP)t	-1.01996	-1.01940	-1.01495	-1.00000
(dLV/dLT)p	1.3627	1.3567	1.2882	1.0000
Cp, KJ/(KG)(K)	8.2837	8.2508	7.5303	2.9418
GAMMAs	1.1449	1.1445	1.1465	1.2723
SON VEL,M/SEC	1592.4	1581.2	1537.4	933.9
MACH NUMBER	0.000	0.413	1.000	4.710
PERFORMANCE PARAMETERS				
Ae/At		1.5800	1.0000	75.000
CSTAR, M/SEC		2332.1	2332.1	2332.1
CF		0.2802	0.6593	1.8863
Ivac, M/SEC		3997.1	2878.5	4554.8
Isp, M/SEC		653.3	1537.4	4399.0
MOLE FRACTIONS				
*H	0.03390	0.03336	0.02747	0.00000
HO2	0.00002	0.00001	0.00001	0.00000
*H2	0.29410	0.29384	0.29358	0.30052
H2O	0.63643	0.63858	0.65337	0.69948
H2O2	0.00001	0.00001	0.00000	0.00000
*O	0.00214	0.00204	0.00130	0.00000
*OH	0.03162	0.03045	0.02314	0.00000
*O2	0.00179	0.00172	0.00113	0.00000

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

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

```
#  EXAMPLE 11:
#      (a)  Rocket problem with an infinite-area combustor (rocket).
#      (b)  Reactants are Li(cr) at 298.15 K and F2(L) at 85.02 K.
#           Enthalpies and "exploded" formulas are to be taken from
#           thermo.lib.  Thus this information is not given.
#      (c)  Relative amounts of reactants are given as moles.
#      (d)  Chamber pressure is 1000 psia (p,psia =1000).
#      (e)  Ionized species are to be included in the products (ions).
#      (f)  Only equilibrium calculations are to be performed (equilibrium).
#      (g)  For exit points, one pressure ratio (pi/p=68.0457), one
#           subsonic area ratio (sub,ae/at=10), and three supersonic area ratios
#           (sup,ae/at=10,20,100) are to be included.

reac   fuel = Li(cr) moles=   1.     t(k)=298.15
       oxid = F2(L)  moles= .5556    t(k)=85.02
prob   case=11 rocket  equilibrium  p,psia=1000 ions
        pi/p=68.0457, sub,ae/at=10,  sup,ae/at=10,20,100
output siunits transport
end

OPTIONS: TP=F  HP=F  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=T  FROZ=F  EQL=T  IONS=T  SIUNIT=T  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=T

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

Pc,BAR =    68.947304

Pc/P =    68.0457

SUBSONIC AREA RATIOS =    10.0000

SUPERSONIC AREA RATIOS =    10.0000    20.0000    100.0000

NFZ=  1  Mdot/Ac= 0.000000E+00  Ac/At= 0.000000E+00

   REACTANT            MOLES     (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
F: Li(cr)            1.000000  -0.298149E-06   298.15  0.0000
       LI 1.00000
O: F2(L)             0.555600  -0.157448E+04    85.02  0.0000
       F  2.00000
```

SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)

l 6/88	*e-	J 6/82	F	J 6/82	F+
J 6/82	F-	tpis89	F2	J12/83	*Li
J12/83	*Li+	J12/68	LiF	J12/68	LiF2-
J12/83	Li2	J12/68	Li2F2	J12/68	Li3F3
tpis82	Li(cr)	tpis82	Li(cr)	tpis82	Li(L)
J12/68	LiF(s)	J12/68	LiF(s)	J12/68	LiF(L)

SPECIES WITH TRANSPORT PROPERTIES

PURE SPECIES

e- F2 Li

BINARY INTERACTIONS

O/F = 3.041496

	EFFECTIVE FUEL	EFFECTIVE OXIDANT	MIXTURE
ENTHALPY	h(2)/R	h(1)/R	h0/R
(KG-MOL)(K)/KG	-0.42954723E-07	-0.41437073E+02	-0.31184169E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*Li	0.14407146E+00	0.00000000E+00	0.35648050E-01
F	0.00000000E+00	0.52636003E-01	0.39612113E-01
*e-	0.00000000E+00	0.00000000E+00	0.00000000E+00

POINT	ITN	T	LI	F	E
1	10	5685.658	-16.270	-19.916	-9.127
Pinf/Pt = 1.760223					
2	4	5334.399	-16.596	-20.296	-9.760
Pinf/Pt = 1.756026					
2	2	5335.817	-16.595	-20.294	-9.757
3	6	3508.754	-19.880	-22.630	-15.648
4	2	5683.383	-16.272	-19.918	-9.131
4	2	5684.563	-16.271	-19.917	-9.129
4	2	5684.330	-16.271	-19.917	-9.129
4	1	5684.303	-16.271	-19.917	-9.129
4	1	5684.303	-16.271	-19.917	-9.129
5	6	3414.068	-20.203	-22.691	-16.205
5	3	3468.547	-20.014	-22.658	-15.879
5	1	3468.466	-20.015	-22.658	-15.880
6	4	2926.255	-22.339	-22.741	-19.920
6	2	2916.483	-22.391	-22.738	-20.011
7	6	1925.971	-30.675	-22.338	-34.299
7	3	1952.523	-30.334	-22.334	-33.731
7	2	1952.608	-30.333	-22.334	-33.729

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM
COMPOSITION DURING EXPANSION FROM INFINITE AREA COMBUSTOR

Pinj = 1000.0 PSIA
CASE = 11

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	Li(cr)	1.0000000	0.000	298.150
OXIDANT	F2(L)	0.5556000	-13091.000	85.020

O/F= 3.04150 %FUEL= 24.743311 R,EQ.RATIO= 0.899928 PHI,EQ.RATIO= 0.899928

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT
Pinf/P	1.0000	1.7560	68.046	1.0021	73.493	188.51	1585.57
P, BAR	68.947	39.263	1.0132	68.804	0.93814	0.36576	0.04348
T, K	5685.66	5335.82	3508.75	5684.30	3468.47	2916.48	1952.61
RHO, KG/CU M	3.1988 0	1.9836 0	8.6962-2	3.1931 0	8.1552-2	3.8114-2	6.9320-3
H, KJ/KG	-259.28	-1422.40	-7051.17	-263.77	-7140.33	-8135.15	-9782.87
U, KJ/KG	-2414.71	-3401.82	-8216.33	-2418.51	-8290.70	-9094.79	-10410.2
G, KJ/KG	-64713.0	-61910.3	-46827.1	-64702.2	-46459.6	-41197.0	-31918.0
S, KJ/(KG)(K)	11.3362	11.3362	11.3362	11.3362	11.3362	11.3362	11.3362
M, (1/n)	21.932	22.413	25.038	21.934	25.069	25.269	25.881
(dLV/dLP)t	-1.08286	-1.07324	-1.00885	-1.08283	-1.00782	-1.00183	-1.02364
(dLV/dLT)p	2.0665	1.9980	1.1726	2.0663	1.1530	1.0248	1.3639
Cp, KJ/(KG)(K)	6.8472	6.6601	2.6365	6.8467	2.5114	1.6054	3.2529
GAMMAs	1.1814	1.1752	1.1967	1.1814	1.2016	1.2714	1.1906
SON VEL,M/SEC	1595.8	1525.2	1180.8	1595.5	1175.7	1104.6	864.2
MACH NUMBER	0.000	1.000	3.121	0.059	3.155	3.593	5.050

TRANSPORT PROPERTIES (GASES ONLY)
CONDUCTIVITY IN UNITS OF MILLIWATTS/(CM)(K)

VISC,MILLIPOISE	1.4392	1.3862	1.0809	1.4390	1.0729	0.95570	0.72997
WITH EQUILIBRIUM REACTIONS							
Cp, KJ/(KG)(K)	6.8472	6.6601	2.6365	6.8467	2.5114	1.6054	3.2529
CONDUCTIVITY	14.6729	13.8861	4.3181	14.6703	4.0680	2.1692	2.7591
PRANDTL NUMBER	0.6716	0.6648	0.6599	0.6716	0.6624	0.7073	0.8606
WITH FROZEN REACTIONS							
Cp, KJ/(KG)(K)	1.5912	1.5704	1.4855	1.5912	1.4844	1.4713	1.4523
CONDUCTIVITY	2.9867	2.8786	2.2503	2.9863	2.2332	1.9786	1.4809
PRANDTL NUMBER	0.7668	0.7562	0.7135	0.7667	0.7132	0.7107	0.7158

PERFORMANCE PARAMETERS

Ae/At	1.0000	9.4392	10.000	10.000	20.000	100.00
CSTAR, M/SEC	2279.0	2279.0	2279.0	2279.0	2279.0	2279.0
CF	0.6692	1.6172	0.0416	1.6278	1.7415	1.9150
Ivac, M/SEC	2823.0	4001.8	22837.2	4019.8	4210.6	4508.0
Isp, M/SEC	1525.2	3685.6	94.7	3709.7	3968.8	4364.3

MOLE FRACTIONS

*e-	0.00292	0.00235	0.00009	0.00292	0.00008	0.00000	0.00000
F	0.21188	0.19608	0.10774	0.21183	0.10670	0.10058	0.10259
F-	0.00465	0.00365	0.00028	0.00465	0.00026	0.00004	0.00000
F2	0.00002	0.00001	0.00000	0.00002	0.00000	0.00000	0.00000
*Li	0.12161	0.10469	0.00840	0.12155	0.00725	0.00041	0.00000
*Li+	0.00758	0.00601	0.00038	0.00757	0.00034	0.00004	0.00000
LiF	0.65001	0.68614	0.88242	0.65015	0.88468	0.89754	0.87248
Li2	0.00022	0.00011	0.00000	0.00022	0.00000	0.00000	0.00000
Li2F2	0.00109	0.00096	0.00068	0.00109	0.00070	0.00140	0.02465
Li3F3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00028

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

F+ LiF2- Li(cr) Li(L) LiF(s)
LiF(L)

```
#  EXAMPLE 12:
#      (a)  Infinite-area rocket problem (rocket).
#      (b)  The fuel is monomethyl hydrazine (CH6N2(L)) and the oxidant is
#           nitrogen tetroxide (N2O4(L)) at 298.15 K.  Enthalpies and
#           "exploded" formulas are to be taken from thermo.lib.
#      (c)  The density of the reactant mixture is desired.  This requires
#           the individual densities be given with the reactant data
#           (rho,g/cc = .874 and rho,g/cc == 1.431).
#      (d)  The oxidant-to-fuel weight ratio is 2.5 (o/f=2.5).
#      (e)  Chamber pressure is 1000 psia (p,psia=1000).
#      (f)  Equilibrium and frozen calculations are to be performed with
#           freezing at the throat (nfz=2).
#      (g)  For exit points one pressure ratio (pi/p=68.0457) and four
#           supersonic area ratios (supersonic=10,50,100,200) are given.

reac fuel = CH6N2(L)      rho,g/cc = .874
     oxid = N2O4(L)       rho,g/cc = 1.431
prob  rocket  case=12  p,psia =1000, pi/p=68.0457,  eql frozen nfz=2
       supersonic=5,10,25,50,75,100,150,200, o/f= 2.5,
only  CO    CO2   H   HNO  HNO2  HO2   H2    H2O   H2O2  N     NO    NO2
     N2    N2O   O  OH  O2    HCO   NH    CH4  NH2  NH3  H2O(L)  C(gr)
output  siunits  massf  plot aeat t p ivac isp mach cf
end

OPTIONS: TP=F  HP=F  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=T  FROZ=T  EQL=T  IONS=F  SIUNIT=T  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

Pc,BAR =     68.947304

Pc/P =     68.0457

SUBSONIC AREA RATIOS =

SUPERSONIC AREA RATIOS =      5.0000     10.0000     25.0000     50.0000     75.0000
  100.0000    150.0000    200.0000

NFZ=  2  Mdot/Ac= 0.000000E+00  Ac/At= 0.000000E+00

WARNING!!  AMOUNT MISSING FOR REACTANT  1.
PROGRAM SETS WEIGHT PERCENT = 100. (REACT)

WARNING!!  AMOUNT MISSING FOR REACTANT  2.
PROGRAM SETS WEIGHT PERCENT = 100. (REACT)

   REACTANT              WT.FRAC    (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
F: CH6N2(L)           1.000000    0.651872E+04    298.15  0.8740
         C  1.00000  H  6.00000  N  2.00000
O: N2O4(L)            1.000000   -0.211065E+04    298.15  1.4310
         N  2.00000  O  4.00000
```

SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)

l 8/88	CH4	tpis79	*CO	l 7/88	*CO2
l 6/94	*H	l12/89	HCO	l12/89	HNO
tpis89	HNO2	l 5/89	HO2	tpis78	*H2
l 8/89	H2O	l 2/93	H2O2	l 6/88	*N
l11/89	*NH	l12/89	NH2	tpis89	NH3
tpis89	*NO	l 7/88	NO2	tpis78	*N2
l 7/88	N2O	l 1/90	*O	tpis78	*OH
tpis89	*O2	x 4/83	C(gr)	x 4/83	C(gr)
x 4/83	C(gr)	l 8/89	H2O(L)		

O/F = 2.500000

	EFFECTIVE FUEL	EFFECTIVE OXIDANT	MIXTURE
ENTHALPY	h(2)/R	h(1)/R	h0/R
(KG-MOL)(K)/KG	0.14148957E+03	-0.22939058E+02	0.24040550E+02
KG-FORM.WT./KG	bi(2)	bi(1)	b0i
C	0.21705101E-01	0.00000000E+00	0.62014573E-02
*H	0.13023060E+00	0.00000000E+00	0.37208744E-01
*N	0.43410201E-01	0.21736513E-01	0.27928995E-01
*O	0.00000000E+00	0.43473025E-01	0.31052161E-01

POINT	ITN	T	C	H	N	O
1	10	3386.569	-17.018	-10.171	-12.866	-15.018
Pinf/Pt = 1.733517						
2	3	3207.237	-17.495	-10.420	-13.029	-15.222
Pinf/Pt = 1.731796						
2	2	3207.551	-17.494	-10.420	-13.029	-15.222
3	5	2173.122	-21.717	-12.457	-14.122	-17.057
4	4	2400.051	-20.495	-11.908	-13.886	-16.543
4	3	2422.435	-20.386	-11.858	-13.861	-16.496
4	1	2422.478	-20.386	-11.858	-13.861	-16.496
5	4	2171.383	-21.727	-12.462	-14.124	-17.061
5	2	2175.478	-21.703	-12.451	-14.120	-17.051
6	4	1843.631	-24.075	-13.429	-14.421	-17.925
6	2	1840.505	-24.102	-13.439	-14.424	-17.934
7	4	1580.708	-27.097	-14.543	-14.630	-18.600
7	2	1583.036	-27.061	-14.530	-14.628	-18.595
8	3	1440.447	-29.620	-15.403	-14.741	-18.819
8	2	1438.100	-29.669	-15.419	-14.743	-18.822

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM

COMPOSITION DURING EXPANSION FROM INFINITE AREA COMBUSTOR

Pinj = 1000.0 PSIA
CASE = 12

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH6N2(L)	1.0000000	54200.000	298.150
OXIDANT	N2O4(L)	1.0000000	-17549.000	298.150

REACTANT DENSITY= 1210.57 KG/CU M

O/F= 2.50000 %FUEL= 28.571429 R,EQ.RATIO= 0.998555 PHI,EQ.RATIO= 0.998555

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
Pinf/P	1.0000	1.7318	68.046	27.260	67.469	219.62	537.92	910.15
P, BAR	68.947	39.813	1.0132	2.5292	1.0219	0.31394	0.12817	0.07575
T, K	3386.57	3207.55	2173.12	2422.48	2175.48	1840.51	1583.04	1438.10
RHO, KG/CU M	5.8414 0	3.6029 0	1.4329-1	3.1771-1	1.4434-1	5.2779-2	2.5095-2	1.6331-2
H, KJ/KG	199.89	-427.33	-3713.93	-3026.58	-3707.90	-4476.65	-4971.56	-5227.72
U, KJ/KG	-980.43	-1532.34	-4421.09	-3822.66	-4415.88	-5071.46	-5482.31	-5691.60
G, KJ/KG	-36876.0	-35543.4	-27505.1	-29547.7	-27524.9	-24626.4	-22302.5	-20971.9
S, KJ/(KG)(K)	10.9479	10.9479	10.9479	10.9479	10.9479	10.9479	10.9479	10.9479
M, (1/n)	23.856	24.135	25.551	25.301	25.549	25.727	25.770	25.776
(dLV/dLP)t	-1.02415	-1.02080	-1.00301	-1.00625	-1.00304	-1.00071	-1.00012	-1.00003
(dLV/dLT)p	1.4608	1.4206	1.0916	1.1700	1.0922	1.0253	1.0051	1.0012
Cp, KJ/(KG)(K)	5.1203	4.9690	2.7893	3.4486	2.7952	2.1078	1.8208	1.7311
GAMMAs	1.1378	1.1352	1.1574	1.1418	1.1572	1.1912	1.2179	1.2297
SON VEL,M/SEC	1158.9	1120.0	904.7	953.4	905.1	841.7	788.7	755.3
MACH NUMBER	0.000	1.000	3.093	2.664	3.089	3.633	4.078	4.362

PERFORMANCE PARAMETERS

Ae/At	1.0000	10.066	5.0000	10.000	25.000	50.000	75.000
CSTAR, M/SEC	1708.6	1708.6	1708.6	1708.6	1708.6	1708.6	1708.6
CF	0.6555	1.6375	1.4868	1.6362	1.7899	1.8823	1.9283
Ivac, M/SEC	2106.6	3050.5	2853.6	3048.9	3252.8	3374.8	3435.5
Isp, M/SEC	1120.0	2797.8	2540.3	2795.6	3058.3	3216.0	3294.7

MASS FRACTIONS

*CO	0.07696	0.06751	0.01018	0.02136	0.01026	0.00214	0.00028	0.00005
*CO2	0.15200	0.16686	0.25693	0.23936	0.25680	0.26956	0.27249	0.27285
*H	0.00044	0.00034	0.00001	0.00005	0.00001	0.00000	0.00000	0.00000
HNO	0.00002	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
HNO2	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
HO2	0.00014	0.00009	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
*H2	0.00314	0.00268	0.00044	0.00085	0.00045	0.00012	0.00002	0.00000
H2O	0.28566	0.29378	0.32967	0.32385	0.32962	0.33382	0.33493	0.33511
H2O2	0.00002	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
*N	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
*NO	0.02214	0.01774	0.00163	0.00373	0.00164	0.00036	0.00009	0.00004
NO2	0.00005	0.00003	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
*N2	0.38082	0.38289	0.39043	0.38945	0.39043	0.39103	0.39115	0.39118
N2O	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
*O	0.00515	0.00387	0.00011	0.00042	0.00011	0.00001	0.00000	0.00000
*OH	0.03288	0.02709	0.00267	0.00621	0.00269	0.00052	0.00009	0.00003
*O2	0.04055	0.03708	0.00792	0.01471	0.00798	0.00243	0.00095	0.00075

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MASS FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

CH4	HCO	*NH	NH2	NH3
C(gr)	H2O(L)			

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

3	3	1337.947	-31.974	-16.184	-14.826	-18.919
3	2	1340.166	-31.918	-16.166	-14.824	-18.918
4	3	1212.262	-35.486	-17.337	-14.938	-19.025
4	2	1210.175	-35.551	-17.358	-14.940	-19.027
5	3	1121.722	-38.528	-18.328	-15.025	-19.105
5	2	1123.659	-38.458	-18.305	-15.023	-19.103

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM
COMPOSITION DURING EXPANSION FROM INFINITE AREA COMBUSTOR

Pinj = 1000.0 PSIA
CASE = 12

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH6N2(L)	1.0000000	54200.000	298.150
OXIDANT	N2O4(L)	1.0000000	-17549.000	298.150

REACTANT DENSITY= 1210.57 KG/CU M
O/F= 2.50000 %FUEL= 28.571429 R,EQ.RATIO= 0.998555 PHI,EQ.RATIO= 0.998555

	CHAMBER	THROAT	EXIT	EXIT	EXIT
Pinf/P	1.0000	1.7318	1322.19	2238.43	3253.04
P, BAR	68.947	39.813	0.05215	0.03080	0.02119
T, K	3386.57	3207.55	1340.17	1210.17	1123.66
RHO, KG/CU M	5.8414 0	3.6029 0	1.2063-2	7.8911-3	5.8480-3
H, KJ/KG	199.89	-427.33	-5395.00	-5611.41	-5752.06
U, KJ/KG	-980.43	-1532.34	-5827.27	-6001.74	-6114.49
G, KJ/KG	-36876.0	-35543.4	-20067.0	-18860.3	-18053.8
S, KJ/(KG)(K)	10.9479	10.9479	10.9479	10.9479	10.9479
M, (1/n)	23.856	24.135	25.778	25.778	25.778
(dLV/dLP)t	-1.02415	-1.02080	-1.00001	-1.00000	-1.00000
(dLV/dLT)p	1.4608	1.4206	1.0004	1.0001	1.0000
Cp, KJ/(KG)(K)	5.1203	4.9690	1.6891	1.6415	1.6099
GAMMAs	1.1378	1.1352	1.2362	1.2446	1.2506
SON VEL,M/SEC	1158.9	1120.0	731.0	697.0	673.2
MACH NUMBER	0.000	1.000	4.576	4.891	5.125

PERFORMANCE PARAMETERS					
Ae/At		1.0000	100.00	150.00	200.00
CSTAR, M/SEC		1708.6	1708.6	1708.6	1708.6
CF		0.6555	1.9578	1.9953	2.0193
Ivac, M/SEC		2106.6	3474.3	3523.7	3555.2
Isp, M/SEC		1120.0	3345.1	3409.2	3450.2
MASS FRACTIONS					
*CO	0.07696	0.06751	0.00001	0.00000	0.00000
*CO2	0.15200	0.16686	0.27291	0.27292	0.27292
*H	0.00044	0.00034	0.00000	0.00000	0.00000
HNO	0.00002	0.00001	0.00000	0.00000	0.00000
HNO2	0.00001	0.00000	0.00000	0.00000	0.00000
HO2	0.00014	0.00009	0.00000	0.00000	0.00000
*H2	0.00314	0.00268	0.00000	0.00000	0.00000
H2O	0.28566	0.29378	0.33515	0.33516	0.33516
H2O2	0.00002	0.00001	0.00000	0.00000	0.00000
*N	0.00001	0.00000	0.00000	0.00000	0.00000
*NO	0.02214	0.01774	0.00002	0.00001	0.00000
NO2	0.00005	0.00003	0.00000	0.00000	0.00000
*N2	0.38082	0.38289	0.39118	0.39119	0.39119
N2O	0.00001	0.00001	0.00000	0.00000	0.00000
*O	0.00515	0.00387	0.00000	0.00000	0.00000
*OH	0.03288	0.02709	0.00001	0.00000	0.00000
*O2	0.04055	0.03708	0.00072	0.00071	0.00072

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MASS FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

CH4	HCO	*NH	NH2	NH3
C(gr)	H2O(L)			

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

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION
AFTER POINT 2

Pinj = 1000.0 PSIA
CASE = 12

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH6N2(L)	1.0000000	54200.000	298.150
OXIDANT	N2O4(L)	1.0000000	-17549.000	298.150

REACTANT DENSITY= 1210.57 KG/CU M

O/F= 2.50000 %FUEL= 28.571429 R,EQ.RATIO= 0.998555 PHI,EQ.RATIO= 0.998555

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
Pinf/P	1.0000	1.7318	68.046	33.323	87.244	302.39	768.78	1327.00
P, BAR	68.947	39.813	1.0132	2.0691	0.79028	0.22801	0.08968	0.05196
T, K	3386.57	3207.55	1630.44	1871.65	1552.50	1204.85	985.62	872.37
RHO, KG/CU M	5.8414 0	3.6029 0	1.8039-1	3.2089-1	1.4776-1	5.4932-2	2.6413-2	1.7288-2
H, KJ/KG	199.89	-427.33	-3393.03	-2962.89	-3529.26	-4117.22	-4468.39	-4642.93
U, KJ/KG	-980.43	-1532.34	-3954.71	-3607.68	-4064.10	-4532.30	-4807.94	-4943.46
G, KJ/KG	-36876.0	-35543.4	-21243.0	-23453.6	-20525.9	-17307.9	-15258.9	-14193.6
S, KJ/(KG)(K)	10.9479	10.9479	10.9479	10.9479	10.9479	10.9479	10.9479	10.9479
M, (1/n)	23.856	24.135	24.135	24.135	24.135	24.135	24.135	24.135
Cp, KJ/(KG)(K)	5.1203	4.9690	1.7572	1.8076	1.7386	1.6393	1.5626	1.5194
GAMMAs	1.1378	1.1352	1.2439	1.2355	1.2471	1.2661	1.2828	1.2932
SON VEL,M/SEC	1158.9	1120.0	835.9	892.5	816.7	724.9	660.0	623.4
MACH NUMBER	0.000	1.000	3.207	2.818	3.344	4.053	4.630	4.992

PERFORMANCE PARAMETERS

Ae/At	1.0000	8.3449	5.0000	10.000	25.000	50.000	75.000
CSTAR, M/SEC	1708.6	1708.6	1708.6	1708.6	1708.6	1708.6	1708.6
CF	0.6555	1.5689	1.4720	1.5984	1.7198	1.7884	1.8215
Ivac, M/SEC	2106.6	2890.2	2771.4	2926.8	3079.7	3166.7	3208.7
Isp, M/SEC	1120.0	2680.6	2515.1	2731.0	2938.4	3055.6	3112.2

MASS FRACTIONS

*CO	0.06751	*CO2	0.16686	*H	0.00034
HNO	0.00001	HO2	0.00009	*H2	0.00268
H2O	0.29378	H2O2	0.00001	*NO	0.01774
NO2	0.00003	*N2	0.38289	N2O	0.00001
*O	0.00387	*OH	0.02709	*O2	0.03708

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MASS FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

CH4	HCO	*NH	NH2	NH3
C(gr)	H2O(L)			

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

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION
AFTER POINT 2

Pinj = 1000.0 PSIA
CASE = 12

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH6N2(L)	1.0000000	54200.000	298.150
OXIDANT	N2O4(L)	1.0000000	-17549.000	298.150

REACTANT DENSITY= 1210.57 KG/CU M

O/F= 2.50000 %FUEL= 28.571429 R,EQ.RATIO= 0.998555 PHI,EQ.RATIO= 0.998555

	CHAMBER	THROAT	EXIT	EXIT	EXIT
Pinf/P	1.0000	1.7318	1955.79	3382.76	4995.07
P, BAR	68.947	39.813	0.03525	0.02038	0.01380
T, K	3386.57	3207.55	798.24	702.08	639.53
RHO, KG/CU M	5.8414 0	3.6029 0	1.2819-2	8.4269-3	6.2651-3
H, KJ/KG	199.89	-427.33	-4754.49	-4895.92	-4985.94
U, KJ/KG	-980.43	-1532.34	-5029.48	-5137.79	-5206.26
G, KJ/KG	-36876.0	-35543.4	-13493.5	-12582.3	-11987.4
S, KJ/(KG)(K)	10.9479	10.9479	10.9479	10.9479	10.9479
M, (1/n)	23.856	24.135	24.135	24.135	24.135
Cp, KJ/(KG)(K)	5.1203	4.9690	1.4902	1.4516	1.4264
GAMMAs	1.1378	1.1352	1.3007	1.3112	1.3184
SON VEL,M/SEC	1158.9	1120.0	598.1	563.1	539.0
MACH NUMBER	0.000	1.000	5.263	5.669	5.975

PERFORMANCE PARAMETERS

Ae/At	1.0000	100.00	150.00	200.00
CSTAR, M/SEC	1708.6	1708.6	1708.6	1708.6
CF	0.6555	1.8423	1.8685	1.8849
Ivac, M/SEC	2106.6	3235.2	3268.2	3288.9
Isp, M/SEC	1120.0	3147.8	3192.4	3220.5

MASS FRACTIONS

*CO	0.06751	*CO2	0.16686	*H	0.00034
HNO	0.00001	HO2	0.00009	*H2	0.00268
H2O	0.29378	H2O2	0.00001	*NO	0.01774
NO2	0.00003	*N2	0.38289	N2O	0.00001
*O	0.00387	*OH	0.02709	*O2	0.03708

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MASS FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

CH4	HCO	*NH	NH2	NH3
C(gr)	H2O(L)			

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

```
!EXAMPLE 13:
!    (a)  Rocket problem with an infinite-area combustor (rocket). This
!         problem was selected to show some unusual derivatives.
!    (b)  Tripropellant.  Fuels are N2H4(L) and Be(L) and oxidant is H2O2(L),
!         all at 298.15 K.
!    (c)  Reactant mixture is given as 67% fuel by weight (%fuel=67.).
!    (d)  Chamber pressure is 3000 psia (p,psia=3000).
!    (e)  Calculations are to be for equilibrium conditions only (equilibrium).
!    (f)  Four exit pressure ratios are assigned (pi/p=3,10,30,300).
!    (g)  BeO(L) is included as possible combustion product for the first
!         point (insert).
!    (h)  Mole fractions > 1.e-10 are to be in e-format (trace=1.e-10).
!    (i)  Units in final tables to be non-SI (calories).


reac fuel = N2H4(L)     wt%= 80   t=298.15
     fuel = Be(a)       wt%= 20   t=298.15
     oxid = H2O2(L)     wt%=100   t=298.15
prob  rocket  case=13  p,psia=3000, pi/p=3,10,30,300,equilibrium   %fuel = 67.

outp  trace= 1.e-10 calories
insert  BeO(L)
end

OPTIONS: TP=F  HP=F  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=T  FROZ=F  EQL=T  IONS=F  SIUNIT=F  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

TRACE= 1.00E-10  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

Pc,BAR =   206.841913

Pc/P =     3.0000    10.0000    30.0000   300.0000

SUBSONIC AREA RATIOS =

SUPERSONIC AREA RATIOS =

NFZ=  1  Mdot/Ac= 0.000000E+00  Ac/At= 0.000000E+00

   REACTANT           WT.FRAC    (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
F: N2H4(L)           0.800000   0.605929E+04   298.15  0.8740
         N  2.00000  H  4.00000
F: Be(a)             0.200000  -0.130953E-05   298.15  1.4310
         BE 1.00000
O: H2O2(L)           1.000000  -0.225846E+05   298.15  0.0000
         H  2.00000  O  2.00000
```

SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)

l 6/94	*Be	tpis81	BeH	j12/60	BeH2
j 6/63	BeN	j12/74	*BEO	j12/75	BeOH
j12/75	BeO2H2	j 9/63	Be2O	j 9/63	Be2O2
j 9/63	Be3O3	j 9/63	Be4O4	j 9/63	Be5O5
j 9/63	Be6O6	l 6/94	*H	l12/89	HNO
tpis89	HNO2	l 4/90	HNO3	l 5/89	HO2
tpis78	*H2	l 8/89	H2O	l 2/93	H2O2
l 6/88	*N	l11/89	*NH	l12/89	NH2
tpis89	NH3	tpis89	NH2OH	tpis89	*NO
l 7/88	NO2	j12/64	NO3	tpis78	*N2
l 5/90	N2H2	tpis89	NH2NO2	l 5/90	N2H4
l 7/88	N2O	l 4/90	N2O3	tpis89	N2O4
l 4/90	N2O5	tpis89	N3	l 7/88	N3H
l 1/90	*O	tpis78	*OH	tpis89	*O2
l 5/90	O3	srd 93	Be(a)	srd 93	Be(a)
srd 93	Be(b)	srd 93	Be(L)	coda89	BeO(a)
coda89	BeO(a)	coda89	BeO(b)	coda89	BeO(L)
J12/75	BeO2H2(b)	l 8/89	H2O(s)	l 8/89	H2O(L)
BeO(L)	INSERTED				

O/F = 0.492537

ENTHALPY	EFFECTIVE FUEL	EFFECTIVE OXIDANT	MIXTURE
	h(2)/R	h(1)/R	h0/R
(KG-MOL)(K)/KG	0.15126831E+03	-0.66396668E+03	-0.11775924E+03
KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*N	0.49929412E-01	0.00000000E+00	0.33452706E-01
*H	0.99858825E-01	0.58798142E-01	0.86308799E-01
*Be	0.22192184E-01	0.00000000E+00	0.14868763E-01
*O	0.00000000E+00	0.58798142E-01	0.19403387E-01

POINT	ITN	T	N	H	BE	O
1	13	3015.477	-12.175	-7.991	-13.104	-20.398
Pinf/Pt = 1.743807						
2	4	2802.203	-12.317	-8.137	-13.670	-21.009
ADD BeO(b)						
2	4	2851.000	-12.349	-8.168	-13.530	-20.860
Pinf/Pt = 1.630416						
2	4	2851.000	-12.315	-8.135	-13.530	-20.860
Pinf/Pt = 1.626685						
2	2	2851.000	-12.314	-8.133	-13.530	-20.860
3	5	2604.969	-12.455	-8.281	-14.318	-21.678
PHASE CHANGE, REPLACE		BeO(L)		WITH BeO(b)		
3	4	2922.003	-12.667	-8.486	-13.245	-20.656
ADD BeO(L)						
3	4	2851.000	-12.621	-8.441	-13.530	-20.859
4	5	2204.200	-12.760	-8.601	-16.149	-23.464
PHASE CHANGE, REPLACE		BeO(L)		WITH BeO(a)		
4	4	2451.195	-12.948	-8.779	-15.487	-22.276
PHASE CHANGE, REPLACE		BeO(a)		WITH BeO(b)		
4	2	2451.586	-12.948	-8.779	-15.484	-22.274
5	5	2061.574	-13.195	-9.042	-18.232	-24.282
PHASE CHANGE, REPLACE		BeO(b)		WITH BeO(a)		
5	2	2067.118	-13.199	-9.046	-18.191	-24.247
6	5	1396.587	-13.721	-9.603	-27.072	-30.583

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM

COMPOSITION DURING EXPANSION FROM INFINITE AREA COMBUSTOR

Pinj = 3000.0 PSIA
CASE = 13

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	TEMP K
FUEL	N2H4(L)	0.8000000	12041.109	298.150
FUEL	Be(a)	0.2000000	0.000	298.150
OXIDANT	H2O2(L)	1.0000000	-44880.497	298.150

O/F= 0.49254 %FUEL= 67.000000 R,EQ.RATIO= 2.990363 PHI,EQ.RATIO= 4.980725

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT
Pinf/P	1.0000	1.6267	3.0000	10.000	30.000	300.00
P, ATM	204.14	125.49	68.046	20.414	6.8046	0.68046
T, K	3015.48	2851.00	2851.00	2451.59	2067.12	1396.59
RHO, G/CC	1.3715-2	8.9279-3	4.8341-3	1.6916-3	6.6969-4	9.9159-5
H, CAL/G	-234.01	-403.86	-612.35	-997.47	-1292.67	-1762.88
U, CAL/G	-594.46	-744.26	-953.24	-1289.71	-1538.74	-1929.07
G, CAL/G	-10112.8	-9743.85	-9952.34	-9028.96	-8064.63	-6338.16
S, CAL/(G)(K)	3.2760	3.2760	3.2760	3.2760	3.2760	3.2760
M, (1/n)	16.625	16.644	16.620	16.670	16.694	16.700
MW, MOL WT	13.372	13.376	13.361	13.370	13.376	13.378
(dLV/dLP)t	-1.00283	-1.00209	-1.00262	-1.00098	-1.00023	-1.00002
(dLV/dLT)p	1.0465	0.0000	0.0000	1.0209	1.0053	1.0001
Cp, CAL/(G)(K)	0.9575	0.0000	0.0000	0.7984	0.7448	0.6649
GAMMAs	1.1546	0.9979	0.9974	1.1829	1.1923	1.2180
SON VEL,M/SEC	1319.6	1192.2	1192.7	1202.7	1108.0	920.3
MACH NUMBER	0.000	1.000	1.492	2.102	2.686	3.887

PERFORMANCE PARAMETERS

Ae/At	1.0000	1.2374	2.4894	5.3398	30.010
CSTAR, FT/SEC	6375.8	6375.8	6375.8	6375.8	6375.8
CF	0.6135	0.9156	1.3006	1.5316	1.8405
Ivac,LB-SEC/LB	243.4	263.2	307.1	338.8	384.6
Isp, LB-SEC/LB	121.6	181.4	257.7	303.5	364.7

MOLE FRACTIONS

*Be	8.681 -6	3.857 -6	7.111 -6	2.586 -7	1.859 -9	1.351-16
BeH	1.104 -6	3.684 -7	4.994 -7	8.737 -9	3.040-11	4.032-19
BeH2	1.171 -5	5.070 -6	5.054 -6	2.194 -7	3.305 -9	7.002-15
BeN	4.457 -8	1.236 -8	1.677 -8	1.685-10	2.807-13	3.873-22
*BEO	3.551 -7	1.342 -7	2.476 -7	5.763 -9	2.341-11	3.240-19
BeOH	1.240 -4	6.727 -5	9.125 -5	6.858 -6	1.620 -7	7.729-13
BeO2H2	2.9966-3	2.5056-3	2.5000-3	7.9244-4	1.6333-4	1.1620-6
Be2O	7.060 -7	2.511 -7	4.630 -7	4.580 -9	5.497-12	1.278-21
Be2O2	3.894 -7	1.728 -7	3.188 -7	6.143 -9	1.750-11	5.868-20
Be3O3	7.665 -7	4.787 -7	8.831 -7	2.536 -8	1.184-10	1.538-18
Be4O4	2.173 -7	1.434 -7	2.646 -7	4.831 -9	1.201-11	2.030-20
Be5O5	6.079 -9	4.184 -9	7.718 -9	8.580-11	1.070-13	1.914-23
Be6O6	3.717-10	2.827-10	5.216-10	4.205-12	3.317-15	1.280-25
*H	7.4008-3	5.5693-3	7.5542-3	2.8642-3	6.2153-4	3.5990-6
HNO	9.938 -8	4.355 -8	4.349 -8	3.791 -9	1.498-10	8.418-15
HNO2	2.406-10	9.046-11	9.038-11	4.939-12	1.004-13	7.126-19
HO2	2.553 -9	1.015 -9	1.379 -9	7.839-11	1.296-12	2.695-18
*H2	5.1230-1	5.1354-1	5.1214-1	5.1486-1	5.1624-1	5.1664-1
H2O	5.7363-2	5.7964-2	5.7835-2	5.9767-2	6.0485-2	6.0664-2
H2O2	5.504 -9	2.426 -9	2.422 -9	2.117-10	7.944-12	3.489-16
*N	4.529 -7	1.904 -7	2.585 -7	1.721 -8	3.711-10	1.810-15
*NH	2.470 -6	1.086 -6	1.084 -6	9.309 -8	3.580 -9	1.671-13
NH2	1.921 -5	9.841 -6	7.222 -6	1.113 -6	1.197 -7	2.226-10
NH3	3.0252-4	2.1058-4	1.1363-4	4.9681-5	2.7432-5	1.3148-5
NH2OH	2.905 -9	1.107 -9	5.975-10	4.397-11	2.287-12	9.065-16
*NO	1.860 -5	1.087 -5	1.476 -5	2.620 -6	2.002 -7	4.479-11
NO2	1.236-10	4.605-11	6.258-11	2.930-12	3.760-14	3.713-20
*N2	2.2349-1	2.2362-1	2.2342-1	2.2360-1	2.2372-1	2.2376-1
N2H2	7.477 -9	2.733 -9	1.476 -9	9.647-11	4.461-12	1.288-15
N2O	9.032 -9	4.103 -9	4.101 -9	3.946-10	1.757-11	1.410-15
N3H	1.480-10	4.527-11	2.447-11	9.231-13	2.001-14	5.124-19
*O	2.448 -6	1.245 -6	2.297 -6	2.389 -7	7.057 -9	5.241-14
*OH	2.7768-4	1.8428-4	2.5007-4	6.4898-5	8.1758-6	8.2744-9
*O2	1.083 -7	5.610 -8	1.036 -7	1.142 -8	3.535-10	2.936-15
BeO(a)	0.0000 0	0.0000 0	0.0000 0	0.0000 0	1.9873-1	1.9892-1
BeO(b)	0.0000 0	1.3853-2	1.5511-1	1.9799-1	0.0000 0	0.0000 0
BeO(L)	1.9567-1	1.8245-1	4.0950-2	0.0000 0	0.0000 0	0.0000 0

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 1.000000E-10 FOR ALL ASSIGNED CONDITIONS

HNO3	NO3	NH2NO2	N2H4	N2O3
N2O4	N2O5	N3	O3	Be(a)
Be(b)	Be(L)	BeO2H2(b)	H2O(s)	H2O(L)

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

```
!  EXAMPLE 14:
!     (a)  Output from this case is used 1) to illustrate the effect of
!          condensed species on volume and molecular weight (see sec.2.2,part I)
!     (b)  Assigned-temperature-and-pressure problem (tp).
!     (c)  Reactants are H2(L) and O2(L) and amounts are specified in moles.
!     (d)  The "exploded" formulas are given to save the program looking them
!          up.  Reactant enthalpies are not needed for assigned temperature
!          problems.
!     (e)  Assigned pressure in atmospheres is p,atm =.05.
!     (f)  Assigned temperatures in kelvin are t,k =1000,500,351,305,304.3,
!          304, 300.
!     (g)  Print intermediate output for the fifth point with debug = 5.

       reac     name H2(L) moles=100   H 2
                name O2(L) moles=60    O 2

       prob     tp  p,atm=.05  case=14
                t,k = 1000,500,350,305,304.3,304.2,304,300,

       output   siunits  debug = 5

       end

OPTIONS: TP=T  HP=F  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=F  FROZ=F  EQL=F  IONS=F  SIUNIT=T  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

T,K =  1000.0000   500.0000   350.0000   305.0000   304.3000   304.2000   304.0000   30

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

P,BAR =      0.050663

   REACTANT            MOLES     (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
N: H2(L)           100.000000   0.000000E+00     0.00  0.8740
         H  2.00000
N: O2(L)            60.000000  -0.156101E+04    90.17  1.4310
         O  2.00000

      SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)

 l 6/94  *H              l 5/89  HO2             tpis78  *H2
 l 8/89  H2O             l 2/93  H2O2            l 1/90  *O
 tpis78  *OH             tpis89  *O2            l 5/90  O3
 l 8/89  H2O(s)          l 8/89  H2O(L)
```

O/F = 0.000000

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.44147845E+02	0.00000000E+00	-0.44147845E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*H	0.94272209E-01	0.00000000E+00	0.94272209E-01
*O	0.56563325E-01	0.00000000E+00	0.56563325E-01

POINT	ITN	T	H	O
1	10	1000.000	-20.527	-15.973
2	3	500.000	-34.596	-15.230
3	1	350.000	-46.944	-15.049
4	1	305.000	-53.061	-15.028

ITERATION 1 MATRIX

0.188544E+00	0.942722E-01	0.942722E-01	-0.114417E+02
0.942722E-01	0.659905E-01	0.565633E-01	-0.600419E+01
0.942722E-01	0.565633E-01	0.000000E+00	-0.586253E+01

SOLUTION VECTOR

H	O	
-0.531707E+02	-0.150274E+02	0.000000E+00

T= 0.30430000E+03 ENN= 0.51849715E-01 ENNL=-0.29594058E+01 PP= 0.50662500E-01
LN P/N=-0.23163446E-01 AMBDA= 0.10000000E+01

	Nj	LN Nj	DEL LN Nj	H0j/RT
		S0j/R	G0j/RT	Gj/RT
*H	0.000000E+00	-0.125204E+03	-0.307497E+00	0.862123E+02
		0.138484E+02	0.723640E+02	-0.528633E+02
HO2	0.000000E+00	-0.604867E+02	-0.121044E+00	0.504603E+01
		0.276408E+02	-0.225947E+02	-0.831046E+02
*H2	0.000000E+00	-0.903810E+02	-0.219421E+00	0.701441E-01
		0.157881E+02	-0.157179E+02	-0.106122E+03
H2O	0.471361E-01	-0.305472E+01	0.177636E-14	-0.954977E+02
		0.227933E+02	-0.118291E+03	-0.121369E+03
H2O2	0.000000E+00	-0.541943E+02	-0.956804E-01	-0.537719E+02
		0.283113E+02	-0.820832E+02	-0.136301E+03
*O	0.000000E+00	-0.938907E+02	-0.226071E+00	0.985373E+02
		0.194248E+02	0.791125E+02	-0.148014E+02
*OH	0.000000E+00	-0.614818E+02	-0.145407E+00	0.156242E+02
		0.221720E+02	-0.654785E+01	-0.680528E+02
*O2	0.471361E-02	-0.535730E+01	-0.639488E-13	0.714483E-01
		0.247458E+02	-0.246744E+02	-0.300549E+02
O3	0.000000E+00	-0.722284E+02	-0.128601E+00	0.561412E+02
		0.288433E+02	0.272979E+02	-0.449537E+02
H2O(s)	0.000000E+00	0.000000E+00	0.000000E+00	-0.115317E+03
		0.550772E+01	-0.120825E+03	-0.172966E+03
H2O(L)	0.000000E+00	0.000000E+00	0.000000E+00	-0.112509E+03
		0.861762E+01	-0.121126E+03	-0.230622E+03

5	1	304.300	-53.171	-15.027

```
H2O(s)              200.000    273.150      0.0000000E+00

H2O(L)              273.150    600.000      0.0000000E+00
[G0j-SUM(Aij*PIi)]/Mj = -0.9021700E-03          MAX NEG DELTA G = -0.9021700E-03
ADD  H2O(L)

ITERATION  0       MATRIX
     0.188544E+00    0.942722E-01    0.200000E+01    0.942722E-01   -0.114417E+02
     0.942722E-01    0.659905E-01    0.100000E+01    0.565633E-01   -0.600419E+01
     0.200000E+01    0.100000E+01    0.000000E+00    0.000000E+00   -0.121385E+03
     0.942722E-01    0.565633E-01    0.000000E+00    0.770217E-15   -0.586253E+01

SOLUTION VECTOR
        H               O
    -0.532195E+02   -0.149462E+02    0.842705E-02   -0.162528E+00

T= 0.30430000E+03 ENN= 0.51849715E-01 ENNL=-0.29594058E+01 PP= 0.50662500E-01
LN P/N=-0.23163446E-01 AMBDA= 0.10000000E+01

                        Nj             LN Nj         DEL LN Nj       H0j/RT
                                          S0j/R            G0j/RT          Gj/RT
 *H                  0.000000E+00   -0.125512E+03   -0.211287E+00    0.862123E+02
                                       0.138484E+02    0.723640E+02   -0.531707E+02
 HO2                 0.000000E+00   -0.606077E+02   -0.487585E-01    0.504603E+01
                                       0.276408E+02   -0.225947E+02   -0.832256E+02
 *H2                 0.000000E+00   -0.906004E+02   -0.260046E+00    0.701441E-01
                                       0.157881E+02   -0.157179E+02   -0.106341E+03
 H2O                 0.471361E-01   -0.305472E+01   -0.178781E+00   -0.954977E+02
                                       0.227933E+02   -0.118291E+03   -0.121369E+03
 H2O2                0.000000E+00   -0.542900E+02   -0.975171E-01   -0.537719E+02
                                       0.283113E+02   -0.820832E+02   -0.136396E+03
 *O                  0.000000E+00   -0.941168E+02   -0.812642E-01    0.985373E+02
                                       0.194248E+02    0.791125E+02   -0.150274E+02
 *OH                 0.000000E+00   -0.616272E+02   -0.130023E+00    0.156242E+02
                                       0.221720E+02   -0.654785E+01   -0.681982E+02
 *O2                 0.471361E-02   -0.535730E+01    0.124345E-12    0.714483E-01
                                       0.247458E+02   -0.246744E+02   -0.300549E+02
 O3                  0.000000E+00   -0.723570E+02    0.812642E-01    0.561412E+02
                                       0.288433E+02    0.272979E+02   -0.450823E+02
 H2O(s)              0.000000E+00    0.000000E+00    0.000000E+00   -0.115594E+03
                                       0.549580E+01   -0.121090E+03   -0.172966E+03
 H2O(L)              0.000000E+00    0.000000E+00    0.842705E-02   -0.112788E+03
                                       0.859679E+01   -0.121385E+03   -0.121385E+03

ITERATION  1       MATRIX
     0.157678E+00    0.788388E-01    0.200000E+01    0.788388E-01   -0.957128E+01
     0.788388E-01    0.582738E-01    0.100000E+01    0.488466E-01   -0.506744E+01
     0.200000E+01    0.100000E+01    0.000000E+00    0.000000E+00   -0.121385E+03
     0.788388E-01    0.488466E-01    0.000000E+00    0.611676E-04   -0.492589E+01

SOLUTION VECTOR
        H               O
    -0.532162E+02   -0.149527E+02   -0.122861E-02    0.131474E-01
```

T= 0.30430000E+03 ENN= 0.44071839E-01 ENNL=-0.31219343E+01 PP= 0.50662500E-01
LN P/N= 0.13936499E+00 AMBDA= 0.10000000E+01

	Nj	LN Nj	DEL LN Nj	H0j/RT
		S0j/R	G0j/RT	Gj/RT
*H	0.000000E+00	-0.125723E+03	0.164343E-01	0.862123E+02
		0.138484E+02	0.723640E+02	-0.532195E+02
HO2	0.000000E+00	-0.606565E+02	0.328686E-02	0.504603E+01
		0.276408E+02	-0.225947E+02	-0.831118E+02
*H2	0.000000E+00	-0.908604E+02	0.197211E-01	0.701441E-01
		0.157881E+02	-0.157179E+02	-0.106439E+03
H2O	0.394194E-01	-0.323350E+01	0.131474E-01	-0.954977E+02
		0.227933E+02	-0.118291E+03	-0.121385E+03
H2O2	0.000000E+00	-0.543875E+02	0.657371E-02	-0.537719E+02
		0.283113E+02	-0.820832E+02	-0.136331E+03
*O	0.000000E+00	-0.941980E+02	0.657371E-02	0.985373E+02
		0.194248E+02	0.791125E+02	-0.149462E+02
*OH	0.000000E+00	-0.617572E+02	0.986057E-02	0.156242E+02
		0.221720E+02	-0.654785E+01	-0.681657E+02
*O2	0.471361E-02	-0.535730E+01	-0.127898E-12	0.714483E-01
		0.247458E+02	-0.246744E+02	-0.298923E+02
O3	0.000000E+00	-0.722758E+02	-0.657371E-02	0.561412E+02
		0.288433E+02	0.272979E+02	-0.448385E+02
H2O(s)	0.000000E+00	0.000000E+00	0.000000E+00	-0.115594E+03
		0.549580E+01	-0.121090E+03	-0.172966E+03
H2O(L)	0.842705E-02	0.000000E+00	-0.122861E-02	-0.112788E+03
		0.859679E+01	-0.121385E+03	-0.121385E+03

ITERATION 2 MATRIX

0.159764E+00	0.798822E-01	0.200000E+01	0.798822E-01	-0.969652E+01
0.798822E-01	0.587955E-01	0.100000E+01	0.493683E-01	-0.513018E+01
0.200000E+01	0.100000E+01	0.000000E+00	0.000000E+00	-0.121385E+03
0.798822E-01	0.493683E-01	0.000000E+00	-0.403867E-06	-0.498922E+01

SOLUTION VECTOR

H	O		
-0.532162E+02	-0.149527E+02	0.126035E-13	-0.856736E-04

```
T= 0.30430000E+03 ENN= 0.44655096E-01 ENNL=-0.31087869E+01 PP= 0.50662500E-01
LN P/N= 0.12621757E+00 AMBDA= 0.10000000E+01

                      Nj            LN Nj        DEL LN Nj      H0j/RT
                                       S0j/R           G0j/RT         Gj/RT
 *H                0.000000E+00  -0.125706E+03  -0.107092E-03   0.862123E+02
                                    0.138484E+02   0.723640E+02  -0.532162E+02
 HO2               0.000000E+00  -0.606532E+02  -0.214184E-04   0.504603E+01
                                    0.276408E+02  -0.225947E+02  -0.831217E+02
 *H2               0.000000E+00  -0.908407E+02  -0.128510E-03   0.701441E-01
                                    0.157881E+02  -0.157179E+02  -0.106432E+03
 H2O               0.399411E-01  -0.322035E+01  -0.856736E-04  -0.954977E+02
                                    0.227933E+02  -0.118291E+03  -0.121385E+03
 H2O2              0.000000E+00  -0.543809E+02  -0.428368E-04  -0.537719E+02
                                    0.283113E+02  -0.820832E+02  -0.136338E+03
 *O                0.000000E+00  -0.941915E+02  -0.428368E-04   0.985373E+02
                                    0.194248E+02   0.791125E+02  -0.149527E+02
 *OH               0.000000E+00  -0.617473E+02  -0.642552E-04   0.156242E+02
                                    0.221720E+02  -0.654785E+01  -0.681690E+02
 *O2               0.471361E-02  -0.535730E+01  -0.284217E-13   0.714483E-01
                                    0.247458E+02  -0.246744E+02  -0.299055E+02
 O3                0.000000E+00  -0.722823E+02   0.428368E-04   0.561412E+02
                                    0.288433E+02   0.272979E+02  -0.448582E+02
 H2O(s)            0.000000E+00   0.000000E+00   0.000000E+00  -0.115594E+03
                                    0.549580E+01  -0.121090E+03  -0.172966E+03
 H2O(L)            0.719845E-02   0.000000E+00   0.126035E-13  -0.112788E+03
                                    0.859679E+01  -0.121385E+03  -0.121385E+03

ITERATION  3      MATRIX
     0.159751E+00   0.798753E-01   0.200000E+01   0.798753E-01  -0.969568E+01
     0.798753E-01   0.587921E-01   0.100000E+01   0.493649E-01  -0.512976E+01
     0.200000E+01   0.100000E+01   0.000000E+00   0.000000E+00  -0.121385E+03
     0.798753E-01   0.493649E-01   0.000000E+00  -0.172989E-10  -0.498880E+01

SOLUTION VECTOR
        H              O
    -0.532162E+02  -0.149527E+02  -0.757420E-14  -0.367002E-08

T= 0.30430000E+03 ENN= 0.44651270E-01 ENNL=-0.31088725E+01 PP= 0.50662500E-01
LN P/N= 0.12630324E+00 AMBDA= 0.10000000E+01
```

	Nj	LN Nj	DEL LN Nj	H0j/RT
		S0j/R	G0j/RT	Gj/RT
*H	0.000000E+00	-0.125707E+03	-0.458755E-08	0.862123E+02
		0.138484E+02	0.723640E+02	-0.532162E+02
HO2	0.000000E+00	-0.606532E+02	-0.917481E-09	0.504603E+01
		0.276408E+02	-0.225947E+02	-0.831216E+02
*H2	0.000000E+00	-0.908408E+02	-0.550507E-08	0.701441E-01
		0.157881E+02	-0.157179E+02	-0.106432E+03
H2O	0.399377E-01	-0.322044E+01	-0.367004E-08	-0.954977E+02
		0.227933E+02	-0.118291E+03	-0.121385E+03
H2O2	0.000000E+00	-0.543810E+02	-0.183496E-08	-0.537719E+02
		0.283113E+02	-0.820832E+02	-0.136338E+03
*O	0.000000E+00	-0.941915E+02	-0.183497E-08	0.985373E+02
		0.194248E+02	0.791125E+02	-0.149527E+02
*OH	0.000000E+00	-0.617474E+02	-0.275250E-08	0.156242E+02
		0.221720E+02	-0.654785E+01	-0.681689E+02
*O2	0.471361E-02	-0.535730E+01	0.746070E-13	0.714483E-01
		0.247458E+02	-0.246744E+02	-0.299054E+02
O3	0.000000E+00	-0.722823E+02	0.183512E-08	0.561412E+02
		0.288433E+02	0.272979E+02	-0.448581E+02
H2O(s)	0.000000E+00	0.000000E+00	0.000000E+00	-0.115594E+03
		0.549580E+01	-0.121090E+03	-0.172966E+03
H2O(L)	0.719845E-02	0.000000E+00	-0.757420E-14	-0.112788E+03
		0.859679E+01	-0.121385E+03	-0.121385E+03
5 3	304.300 -53.216	-14.953		

H2O(s)	200.000	273.150	0.0000000E+00
H2O(L)	273.150	600.000	0.7198445E-02

T DERIV MATRIX

0.159751E+00	0.798753E-01	0.200000E+01	0.798753E-01	-0.762791E+01
0.798753E-01	0.587921E-01	0.100000E+01	0.493649E-01	-0.381328E+01
0.200000E+01	0.100000E+01	0.000000E+00	0.000000E+00	-0.112788E+03
0.798753E-01	0.493649E-01	0.000000E+00	0.000000E+00	-0.381362E+01

SOLUTION VECTOR

H	O		
-0.930373E+02	0.732862E+02	0.654145E+01	-0.146501E+03

P DERIV MATRIX

0.159751E+00	0.798753E-01	0.200000E+01	0.798753E-01	0.798753E-01
0.798753E-01	0.587921E-01	0.100000E+01	0.493649E-01	0.493649E-01
0.200000E+01	0.100000E+01	0.000000E+00	0.000000E+00	0.000000E+00
0.798753E-01	0.493649E-01	0.000000E+00	0.000000E+00	0.446513E-01

SOLUTION VECTOR

H	O		
-0.236821E+01	0.473642E+01	0.378323E+00	-0.847284E+01

POINT= 5 P= 0.506625E-01 T= 0.304300E+03
H/R=-0.140755E+04 S/R= 0.123707E+01
M= 0.223958E+02 CP/R= 0.113349E+03 DLVPT=-0.947284E+01
DLVTP= 0.147501E+03 GAMMA(S)= 0.110818E+01 V= 0.222990E+07

6	3	304.200	-53.247	-14.929
7	4	304.000	-53.305	-14.886
8	6	300.000	-54.288	-14.426

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
TEMPERATURE AND PRESSURE

CASE = 14

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
NAME	H2(L)	100.0000000	0.000	0.000
NAME	O2(L)	60.0000000	-12979.000	90.170

REACTANT DENSITY= 1349.29 KG/CU M

O/F= 0.00000 %FUEL= 0.000000 R,EQ.RATIO= 0.833333 PHI,EQ.RATIO= 0.000000

THERMODYNAMIC PROPERTIES

P, BAR	0.05066	0.05066	0.05066	0.05066	0.05066	0.05066	0.05066	0.05066
T, K	1000.00	500.00	350.00	305.00	304.30	304.20	304.00	300.00
RHO, KG/CU M	1.1752-2	2.3504-2	3.3577-2	3.8530-2	4.4845-2	4.7014-2	5.1325-2	1.3024-1
H, KJ/KG	-10066.0	-11043.6	-11309.1	-11386.9	-11703.1	-11792.8	-11948.7	-12988.1
U, KJ/KG	-10497.1	-11259.2	-11460.0	-11518.4	-11816.0	-11900.5	-12047.4	-13027.0
G, KJ/KG	-23601.6	-17139.8	-15355.8	-14840.7	-14833.0	-14831.9	-14830.0	-14801.2
S, KJ/(KG)(K)	13.5356	12.1924	11.5619	11.3239	10.2856	9.9907	9.4781	6.0435
M, (1/n)	19.287	19.287	19.287	19.287	22.396	23.471	25.607	64.125
MW, MOL WT	19.287	19.287	19.287	19.287	19.287	19.287	19.287	19.287
(dLV/dLP)t	-1.00000	-1.00000	-1.00000	-1.00000	-9.47284	-9.03875	-8.28504	-3.30842
(dLV/dLT)p	1.0000	1.0000	1.0000	1.0000	147.5009	140.0542	127.1235	41.6525
Cp, KJ/(KG)(K)	2.1108	1.8069	1.7370	1.7233	942.4445	854.1858	711.2554	96.0625
GAMMAs	1.2567	1.3133	1.3301	1.3336	1.1082	1.1061	1.1019	1.0345
SON VEL,M/SEC	736.0	532.1	448.0	418.8	353.8	345.2	329.8	200.6

MOLE FRACTIONS

H2O	0.90909	0.90909	0.90909	0.90909	0.77026	0.73080	0.66228	0.20986
*O2	0.09091	0.09091	0.09091	0.09091	0.09091	0.09091	0.09091	0.09091
H2O(L)	0.00000	0.00000	0.00000	0.00000	0.13883	0.17830	0.24681	0.69923

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*H	HO2	*H2	H2O2	*O
*OH	O3	H2O(s)		

References

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13. ABSTRACT (*Maximum 200 words*)

This users manual is the second part of a two-part report describing the NASA Lewis CEA (Chemical Equilibrium with Applications) program. The program obtains chemical equilibrium compositions of complex mixtures with applications to several types of problems. The topics presented in this manual are (1) details for preparing input data sets; (2) a description of output tables for various types of problems; (3) the overall modular organization of the program with information on how to make modifications; (4) a description of the function of each subroutine; (5) error messages and their significance; and (6) a number of examples that illustrate various types of problems handled by CEA and that cover many of the options available in both input and output. Seven appendixes give information on the thermodynamic and thermal transport data used in CEA; some information on common variables used in or generated by the equilibrium module; and output tables for 14 example problems. The CEA program was written in ANSI standard FORTRAN 77. CEA should work on any system with sufficient storage. There are about 6300 lines in the source code, which uses about 225 kilobytes of memory. The compiled program takes about 975 kilobytes.

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Chemical equilibrium; Combustion products; Combustion temperatures; Computer program; Thermodynamic mixture properties; Thermal transport properties; Rocket performance

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