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CHEMKIN: A General-Purpose, Problem-Independent, Transportable, Fortran Chemical Kinetics Code Package

R. J. Kee, J. A. Miller, T. H. Jefferson

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CHEMKIN: A GENERAL-PURPOSE, PROBLEM-INDEPENDENT, TRANSPORTABLE, FORTRAN CHEMICAL KINETICS CODE PACKAGE

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ABSTRACT

The CHEMKIN package is comprised of two major components--the INTERPRETER and the gas-phase subroutine library. The INTERPRETER is a FORTRAN code which is used to read a symbolic description of an arbitrary, user-specified chemical reaction mechanism. The output of the INTERPRETER is a data file which forms a link to the gas-phase subroutine library. This library is a collection of about 200 modular FORTRAN subroutines which may be called to return thermodynamic properties, chemical production rates, derivatives of thermodynamic properties, derivatives of chemical production rates, or sensitivity parameters. Thermodynamic properties for the chemical species are given in terms of polynomial fits to the specific heats, and are stored on a thermodynamic data base. The data base is in exactly the same format as the one used in the NASA chemical equilibrium code. Therefore, the user may either supply his own data base or use the NASA data base directly.

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NOMENCLATURE

		CGS UNITS
a_{nk}	Coefficients to fits of thermodynamic data	depends on n
a_k^o	Standard state specific Helmholtz free energy for the kth species	ergs/g
$\bar{a}^o$	Mass-weighted mean standard state Helmholtz free energy	ergs/g
A_k^o	Standard state Helmholtz free energy for the kth species	ergs/mole
$\bar{A}^o$	Molar-weighted mean standard state Helmholtz free energy	ergs/mole
A_i	Pre-exponential factor in the rate constant of the ith reaction	depends on reaction
c_{p_k}	Specific heat at constant pressure of the kth species	ergs/(g K)
$\bar{c}_p$	Mass-weighted mean specific heat at constant pressure	ergs/(g K)
$C_{p_k}^o$	Standard state specific heat at constant pressure of the kth species	ergs/(mole K)
C_{p_k}	Specific heat at constant pressure of the kth species	ergs/(mole K)
$\bar{C}_p$	Molar-weighted mean specific heat at constant pressure	ergs/(mole K)
c_{v_k}	Specific heat at constant volume of the kth species	ergs/(g K)
$\bar{c}_v$	Mass-weighted mean specific heat at constant volume	ergs/(g K)

		CGS UNITS
C_{v_k}	Specific heat at constant volume of the kth species	ergs/(mole K)
$\bar{C}_v$	Molar-weighted mean specific heat at constant volume	ergs/(mole K)
$\dot{C}_k$	Chemical creation rate of the kth species	moles/(cm^3 sec)
$\dot{D}_k$	Chemical destruction rate of the kth species	moles/(cm^3 sec)
E_i	Activation energy in the rate constant of the ith reaction [defined in Eq. (II.5.5)]	[cal/mole]
g_k^o	Standard state specific Gibbs free energy for the kth species	ergs/g
$\bar{g}^o$	Mass-weighted mean standard state Gibbs free energy	ergs/g
G_k^o	Standard state Gibbs free energy for the kth species	ergs/mole
$\bar{G}^o$	Molar-weighted mean standard state Gibbs free energy	ergs/mole
h_k	Specific enthalpy of the kth species	ergs/g
$\bar{h}$	Mass-weighted mean specific enthalpy	ergs/g
H_k^o	Standard state enthalpy of the kth species	ergs/mole
H_k	Enthalpy of the kth species	ergs/mole
$\bar{H}$	Molar-weighted mean enthalpy	ergs/mole
i	Reaction index	
I	Total number of reactions	
k	Species index	
k_{f_i}	Forward rate constant of the ith reaction	depends on reaction
k_{r_i}	Reverse rate constant of the ith reaction	depends on reaction

		CGS UNITS
K	Total number of species	
K_{c_i}	Equilibrium constant in concentration units for the ith reaction	depends on reaction
K_{p_i}	Equilibrium constant in pressure units for the ith reaction	depends on reaction
N	Number of coefficients in polynomial fits to C_p^o/R	
P	Pressure	dynes/cm^2
P_{atm}	Pressure of one standard atmosphere	dynes/cm^2
q_i	Rate of progress of the ith reaction	moles/(cm^{3}sec)
R	Universal gas constant	ergs/(mole K)
R_c	Universal gas constant, in same units as activation energy E_i	[cal/(mole K)]
s_k^o	Standard state specific entropy of the kth species	ergs/(g K)
$\bar{s}^o$	Mass-weighted mean standard state specific entropy	ergs/(g K)
S_k^o	Standard state entropy of the kth species	ergs/(mole K)
S_k	Entropy of the kth species	ergs/(mole K)
$\bar{S}^o$	Molar-weighted mean standard state entropy	ergs/(mole K)
T	Temperature	K
u_k	Specific internal energy of the kth species	ergs/g
$\bar{u}$	Mass-weighted mean specific internal energy	ergs/g
U_k	Internal energy of the kth species	ergs/mole
$\bar{U}$	Molar-weighted mean internal energy	ergs/mole
Y_k	Mass fraction of the kth species	
X_k	Mole fraction of kth species	

		CGS UNITS
$[X_k]$	Molar concentration of kth species	moles/cm^3
W_k	Molecular weight of kth species	g/mole
$\bar{W}$	Mean molecular weight	g/mole

GREEK

α_{ki}	Enhanced third body efficiencies of the kth species in the ith reaction.	
β_i	Temperature exponent in the rate constant of the ith reaction.	
δ_{ij}	Kronecker delta; $\delta_{ij} = 0$ for $i \neq j$, $\delta_{ij} = 1$ for $i = j$.	
ρ	Mass density.	g/cm^3
τ_k	Characteristic chemical destruction time of the kth species.	sec
ν_{ki}	Stoichiometric coefficients of the kth species in the ith reaction, $\nu_{ki} = \nu''_{ki} - \nu'_{ki}$.	
ν'_{ki}	Stoichiometric coefficients of the kth reactant species in the ith reaction.	
ν''_{ki}	Stoichiometric coefficients of the kth product species in the ith reaction.	
$\dot{\omega}_k$	Chemical production rate of the kth species.	mole/(cm^3 sec)

CHEMKIN: A GENERAL-PURPOSE, PROBLEM-INDEPENDENT, TRANSPORTABLE, FORTRAN CHEMICAL KINETICS CODE PACKAGE

I. Introduction

1. Overview

CHEMKIN is a package of FORTRAN programs which are designed to facilitate a chemist's interaction with the computer in modeling chemical kinetics. The modeling process requires that the chemist formulate an applicable reaction mechanism (with rate constants) and that he formulate and solve an appropriate system of governing equations. Once the mechanism and governing equations are defined, CHEMKIN provides a means to describe symbolically the reaction mechanism (the INTERPRETER) and a means to describe computationally an arbitrary system of governing equations (The Gas-Phase Subroutine Library). CHEMKIN does not provide a means to solve the governing equations; therefore selection and implementation of a solution method is left to the user.

Input to the INTERPRETER may be any number of reversible or irreversible reactions, including those with arbitrary third bodies, photons, or ionic species as reactants or products. Also, enhanced third body efficiencies may be specified for any of the species in three body reactions. The input to the INTERPRETER is in familiar chemical, not computational, notation. In this aspect CHEMKIN may be considered to be a computer language which translates chemical reaction nomenclature into FORTRAN code. As a result the definition and modification of a mechanism is easy, and feedback on the effect of a change is rapid. Moreover, since the language is familiar, the chances of error associated with writing and debugging new FORTRAN code are significantly reduced.

The Gas-Phase Subroutine Library is a collection of about 200 modular FORTRAN subroutines which may be called to return equation of state variables,

thermodynamic properties, chemical production rates, derivatives of equation of state variables, derivatives of thermodynamic properties, derivatives of chemical production rates, and sensitivity parameters. The variables returned from these subroutines may be combined by the user in his FORTRAN code to form any set of governing equations.

There are a number of other general purpose chemical kinetics codes available. The NASA general chemical kinetics code by Bittker and Scullin[1] and the SETKIN code by Dickinson and Gelinas[2] are notable examples. However, the concept and construction of CHEMKIN is quite different from these other codes, which were written primarily to solve a problem or a class of problems. The CHEMKIN package is not intended to solve a single class of problems but, instead, it is intended to allow the creation of a general framework from which any problem involving a complex chemical mechanism may be formulated. In other words, CHEMKIN is designed for efficient handling of physical problems regardless of the chemical reaction mechanism and the governing equations.

Because the CHEMKIN package is not designed to solve a single type of problem directly, the user must write some FORTRAN code to describe his particular set of governing equations. However, the programming is minimal. A user need only call CHEMKIN subroutines that define those terms in his equations that relate to equation of state, chemical production, and thermodynamics, and then combine the results to define his problem. In addition to problems in chemical kinetics which lead to systems of ordinary differential equations we anticipate that a major use of the package will be to define the chemical rate terms in systems of partial differential equations which also describe fluid transport. The solution methods are of the user's choosing and are independent of the CHEMKIN package.

An important advantage of the general-purpose and problem-independent structure of CHEMKIN is that it allows the chemist to work with the same input nomenclature regardless of his particular problem. Thus there is no need to remember a different input protocol for different problems, and consequently the time required to switch between problems or to begin a new problem is minimized. Additionally, by having made CHEMKIN easily transportable between computers, we hope to facilitate the exchange of applications codes between

different sites. Currently such exchanges are often hampered by machine-dependent or problem-specific coding.

2. Structure of CHEMKIN

The CHEMKIN package is composed of four important pieces: the INTERPRETER, the Thermodynamic Data Base, the Linking File, and the Gas-Phase Subroutine Library. The INTERPRETER is a program which first reads the user's symbolic description of the reaction mechanism. It then extracts the appropriate thermodynamic information for the species involved from the Thermodynamic Data Base. The Data Base has exactly the same format as that used by the NASA complex chemical equilibrium code by Gordon and McBride[3]. The output of the INTERPRETER is the Linking File which contains all the pertinent information on the elements, species, and reactions in the mechanism.

The Linking File is read by an initialization subroutine which is called from the user code. The purpose of initialization is to create two data arrays (one integer and one floating point) for use internally by the other CHEMKIN gas-phase subroutines.

The CHEMKIN gas-phase subroutines, of which there are over 100, are called to return information on the elements, species, reactions, equation of state, thermodynamic properties, chemical production rates, sensitivity parameters, derivatives of chemical production rates, and derivatives of thermodynamic properties. Generally the input to these routines will be the state variables of the gas--pressure or density, temperature, and the species composition. All routines can be called with the species composition defined as mass fractions, mole fractions, or molar concentration.

3. Example

As an example of the use of the CHEMKIN package consider a hydrogen oxidation mechanism. We must first define the elements and species which appear in the mechanism, and then describe the reaction mechanism itself. A sample of the card input needed for the INTERPRETER is shown in Figure 1. The input is essentially format free. The elements and species need only be separated by blank spaces. The reaction descriptions appear first and are

```
END
 OH+N=NO+H                                  4.0E13     0.000        0.
 N+O2=NO+O                                  6.4E09     1.000     6280.
 O+N2=NO+N                                  1.4E14     0.000    75800.
 H+HO2=H2+O2                                1.3E13     0.000        0.
 H2O/20.0/
 H+OH+M=H2O+M                               7.5E23    -2.600        0.
 O2+M=2O+M                                  1.83E11    0.500    95560.
 H2O/5/
 H2+M=2H+M                                  2.23E12    0.500    92600.
 2OH=O+H2O                                  1.7E06     2.030    -1190.
 O+HO2=O2+OH                                1.0E13     0.000        0.
 H+HO2=2OH                                  6.0E13     0.000        0.
 OH+HO2=H2O+O2                              1.2E13     0.000        0.
 H2O / 20./
 H+O2+M=HO2+M                               2.0E15     0.000     -870.
 O+H2=OH+H                                  1.8E10     1.000     8826.
 H+O2=OH+O                                  1.22E17   -0.907    16620.
 H2+OH=H2O+H                                5.2E13     0.000     6300
 H2+O2=2OH                                  1.7E13     0.000    47780.
REACTIONS
END
 H2  O2  N2  H  O  M  OH  HO2  H2O  NO
SPECIES
END
 H   O   N
ELEMENTS
```

Figure 1. Example of Card Image Input to CHEMKIN

followed by the three Arrhenius coefficients (pre-exponential factor, temperature exponent, and activation energy). Enhanced third body efficiencies for selected species can be specified in the card following that for a reaction which has an arbitrary third body specified.

Assume the governing equation we wish to study is the energy conservation equation for a constant-pressure environment:

$$\frac{\partial T}{\partial t} = -\frac{1}{\rho \bar{c}_p} \sum_{k=1}^{K} h_k \dot{\omega}_k W_k$$

where T is the temperature, ρ the mass density, and $\bar{c}_p$ the mean specific heat; h_k, $\dot{\omega}_k$, and W_k are the specific enthalpies, molar production rates, and molecular weights of the species, respectively. The representation of this equation begins with CHEMKIN subroutine calls of the following form, where the output variables are underlined:

```
CALL CKINIT(LENIWK,LENWK,LINK,LOUT,IWORK,WORK)
CALL CKINDX(IWORK,WORK,MM,KK,II,LENEL,LENSYM,NFIT)
CALL CKRHOY(P,T,Y,IWORK,WORK,RHO)
CALL CKCPBY(T,Y,IWORK,WORK,CPB)
CALL CKHY(T,Y,IWORK,WORK,H)
CALL CKWYP(P,T,Y,IWORK,WORK,WDOT)
CALL CKWT(IWORK,WORK,WT)
```

The complete details on these calls are explained in later sections of the this document, the object here being to illustrate the relative simplicity of the use of CHEMKIN. Briefly, the first call is to the initialization subroutine, CKINIT, which reads the Linking File that was created by the INTERPRETER for the hydrogen-air reaction mechanism. LENIWK and LENWK are the actual dimensions provided by the user for the data arrays, IWORK and WORK, LINK is the logical file number of the Linking File, and LOUT is the logical file number for printed error messages. In the remaining calls, the pressure, temperature, and mass fraction distribution are input as P, T, and Y. The output variables

(underlined), correspond to the various terms for describing the equation, i.e., RHO = ρ, CPB = $\bar{c}_p$, H = h_k, WDOT = $\dot{\omega}_k$, WT = W_k. The total number of species is denoted by KK because the running index k becomes "K" in FORTRAN (see below).

The FORTRAN representation of the governing equation, given by combining the results of the above subroutine calls, is simply

```
      SUM=0.
      DO 100 K=1,KK
      SUM=SUM + H(K)*WDOT(K)*WT(K)
  100 CONTINUE
      DTDT=-SUM/(RHO*CPB)
```

One can see from this example that only a minimum of programming effort is required to form an arbitrary governing equation from an arbitrary reaction mechanism.

4. Transportability

The CHEMKIN package was developed on a CDC 6600 computer using the NOS-BE operating system. However, we have not taken advantage of any special CDC features. Written entirely in ANSI standard FORTRAN, the code should be easily transportable to other computer systems. The machine word length is not important in any of the CHEMKIN subroutines so there should not not be any need to change variables to double precision on small-word-length computers.

5. Organization of the Report

Chapter II is a compendium of important equations in gas phase chemical kinetics. Many of the equations are simply definitions, but in any case derivations are either very sketchy or not given. Although most readers will find all the equations quite familar, it is useful to have these equations

stated concisely in one document. For most of the equations the package contains a subroutine which, when given the variables on the right-hand side, returns the variable on the left. Below the equation number is stated (in brackets) the name of the subroutine which provides information about that equation. For example, Eq. (II.2.3) gives mean molecular weight in terms of the mass fractions. Subroutine CKMMWY would therefore be called to return this information.

Chapter III explains the mechanics of using CHEMKIN and provides a description of the job control logic for running a problem. Chapter IV explains the CHEMKIN INTERPRETER and how to set up the required symbolic input to define a reaction mechanism. Chapters V and VI describe the CHEMKIN gas-phase subroutines, V being composed of short descriptions for quick reference and VI, an alphabetical listing, explaining the input and output in the call sequence and cross referencing each subroutine to equation numbers in Chapter II. To demonstrate CHEMKIN explicitly Chapter VII goes through a sample problem in detail.

Appendix A defines the allocation of two work arrays which are created from the Linking File. With this information, subroutines can be readily created for problems not presently covered in the current version of the Gas-Phase Subroutine Library. Since the INTERPRETER is more general than the current Gas-Phase Subroutine Library, there is room for expansion of the package.

Appendix B provides information on the structure and content of the thermodynamic data base. Appendix C is a microfiche listing of the INTERPRETER and the Gas-Phase Subroutine Library.

II. Thermodynamics and Chemical Rate Expressions

1. Choice of Variables

The formulation of any problem requires that a set of dependent variables be chosen. Unfortunately there is no clear choice that is generally superior for all problems. In the CHEMKIN package we have decided to allow the user to select either pressure or density, temperature, and either mass fraction, mole fraction, or molar concentration. In other words, to define the state of a gas, one variable must be selected from each column of the diagram below.

$$\left\{ \begin{array}{ccc} p & T & Y_k \\ \rho & & X_k \\ & & [X_k] \end{array} \right\}$$

In making these options available from among the many possible, we have attempted to provide combinations of variables which are natural ones for a wide class of problems. In particular, pressure is a natural choice in situations where pressure is held fixed, and density is a natural variable in a system where volume is fixed. Moreover, density is a natural variable in many problems involving fluid mechanics because density is determined directly from the mass continuity equation. Temperature is always taken as a natural variable because both the thermodynamic properties and the chemical rate constants depend directly on temperature. Mass fraction and mole fraction are both convenient variables to describe the composition of a gas. Molar concentration is usually less convenient but it is often a natural variable because the rate of progress of chemical reactions depends directly on the molar concentration of the reactants and products.

From the standpoint of evaluating properties or chemical rate expressions the choice of variables is really just a matter of convenience since one set of variables can readily be converted to another. However, in evaluating partial derivatives the choice is more important, because there the choice dictates what is being held constant in the differentiation.

2. Equation of State

The equation of state used is that of a perfect gas:

$$P = \frac{\rho R T}{\overline{W}} \qquad \text{(II.2.1)*} \quad \text{[CKPY,CKPX,CKPC]}$$

$$\rho = \frac{P\overline{W}}{RT} \qquad \text{(II.2.2)} \quad \text{[CKRHOY,CKRHOX,CKRHOC]}$$

The mean molecular weight $\overline{W}$ is defined variously as

$$\overline{W} = \frac{1}{\sum_{k=1}^{K} \frac{Y_k}{W_k}} \qquad \text{(II.2.3)} \quad \text{[CKMMWY]}$$

$$\overline{W} = \sum_{k=1}^{K} X_k W_k \qquad \text{(II.2.4)} \quad \text{[CKMMWX]}$$

$$\overline{W} = \frac{\sum_{k=1}^{K} [X_k] W_k}{\sum_{k=1}^{K} [X_k]} \qquad \text{(II.2.5)} \quad \text{[CKMMWC]}$$

3. Mole-Mass Conversions

Use of the CHEMKIN subroutines requires that the species distribution be specified either as mass fraction, mole fraction, or molar concentration. In this section we state conversion formulas between these various ways to describe the make up of the mixtures. Also, in the case of conversion to molar concentration we state the formulas both in terms of pressure and density.

---

*The names in brackets refer to subroutines which are described in Chapters V and VI. Mnemonic devices used for the naming conventions are described at the beginning of Chapter V.

Mass Fraction to Mole Fraction--

$$X_k = \frac{Y_k}{W_k \sum_{j=1}^{K} \frac{Y_j}{W_j}} = \frac{Y_k \overline{W}}{W_k} \qquad \text{(II.3.1) [CKYTX]}$$

Mass Fraction to Molar Concentration--

$$[X_k] = \frac{P\left(\frac{Y_k}{W_k}\right)}{RT \sum_{j=1}^{K} \frac{Y_j}{W_j}} = \left(\frac{P\overline{W}}{RT}\right) \frac{Y_k}{W_k} \qquad \text{(II.3.2) [CKYTCP]}$$

$$[X_k] = \rho \frac{Y_k}{W_k} \qquad \text{(II.3.3) [CKYTCR]}$$

Mole Fraction to Mass Fraction--

$$Y_k = \frac{X_k W_k}{\sum_{j=1}^{K} X_j W_j} = \frac{X_k W_k}{\overline{W}} \qquad \text{(II.3.4) [CKXTY]}$$

Mole Fraction to Molar Concentration--

$$[X_k] = X_k \frac{P}{RT} \qquad \text{(II.3.5) [CKXTCP]}$$

$$[X_k] = X_k \frac{\rho}{\overline{W}} \qquad \text{(II.3.6) [CKXTCR]}$$

Molar Concentration to Mass Fraction--

$$Y_k = \frac{[X_k]W_k}{\sum_{j=1}^{K} [X_j]W_j} \qquad \text{(II.3.7)}$$

[CKCTY]

Molar Concentration to Mole Fraction--

$$X_k = \frac{[X_k]}{\sum_{j=1}^{K} [X_j]} \qquad \text{(II.3.8)}$$

[CKCTX]

4. Thermodynamic Properties

Thermodynamic properties are taken to be in the form of polynomial fits to the specific heat at constant pressure.

$$\frac{C^o_{p_k}}{R} = \sum_{n=1}^{N} a_{nk} T^{(n-1)} \qquad \text{(II.4.1)}$$

[CKATHM,CKCPOR,CKCPML]

The superscript o refers to the standard state one atmosphere. For perfect gases, however, the heat capacities are independent of pressure; the standard state values are the actual values. Other thermodynamic properties are given in terms of the fits to C^o_p. First, the enthalpy is given by

$$\frac{H^o_k}{R} = \int_0^T C^o_{p_k} \, dT \qquad \text{(II.4.2)}$$

so that

$$\frac{H^o_k}{RT} = \sum_{n=1}^{N} \frac{a_{nk} T^{(n-1)}}{n} + \frac{a_{N+1,k}}{T} \qquad \text{(II.4.3)}$$

[CKATHM,CKHORT,CKHML]

where the constant of integration, $a_{N+1,k}*R$, is the standard formation enthalpy at 0 K. Additionally, the standard state entropy is written as

$$\frac{S_k^o}{R} = \int_0^T \frac{C_{p_k}^o}{T} \, dT \qquad \text{(II.4.4)}$$

so that

$$\frac{S^o_k}{R} = a_{1k} \ln T + \sum_{n=2}^{N} \frac{a_{nk} \, T^{(n-1)}}{(n-1)} + a_{N+2,k} \qquad \text{(II.4.5)}$$

[CKATHM,CKSOR,CKSML]

where the constant of integration, $a_{N+2,k}*R$, is the standard formation entropy at 0 K.

Although the programming is done in general for an arbitrary order polynomial fit, the data base normally used in the CHEMKIN package is that of the NASA fits[3] to the JANNAF data. In this case seven coefficients are needed for two temperature ranges. These fits are given in the following form:

$$\frac{C_{p_k}^o}{R} = a_{1k} + a_{2k}T + a_{3k}T^2 + a_{4k}T^3 + a_{5k}T^4 \qquad \text{(II.4.6)}$$

[CKCPOR]

$$\frac{H_k^o}{RT} = a_{1k} + \frac{a_{2k}}{2} T + \frac{a_{3k}}{3} T^2 + \frac{a_{4k}}{4} T^3 + \frac{a_{5k}}{5} T^4 + \frac{a_{6k}}{T} \qquad \text{(II.4.7)}$$

[CKHORT]

$$\frac{S_k^o}{R} = a_{1k} \ln T + a_{2k} T + \frac{a_{3k}}{2} T^2 + \frac{a_{4k}}{3} T^3 + \frac{a_{5k}}{4} T^4 + a_{7k} \qquad \text{(II.4.8)}$$

[CKSOR]

Other thermodynamic properties are easily given in terms of C_p^o, H^o, and S^o. The specific heat at constant volume, C_v, is stated as

$$C_v = C_p - R \qquad \text{(II.4.9)}$$

[CKCVML]

The internal energy U is given as

$$U = H - RT \qquad \text{(II.4.10) [CKUML]}$$

The standard state Gibbs free energy G^o is written as

$$G^o = H - TS^o \qquad \text{(II.4.11) [CKGML]}$$

and, the standard state Helmholtz free energy A^o is defined to be

$$A^o = U - TS^o \qquad \text{(II.4.12) [CKAML]}$$

For C_p, C_v, H, and U the standard state values (i.e., superscript o) are the actual values for perfect gases. However, to obtain S, G, and A from the standard state values one must add the appropriate pressure and entropy of mixing terms, i.e.

$$S_k = S_k^o - R \ln X_k - R \ln(P/P_{atm})$$

In the CHEMKIN Gas-Phase subroutine library we provide only standard state quantities.

Often specific thermodynamic properties are needed in mass units rather than molar units. These are determined simply by dividing the property in molar units by the molecular weight. The specific properties are thus given as

$$c_{pk} = \frac{C_{pk}}{W_k} \qquad \text{(II.4.13) [CKCPMS]}$$

$$h_k = \frac{H_k}{W_k} \qquad \text{(II.4.14) [CKHMS]}$$

$$s_k^o = \frac{S_k^o}{W_k} \qquad \text{(II.4.15) [CKSMS]}$$

$$c_{v_k} = \frac{C_{v_k}}{W_k}$$ (II.4.16) [CKCVMS]

$$u_k = \frac{U_k}{W_k}$$ (II.4.17) [CKUMS]

$$g_k^o = \frac{G_k^o}{W_k}$$ (II.4.18) [CKGMS]

$$a_k^o = \frac{A_k^o}{W_k}$$ (II.4.19) [CKAMS]

In addition one may need average thermodynamic properties. The CHEMKIN thermodynamics subroutines return molar averaged properties if the variable is in molar units and mass averaged properties if the variable is in mass units. For example

$$\bar{C}_p = \sum_{k=1}^{K} C_{p_k} X_k$$ (II.4.20) [CKCPBL]

$$\bar{c}_p = \sum_{k=1}^{K} c_{p_k} Y_k$$ (II.4.21) [CKCPBS]

All the other thermodynamic variables are averaged in the same way.

$$\bar{H} = \sum_{k=1}^{K} H_k X_k$$ (II.4.22) [CKHBML]

$$\bar{h} = \sum_{k=1}^{K} h_k Y_k$$ (II.4.23) [CKHBMS]

$$\bar{S}^o = \sum_{k=1}^{K} S_k^o X_k$$ (II.4.24) [CKSBML]

$$\bar{s}^o = \sum_{k=1}^{K} s_k^o Y_k \qquad \text{(II.4.25) [CKSBMS]}$$

$$\bar{C}_v = \sum_{k=1}^{K} C_{v_k} X_k \qquad \text{(II.4.26) [CKCVBL]}$$

$$\bar{c}_v = \sum_{k=1}^{K} c_{v_k} Y_k \qquad \text{(II.4.27) [CKCVBS]}$$

$$\bar{U} = \sum_{k=1}^{K} U_k X_k \qquad \text{(II.4.28) [CKUBML]}$$

$$\bar{u} = \sum_{k=1}^{K} u_k Y_k \qquad \text{(II.4.29) [CKUBMS]}$$

$$\bar{G}^o = \sum_{k=1}^{K} G_k^o X_k \qquad \text{(II.4.30) [CKGBML]}$$

$$\bar{g}^o = \sum_{k=1}^{K} g_k^o Y_k \qquad \text{(II.4.31) [CKGBMS]}$$

$$\bar{A}^o = \sum_{k=1}^{K} A_k^o X_k \qquad \text{(II.4.32) [CKABML]}$$

$$\bar{a}^o = \sum_{k=1}^{K} a_k^o Y_k \qquad \text{(II.4.33) [CKABMS]}$$

5. Chemical Rate Expressions

Consider I elementary reversible (or irreversible) reactions involving K chemical species which can be represented in the general form given below,

$$\sum_{k=1}^{K} \nu'_{ki} X_k \rightleftarrows \sum_{k=1}^{K} \nu''_{ki} X_k \quad (i = 1,\ldots,I) \qquad \text{(II.5.1) [CKITR]}$$

The stoichiometric coefficients ν_{ki} are integers and X_k is the chemical symbol for the kth species. Normally a reaction involves only three or four species; hence the ν_{ki} matrix is quite sparse for a large set of reactions.

The production rate $\dot{\omega}_k$ of the kth species can be written as a summation of the rate of progress variables for all reactions involving the kth species:

$$\dot{\omega}_k = \sum_{i=1}^{I} \nu_{ki}\, q_i \qquad (k=1,\ldots,K) \qquad \text{(II.5.2)}$$

[CKWYP,CKWYR,CKWXP,CKWXR,CKWC, CKCONT]

where

$$\nu_{ki} = (\nu''_{ki} - \nu'_{ki}) \qquad \text{(II.5.3)}$$

[CKNU]

The rate of progress variable, q_i, for the ith reaction is given by the difference of the forward rates minus the reverse rates as

$$q_i = k_{f_i} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{r_i} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}} \qquad \text{(II.5.4)}$$

[CKQYP,CXQYR,CKQXP,CKQXR,CKQC, CKCONT]

where $[X_k]$ is the molar concentration of the kth species and k_{f_i} and k_{r_i} are the forward and reverse* rate constants of the ith reaction. The forward rate constants for the I reactions are assumed to have the following Arrhenius temperature dependence:**

$$k_{f_i} = A_i\, T^{\beta_i} \exp(-E_i/R_c T) \qquad \text{(II.5.5)}$$

[CKABE]

where the pre-exponential factor A_i, the temperature exponent β_i, and the activation energy E_i usually come from experiment. For all reactions the parameters in Eq. (II.5.5) are required input to the CHEMKIN package for each reaction.

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*If the reaction is irreversible, then k_{r_i} is of course zero.

**Two gas constants, R and R_c, are used throughout this report and the CHEMKIN code. R_c is used only in conjunction with the activation energy, E_i, and has compatible units. The reason for the duality is because we find that many users would rather use different units (say cal/mole) for activation energies even though other units (say cgs) are used otherwise.

The reverse rate constants k_{r_i} are related to the forward rate constants through the equilibrium constants as

$$k_{r_i} = \frac{k_{f_i}}{K_{c_i}} \qquad \text{(II.5.6)}$$

Although K_{c_i} is given in concentration units, the equilibrium constants are more easily determined from the thermodynamic properties in pressure units; they are related by

$$K_{c_i} = K_{p_i} \left(\frac{P_{atm}}{RT}\right)^{\sum_{k=1}^{K} \nu_{ki}} \qquad \text{(II.5.7)}$$

[CKEQYP,CKEQYR,CKEQXP,CKEQXR,CKEQC]

where P_{atm} denotes atmospheric pressure. The equilibrium constants K_{p_i} are obtained with the relationship

$$K_{p_i} = \exp\left(\frac{\Delta S_i^o}{R} - \frac{\Delta H_i^o}{RT}\right) \qquad \text{(II.5.8)}$$

The Δ refers to the change that occurs in passing completely from reactants to products by the ith reaction. More specifically

$$\frac{\Delta S_i^o}{R} = \sum_{k=1}^{K} \nu_{ki} \frac{S_k^o}{R} \qquad \text{(II.5.9)}$$

$$\frac{\Delta H_i^o}{RT} = \sum_{k=1}^{K} \nu_{ki} \frac{H_k^o}{RT} \qquad \text{(II.5.10)}$$

Three Body Reactions--

In some reactions a third body is required for the reaction to proceed; this is often the case in dissociation or recombination reactions. When a third body is needed, the rate of progress variable is different from Eq(II.5.4) by first factor in the equation below.

$$q_i = \left(\sum_{k=1}^{K} \alpha_{ki}[X_k]\right)\left(k_{f_i} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{r_i} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}}\right) \qquad \text{(II.5.11)}$$

[CKQYP,CKQYR,CKQXP, CKQXR,CKQC,CKTHB]

If all species contribute equally as third bodies, then all $\alpha_{ki} = 1$, and the first factor is the total concentration of the mixture:

$$\sum_{k=1}^{K} [X_k] = \frac{P}{RT} \qquad \text{(II.5.12)}$$

However, it is often the case that some species act more efficiently as third bodies than do others. The α_{ki} coefficients are then used to specify the increased efficiency of the kth species in the ith reaction. Note also that if a species is to be excluded from acting as a third body, then $\alpha_{ki} = 0$ for that species. Any α_{ki} which differ from 1 must be input to the CHEMKIN INTERPRETER.

Special Forms--

Some numerical methods require the species production rates to be divided into a creation rate and a destruction rate, i.e.,

$$\dot{\omega}_k = \dot{C}_k - \dot{D}_k \qquad \text{(II.5.13)}$$

[CKCDYP,CKCDYR, CKCDXP,CKCDXR,CKCDC]

where, for non-three body reactions,

$$\dot{C}_k = \sum_{i=1}^{I} \nu'_{ki}\, k_{r_i} \prod_{j=1}^{K} [X_j]^{\nu''_{ji}} + \sum_{i=1}^{I} \nu''_{ki}\, k_{f_i} \prod_{j=1}^{K} [X_j]^{\nu'_{ji}} \qquad \text{(II.5.14)}$$

and

$$\dot{D}_k = \sum_{i=1}^{I} \nu'_{ki}\, k_{f_i} \prod_{j=1}^{K} [X_j]^{\nu'_{ji}} + \sum_{i=1}^{I} \nu''_{ki}\, k_{r_i} \prod_{j=1}^{K} [X_j]^{\nu''_{ji}} \qquad \text{(II.5.15)}$$

When third body reactions are involved, each sum in the above equation is multiplied by the factor

$$\sum_{k=1}^{K} \alpha_{ki} [X_k]$$

Another useful form for the chemical production rates is found by defining a creation rate and a characteristic time for the destruction rate, i.e.

$$\dot{\omega}_k = \dot{C}_k - \frac{[X_k]}{\tau_k} \qquad \text{(II.5.16)}$$

[CKCTYP,CKCTYR,CKCTXP, CKCTXR,CKCTC]

Here the characteristic time is given simply in terms of $\dot{D}_k$ as

$$\tau_k = \frac{[X_k]}{\dot{D}_k} \qquad \text{(II.5.17)}$$

As a precaution against $[X_k]$ and $\dot{D}_k$ simultaneously approaching zero, the coding is written as

$$\tau_k = \frac{[X_k]}{(\dot{D}_k + \varepsilon)} \qquad \text{(II.5.18)}$$

[CKCTYP,CKCTYR,CKCTXP, CKCTXR,CKCTC]

where ε is a very small number which has been programmed to be 1×10^{-99}.

6. The Partial Derivatives

Often the differential equations governing chemical rate behavior are classified as numerically stiff. In such cases, implicit numerical methods are normally required for their efficient solution. Implicit solution algorithms usually rely on having Jacobian matrices, i.e., the partial derivatives of the rate equations with respect to the dependent variables. It is for this reason that the partial derivative subroutines are included in the CHEMKIN package.

To use the derivative routines the user must first derive the terms in the Jacobian for his particular problem. This procedure usually amounts to writing out the terms by use of chain rule differentiation. Then the various CHEMKIN subroutines are called to form each term of the Jacobian.

Unfortunately, one must be very careful in deriving and using Jacobian matrices. It is important to specify what is being held constant in the differentiation. We have tried to be explicit in stating how the derivatives are taken in each of the equations in the following sections.

One of the problems in differentiating with respect to species composition is that the concentrations are not independent. Suppose, for example, that a function f depends on pressure, temperature, and the mole fractions of K species, i.e.,

$$f = f(P,T,X_1,X_2,\ldots X_K) \tag{II.6.1}$$

However, since the mole fractions are constrained to sum to 1, X_K can be considered to depend on the other X_k, i.e.,

$$X_K = X_K(X_1,X_2,\ldots,X_{K-1}) \tag{II.6.2}$$

Therefore (II.6.3)

$$\left.\frac{\partial f}{\partial X_k}\right)_{P,T,X_1,\ldots,X_{k-1},X_{k+1},\ldots X_{K-1}} = \left[\left.\frac{\partial f}{\partial X_k}\right)_{P,T,X_1,\ldots X_{k-1},X_{k+1},\ldots X_K}\right]$$

$$+ \sum_{k=1}^{K-1}\left[\left.\frac{\partial f}{\partial X_K}\right)_{P,T,X_1,\ldots X_{K-1}}\right]\left[\left.\frac{\partial X_K}{\partial X_k}\right)_{P,T,X_1,\ldots X_{k-1},X_{k+1},\ldots X_{K-1}}\right]$$

If, for example, the Kth species is given by

$$X_K = 1 - \sum_{k=1}^{K-1} X_k \tag{II.6.4}$$

then,

$$\left.\frac{\partial X_K}{\partial X_k}\right)_{P,T,X_1,\ldots X_{k-1},\ X_{k+1},\ldots X_{K-1}} = -\delta_{kK} \tag{II.6.5}$$

Thus, the constrained derivative, (II.6.6)

$$\left.\frac{\partial f}{\partial X_k}\right)_{P,T,X_1,\ldots X_{k-1},X_{k+1},\ldots X_{K-1}} = \left[\left.\frac{\partial f}{\partial X_k}\right)_{P,T,X_1,\ldots X_{k-1},X_{k+1},\ldots X_K}\right]$$

$$-\left[\left.\frac{\partial f}{\partial X_K}\right)_{P,T,X_1,\ldots X_{K-1}}\right]$$

The CHEMKIN subroutines always return unconstrained derivatives. That is, it is assumed for the purpose of differentiation that all X_k are independent. Thus, the information returned from CHEMKIN is always in the form of the first term on the right hand side of Eq. (II.6.3).

We have chosen to write the coding in this way because we believe it is the most general approach. The choice of how the constraint is handled is thus left to the user. Equation (II.6.4) is one way to impose the constraint but it is by no means the most general way. Even if Eq. (II.6.4) is the one used, a choice must be made as to which species is the dependent one.

7. Equation of State Derivatives

In this section are presented the partial derivatives of density, pressure, and mean molecular weight with respect to temperature, mass fraction, mole fraction and concentration.

Mean Molecular Weight--

$$\left.\frac{\partial \overline{W}}{\partial Y_k}\right)_{Y_{j,j\neq k}} = -\frac{\overline{W}^2}{W_k} \qquad \text{(II.7.1) [CKDWBY]}$$

$$\left.\frac{\partial \overline{W}}{\partial X_k}\right)_{X_{j,j\neq k}} = W_k \qquad \text{(II.7.2) [CKDWBX]}$$

$$\left.\frac{\partial \overline{W}}{\partial [X_k]}\right)_{[X_j]_{j\neq k}} = \frac{(W_k - \overline{W})}{\sum_{n=1}^{K} [X_n]} \qquad \text{(II.7.3) [CXDWBC]}$$

Density--

$$\left.\frac{\partial \rho}{\partial T}\right)_{P,Y_k} = -\frac{P\overline{W}}{RT^2} \qquad \text{(II.7.4) [CRDRTY]}$$

$$\left.\frac{\partial \rho}{\partial T}\right)_{P,X_k} = -\frac{P\overline{W}}{RT^2} \qquad \text{(II.7.5) [CKDRTX]}$$

$$\left.\frac{\partial \rho}{\partial T}\right)_{P,[X_k]} = -\frac{P\overline{W}}{RT^2}$$ (II.7.6) [CKDRTC]

$$\left.\frac{\partial \rho}{\partial Y_k}\right)_{P,T,Y_{j,j\neq k}} = -\frac{P\overline{W}^2}{RTW_k}$$ (II.7.7) [CKDRDY]

$$\left.\frac{\partial \rho}{\partial X_k}\right)_{P,T,X_{j,j\neq k}} = \frac{PW_k}{RT}$$ (II.7.8) [CKDRDX]

$$\left.\frac{\partial \rho}{\partial [X_k]}\right)_{P,T,[X_j]_{j\neq k}} = \frac{P}{RT}\;\frac{\left(W_k - \overline{W}\right)}{\sum_{n=1}^{K}[X_n]}$$ (II.7.9) [CKDRDC]

<u>Pressure</u>--

$$\left.\frac{\partial P}{\partial T}\right)_{\rho,Y_k} = \frac{\rho R}{\overline{W}}$$ (II.7.10) [CKDPTY]

$$\left.\frac{\partial P}{\partial T}\right)_{\rho,X_k} = \frac{\rho R}{\overline{W}}$$ (II.7.11) [CKDPTX]

$$\left.\frac{\partial P}{\partial T}\right)_{\rho,[X_k]} = \frac{\rho R}{\overline{W}}$$ (II.7.12) [CKDPTC]

$$\left.\frac{\partial P}{\partial Y_k}\right)_{\rho,T,Y_{j,j\neq k}} = \frac{\rho RT}{W_k}$$ (II.7.13) [CKDPDY]

$$\left.\frac{\partial P}{\partial X_k}\right)_{\rho,T,X_{j,j\neq k}} = -\frac{\rho RTW_k}{\overline{W}^2}$$ (II.7.14) [CKDPDX]

$$\left.\frac{\partial P}{\partial [X_k]}\right)_{\rho,T,[X_j]_{j\neq k}} = - \frac{\rho RT}{\overline{W}^2} \frac{(W_k - \overline{W})}{\sum_{n=1}^{K} [X_n]} \qquad \text{(II.7.15) [CKDPDC]}$$

8. Mole-Mass Conversion Derviatives

The following derivative functions are found to be useful when constructing chain rule expansions. As written here, all derivatives taken with respect to one species assume that all other species are held fixed. Since the species concentrations are not independent some care need be exercised in intepreting the results. The reader may refer to section 6 for a further discussion of the partial derviatives.

Mass Fraction with Respect to Mole Fraction--

$$\left.\frac{\partial Y_k}{\partial X_n}\right)_{X_{j,j\neq n}} = \delta_{kn} \frac{W_k}{\overline{W}} - \frac{X_k W_k W_n}{\overline{W}^2} \qquad \text{(II.8.1) [CKDYDX]}$$

Mole Fraction with Respect to Mass Fraction--

$$\left.\frac{\partial X_k}{\partial Y_n}\right)_{Y_{j,j\neq n}} = \delta_{kn} \frac{\overline{W}}{W_k} - \frac{Y_k \overline{W}^2}{W_k W_n} \qquad \text{(II.8.2) [CKDXDY]}$$

Molar Concentration with Respect to Mass Fraction, Pressure Fixed--

$$\left.\frac{\partial [X_k]}{\partial Y_n}\right)_{P,T,Y_{j,j\neq n}} = \frac{P}{RT}\left(\delta_{kn} \frac{\overline{W}}{W_k} - \frac{Y_k \overline{W}^2}{W_k W_n}\right) \qquad \text{(II.8.3) [CKDCYP]}$$

Molar Concentration with Respect to Mass Fraction, Density Fixed--

$$\left.\frac{\partial[X_k]}{\partial Y_n}\right)_{\rho,T,Y_{j,j\neq n}} = \delta_{kn}\ \frac{\rho}{W_k} \qquad \text{(II.8.4) [CKDCYR]}$$

Molar Concentration with Respect to Mole Fraction, Pressure Fixed--

$$\left.\frac{\partial[X_k]}{\partial X_n}\right)_{P,T,X_{j,j\neq n}} = \delta_{kn}\ \frac{P}{RT} \qquad \text{(II.8.5) [CXDCXP]}$$

Molar Concentration with Respect to Mole Fraction, Density Fixed--

$$\left.\frac{\partial[X_k]}{\partial X_n}\right)_{\rho,T,X_{j,j\neq n}} = \frac{\rho}{\overline{W}}\left(\delta_{kn} - \frac{X_k W_n}{\overline{W}}\right) \qquad \text{(II.8.6) [CKDCXR]}$$

Molar Concentration with Respect to Temperature, Pressure and Mass Fraction Fixed--

$$\left.\frac{\partial[X_k]}{\partial T}\right)_{P,Y_k} = -\frac{PY_k\overline{W}}{RT^2W_k} \qquad \text{(II.8.7) [CKDCTY]}$$

Molar Concentration with Respect to Temperature, Pressure and Mole Fraction Fixed--

$$\left.\frac{\partial[X_k]}{\partial T}\right)_{P,X_k} = -\frac{PX_k}{RT^2} \qquad \text{(II.8.8) [CKDCTX]}$$

Molar Concentration with Respect to Temperature, Density Fixed

$$\left.\frac{\partial[X_k]}{\partial T}\right)_{\rho,Y_k} = \left.\frac{\partial[X_k]}{\partial T}\right)_{\rho,X_k} = 0 \qquad \text{(II.8.9)}$$

Molar Concentration with Respect to Density, Temperature and Mass Fraction Fixed

$$\left.\frac{\partial[X_k]}{\partial \rho}\right)_{T,Y_k} = \frac{Y_k}{W_k} \qquad \text{(II.8.10) [CKDCRY]}$$

Molar Concentration with Respect to Density, Temperature and Mole Fraction Fixed

$$\left.\frac{\partial[X_k]}{\partial \rho}\right)_{T,X_k} = \frac{X_k}{\overline{W}} \qquad \text{(II.8.11) [CKDCRX]}$$

Molar Concentration with Respect to Pressure, Temperature and Mass Fraction Fixed

$$\left.\frac{\partial[X_k]}{\partial P}\right)_{T,Y_k} = \frac{\overline{W}\ Y_k}{RTW_k} \qquad \text{(II.8.12) [CKDCPY]}$$

Molar Concentration with Respect to Pressure, Temperature and Mole Fraction Fixed

$$\left.\frac{\partial[X_k]}{\partial P}\right)_{T,X_k} = \frac{X_k}{RT} \qquad \text{(II.8.13) [CKDCPX]}$$

9. Thermodynamic Property Derivatives

Since the standard state thermodynamic properties are functions of temperature alone, only temperature derivatives need to be considered. They are given in the following equations in molar units.

$$\frac{\partial C_{p_k}}{\partial T} = R \sum_{n=2}^{N} (n-1)\, a_{nk}\, T^{(n-2)} \qquad \text{(II.9.1) [CKDCPL]}$$

$$\frac{\partial H_k}{\partial T} = R \sum_{n=1}^{N} a_{nk}\, T^{(n-1)} \qquad \text{(II.9.2) [CKDHML]}$$

$$\frac{\partial S_k^o}{\partial T} = R \frac{a_{1k}}{T} + R \sum_{n=2}^{N} a_{nk}\, T^{(n-2)} \qquad \text{(II.9.3) [CKDSML]}$$

The other thermodynamic properties are written in terms of the above three.

$$\frac{\partial C_{v_k}}{\partial T} = \frac{\partial C_{p_k}}{\partial T} \qquad \text{(II.9.4) [CKDCVL]}$$

$$\frac{\partial U_k}{\partial T} = \frac{\partial H_k}{\partial T} - R \qquad \text{(II.9.5) [CKDUML]}$$

$$\frac{\partial G_k^o}{\partial T} = \frac{\partial H_k}{\partial T} - T \frac{\partial S_k^o}{\partial T} - S_k^o \qquad \text{(II.9.6) [CKDGML]}$$

$$\frac{\partial A_k^o}{\partial T} = \frac{\partial U_k}{\partial T} - T \frac{\partial S_k^o}{\partial T} - S_k^o \qquad \text{(II.9.7) [CKDAML]}$$

The property derivatives in mass units are determined simply by dividing the derivatives in molar units by the molecular weights, i.e.,

$$\frac{\partial c_{p_k}}{\partial T} = \frac{1}{W_k} \frac{\partial C_{p_k}}{\partial T}$$ (II.9.8) [CKDCPS]

$$\frac{\partial h_k}{\partial T} = \frac{1}{W_k} \frac{\partial H_k}{\partial T}$$ (II.9.9) [CKDHMS]

$$\frac{\partial s_k^o}{\partial T} = \frac{1}{W_k} \frac{\partial S_k^o}{\partial T}$$ (II.9.10) [CKDSMS]

$$\frac{\partial c_{v_k}}{\partial T} = \frac{1}{W_k} \frac{\partial C_{v_k}}{\partial T}$$ (II.9.11) [CKDCVS]

$$\frac{\partial u_k}{\partial T} = \frac{1}{W_k} \frac{\partial U_k}{\partial T}$$ (II.9.12) [CKDUMS]

$$\frac{\partial g_k^o}{\partial T} = \frac{1}{W_k} \frac{\partial G_k^o}{\partial T}$$ (II.9.13) [CKDGMS]

$$\frac{\partial a_k^o}{\partial T} = \frac{1}{W_k} \frac{\partial A_k^o}{\partial T}$$ (II.9.14) [CKDAMS]

10. Chemical Rate Expression Derivatives

In this section we give the partial derivatives of the chemical production rates with respect to temperature, pressure, density mass fraction, mole fraction, and concentration.

Temperature Derivatives, Pressure and Either Mass Fraction or Mole Fraction Held Fixed--

The temperature derivatives of the chemical production rates are found from differentiation of Eq. (II.5.2):

$$\frac{\partial \dot{\omega}_k}{\partial T} = \sum_{i=1}^{I} \nu_{ki} \frac{\partial q_i}{\partial T}$$ (II.10.1) [CKDTYP,CKDTYR,CKDTXP, CKDTXR,CKDTC]

Referring to Eq. (II.5.4) it may be seen

$$\frac{\partial q_i}{\partial T} = \frac{\partial k_{f_i}}{\partial T} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - \frac{\partial k_{r_i}}{\partial T} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}}$$

$$+ k_{f_i} \frac{\partial}{\partial T} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{r_i} \frac{\partial}{\partial T} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}} \qquad \text{(II.10.2)}$$

Since the concentrations are functions of the state of the gas, care must be taken in specifying which variables are being held constant. The rate constants, which are functions of temperature alone, may be differentiated as follows.

$$\frac{\partial k_{f_i}}{\partial T} = \frac{\partial}{\partial T}\left[A_i \; T^{\beta_i} \; e^{-(E_i/R_c T)}\right]$$

$$= A_i \; \beta_i \; T^{\beta_i - 1} \; e^{-(E_i/R_c T)} + A_i \; T^{\beta_i} \left(\frac{E_i}{R_c T^2}\right) e^{-(E_i/R_c T)}$$

$$= \frac{k_{f_i}}{T}\left(\beta_i + \frac{E_i}{R_c T}\right) \qquad \text{(II.10.3)}$$

The reverse rate constants, defined by Eq. (II.5.6), are also functions of temperature alone and are differentiated below.

$$\frac{\partial k_{r_i}}{\partial T} = \frac{1}{K_{c_i}} \frac{\partial k_{f_i}}{\partial T} - \frac{k_{f_i}}{K_{c_i}^2} \frac{\partial K_{c_i}}{\partial T} \qquad \text{(II.10.4)}$$

where, from Eq. (II.5.7), it may be seen that:

$$\frac{\partial K_{c_i}}{\partial T} = \frac{\partial K_{p_i}}{\partial T} \left(\frac{P_{atm}}{RT}\right)^{\sum_{k=1}^{K} \nu_{ki}} - K_{p_i}\left(\sum_{k=1}^{K} \nu_{ki}\right)\left(\frac{P_{atm}}{RT}\right)\left[\left(\sum_{k=1}^{K} \nu_{ki}\right) - 1\right]\left(\frac{P_{atm}}{RT^2}\right)$$

which is condensed to

$$\frac{\partial K_{c_i}}{\partial T} = \left(\frac{P_{atm}}{RT}\right)^{\sum_{k=1}^{K} \nu_{ki}} \left[\frac{\partial K_{p_i}}{\partial T} - \frac{K_{p_i}}{T} \sum_{k=1}^{K} \nu_{ki}\right] \tag{II.10.5}$$

From its definition, Eq. (II.5.8), K_{p_i} is differentiated as follows.

$$\frac{\partial K_{p_i}}{\partial T} = \frac{\partial}{\partial T}\left[\exp\left(\frac{\Delta S_i^o}{R} - \frac{\Delta H_i^o}{RT}\right)\right]$$

$$= K_{p_i}\left[\frac{\partial}{\partial T}\left(\frac{\Delta S_i^o}{R} - \frac{\Delta H_i^o}{RT}\right)\right] \tag{II.10.6}$$

where

$$\frac{\partial}{\partial T}\left(\frac{\Delta S_i^o}{R} - \frac{\Delta H_i^o}{RT}\right) = \sum_{k=1}^{K} \nu_{ki} \frac{\partial}{\partial T}\left(\frac{S_k^o}{R} - \frac{H_k^o}{RT}\right) \tag{II.10.7}$$

Then from Eqs. (II.9.2) and (II.9.3) it may be found that

$$\frac{\partial}{\partial T}\left(\frac{S_k^o}{R} - \frac{H_k^o}{RT}\right) = \sum_{n=1}^{N} \frac{a_{nk} T^{(n-2)}}{n} + \frac{a_{N+1,k}}{T^2} \tag{II.10.8}$$

Consider now the temperature derivatives of the molar concentration products which appear in Eq. (II.10.2).

$$\frac{\partial}{\partial T} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} = \sum_{k=1}^{K} \nu'_{ki} [X_k]^{(\nu'_{ki}-1)} \frac{\partial [X_k]}{\partial T} \prod_{\substack{j=1 \\ j\neq k}}^{K} [X_j]^{\nu'_{ji}} \tag{II.10.9}$$

A similar expression is found for the last term in Eq. (II.10.2) except that ν'_{ki} is replaced by ν''_{ki}. Note also that if no $[X_k]$'s are zero then Eq. (II.10.9) may be reduced to

$$\frac{\partial}{\partial T}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} = \left(\sum_{k=1}^{K}\nu'_{ki}[X_k]^{-1}\frac{\partial[X_k]}{\partial T}\right)\left(\prod_{k=1}^{K}[X_k]^{\nu'_{ki}}\right) \qquad \text{(II.10.10)}$$

The temperature derivatives of concentration, depending on what is being held constant, are given by Eqs. (II.8.7) through (II.8.9).

Consider now the slightly more complicated form of the rate of progress variable when third body interactions are included. In this case Eq. (II.5.11) is differentiated as follows.

$$\frac{\partial q_i}{\partial T} = \frac{\partial}{\partial T}\left(\sum_{k=1}^{K}\alpha_{ki}[X_k]\right)\left(k_{f_i}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} - k_{r_i}\prod_{k=1}^{K}[X_k]^{\nu''_{ki}}\right) \qquad \text{(II.10.11)}$$

$$+\left(\sum_{k=1}^{K}\alpha_{ki}[X_k]\right)\frac{\partial}{\partial T}\left(k_{f_i}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} - k_{r_i}\prod_{k=1}^{K}[X_k]^{\nu''_{ki}}\right)$$

All terms in the above expression have already been evaluated except

$$\frac{\partial}{\partial T}\left(\sum_{k=1}^{K}\alpha_{ki}[X_k]\right) = \sum_{k=1}^{K}\alpha_{ki}\frac{\partial[X_k]}{\partial T} \qquad \text{(II.10.12)}$$

All the intermediate steps needed to evaluate the temperature derivatives of the production rates of the kth species, Eq. (II.10.1), have now been completed.

Mass Fraction Derivatives, Temperature and Either Pressure or Density Held Fixed--

To obtain the mass fraction derivatives of the species production rates differentiate Eq. (II.5.2) as

$$\frac{\partial\dot{\omega}_k}{\partial Y_n} = \sum_{i=1}^{I}\nu_{ki}\frac{\partial q_i}{\partial Y_n} \qquad \text{(II.10.13)}$$

[CKDWYP,CKDWYR]

Differentiation of Eq. (II.5.4), noting that k_{f_i} and k_{r_i} are functions of temperature alone, yields

$$\frac{\partial q_i}{\partial Y_n} = k_{f_i} \frac{\partial}{\partial Y_n} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{r_i} \frac{\partial}{\partial Y_n} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}} \tag{II.10.14}$$

where

$$\frac{\partial}{\partial Y_n} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} = \sum_{k=1}^{K} \nu'_{ki} [X_k]^{(\nu'_{ki}-1)} \frac{\partial [X_k]}{\partial Y_n} \prod_{\substack{j=1 \\ j\neq k}}^{K} [X_j]^{\nu'_{ji}} \tag{II.10.15}$$

A similar expression is of course found for the second term in Eq. (II.10.15) where ν'_{ki} is replaced by ν''_{ki}. As with the temperature derivatives, note that if none of the $[X_k]$ are zero then Eq. (II.10.15) may be reduced to

$$\frac{\partial}{\partial Y_n} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} = \left(\sum_{k=1}^{K} \nu'_{ki} [X_k]^{-1} \frac{\partial [X_k]}{\partial Y_n} \right) \left(\prod_{k=1}^{K} [X_k]^{\nu'_{ki}} \right) \tag{II.10.16}$$

In the above equations the mass fraction derivatives of molar concentration are given by either Eq. (II.8.3) or (II.8.4) depending on whether pressure or density is held fixed.

The derivatives of the rate of progress variable when third body interactions are included are given by differentiation of Eq. (II.5.11).

$$\frac{\partial q_i}{\partial Y_n} = \frac{\partial}{\partial Y_n} \left(\sum_{k=1}^{K} \alpha_{ki} [X_k] \right) \left(k_{f_i} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{r_i} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}} \right)$$

$$+ \left(\sum_{k=1}^{K} \alpha_{ki} [X_k] \right) \left(k_{f_i} \frac{\partial}{\partial Y_n} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{r_i} \frac{\partial}{\partial Y_n} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}} \right) \tag{II.10.17}$$

All terms in the above expression have already been evaluated except

$$\frac{\partial}{\partial Y_n}\left(\sum_{k=1}^{K} \alpha_{ki}\,[X_k]\right) = \sum_{k=1}^{K} \alpha_{ki}\,\frac{\partial [X_k]}{\partial Y_n} \qquad \text{(II.10.18)}$$

where $\partial[X_k]/\partial Y_n$ is given by either Eq. (II.8.3) or (II.8.4) depending on whether pressure or density is held fixed.

Mole Fraction Derivatives, Temperature and Either Pressure or Density Held Fixed--

Mole fraction derivatives of the species production rates are found by differentiation of Eq. (II.5.2) as

$$\frac{\partial \dot{\omega}_k}{\partial X_n} = \sum_{i=1}^{I} \nu_{ki}\,\frac{\partial q_i}{\partial X_n} \qquad \text{(II.10.19)}$$

[CKDWXP,CKDWXR]

Noting that k_{f_i} and k_{r_i} are functions of temperature alone, Eq. (II.4.4) is differentiated as follows

$$\frac{\partial q_i}{\partial X_n} = k_{f_i}\,\frac{\partial}{\partial X_n}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} - k_{r_i}\,\frac{\partial}{\partial X_n}\prod_{k=1}^{K}[X_k]^{\nu''_{ki}} \qquad \text{(II.10.20)}$$

where

$$\frac{\partial}{\partial X_n}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} = \sum_{k=1}^{K} \nu'_{ki}\,[X_k]^{(\nu'_{ki}-1)}\,\frac{\partial [X_k]}{\partial X_n}\prod_{\substack{j=1\\ j\neq k}}^{K}[X_j]^{\nu'_{ji}} \qquad \text{(II.10.21)}$$

A similar expression is found for the second term in Eq. (II.10.20) where ν'_{ki} is replaced by ν''_{ki}. Again note that if all $[X_k]$ are non-zero then Eq. (II.10.21) may be reduced to

$$\frac{\partial}{\partial X_n}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} = \left(\sum_{k=1}^{K} \nu'_{ki}\,[X_k]^{-1}\,\frac{\partial [X_k]}{\partial X_n}\right)\left(\prod_{k=1}^{K}[X_k]^{\nu'_{ki}}\right) \qquad \text{(II.10.22)}$$

In the above equations the mole fraction derivatives of molar concentration are given by either Eq. (II.8.5) or (II.8.6) depending on whether pressure or density is held fixed. The derivatives of the rate of progress variable

when third body interactions are included are given by differentiations of Eq. (II.5.11).

$$\frac{\partial q_i}{\partial X_n} = \frac{\partial}{\partial X_n}\left(\sum_{k=1}^{K} \alpha_{ki}\,[X_k]\right)\left(k_{f_i}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} - k_{r_i}\prod_{k=1}^{K}[X_k]^{\nu''_{ki}}\right)$$

$$+\left(\sum_{k=1}^{K} \alpha_{ki}\,[X_k]\right)\left(k_{f_i}\frac{\partial}{\partial X_n}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} - k_{r_i}\frac{\partial}{\partial X_n}\prod_{k=1}^{K}[X_k]^{\nu''_{ki}}\right) \qquad \text{(II.10.23)}$$

All terms in the above expression have already been evaluated except

$$\frac{\partial}{\partial X_n}\left(\sum_{k=1}^{K} \alpha_{ki}\,[X_k]\right) = \sum_{k=1}^{K} \alpha_{ki}\,\frac{\partial [X_k]}{\partial X_n} \qquad \text{(II.10.24)}$$

where $\partial[X_k]/\partial X_n$ is given by either Eq. (II.8.5) or (II.8.6) depending on whether pressure or density is held fixed.

Concentration Derivatives, Temperature and Either Pressure or Density Held Fixed

To obtain molar concentration derivatives of the species production rates differentiate Eq. (II.5.2) as follows.

$$\frac{\partial \dot{\omega}_k}{\partial [X_n]} = \sum_{i=1}^{I} \nu_{ki}\,\frac{\partial q_i}{\partial [X_n]} \qquad \text{(II.10.25) [CKDWC]}$$

Since k_{f_i} and k_{r_i} are functions of temperature alone, differentiation of Eq. (II.5.4) yields

$$\frac{\partial q_i}{\partial [X_n]} = k_{f_i}\,\frac{\partial}{\partial [X_n]}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} - k_r\,\frac{\partial}{\partial [X_n]}\prod_{k=1}^{K}[X_K]^{\nu''_{ki}} \qquad \text{(II.10.26)}$$

where

$$\frac{\partial}{\partial [X_n]}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} = \sum_{k=1}^{K} \nu'_{ki}\,[X_k]^{\nu'_{ki}-1}\,\frac{\partial [X_k]}{\partial [X_n]}\prod_{\substack{j=1\\ j\neq k}}^{K}[X_j]^{\nu'_{ji}} \qquad \text{(II.10.27)}$$

A similar expression is of course found for the second term in Eq. (II.10.26) where ν'_{ki} is replaced by ν''_{ki}. Since $\partial[X_k]/\partial[X_n]$ equals 0 for $k \neq n$ and 1 for $k=n$, the summation is not needed, thus

$$\frac{\partial}{\partial[X_n]} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} = \nu'_{ni} [X_n]^{\nu'_{ni}-1} \prod_{\substack{j=1 \\ j \neq n}}^{K} [X_j]^{\nu'_{ji}} \tag{II.10.28}$$

Furthermore, if all $[X_k]$ are non-zero the expression can be reduced to

$$\frac{\partial}{\partial[X_n]} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} = \nu'_{ni} [X_n]^{-1} \prod_{j=1}^{K} [X_j]^{\nu'_{ji}} \tag{II.10.29}$$

The derivatives of the rate of progress variable when third body interactions are included are given by differentiation of Eq. (II.5.11)

$$\frac{\partial q_i}{\partial[X_n]} = \frac{\partial}{\partial[X_n]}\left(\sum_{k=1}^{K} \alpha_{ki} [X_k]\right)\left(k_{f_i} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{r_i} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}}\right) \tag{II.10.30}$$

$$+ \left(\sum_{k=1}^{K} \alpha_{ki} [X_k]\right)\left(k_{f_i} \frac{\partial}{\partial[X_n]} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{r_i} \frac{\partial}{\partial[X_n]} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}}\right)$$

All terms in the above expression have already been evaluated except

$$\frac{\partial}{\partial[X_n]}\left(\sum_{k=1}^{K} \alpha_{ki} [X_k]\right) = \alpha_{ni} \tag{II.10.31}$$

<u>Pressure Derivatives, Temperature and Either Mass Fraction or Mole Fraction Held Fixed--</u>

To obtain the pressure derivatives of the species production rates differentiate Eq. (II.5.2) as

$$\frac{\partial \dot{\omega}_k}{\partial P} = \sum_{i=1}^{I} \nu_{ki} \frac{\partial q_i}{\partial P} \tag{II.10.32}$$

[CKDWPY,CKDWPX]

Differentiation of Eq. (II.5.4), noting that k_{f_i} and k_{r_i} are functions of temperature alone, yields

$$\frac{\partial q_i}{\partial p} = k_{f_i} \frac{\partial}{\partial p} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{r_i} \frac{\partial}{\partial p} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}} \tag{II.10.33}$$

where

$$\frac{\partial}{\partial p} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} = \sum_{k=1}^{K} \nu'_{ki} [X_k]^{(\nu'_{ki}-1)} \frac{\partial [X_k]}{\partial p} \prod_{\substack{j=1 \\ j \neq k}}^{K} [X_j]^{\nu'_{ji}} \tag{II.10.34}$$

A similar expression is of course found for the second term in Eq. (II.10.34) where ν'_{ki} is replaced by ν''_{ki}. As with the temperature derivatives, note that if none of the $[X_k]$ are zero then Eq. (II.10.34) may be reduced to

$$\frac{\partial}{\partial p} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} = \left(\sum_{k=1}^{K} \nu'_{ki} [X_k]^{-1} \frac{\partial [X_k]}{\partial p} \right) \left(\sum_{k=1}^{K} [X_k]^{\nu'_{ki}} \right) \tag{II.10.35}$$

In the above equations the pressure derivatives of molar concentration are given by either Eq. (II.8.12) or (II.8.13) depending on whether mass fraction or mole fraction is held fixed.

The derivatives of the rate of progress variable when third body interactions are included are given by differentiation of Eq. (II.5.11).

$$\frac{\partial q_i}{\partial p} = \frac{\partial}{\partial p} \left(\sum_{k=1}^{K} \alpha_{ki} [X_k] \right) \left(k_{f_i} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{r_i} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}} \right)$$

$$+ \left(\sum_{k=1}^{K} \alpha_{ki} [X_k] \right) \left(k_{f_i} \frac{\partial}{\partial p} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{r_i} \frac{\partial}{\partial p} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}} \right) \tag{II.10.36}$$

All terms in the above expression have already been evaluated except

$$\frac{\partial}{\partial p} \left(\sum_{k=1}^{K} \alpha_{ki} [X_k] \right) = \sum_{k=1}^{K} \alpha_{ki} \frac{\partial [X_k]}{\partial p} \tag{II.10.37}$$

where $\partial[X_k]/\partial P$ is given by either Eq. (II.8.12) or (II.8.13) depending on whether mass fraction or mole fraction is held fixed.

Density Derivatives, Temperature and Either Mass Fraction or Mole Fraction Held Fixed--

To obtain the density derivatives of the species production rates differentiate Eq. (II.5.2) as

$$\frac{\partial \dot{\omega}_k}{\partial \rho} = \sum_{i=1}^{I} \nu_{ki} \frac{\partial q_i}{\partial \rho} \qquad \text{(II.10.38)}$$

[CKDWRY,CKDWRX]

Differentiation of Eq. (II.5.4), noting that k_{f_i} and k_{r_i} are functions of temperature alone, yields

$$\frac{\partial q_i}{\partial \rho} = k_{f_i} \frac{\partial}{\partial \rho} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{r_i} \frac{\partial}{\partial \rho} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}} \qquad \text{(II.10.39)}$$

where

$$\frac{\partial}{\partial \rho} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} = \sum_{k=1}^{K} \nu'_{ki} [X_k]^{(\nu'_{ki}-1)} \frac{\partial [X_k]}{\partial \rho} \prod_{\substack{j=1 \\ j \neq k}}^{K} [X_j]^{\nu'_{ji}} \qquad \text{(II.10.40)}$$

A similar expression is of course found for the second term in Eq. (II.10.40) where ν'_{ki} is replaced by ν''_{ki}. As with the temperature derivatives, note that if none of the $[X_k]$ are zero then Eq. (II.10.40) may be reduced to

$$\frac{\partial}{\partial \rho} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} = \left(\sum_{k=1}^{K} \nu'_{ki} [X_k]^{-1} \frac{\partial [X_k]}{\partial \rho} \right) \left(\prod_{k=1}^{K} [X_k]^{\nu'_{ki}} \right) \qquad \text{(II.10.41)}$$

In the above equations the density derivatives of molar concentration are given by either Eq. (II.8.10) or (II.8.11) depending on whether mass fraction or mole fraction is held fixed.

The derivatives of the rate of progress variable when third body interactions are included are given by differentiation of Eq. (II.5.11).

$$\frac{\partial q_i}{\partial \rho} = \frac{\partial}{\partial \rho}\left(\sum_{k=1}^{K} \alpha_{ki}\,[X_k]\right)\left(k_{f_i}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} - k_{r_i}\prod_{k=1}^{K}[X_k]^{\nu''_{ki}}\right)$$

$$+\left(\sum_{k=1}^{K} \alpha_{ki}\,[X_k]\right)\left(k_{f_i}\frac{\partial}{\partial \rho}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} - k_{r_i}\frac{\partial}{\partial \rho}\prod_{k=1}^{K}[X_k]^{\nu''_{ki}}\right) \qquad \text{(II.10.42)}$$

All terms in the above expression have already been evaluated except

$$\frac{\partial}{\partial \rho}\left(\sum_{k=1}^{K} \alpha_{ki}\,[X_k]\right) = \sum_{k=1}^{K} \alpha_{ki}\,\frac{\partial [X_k]}{\partial \rho} \qquad \text{(II.10.43)}$$

where $\partial[X_k]/\partial\rho$ is given by either Eq. (II.8.10) or (II.8.11) depending on whether mass fraction or mole fraction is held fixed.

11. Sensitivity Parameters

There is often a great deal of uncertainty in the rate constants for a reaction mechanism. It is, therefore, desirable to have an ability to quantify the effect of an uncertain parameter on the solution to a problem. Sensitivity analysis (cf., Ref. 4 or 5) is a technique which is used to help achieve this end. To apply a sensitivity analysis to a chemical rate mechanism it is necessary to have partial derivatives of the production rates of the K species with respect to parameters in the rate constants for the I chemical reactions.

Consider differentiating the chemical production rate of the kth species, $\dot{\omega}_k$, with respect to the forward rate constant of the ith reaction, k_{f_i}. Begin by rewriting Eqs. (II.5.2) through (II.5.6) to yield an expression for the production rate of the kth species in terms of k_{f_i}

$$\dot{\omega}_k = \sum_{i=1}^{I} \nu_{ki}\left(k_{f_i}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} - \frac{k_{f_i}}{K_{c_i}}\prod_{k=1}^{K}[X_k]^{\nu''_{ki}}\right) \qquad \text{(II.11.1)}$$

Differentiation with respect to k_{f_i} readily yields

$$\frac{\partial \dot{\omega}_k}{\partial k_{f_i}} = \nu_{ki}\left(\prod_{k=1}^{k} [X_k]^{\nu'_{ki}} - \frac{1}{K_{c_i}} \prod_{k=1}^{k} [X_k]^{\nu''_{ki}}\right) \qquad \text{(II.11.2)}$$

[CKSKYP,CKSKYR,CXSKXP, CXSKXR,CKSKC]

Since the rate constant k_{f_i} is specified in terms of the parameters A_i, β_i, and E_i in Eq. (II.5.5) it may be useful to have the partial derivatives with respect to these parameters besides with respect to the overall rate constant. Differentiation of Eq. (II.5.5), together with Eq. (II.11.2), easily yields the required relationships

$$\frac{\partial \dot{\omega}_k}{\partial A_i} = \frac{\partial \dot{\omega}_k}{\partial k_{f_i}} \frac{\partial k_{f_i}}{\partial A_i} = T^{\beta_i} \exp(-E_i/R_c T) \frac{\partial \dot{\omega}_k}{\partial k_{f_i}} \qquad \text{(II.11.3)}$$

[CKSAYP,CKSAYR,CKSAXP, CKSAXR,CKSAC]

$$\frac{\partial \dot{\omega}_k}{\partial \beta_i} = \frac{\partial \dot{\omega}_k}{\partial k_{f_i}} \frac{\partial k_{f_i}}{\partial \beta_i} = A_i T^{\beta_i} \ln (T) \exp(-E_i/R_c T) \frac{\partial \dot{\omega}_k}{\partial k_{f_i}} \qquad \text{(II.11.4)}$$

[CKSBYP,CKSBYR,CKSBXP, CKSBXR,CKSBC]

$$\frac{\partial \dot{\omega}_k}{\partial E_i} = \frac{\partial \dot{\omega}_k}{\partial k_{f_i}} \frac{\partial k_{f_i}}{\partial E_i} = - \frac{A_i}{RT} T^{\beta_i} \exp(-E_i/R_c T) \frac{\partial \dot{\omega}_k}{\partial k_{f_i}} \qquad \text{(II.11.5)}$$

[CKSEYP,CKSEYR,CKSEXP, CKSEXR,CKSEC]

Note that if a reaction is a three body reaction then Eq. (II.11.1) would be modified as in Eq. (II.5.11) to be

$$\dot{\omega}_k = \sum_{i=1}^{I} \nu_{ik} \left(\sum_{k=1}^{K} \alpha_{ki} [X_k]\right)\left(k_{f_i} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - \frac{k_{f_i}}{K_{c_i}} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}}\right) \qquad \text{(II.11.6)}$$

Eq. (II.9.2) would therefore be modified as

$$\frac{\partial \dot{\omega}_k}{\partial k_{f_i}} = \nu_{ki}\left(\sum_{k=1}^{K} \alpha_{ki}[X_k]\right)\left(\prod_{k=1}^{K} [X_k]^{\nu_{ki}} - \frac{1}{K_{c_i}} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}}\right) \qquad \text{(II.11.7)}$$

for third body reactions.

III. The Mechanics of Using CHEMKIN

Using the CHEMKIN package requires the manipulation of a number of programs, subroutines, and data files. This chapter describes the structure of the package and the job control logic which is required to execute a program using the package. In Chapter IV are details on how to specify reaction and thermodynamic information. The subroutine descriptions for the Gas-Phase Subroutine Library are given in Chapters V and VI.

1. Structure of CHEMKIN

The general structure of the CHEMKIN package is shown in Figure 2. The INTERPRETER is a program which reads a symbolic description of a reaction mechanism, and then extracts the needed thermodynamic data for each species involved from the Thermodynamic Data Base. The primary output from the INTERPRETER is a binary file which we call the Linking File. This file contains numerical information which describes the elements, species, and reaction mechanism.

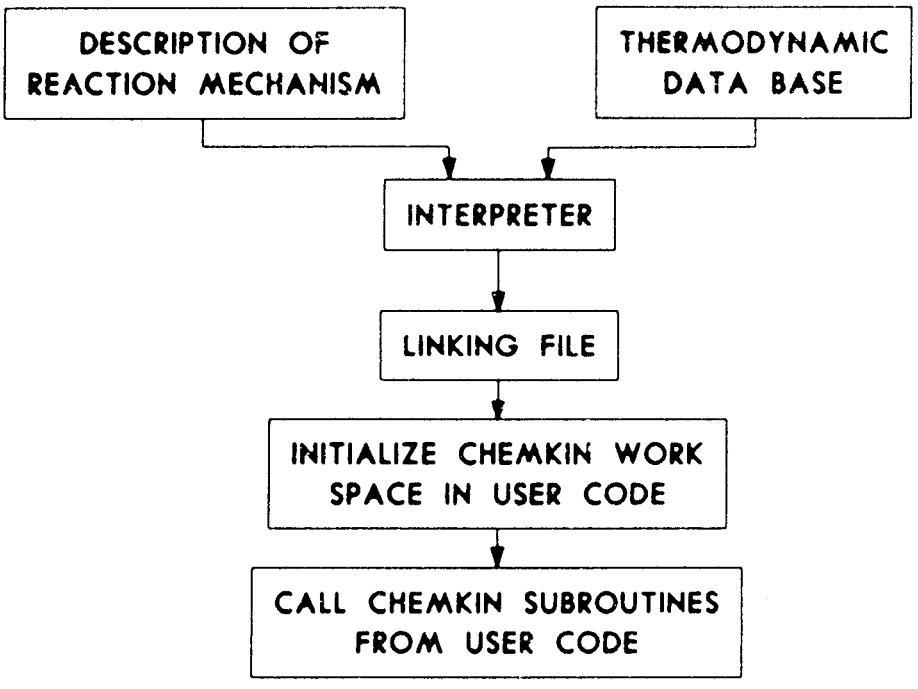

Figure 2. Structure of the CHEMKIN package

In addition to the Linking File, four other files are needed by the INTERPRETER. The input to the INTERPRETER is read from file LIN (programmed as TAPE5) and printed output is directed to LOUT (programmed as TAPE6). The printed output contains a listing of the elements, species, and the reaction mechanism, and it provides diagnostic error messages if they should be needed.

The Linking File is written on LINK (programmed as TAPE95). The logical file number for LINK must be declared both in the INTERPRETER (so it can be written) and in the user code (so that it can be read by the initialization subroutine).

At least one, but usually two, files are needed by the INTERPRETER to manipulate the thermodynamic data. Details on the format of the thermodynamic data are found in Section IV.2. The Thermodynamic Data Base is assumed to be on file LTHRM (programmed as TAPE91). Internal to the INTERPRETER the thermodynamic properties are manipulated on LDATA (programmed as TAPE93). LTHRM can be a large file which contains information on many species, most of which are not needed for any given problem. Data can also be read from input which will add to or override data on LTHRM. Also, all the thermodynamic data can be read from input and the Thermodynamic Data Base does not need to be used. The file LDATA is used by the INTERPRETER to store properties of only those species which appear in the particular reaction mechanism which is being considered.

Once the INTERPRETER has been executed and the Linking File created,* the user is ready to use the Gas-Phase Subroutine Library. These subroutines are called from the user's FORTRAN code. The user's first step must be to dimension two work arrays (one integer and one floating point) and then call the initialization subroutine, CKINIT, (see Section V.1) to create the work arrays from the Linking File. These work arrays are required input to every other subroutine in the CHEMKIN package.

Selection of which of the CHEMKIN subroutines are needed for any given problem begins by finding the appropriate equations in Chapter II. Most

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*The Linking File will not be created if there are errors in the INTERPRETER input.

equations give a reference to a subroutine name for which the input and output lists are described in Chapters V and VI. Normally only a few of the subroutines in the package would be called for any one problem. Therefore, the subroutine package should be implemented in a library format so that only those routines which are actually called by the user's code are loaded at the time of execution.

2. Job Control

Listed here is a brief outline of the required steps to run a program using CHEMKIN. It is assumed that the INTERPRETER is already in a compiled form and that a library of the precompiled CHEMKIN gas-phase subroutines has been created.

1. Execute the INTERPRETER

   File declaration:

   Input

   LIN (default TAPE5) - Card image input
   LTHRM (default TAPE91) - Thermodynamic Data Base
   (If all thermodynamic data come from input, LIN, then LTHRM need not be present.)

   Scratch

   LDATA (default TAPE93) - Coded

   Output

   LOUT (default TAPE6) - Print file
   LINK (default TAPE95) - Binary file used later as input to the gas-phase subroutine package

2. Compile user's code

3. Execute user's code along with any Referenced CHEMKIN subroutines.

   The CHEMKIN subroutines should be in a library in precompiled form.

   File declaration:

   Input

   LINK (default TAPE95) - The binary file created by the INTERPRETER.

   Any other files needed by the user code.

The following is an example of the NOS-BE control cards which are needed to execute a program that uses CHEMKIN.

Instruction	Meaning
ATTACH,INTERP,ID=INTERP.	Get INTERPRETER
ATTACH,TAPE91,THRMDAT,ID=THRMDAT.	Get Thermodynamic Data Base
INTERP.	Execute INTERPRETER and create Linking File
FTN.	Compile Users Code
ATTACH,CKLIB,ID=CKLIB.	Get Gas-Phase Subroutine Library
LDSET(LIB=CKLIB)	Collect and load CHEMKIN subroutines which are referenced in User's Code
LGØ.	Execute User's Code

(end of record)

CHEMKIN INTERPRETER input

(end of record)

User's Fortran Code

(end of record)

User's input

(end of record)

IV. Using the INTERPRETER

The INTERPRETER is used to read (from file LIN) a symbolic description of an elementary chemical reaction mechanism, and create a file (LINK) of numerical information about that mechanism. The LINK file is subsequently accessed by various subroutines to provide information on equation of state, thermodynamic properties, and chemical production rates. The four types of input required to the INTERPRETER are information on elements, thermodynamic data, species, and the reaction mechanism.

Input information on file LIN is given in 80-column card image format. Element Cards are read first. THERMO cards (if used) are second, followed by Species Cards, with Reaction Cards last. The THERMO cards are optional. The Thermodynamic data for the species may come from input (file LIN) or it may come entirely from a data base (file LTHRM). The syntax for the four types of input is described in the following sections.

With the exception of the thermodynamic data all input is format free. For the thermodynamic data we have chosen to use the same format as used in the NASA Chemical Equilibrium code by Gordon and McBride.[3] Since this code is already in wide use, the data base provided with it is an excellent source of thermodynamic data.

1. Element Cards

All chemical species in the reaction mechanism must be composed of chemical elements or isotopes of chemical elements. Each element and isotope must be identified on an Element Card (or cards). The elements and isotopes are all identified by one- or two-character symbols. The purpose of the Element Cards is to associate atomic weights of the elements with their character symbol representations, and to identify the order in which arrays of element information in the Gas-Phase Subroutine Library are referenced. For example, an array of atomic weights for the elements would be in exactly the same order in which the elements were declared on the Element Cards. In other

words if the atomic weights were stored in an array AWT, then AWT(3) would be the atomic weight of the third element declared on the Element Cards.

For the elements which appear on the periodic chart,* the INTERPRETER has the atomic weight (g/mole) stored internally. For isotopes a one- or two-character symbol must be defined to identify the isotope, and both the symbol and the atomic weight (g/mole) of the isotope must be read in. The same symbol must be used in the thermodynamic data to identify the elemental make-up of species involving the isotope. Once an isotope has been so defined, it is treated exactly as a new element.

The first Element Card must contain the word ELEMENTS starting in Column 1. It is then followed by any number of cards which specify the elements. Element symbols may appear anywhere on the cards, but elements on the same card must be separated by blanks. After all elements are stated, the following card must contain the word END starting in Column 1.

If an element is on the periodic chart, then only the symbol identifying the element need appear on the Element Card. For isotopes the atomic weights must follow the identifying symbol and be delimited by slashes (/). The atomic weights may be in integer, floating point, or E format (e.g., 2, 2.0, .2E1). For example, the isotope deuterium could be identified as D/2.014/. In addition, if desired, the atomic weight of an element in the periodic chart may be altered by including the atomic weight as input just as though the element were an isotope.

Several equivalent ways to describe element information are shown in Figure 3. In this example the elements are hydrogen, oxygen and nitrogen, and the isotope deuterium. Table I summarizes the rules for Element Cards.

---

*The elements that CHEMKIN recognizes are:

H	HE	LI	BE	B	C	N	O	F	NE
NA	MG	AL	SI	P	S	CL	AR	K	CA
SC	TI	V	CR	MN	FE	CO	NI	CU	ZN
GA	GE	AS	SE	BR	KR	RB	SR	Y	ZR
NB	MO	TC	RU	RH	PD	AG	CD	IN	SN
SB	TE	I	XE	CS	BA	LA	CE	PR	ND
PM	SM	EU	GD	TB	DY	HO	ER	TM	YB
LU	HF	TA	W	RE	OS	IR	PT	AU	HG
TL	PB	BI	PO	AT	RN	FR	RA	AC	TH
PA	U	NP	PU	AM	CM	BK	CF	ES	FM

```
ELEMENTS
H          D  /2.014/        O        N
END


ELEMENTS
     H       D/2.014/
           O        N
END
```

Figure 3. Equivalent Ways to Describe Element Information

TABLE I. SUMMARY OF THE RULES FOR ELEMENT CARDS

1. The first (last) Element Card must contain the word ELEMENTS (END) starting in Column 1. All other columns on this card are ignored.
2. Element or isotope names are either one- or two-character symbols.
3. An isotope name (i.e., a name not on the periodic chart) must be followed by its atomic weight (g/mole) delimited by slashes.
4. Each element or isotope may be declared only once.
5. The element or isotope declarations may appear anywhere on the cards.
6. Any number of element or isotope declarations may appear on a card. Thus more than one card may be used.
7. Element or isotope declarations which appear on the same card must be separated by at least one blank space.
8. An element or isotope declaration which begins on one card may not continue to the next card.
9. An element or isotope declaration may end in Column 80 of one card and the next declaration may begin in Column 1 of the next card.
10. Any blank spaces between the isotope symbol and the first slash are ignored and any blank spaces between the slashes and the atomic weight are also ignored. However, no blank spaces are allowed within the atomic weight.

2. Thermodynamic Data

Any chemical species which appears in a problem must have thermodynamic data associated with it. These data may be either extracted from a data base (file LTHRM), or read from input (file LIN), or a combination of both. If all the thermodynamic data are to be extracted from the data base, then no thermodynamic card input is required. However, if the user wishes to override information in the data base or to provide data on species not in the data base, then card input is needed. In any case the format for the information is always the same.

The format used (see Table II) is a minor modification of that used by Gordon and McBride[3] for the thermodynamic data base in the NASA Chemical Equilibrium code. Our modification allows for the possibility of a different midpoint temperature for the fits to the properties of each chemical species. We also allow a species to be composed of a maximum of five elements, not four. However, the formatting is such that the CHEMKIN INTERPRETER can use the NASA data base directly without any modification.

As indicated in Table II, the pertinent information includes the species name, the elemental make up of the species, and the temperature ranges over which the polynomial fits to thermodynamic data are valid. The fits to C_p°/R, H°/RT, and S°/R consist of seven coefficients for two temperature ranges [see Eqs. (II.4.6) through (II.4.8)].

When thermodynamic card input is required, it must immediately follow the Element Cards. The first thermodynamic card must contain the word THERMO starting in Column 1. If all the thermodynamic data are in card input, then the first card must read THERMO ALL and the code will not expect a thermodynamic data base from file LTHRM. The subsequent thermodynamic cards are in the format of Cards 3 through 6 of Table II. If the THERMO ALL option is used, the following card must be Card 2 of Table II. For the THERMO option the midpoint temperature is taken from the Card 2 information already given in the data base. As many species as needed can be included as THERMO input. The card following the last thermodynamic input must contain the word END beginning in Column 1.

TABLE II. FORMAT FOR THERMODYNAMIC DATA

Card Number	Contents	Format	Card Column
1	THERMO (or THERMO ALL[a])	6A1	1 to 6 (and 8 to 10[a])
2[b]	Temperature ranges for 2 sets of coefficients: lowest T, common T, and highest T	3F10.0	1 to 30
3	Species name (must start in Column 1)	18A1	1 to 18
	Date (not used in the code)	6A1	19 to 24
	Atomic symbols and formula	4(2A1,I3)	25 to 44
	Phase of species (S,L, or G for solid liquid, or gas, respectively)	A1	45
	Low temperature	E10.0	46 to 55
	High temperature	E10.0	56 to 65
	Common temperature (if needed) (blank for default)	E8.0	66 to 73
	Atomic symbols and formula (if needed) (blank for default)	2A1,I3	74 to 78
	The integer "1"	I1	80
4	Coefficients a_1-a_5, in Eqs. (II.4.6)-(II.4.8), for upper temperature interval	5(E15.0)	1 to 75
	The integer "2"	I1	80
5	Coefficients a_6, a_7 for upper temperature interval, and a_1, a_2, and a_3 for lower	5(E15.0)	1 to 75
	The integer "3"	I1	80
6	Coefficients a_4, a_5, a_6, a_7 for lower temperature interval	4(E15.0)	1 to 60
	The integer "4"	I1	80
(a)	Repeat Cards 3 through 6 for each species		
(Final card)	END (Indicates end of thermodynamic data)	3A1	1 to 3

[a]Use only when all the thermodynamic data are to be taken from card input.

[b]Card 2 is needed in the Data Base, and on input only if the THERMO ALL option is used.

Figure 4 shows some examples of thermodynamic property input. In these three examples for OH, OH+, and OH-, it is seen from Columns 25 through 34 that the elemental composition of each molecule is one O atom and one H atom. In addition, Columns 35 through 39 indicate that two of the species, OH+ and OH-, are ionic since they contain -1 and +1 free electrons (E), respectively. The G in Column 45 indicates that all three species are gaseous. The 1100. in Columns 66 to 73 for OH+ indicates that the common temperature between the high- and low-temperature fits is 1100.0 K. If Columns 66 to 73 are left blank, as they are for OH and OH-, then the common temperature is that given in Columns 21 to 30 of card 2 in Table II, which, in this example, is in the thermodynamic data base.

```
THERMO
OH                  J12/70O   1H   1O   00   0G   300.000  5000.000                1
 0.29131230E+01 0.95418248E-03-0.19084325E-06 0.12730795E-10 0.24803941E-15        2
 0.39647060E+04 0.54288735E+01 0.38365518E+01-0.10702014E-02 0.94849757E-06        3
 0.20843575E-09-0.23384265E-12 0.36715807E+04 0.49805456E+00                       4
OH+                 J12/70O   1H   1E  -1O   0G   300.000  5000.000  1100.         1
 0.27381495E+01 0.14613173E-02-0.46950536E-06 0.73663560E-10-0.41410922E-14        2
 0.15761683E+06 0.61343811E+01 0.35365969E+01-0.47029254E-04-0.62344259E-06        3
 0.17601461E-08-0.82678699E-12 0.15736677E+06 0.18477172E+01                       4
OH-                 J12/70O   1H   1E   1O   0G   300.000  5000.000                1
 0.28881148E+01 0.96560229E-03-0.19659254E-06 0.14053802E-10 0.12080617E-15        2
-0.18086455E+05 0.41896259E+01 0.34621427E+01 0.40525802E-03-0.13516992E-05        3
 0.17899459E-08-0.63434810E-12-0.18312355E+05 0.92893220E+00                       4
END
```

Figure 4. Examples of Thermodynamic Data Input

The following is a summary of the possibilities for specifying thermodynamic data.

Case 1--All thermodynamic data from Data Base

1. Attach the data base as file LTHRM (default TAPE91)
2. No THERMO cards required as input

Case 2--Thermodynamic data both from Data Base and Input

1. Attach the data base as file LTHRM (default TAPE91)
2. Include the following cards

   THERMO

   Data in Table II format (cards 3 through 6 repeated) for species in addition to Data Base or to override species in Data Base

   END

Case 3--All thermodynamic data from Input

1. Do not attach a Data Base

2. Include the following cards

THERMO ALL

Card 2 (Table II) must be the next card, giving the low temperature, common temperature, and high temperature for the fits

Thermodynamic data cards, Cards 3 through 6 (Table II), repeated for at least all species in the problem.

END

3. Species Cards

Each chemical species in a problem must be identified on a Species Card (or cards). Any set of up to 10 characters* can be used as a species name, and thermodynamic data (previous section) must be available for each species included. In addition, each species must be composed of elements which have been identified on the Element Card(s), and the elemental composition of the species is that specified in the thermodynamic data. As with the Element Cards, one of the primary purposes of the Species Cards is to identify the order in which arrays of species information are referenced in the Gas-Phase Subroutine Library.

The first Species Card must contain the word SPECIES starting in Column 1. It is then followed by any number of cards which identify the species. Species symbols may appear anywhere on the card, and those on the same card must be separated by blank spaces. After all the species have been given, the following card must contain the word END starting in Column 1. Two equivalent ways to specify species information for a problem which might arise in hydrogen-air combustion are shown in Figure 5. The rules for Species Cards are summarized in Table III.

```
SPECIES
  H2    O2    H    O    OH    HO2    H2O    N2    N     NO
END

SPECIES
     H2        O2
       H        O        OH        HO2
 H2O
N2 N       NO
END
```

Figure 5. Equivalent Ways to Describe Species Information

*Species names must begin with a letter. Also, up to 18 characters may be used by changing the value of LENSYM in the INTERPRETER.

TABLE III. SUMMARY OF THE RULES FOR SPECIES CARDS

1. The first (last) Species Card must contain the word SPECIES (END) starting in Column 1. All other columns on this card are ignored.

2. Species names are composed of up to 10-character symbols. The names cannot begin with the characters +, -, =, a parenthesis, or a number.

3. Each species must be declared only once.

4. Each species which subsequently appears in a reaction must be declared.

5. The species declarations may appear anywhere on the cards.

6. Any number of species declarations may appear on a card. Thus, more than one card may be used.

7. Species declarations which appear on the same card must be separated by are least one blank space.

8. A species declaration which begins on one card may not continue to the next card.

9. One species declaration may end in Column 80 of one card and the next declaration may begin in Column 1 of the next card.

4. Reaction Mechanism Description

The reaction mechanism may involve any number of chemical reactions involving the species named on the Species Cards.* The reactions may be reversible or irreversible, they may be three body reactions with an arbitrary third body--including the effects of enhanced third body efficiencies, and they may involve photon radiation as either a reactant or product.

The first Reaction Card must contain the word REACTIONS starting in Column 1. The following cards contain the reaction description together with the Arrhenius rate coeficients [Eq. (II.5.5)]. The reaction description is made up of Reaction Cards and perhaps Auxiliary Information Cards. The last card of the reaction description must contain the word END starting in Column 1.

*If more than 6 species appear in a reaction, some dimensioning needs to be changed in the INTERPRETER (see opening statements in program on microfiche).

Reaction Cards--Each Reaction Card is divided into two fields. The first field contains the symbolic description of the reaction while the second contains the Arrhenius rate coefficients. Both fields are format free, and blank spaces are ignored (except within a number or a species symbol).

The reaction description, given in the first field, must be composed of the species symbols, coefficients, delimiters, and special symbols as summarized below.

Species Symbols--Each species in a reaction is described with the unique sequence of characters exactly as they appear in the Species Cards and the THERMO cards.

Coefficients--Any species symbol may be preceded by an integer coefficient. The coefficient simply has the meaning that there are that many moles of the particular species present as either reactants or products; e.g., 2OH is equivalent to OH + OH (a real coefficient is not allowed).

Delimiters--

+ A plus sign is the delimiter between the reactant species and between the product species

= An equality sign is the delimiter between the reactants and products for a reversible reaction

- A minus sign is the delimiter between the reactants and products for an irreversible reaction

Special Symbols--

M The symbol M stands for an arbitrary third body. Normally it would appear as both a reactant and a product. However, it has the identical meaning even if it appears only as a reactant or a product. In other words, an M anywhere in the reaction description indicates that a third body is participating in the reaction. In any reaction containing an M, species can be specified to have enhanced third body efficiencies, in which case the next card(s) must be Auxiliary Information cards (described below). If no enhanced third body efficiencies are specified, then an M means that all species act equally as third bodies and the total concentration of the mixture is the effective concentration of the third body.

HV The symbol HV indicates that photon radiation ($h\nu$) is present as either a reactant or a product. If an HV appears in a reaction description, the wavelength of the radiation may be specified on an Auxiliary Information Card (described later).

E The symbol E is used to represent an electron. Electrons are treated just like any other species except that they are not composed of elements. Thus they only affect the charge balance and not element balance. If an E appears in any reaction, then it must be declared as a species in the Species Cards and thermodynamic data must be supplied for it.

(An open parenthesis means that any following characters through the beginning of the numbers for the Arrhenius coefficients are comments on the reaction. For example the comment may be used to give a reference to the source of the reaction and rate data.

A special case for reaction descriptions occurs if two or more species names are identical except for the last character in one of the names being a +, -, or = (e.g. CH, CH+, CH++). The INTERPRETER always seeks to find the longest possible species name between delimiters (+, -, =). Therefore the species CH may not be followed directly by a + as a delimiter since this would be confused with the species CH+. To prevent this problem the species CH must be separated from the delimiter + by at least one blank space (e.g., CH+M = C+H+M must be written as CH +M = C+H+M). However, CH++ +M+2E = C+H+M may just as well be written as CH+++M+2E = C+H+M so long as CH+++ is not a species). There is no ambiguity in the convention and the worst that can happen if the blank is not included before the delimiter is that an error message will be written from the INTERPRETER. The blank will have to be inserted by the user, but there is no possibly of having a reaction misinterpreted by the code and proceeeding with an incorrect reaction.

The second field of the reaction card is used to define the Arrhenius rate coefficients A_i, β_i, and E_i as given by Eq. (II.5.5). The three numbers must appear in order, the first number being A_i, the second being β_i, and the third being E_i. At least one blank space must separate the first number and the last symbol in the reaction or the comment. The three numbers must be separated by at least one blank space; be stated in either integer, floating point, or E format (e.g., 123 or 123.0 or 12.3E1); and

have units associated with them. The default units for A_i are cgs (cm, sec, K, and moles), the exact units depending on the reaction. The factor β_i is dimensionless. The default units for the activation energies are cal/mole.

Table IV is a summary of the Reaction Card rules, and examples of some reaction cards are shown in Figure 6.

TABLE IV. SUMARY OF THE RULES FOR REACTION CARDS

1. The first (last) Reaction Card must contain the word REACTIONS (END) starting in Column 1. All other columns of this card are ignored. (The END card would follow the last Auxiliary Information Card, if one was used for the last reaction).

2. The reaction description can begin anywhere on the card. All blank spaces, except those within species symbols and within coefficients, are ignored.

3. If some species names end with either the characters +, -, or =, and there are other species names which are identical to these except that they don't end in a +, -, or =, then in the reaction description the latter species names must be separated from +, -, or = delimiters by at least one blank space.

4. Each reaction description must use only one card and may not continue onto the next card.

5. Three numbers for the Arrhenius coefficients: must appear on each Reaction Card; must occupy the last non-blank entries on the card; must be separated from the reaction description by at least one blank space; must be in order, (A_i, β_i, and E_i); and must be separated by at least one blank space. No blanks are allowed within the numbers themselves.

6. Comments are any characters following an open parenthesis and up to within one blank space of the first Arrhenius coefficient. The comments are written on LOUT along with the reaction description, but are otherwise ignored within the code.

```
REACTIONS
H2+O2=2OH                                    1.7E13  0  47780.
H2+O2= OH + OH      (REF. 21)                1.7E13  0  47780.
H+O2+M=HO2+M                                         2.0E15     0.000     -870.
H+O2+M=HO2                                           2.0E15     0.000     -870.
H+O2  =HO2+M                                         2.0E15     0.000     -870.
OH+ + H +E-H2O                                   1.E19   0    0.0
OH++H+E=H2O                                  1.E19   0.   0.
O  +  HV  =  O(*)   (REF.  99)  1.E15  0.      0.
END
```

Figure 6. Examples of Reaction Cards

The units in the CHEMKIN code can be changed to any consistent set of units the user desires by a call to SUBROUTINE CKUNIT. This subroutine resets the values of the gas constants R and R_c, and the pressure of one standard atmosphere P_{atm}. The gas constant R is used everywhere except in conjunction with the activation energy, where R_c is used. If the units are changed in the CHEMKIN subroutine package, then the units on the reaction card input must be changed accordingly.

Auxiliary Information Cards--If a reaction contains an M as third body and/or it contains an HV to denote radiation, the card or cards following that reaction card may be Auxiliary Information Cards. These cards specify enhanced third body efficiences of certain species [i.e., α_{ki}, Equation (II.5.11)] or specify radiation wavelength (in angstroms). Any species which acts as an enhanced third body must be declared as one of the species on the Species Cards.

The format of the card is a name (either a species name or the characters HV) followed by a number (either integer, floating point, or E format) delimited by slashes (/). For enhanced third body efficiencies the name is the species name of the enhanced third body and the number is its enhanced efficiency factor. For wavelength specification the symbols HV are followed by the wavelength in angstroms.

Any number of enhanced third bodies may be included,* and each Auxiliary Information Card may contain one or more enhanced efficiency factors. Also, the radiation wavelength may appear on a separate card, or it may be on the same card as an enhanced third body specification. Thus, more than one Auxiliary Information Card may be used for any one reaction.

Examples of equivalent ways to state auxiliary information are shown in Figure 7. The above rules are summarized in Table V.

*If more than 6 species have enhanced third body efficiencies in any one reaction, some dimensioning needs to be changed in the INTERPRETER (see program on microfiche).

```
H+O2+M=HO2+M                                          2.0E15     0.000     -870.
     H2O /  20./        H2/2/        N2/.9/

H+O2+M=HO2+M                                          2.0E15     0.000     -870.
  H2O/2.0E1/      H2/2.0/
 N2   /  9.0E-1/

O+HV-O(*)            1.E+15     0.        0.
     HV    /4880/
```

Figure 7. Examples of Auxiliary Information Definitions

TABLE V. SUMMARY OF THE RULES FOR AUXILIARY INFORMATION CARDS

1. Auxiliary Information Cards may only follow Reaction Cards which contain an M or an HV.

2. A species may have only one enhanced third body efficiency associated with it in any one reaction.

3. Only one radiation wavelength may be declared in a reaction.

4. The order in which the enhanced third body declarations are given is the order in which arrays of enhanced third body information are referenced in the subroutine package. The order in which the radiation wavelength appears with respect to enhanced third body information is unimportant.

5. Enhanced third body (or wavelength) information may appear anywhere on the card.

6. Any number of enhanced third body efficiences may appear on a card. Thus more than one card may be used.

7. Enhanced third body declarations or radiation wavelength specifications which appear on the same card must be separated by at least one blank space.

8. An enhanced third body (or wavelength) declaration which begins on one card may not continue to the next card.

9. One declaration (enhanced third body or wavelength) may end in column 80 of one card and the next declaration may begin in Column 1 of the next card.

10. Any blank spaces between the species symbol (or HV) and the first slash are ignored and any blanks between the slashes and the enhanced efficiency factor (or wavelength) are also ignored. However, no blank spaces are allowed within the factor (or wavelength).

Problems Having No Reactions--In some problems only information about the elements and species is needed (e.g., chemical equilibrium computations). In these cases it is not necessary to include Reaction Cards. The INTERPRETER will create the LINK file, but of course it will not contain any reaction information. Therefore, no subroutines in the Gas-Phase Subroutine Library which deal with chemical reactions (e.g., chemical production rates) may be used.

5. Error Checks

The INTERPRETER checks each input card for proper syntax and writes self-explanatory diagnostic messages on logical file LOUT if bad syntax is encountered. In addition, each reaction is checked for both element and charge balance. If a reaction does not balance, a message is written on LOUT. If any errors are encountered, the INTERPRETER does not create the linking file. Therefore, the input must be error free before any of the CHEMKIN subroutines can be called.

6. Access to INTERPRETER Output

Information about elements, species, and reactions which is produced by the INTERPRETER may be obtained from the Gas-Phase Subroutine Library in two ways. The first way, and the most convenient, is to call subroutines given in Sections V.2 through V.5. It is also possible to extract information directly from the work arrays, whose structure is described in Appendix A. Using the work arrays directly will require less storage than calling the high-level subroutines. However, dealing with the work arrays may be cumbersome for many users.

V. Quick Reference Guide to the Gas-Phase Subroutine Library

This chapter is arranged by topical area and it provides a quick reference to each of the Gas-Phase Library subroutines. Along with the actual subroutine statement is given a short description of the routine which, where appropriate, refers to an equation number in Chapter II. The page number given for each subroutine refers to the page in Chapter VI where a detailed description of the subroutine call list may be found.

Mnemonics

There are no firm general rules for explaining the mnemonics used in naming subroutines, but there are some good rules of thumb. All subroutines begin with the letters CK so that CHEMKIN subroutines are easily recognized, and so that they are likely unique from any user subroutine names. The remaining four letters are used to identify the purpose of the subroutine. The first one or two letters after CK usually refer to the variable which is being computed. The last letters refer to either the input variables, the units, or what is being held fixed in a differentiation.

State variables are denoted by: P pressure, T temperature, Y mass fractions, X mole fractions, and C molar concentrations. Thermodynamic properties are referred to by: CP and CV specific heats, H enthalpy, S entropy, U internal energy, G Gibbs free energy, and A Helmholtz free energy. The thermodynamic subroutines may be called to return properties in mass units, denoted by MS or S as the last letters, or in molar units, denoted by ML or L as the last letters. A B in a thermodynamic property subroutine name indicates that it returns mean properties.

Subroutines which return chemical production rates have a W following the CK, and routines which return creation rates and destruction rates or creation rates and destruction times have a CD or a CT, respectively, following the CK. Rate of progress variables are denoted by Q and equilibrium constants by EQ.

A D following the CK indicates that the suroutine is used to compute a derivative. If an S follows the CK then the subroutine is used to find sensitivity matrices.

The mnemonics used for the variable names in the subroutine calls are roughly the same as for the subroutine names. However, because six letters can be used (only four in the subroutine names because CK occupies two), the mnemonics can be more explicit, and thus more immediately recognizable.

1. INITIALIZATION.

SUBROUTINE CKINDX (IWORK,WORK,MM,KK,II,LENEL,LENSYM,NFIT) PAGE 136
THIS SUBROUTINE RETURNS A GROUP OF INDICES DEFINING THE SIZE OF THE PARTICULAR REACTION MECHANISM.

SUBROUTINE CKINIT (LENIWK,LENWK,LINK,LOUT,IWORK,WORK) PAGE 137
THIS SUBROUTINE SERVES TO READ THE LINKING FILE AND CREATE THE INTERNAL WORK ARRAYS, IWORK AND WORK. CKINIT MUST BE CALLED BEFORE ANY OTHER CHEMKIN SUBROUTINE IS CALLED. THE WORK ARRAYS MUST THEN BE MADE AVAILABLE AS INPUT TO THE OTHER CHEMKIN SUBROUTINES.

2. INFORMATION ABOUT ELEMENTS.

SUBROUTINE CKAWT (IWORK,WORK,AWT) PAGE 90
THIS SUBROUTINE RETURNS THE ATOMIC WEIGHTS OF THE ELEMENTS.

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SUBROUTINE CKRHOX (P,T,X,IWORK,WORK,RHO) PAGE 146
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SUBROUTINE CKYTCR (RHO,T,Y,IWORK,WORK,C) PAGE 171
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SUBROUTINE CKCPOR (T,IWORK,WORK,CPOR) PAGE 95
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SUBROUTINE CKHORT (T,IWORK,WORK,HORT) PAGE 136
THIS SUBROUTINE RETURNS THE NONDIMENSIONAL ENTHALPIES. REFERENCE EQUATION (II.4.3) OR (II.4.7).

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SUBROUTINE CKAMS (T,IWORK,WORK,AMS) PAGE 89
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SUBROUTINE CKCPMS (T,IWORK,WORK,CPMS) PAGE 95
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SUBROUTINE CKHMS (T,IWORK,WORK,HMS) PAGE 136
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SUBROUTINE CKSMS (T,IWORK,WORK,SMS) PAGE 161
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SUBROUTINE CKUMS (T,IWORK,WORK,UMS) PAGE 164
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10. THERMODYNAMIC PROPERTIES (MOLAR UNITS)

SUBROUTINE CKAML (T,IWORK,WORK,AML) PAGE 88
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SUBROUTINE CKCPML (T,IWORK,WORK,CPML) PAGE 95
THIS SUBROUTINE RETURNS THE SPECIFIC HEATS AT CONSTANT PRESSURE IN MOLAR UNITS. REFERENCE EQUATION (II.4.1).

SUBROUTINE CKCVML (T,IWORK,WORK,CVML) PAGE 101
THIS SUBROUTINE RETURNS THE SPECIFIC HEATS IN CONSTANT VOLUME IN MOLAR UNITS. REFERENCE EQUATION (II.4.9).

SUBROUTINE CKGML (T,IWORK,WORK,GML) PAGE 134
THIS SUBROUTINE RETURNS THE STANDARD STATE GIBBS FREE ENERGIES IN MOLAR UNITS. REFERENCE EQUATION (II.4.11).

SUBROUTINE CKHML (T,IWORK,WORK,HML) PAGE 135
THIS SUBROUTINE RETURNS THE ENTHALPIES IN MOLAR UNITS. REFERENCE EQUATION (II.4.3).

SUBROUTINE CKSML (T,IWORK,WORK,SML) PAGE 160
THIS SUBROUTINE RETURNS THE STANDARD STATE ENTROPIES IN MOLAR UNITS. REFERENCE EQUATION (II.4.5).

SUBROUTINE CKUML (T,IWORK,WORK,UML) PAGE 164
THIS SUBROUTINE RETURNS THE INTERNAL ENERGIES IN MOLAR UNITS. REFERENCE EQUATION (II.4.10).

11. MEAN THERMODYNAMIC PROPERTIES (MASS UNITS).

SUBROUTINE CKABMS (T,Y,IWORK,WORK,ABMS) PAGE 88
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SUBROUTINE CKCPBS (T,Y,IWORK,WORK,CPBMS) PAGE 95
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SUBROUTINE CKCVBS (T,Y,IWORK,WORK,CVBMS) PAGE 100
THIS SUBROUTINE RETURNS THE MASS WEIGHTED MEAN SPECIFIC HEAT AT CONSTANT VOLUME IN MASS UNITS. REFERENCE EQUATION (II.4.27).

SUBROUTINE CKGBMS (T,Y,IWORK,WORK,GBMS) PAGE 133
THIS SUBROUTINE RETURNS THE MASS WEIGHTED MEAN STANDARD STATE GIBBS FREE ENERGY OF THE MIXTURE IN MASS UNITS. REFERENCE EQUATION (II.4.21).

SUBROUTINE CKHBMS (T,Y,IWORK,WORK,HBMS) PAGE 135
THIS SUBROUTINE RETURNS THE MASS WEIGHTED MEAN ENTHALPY OF THE MIXTURE IN MASS UNITS. REFERENCE EQUATION (II.4.23).

SUBROUTINE CKSBMS (T,Y,IWORK,WORK,SBMS) PAGE 151
THIS SUBROUTINE RETURNS THE MASS WEIGHTED MEAN STANDARD STATE ENTROPY OF THE MIXTURE IN MASS UNITS. REFERENCE EQ. (II.4.25)

SUBROUTINE CKUBMS (T,Y,IWORK,WORK,UBMS) PAGE 164
THIS SUBROUTINE RETURNS THE MASS WEIGHTED MEAN INTERNAL ENERGY OF THE MIXTURE IN MASS UNITS. REFERENCE EQUATION (II.4.29).

12. MEAN THERMODYNAMIC PROPERTIES (MOLAR UNITS).

SUBROUTINE CKABML (T,X,IWORK,WORK,ABML) PAGE 87
THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN STANDARD STATE HELMHOLTZ FREE ENERGY OF THE MIXTURE IN MOLAR UNITS. REFERENCE EQUATION (II.4.32).

SUBROUTINE CKCPBL (T,X,IWORK,WORK,CPBML) PAGE 94
THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN SPECIFIC HEAT AT CONSTANT PRESSURE. REFERENCE EQUATION (II.4.20).

SUBROUTINE CKCVBL (T,X,IWORK,WORK,CVBML) PAGE 100
THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN SPECIFIC HEAT AT CONSTANT VOLUME IN MOLAR UNITS. REFERENCE EQUATION (II.4.26).

SUBROUTINE CKGBML (T,X,IWORK,WORK,GBML) PAGE 133
THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN STANDARD STATE GIBBS FREE ENERGY OF THE MIXTURE IN MOLAR UNITS. REFERENCE EQUATION (II.4.30).

SUBROUTINE CKHBML (T,X,IWORK,WORK,HBML) PAGE 134
THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN ENTHALPY OF THE MIXTURE IN MOLAR UNITS. REFERENCE EQUATION (II.4.22).

SUBROUTINE CKSBML (T,X,IWORK,WORK,SBML) PAGE 151
THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN STANDARD STATE ENTROPY OF THE MIXTURE IN MOLAR UNITS. REFERENCE EQ. (II.4.24)

SUBROUTINE CKUBML (T,X,IWORK,WORK,UBML) PAGE 163
THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN INTERNAL ENERGY OF THE MIXTURE IN MOLAR UNITS. REFERENCE EQUATION (II.4.28).

13. CHEMICAL PRODUCTION RATES.

SUBROUTINE CKCDC (T,C,IWORK,WORK,CDOT,DDOT) PAGE 90
THIS SUBROUTINE RETURNS THE MOLAR CREATION AND DESTRUCTION RATES OF THE SPECIES GIVEN THE TEMPERATURE AND MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.5.13).

SUBROUTINE CKCDXP (P,T,X,IWORK,WORK,CDOT,DDOT) PAGE 91
THIS SUBROUTINE RETURNS THE MOLAR CREATION AND DESTRUCTION RATES OF THE SPECIES GIVEN PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.5.13).

SUBROUTINE CKCDXR (RHO,T,X,IWORK,WORK,CDOT,DDOT) PAGE 91
THIS SUBROUTINE RETURNS THE MOLAR CREATION AND DESTRUCTION RATES OF THE SPECIES GIVEN THE MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.5.13).

SUBROUTINE CKCDYP (P,T,Y,IWORK,WORK,CDOT,DDOT) PAGE 92
THIS SUBROUTINE RETURNS THE MOLAR CREATION AND DESTRUCTION RATES OF THE SPECIES GIVEN MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.5.13).

SUBROUTINE CKCDYR (RHO,T,Y,IWORK,WORK,CDOT,DDOT) PAGE 92
THIS SUBROUTINE RETURNS THE MOLAR CREATION AND DESTRUCTION RATES OF THE SPECIES GIVEN THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.5.13)

SUBROUTINE CKCONT (K,ROP,IWORK,WORK,CIK) PAGE 94
THIS SUBROUTINE RETURNS THE CONTRIBUTION OF THE II REACTIONS TO THE MOLAR PRODUCTION RATE OF THE K TH SPECIES.

SUBROUTINE CKCTC (T,C,IWORK,WORK,CDOT,TAU) PAGE 96
THIS SUBROUTINE RETURNS THE MOLAR CREATION RATES AND CHARACTERISTIC DESTRUCTION TIMES OF THE SPECIES GIVEN THE TEMPERATURE AND MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.5.16).

SUBROUTINE CKCTXP (P,T,X,IWORK,WORK,CDOT,TAU) PAGE 97
THIS SUBROUTINE RETURNS THE MOLAR CREATION RATES AND CHARACTERISTIC DESTRUCTION TIMES OF THE SPECIES GIVEN THE PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.5.16).

SUBROUTINE CKCTXR (RHO,T,X,IWORK,WORK,CDOT,TAU) PAGE 98
THIS SUBROUTINE RETURNS THE MOLAR CREATION RATES AND CHARACTERISTIC DESTRUCTION TIMES OF THE SPECIES GIVEN THE MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.5.16).

SUBROUTINE CKCTYP (P,T,Y,IWORK,WORK,CDOT,TAU) PAGE 99
THIS SUBROUTINE RETURNS THE MOLAR CREATION RATES AND CHARACTERISTIC DESTRUCTION TIMES OF THE SPECIES GIVEN THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.5.16).

SUBROUTINE CKCTYR (RHO,T,Y,IWORK,WORK,CDOT,TAU) PAGE 99
THIS SUBROUTINE RETURNS THE MOLAR CREATION RATES AND CHARACTERISTIC DESTRUCTION TIMES OF THE SPECIES GIVEN THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.5.16)

SUBROUTINE CKWC (T,C,IWORK,WORK,WDOT) PAGE 165
THIS SUBROUTINE RETURNS THE MOLAR PRODUCTION RATES OF THE SPECIES GIVEN THE TEMPERATURE AND MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.5.2.)

SUBROUTINE CKWXP (P,T,X,IWORK,WORK,WDOT) PAGE 167
THIS SUBROUTINE RETURNS THE MOLAR PRODUCTION RATES OF THE SPECIES GIVEN THE PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.5.2).

SUBROUTINE CKWXR (RHO,T,X,IWORK,WORK,WDOT) PAGE 167
THIS SUBROUTINE RETURNS THE MOLAR PRODUCTION RATES OF THE SPECIES GIVEN THE MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.5.2).

SUBROUTINE CKWYP (P,T,Y,IWORK,WORK,WDOT) PAGE 168
THIS SUBROUTINE RETURNS THE MOLAR PRODUCTION RATES OF THE SPECIES GIVEN THE PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.5.2).

SUBROUTINE CKWYR (RHO,T,Y,IWORK,WORK,WDOT) PAGE 168
THIS SUBROUTINE RETURNS THE MOLAR PRODUCTION RATES OF THE SPECIES GIVEN THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.5.2).

14. EQUILIBRIUM CONSTANTS AND RATE OF PROGRESS VARIABLES.

SUBROUTINE CKEQC (T,C,IWORK,WORK,EQKC) PAGE 130
THIS SUBROUTINE RETURNS THE EQUILIBRIUM CONSTANTS OF THE REACTIONS GIVEN TEMPERATURE, AND MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.5.7).

SUBROUTINE CKEQXP (P,T,X,IWORK,WORK,EQKC) PAGE 131
THIS SUBROUTINE RETURNS THE EQUILIBRIUM CONSTANTS FOR THE REACTIONS GIVEN PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.5.7).

SUBROUTINE CKEQXR (RHO,T,X,IWORK,WORK,EQKC) PAGE 131
THIS SUBROUTINE RETURNS THE EQUILIBRIUM CONSTANTS OF THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.5.7).

SUBROUTINE CKEQYP (P,T,Y,IWORK,WORK,EQKC) PAGE 132
THIS SUBROUTINE RETURNS THE EQUILIBRIUM CONSTANTS FOR THE REACTIONS GIVEN PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.5.7).

SUBROUTINE CKEQYR (RHO,T,Y,IWORK,WORK,EQKC) PAGE 132
THIS SUBROUTINE RETURNS THE EQUILIBRIUM CONSTANTS OF THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.5.7).

SUBROUTINE CKQC (T,C,IWORK,WORK,ROP) PAGE 143
THIS SUBROUTINE RETURNS THE RATE OF PROGRESS VARIABLES FOR THE REACTIONS GIVEN TEMPERATURE AND MOLAR CONCENTRATIONS. REFERENCE EQUATIONS (II.5.4) AND (II.5.11).

SUBROUTINE CKQXP (P,T,X,IWORK,WORK,ROP) PAGE 143
THIS SUBROUTINE RETURNS THE RATE OF PROGRESS VARIABLES FOR THE REACTIONS GIVEN PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATIONS (II.5.4) AND (II.5.11).

SUBROUTINE CKQXR (RHO,T,X,IWORK,WORK,ROP) PAGE 144
THIS SUBROUTINE RETURNS THE RATE OF PROGRESS VARIABLES FOR THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATIONS (II.5.4) AND (II.5.11).

SUBROUTINE CKQYP (P,T,Y,IWORK,WORK,ROP) PAGE 144
THIS SUBROUTINE RETURNS THE RATE OF PROGRESS VARIABLES FOR THE REACTIONS GIVEN PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATIONS (II.5.4) AND (II.5.11).

SUBROUTINE CKQYR (RHO,T,Y,IWORK,WORK,ROP) PAGE 145
THIS SUBROUTINE RETURNS THE RATE OF PROGRESS VARIABLES FOR THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATIONS (II.5.4) AND (II.5.11).

15. SENSITIVITY PARAMETERS.

SUBROUTINE CKSAC (T,C,KDIM,IWORK,WORK,DWKDAI) PAGE 147
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE PRE-EXPONENTIAL CONSTANTS OF THE REACTIONS GIVEN TEMPERATURE AND MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.11.3).

SUBROUTINE CKSAXP (P,T,X,KDIM,IWORK,WORK,DWKDAI) PAGE 143
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE PRE-EXPONENTIAL CONSTANTS OF THE REACTIONS GIVEN PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.11.3).

SUBROUTINE CKSAXR (RHO,T,X,KDIM,IWORK,WORK,DWKDAI) PAGE 148
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE PRE-EXPONENTIAL CONSTANTS OF THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.11.3).

SUBROUTINE CKSAYP (P,T,Y,KDIM,IWORK,WORK,DWKDAI) PAGE 149
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE PRE-EXPONENTIAL CONSTANTS OF THE REACTIONS GIVEN PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.11.3).

SUBROUTINE CKSAYR (RHO,T,Y,KDIM,IWORK,WORK,DWKDAI) PAGE 149
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE PRE-EXPONENTIAL CONSTANTS OF THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.11.3).

SUBROUTINE CKSBC (T,C,KDIM,IWORK,WORK,DWKDBI) PAGE 150
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE TEMPERATURE EXPONENTS OF THE REACTIONS GIVEN TEMPERATURE AND MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.11.4).

SUBROUTINE CKSBXP (P,T,X,KDIM,IWORK,WORK,DWKDBI) PAGE 152
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE TEMPERATURE EXPONENTS OF THE REACTIONS GIVEN PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.11.4).

SUBROUTINE CKSBXR (RHO,T,X,KDIM,IWORK,WORK,DWKDBI) PAGE 152
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE TEMPERATURE EXPONENTS OF THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.11.4).

SUBROUTINE CKSBYP (P,T,Y,KDIM,IWORK,WORK,DWKDBI) PAGE 153
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE TEMPERATURE EXPONENTS OF THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.11.4).

SUBROUTINE CKSBYR (RHO,T,Y,KDIM,IWORK,WORK,DWKDBI) PAGE 153
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE TEMPERATURE EXPONENTS OF THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.11.4)

SUBROUTINE CKSEC (T,C,KDIM,IWORK,WORK,DWKDEI) PAGE 154
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE ACTIVATION ENERGY OF THE REACTIONS GIVEN TEMPERATURE AND MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.11.5).

SUBROUTINE CKSEXP (P,T,X,KDIM,IWORK,WORK,DWKDEI) PAGE 155
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE ACTIVATION ENERGY OF THE REACTIONS GIVEN PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.11.5).

SUBROUTINE CKSEXR (RHO,T,X,KDIM,IWORK,WORK,DWKDEI) PAGE 155
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE ACTIVATION ENERGY OF THE REACTIONS GIVEN MASS DENSITY TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.11.5).

SUBROUTINE CKSEYP (P,T,Y,KDIM,IWORK,WORK,DWKDEI) PAGE 156
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE ACTIVATION ENERGY OF THE REACTIONS GIVEN PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.11.5).

SUBROUTINE CKSEYR (RHO,T,Y,KDIM,IWORK,WORK,DWKDEI) PAGE 156
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE ACTIVATION ENERGY OF THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.11.5).

SUBROUTINE CKSKC (T,C,KDIM,IWORK,WORK,DWKDKI) PAGE 157
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE FORWARD RATE CONSTANTS OF THE REACTIONS GIVEN TEMPERATURE AND MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.11.2).

SUBROUTINE CKSKXP (P,T,X,KDIM,IWORK,WORK,DWKDKI) PAGE 158
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE FORWARD RATE CONSTANTS OF THE REACTIONS GIVEN PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.11.2).

SUBROUTINE CKSKXR (RHO,T,X,KDIM,IWORK,WORK,DWKDKI) PAGE 158
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE FORWARD RATE CONSTANTS OF THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.11.2).

SUBROUTINE CKSKYP (P,T,Y,KDIM,IWORK,WORK,DWKDKI) PAGE 159
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE FORWARD RATE CONSTANTS OF THE REACTIONS GIVEN PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.11.2).

SUBROUTINE CKSKYR (RHO,T,Y,KDIM,IWORK,WORK,DWKDKI) PAGE 159
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE FORWARD RATE CONSTANTS OF THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.11.2).

16. DERIVATIVES OF EQUATION OF STATE.

SUBROUTINE CKDPDC (RHO,T,C,IWORK,WORK,DPDC) PAGE 112
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE PRESSURE WITH RESPECT TO THE MOLAR CONCENTRATIONS GIVEN THE MASS DENSITY, TEMPERATURE AND MOLAR CONCENTRATIONS, REFERENCE EQUATION (II.7.15).

SUBROUTINE CKDPDX (RHO,T,X,IWORK,WORK,DPDX) PAGE 113
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE PRESSURE WITH RESPECT TO MOLE FRACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.7.14).

SUBROUTINE CKDPDY (RHO,T,Y,IWORK,WORK,DPDY) PAGE 113
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF PRESSURE WITH RESPECT TO THE MASS FRACTIONS GIVEN THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.7.13).

SUBROUTINE CKDPTC (RHO,T,C,IWORK,WORK,DPDT) PAGE 114
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE PRESSURE WITH RESPECT TO TEMPERATURE GIVEN THE MASS DENSITY, TEMPERATURE AND MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.7.12).

SUBROUTINE CKDPTX (RHO,T,X,IWORK,WORK,DPDT) PAGE 114
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE PESSURE WITH RESPECT TO TEMPERATURE GIVEN THE MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.7.11)

SUBROUTINE CKDPTY (RHO,T,Y,IWORK,WORK,DPDT) PAGE 115
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE PRESSURE WITH RESPECT TO TEMPERATURE GIVEN THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.7.10)

SUBROUTINE CKDRDC (P,T,C,IWORK,WORK,DRHODC) PAGE 115
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MASS DENSITY WITH RESPECT TO THE MOLAR CONCENTRATIONS GIVEN THE PRESSURE, TEMPERATURE AND MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.7.9).

SUBROUTINE CKDRDX (P,T,X,IWORK,WORK,DRHODX) PAGE 116
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MASS DENSITY WITH RESPECT TO THE MOLE FRACTIONS GIVEN THE PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.7.8).

SUBROUTINE CKDRDY (P,T,Y,IWORK,WORK,DRHODY) PAGE 116
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MASS DENSITY WITH RESPECT TO MASS FRACTIONS GIVEN PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.7.7).

SUBROUTINE CKDRTC (P,T,C,IWORK,WORK,DRHODT) PAGE 117
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE MASS DENSITY WITH RESPECT TO TEMPERATURE GIVEN PRESSURE, TEMPERATURE AND MOLAR CONCENTRATION. REFERENCE EQUATION (II.7.6).

SUBROUTINE CKDRTX (P,T,X,IWORK,WORK,DRHODT) PAGE 117
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE MASS DENSITY WITH RESPECT TO TEMPERATURE GIVEN PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.7.5)

SUBROUTINE CKDRTY (P,T,Y,IWORK,WORK,DRHODT) PAGE 118
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE MASS DENSITY WITH RESPECT TO TEMPERATURE GIVEN THE PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.7.4)

SUBROUTINE CKDWBC (C,IWORK,WORK,DWBDC) PAGE 123
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MEAN MOLECULAR WEIGHT WITH RESPECT TO THE MOLAR CONCENTRATIONS GIVEN THE MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.7.3).

SUBROUTINE CKDWBX (X,IWORK,WORK,DWBDX) PAGE 123
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE MEAN MOLECULAR WEIGHT WITH RESPECT TO THE MOLE FRACTIONS GIVEN THE MOLE FRACTIONS. REFERENCE EQUATION (II.7.2).

SUBROUTINE CKDWBY (Y,IWORK,WORK,DWBDY) PAGE 124
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE MEAN MOLECULAR WEIGHT WITH RESPECT TO THE MASS FRACTIONS GIVEN THE MASS FRACTIONS. REFERENCE EQUATION (II.7.1).

17. MOLE-MASS CONVERSION DERIVATIVES.

SUBROUTINE CKDCXP (P,T,X,KDIM,IWORK,WORK,DCKDXN) PAGE 108
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR CONCENTRATIONS WITH RESPECT TO THE MOLE FRACTIONS GIVEN THE PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.8.5).

SUBROUTINE CKDCXR (RHO,T,X,KDIM,IWORK,WORK,DCKDXN) PAGE 108
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR CONCENTRATIONS WITH RESPECT TO THE MOLE FRACTIONS GIVEN THE MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.6.6).

SUBROUTINE CKDCYP (P,T,Y,KDIM,IWORK,WORK,DCKDYN) PAGE 109
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR CONCENTRATIONS WITH RESPECT TO THE MASS FRACTIONS GIVEN THE PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.8.3).

SUBROUTINE CKDCYR (RHO,T,Y,KDIM,IWORK,WORK,DCKDYN) PAGE 110
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR CONCENTRATIONS WITH RESPECT TO THE MASS FRACTIONS GIVEN THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.8.4).

SUBROUTINE CKDXDY (Y,KDIM,IWORK,WORK,DXKDYN) PAGE 129
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLE FRACTIONS WITH RESPECT TO THE MASS FRACTIONS GIVEN THE MASS FRACTIONS. REFERENCE EQUATION (II.8.2).

SUBROUTINE CKDYDX (X,KDIM,IWORK,WORK,DYKDXN) PAGE 130
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MASS FRACTIONS WITH RESPECT TO THE MOLE FRACTIONS GIVEN THE MOLE FRACTIONS. REFERENCE EQUATION (II.8.1).

18. DERIVATIVES OF THE MOLAR CONCENTRATIONS.

SUBROUTINE CKDCPX (P,T,X,IWORK,WORK,DCDPTX) PAGE 104
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR CONCENTRATIONS WITH RESPECT TO PRESSURE GIVEN PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.8.12).

SUBROUTINE CKDCPY (P,T,Y,IWORK,WORK,DCDPTY) PAGE 104
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR CONCENTRATIONS WITH RESPECT TO PRESSURE GIVEN PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.8.12).

SUBROUTINE CKDCRX (RHO,T,X,IWORK,WORK,DCDRTX) PAGE 105
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR CONCENTRATIONS WITH RESPECT TO MASS DENSITY GIVEN MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.8.11).

SUBROUTINE CKDCRY (RHO,T,Y,IWORK,WORK,DCDRTY) PAGE 105
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR CONCENTRATIONS WITH RESPECT TO MASS DENSITY GIVEN MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.8.10).

SUBROUTINE CKDCTX (P,T,X,IWORK,WORK,DCDTPX) PAGE 105
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR CONCENTRATIONS WITH RESPECT TO TEMPERATURE GIVE THE PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.8.8).

SUBROUTINE CKDCTY (P,T,Y,IWORK,WORK,DCDTPY) PAGE 106
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR CONCENTRATIONS WITH RESPECT TO TEMPERATURE GIVEN THE PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.8.7).

19. DERIVATIVES OF THE THERMODYNAMIC PROPERTIES (MASS UNITS).

SUBROUTINE CKDAMS (T,IWORK,WORK,DADTMS) PAGE 102
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE STANDARD STATE HELMHOLTZ FREE ENERGIES IN MASS UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.14).

SUBROUTINE CKDCPS (T,IWORK,WORK,DCPTMS) PAGE 103
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE SPECIFIC HEATS AT CONSTANT PRESSURE IN MASS UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.8).

SUBROUTINE CKDCVS (T,IWORK,WORK,DCVTMS) PAGE 107
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE SPECIFIC HEATS AT CONSTANT VOLUME IN MASS UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.11).

SUBROUTINE CKDGMS (T,IWORK,WORK,DGDTMS) PAGE 111
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE STANDARD STATE GIBBS ENERGIES IN MASS UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.13).

SUBROUTINE CKDHMS (T,IWORK,WORK,DHDTMS) PAGE 112
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE ENTHALPIES IN MASS UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.9).

SUBROUTINE CKDSMS (T,IWORK,WORK,DSDTMS) PAGE 119
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE STANDARD STATE ENTROPIES IN MASS UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.10).

SUBROUTINE CKDUMS (T,IWORK,WORK,DUDTMS) PAGE 122
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE INTERNAL ENERGIES IN MASS UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.12).

20. DERIVATIVES OF THE THERMODYNAMIC PROPERTIES (MOLAR UNITS).

SUBROUTINE CKDAML (T,IWORK,WORK,DADTML) PAGE 102
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE HELMHOLTZ FREE ENERGIES IN MOLAR UNITS WITH RESPECT TO RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.7).

SUBROUTINE CKDCPL (T,IWORK,WORK,DCPTML) PAGE 103
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE SPECIFIC HEATS AT CONSTANT PRESSURE IN MOLAR UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.1).

SUBROUTINE CKDCVL (T,IWORK,WORK,DCVTML) PAGE 107
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE SPECIFIC HEATS AT CONSTANT VOLUME IN MOLAR UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.4).

SUBROUTINE CKDGML (T,IWORK,WORK,DGDTML) PAGE 110
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE GIBBS STATE GIBBS FREE ENERGIES IN MOLAR UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.6).

SUBROUTINE CKDHML (T,IWORK,WORK,DHDTML) PAGE 111
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE ENTHALPIES IN MOLAR UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.2).

SUBROUTINE CKDSML (T,IWORK,WORK,DSDTML) PAGE 118
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE STANDARD STATE ENTROPIES IN MOLAR UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.3).

SUBROUTINE CKDUML (T,IWORK,WORK,DUDTML) PAGE 122
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE INTERNAL ENERGIES IN MOLAR UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.5).

21. DERIVATIVES OF THE CHEMICAL PRODUCTION RATES.

SUBROUTINE CKDTC (T,C,IWORK,WORK,DWDTC) PAGE 119
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO TEMPERATURE GIVEN THE TEMPERATURE AND MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.10.1).

SUBROUTINE CKDTXP (P,T,X,IWORK,WORK,DWDTPX) PAGE 120
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO TEMPERATURE GIVEN THE PRESSURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.10.1).

SUBROUTINE CKDTXR (RHO,T,X,IWORK,WORK,DWDTRX) PAGE 120
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO TEMPERATURE GIVEN THE MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.10.1).

SUBROUTINE CKDTYP (P,T,Y,IWORK,WORK,DWDTPY) PAGE 121
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO TEMPERATURE GIVEN THE PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.10.1).

SUBROUTINE CKDTYR (RHO,T,Y,IWORK,WORK,DWDTRY) PAGE 121
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO TEMPERATURE GIVEN THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.10.1).

SUBROUTINE CKDWC (T,C,KDIM,IWORK,WORK,DWDCT) PAGE 124
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO MOLAR CONCENTRATIONS GIVEN THE TEMPERATURE AND MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.10.25).

SUBROUTINE CKDWPX (P,T,X,IWORK,WORK,DWDPTX) PAGE 125
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO PRESSURE GIVEN THE PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.10.32).

SUBROUTINE CKDWPY (P,T,Y,IWORK,WORK,DWDPTY) PAGE 125
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO PRESSURE GIVEN THE PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.10.32).

SUBROUTINE CKDWRX (RHO,T,X,IWORK,WORK,DWDRTX) PAGE 126
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE MASS DENSITY GIVEN THE MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.10.38).

SUBROUTINE CKDWRY (RHO,T,Y,IWORK,WORK,DWDRTY) PAGE 126
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE MASS DENSITY GIVEN THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.10.38).

SUBROUTINE CKDWXP (P,T,X,KDIM,IWORK,WORK,DWDXPT) PAGE 127
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO MOLE FRACTIONS GIVEN THE PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.10.19).

SUBROUTINE CKDWXR (RHO,T,X,KDIM,IWORK,WORK,DWDXRT) PAGE 127
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO MOLE FRACTIONS GIVEN THE MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE EQUATION (II.10.19).

SUBROUTINE CKDWYP (P,T,Y,KDIM,IWORK,WORK,DWDYPT) PAGE 128
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE MASS FRACTIONS GIVEN THE PRESSURE, TEMPERATURE AND MASS FRACTION. REFERENCE EQUATION (II.10.13).

SUBROUTINE CKDWYR (RHO,T,Y,KDIM,IWORK,WORK,DWDYRT) PAGE 129
THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE MASS FRACTIONS GIVEN THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE EQUATION (II.10.13).

VI. Alphabetical Listing of the Gas-Phase Subroutine Library with Detailed Instructions

Each of the Gas-Phase Library subroutines is described in this chapter, together with a detailed description of the parameters in the call list. For all arrays, information is given on the required dimensioning in the calling program. For all variables having units, the cgs units are stated. In many cases, a reference to the most applicable equation in Chapter II is also given.

```
SUBROUTINE CKABE (IWORK,WORK,RA,RB,RE)

   THIS SUBROUTINE RETURNS THE ARRHENIUS COEFFICIENTS FOR
   THE REACTIONS. REFERENCE EQUATION (II.5.5).

 INPUT
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   RA     - ARRAY OF PRE-EXPONENTIAL CONSTANTS FOR THE II
            REACTIONS.
               CGS UNITS - DEPENDS ON REACTION.
               DIMENSION RA(*) AT LEAST II.
   RB     - ARRAY OF TEMPERATURE DEPENDENCE EXPONENTS FOR THE II
            REACTIONS.
               CGS UNITS - NONE.
               DIMENSION RB(*) AT LEAST II.
   RE     - ARRAY OF ACTIVATION ENERGIES FOR THE II REACTIONS.
               PREFERRED UNITS - CAL/MOLE.  UNITS ON RE MUST BE
               COMPATIBLE WITH THE UNITS GIVEN FOR RUC.
               DIMENSION RE(*) AT LEAST II.


CKABML      CKABML      CKABML      CKABML      CKABML      CKABML
               ************************************
                     ***************************
                           *************
SUBROUTINE CKABML (T,X,IWORK,WORK,ABML)

   THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN
   STANDARD STATE HELMHOLTZ FREE ENERGY OF THE MIXTURE IN MOLAR
   UNITS.  REFERENCE EQUATION (II.4.32).

 INPUT
   T      - TEMPERATURE.
               CGS UNITS - K
   X      - MOLE FRACTIONS OF THE KK SPECIES.
               CGS UNITS - NONE.
               DIMENSION X(*) AT LEAST KK.
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
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                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   ABML    - MOLAR WEIGHTED MEAN STANDARD STATE HELMHOLTZ FREE
             ENERGY IN MOLAR UNITS.
                CGS UNITS - ERGS/MOLE.


CKABMS       CKABMS       CKABMS       CKABMS       CKABMS       CKABMS
                ************************************
                      *************************
                            *************
SUBROUTINE CKABMS (T,Y,IWORK,WORK,ABMS)

   THIS SUBROUTINE RETURNS THE MASS WEIGHTED MEAN
   STANDARD STATE HELMHOLTZ FREE ENERGY OF THE MIXTURE IN MASS
   UNITS.  REFERENCE EQUATION (II.4.33).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   ABMS    - MASS WEIGHTED MEAN STANDARD STATE HELMHOLTZ FREE
             ENERGY IN MASS UNITS.
                CGS UNITS - ERGS/GM.


CKAML        CKAML        CKAML        CKAML        CKAML        CKAML
                ************************************
                      *************************
                            *************
SUBROUTINE CKAML (T,IWORK,WORK,AML)

   THIS SUBROUTINE RETURNS THE STANDARD STATE HELMHOLTZ FREE
   ENERGIES IN MOLAR UNITS. REFERENCE EQUATION (II.4.12).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   AML     - ARRAY OF STANDARD STATE HELMHOLTZ FREE ENERGIES IN
             MOLAR UNITS FOR THE KK SPECIES.
                CGS UNITS - ERGS/MOLE.
                DIMENSION AML(*) AT LEAST KK.
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CKAMS        CKAMS        CKAMS        CKAMS        CKAMS        CKAMS
                 ************************************
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                           *************
SUBROUTINE CKAMS (T,IWORK,WORK,AMS)

   THIS SUBROUTINE RETURNS THE STANDARD STATE HELMHOLTZ FREE
   ENERGIES IN MASS UNITS. REFERENCE EQUATION (II.4.19).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   AMS     - ARRAY OF STANDARD STATE HELMHOLTZ FREE ENERGIES IN
             MASS UNITS FOR THE KK SPECIES.
                CGS UNITS - ERGS/GM.
                DIMENSION AMS(*) AT LEAST KK.


CKATHM       CKATHM       CKATHM       CKATHM       CKATHM       CKATHM
                 ************************************
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                           *************
SUBROUTINE CKATHM (NDIM1,NDIM2,IWORK,WORK,TMID,A)

   THIS SUBROUTINE RETURNS THE COEFFICIENTS OF THE FITS FOR THE
   THERMODYNAMIC PROPERTIES OF THE SPECIES. REFERENCE EQUATIONS
   (II.4.1) THROUGH (II.4.8).

 INPUT
   NDIM1   - ACTUAL FIRST DIMENSION OF ARRAY OF THERMODYNAMIC FIT
             COEFFICIENTS. NDIM1 MUST BE AT LEAST NCP2, THE TOTAL
             NUMBER OF COEFFICIENTS FOR ONE TEMPERATURE RANGE
   NDIM2   - ACTUAL SECOND DIMENSION OF ARRAY OF THERMODYNAMIC FIT
             COEFFICIENTS. NDIM2 MUST BE AT LEAST 2 SINCE THERE ARE
             2 TEMPERATURE RANGES.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   TMID    - ARRAY OF COMMON TEMPERATURES DIVIDING THE HIGH AND
             LOW TEMPERATURE THERMODYNAMIC FITS TO THE
             THERMODYNAMIC DATA.
                CGS UNITS - K.
                DIMENSION TMID(*) AT LEAST KK.
   A       - THREE DIMENSIONAL ARRAY OF FIT COEFFICIENTS TO THE
             THERMODYNAMIC DATA FOR THE KK SPECIES.
             THE INDICIES IN  A(N,L,K) MEAN-
             N = 1,NN REPRESENT POLYNOMIAL COEFFICIENTS IN CP/R
               CP/R(K)=A(1,L,K) + A(2,L,K)*T + A(3,L,K)*T**2 + ...
             N = NN+1 IS FOR THE FORMATION ENTHALPIES, I.E.,
               HO/P = A(NN+1,L,K)
             N = NN+2 IS FOR THE STANDARD STATE FORMATION
                 ENTORPIES, I.E.,
               SO/R = A(NN+2,L,K)
             L = 1 IS FOR THE LOW TEMPERATURE RANGE
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            L = 2 IS FOR THE HIGH TEMPERATURES RANGE
            K  IS  THE  SPECIES INDEX
               DIMENSION A(NDIM1,NDIM2,*) EXACTLY NDIM1 AND NDIM2
               FOR THE FIRST AND SECOND DIMENSIONS AND AT LEAST
               KK FOR THE THIRD.


CKAWT        CKAWT        CKAWT        CKAWT        CKAWT        CKAWT
               ************************************
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                           *************
SUBROUTINE CKAWT (IWORK,WORK,AWT)

   THIS SUBROUTINE RETURNS THE ATOMIC WEIGHTS OF THE ELEMENTS.

 INPUT
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   AWT    - ARRAY OF ATOMIC WEIGHTS FOR THE MM ELEMENTS.
               CGS UNITS - GM/MOLE.
               DIMENSION AWT(*) AT LEAST MM.


CKCDC        CKCDC        CKCDC        CKCDC        CKCDC        CKCDC
               ************************************
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                           *************
SUBROUTINE CKCDC (T,C,IWORK,WORK,CDOT,DDOT)

   THIS SUBROUTINE RETURNS THE MOLAR CREATION AND DESTRUCTION
   RATES OF THE SPECIES GIVEN THE TEMPERATURE AND MOLAR
   CONCENTRATIONS. REFERENCE EQUATION (II.5.13).

 INPUT
   T      - TEMPERATURE.
               CGS UNITS - K
   C      - MOLAR CONCENTRATIONS OF THE KK SPECIES.
               CGS UNITS - MOLE/CM**3
               DIMENSION C(*) AT LEAST KK.
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

OUTPUT
   CDOT   - ARRAY OF CHEMICAL MOLAR CREATION RATES FOR THE KK
            SPECIES.
               CGS UNITS - MOLE/(CM**3*SEC).
               DIMENSION CDOT(*) AT LEAST KK.
   DDOT   - ARRAY OF CHEMICAL MOLAR DESTRUCTION RATES FOR THE
            KK SPECIES.
               CGS UNITS - MOLES/(CM**3*SEC).
               DIMENSION DDOT(*) AT LEAST KK.
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CKCDXP      CKCDXP      CKCDXP      CKCDXP      CKCDXP      CKCDXP
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                             *************
SUBROUTINE CKCDXP (P,T,X,IWORK,WORK,CDOT,DDOT)

   THIS SUBROUTINE RETURNS THE MOLAR CREATION AND DESTRUCTION
   RATES OF THE SPECIES GIVEN PRESSURE, TEMPERATURE AND
   MOLE FRACTIONS. REFERENCE EQUATION (II.5.13).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CDOT    - ARRAY OF CHEMICAL MOLAR CREATION RATES FOR THE KK
             SPECIES.
                CGS UNITS - MOLE/(CM**3*SEC).
                DIMENSION CDOT(*) AT LEAST KK.
   DDOT    - ARRAY OF CHEMICAL MOLAR DESTRUCTION RATES FOR THE
             KK SPECIES.
                CGS UNITS - MOLES/(CM**3*SEC).
                DIMENSION DDOT(*) AT LEAST KK.


CKCDXR      CKCDXR      CKCDXR      CKCDXR      CKCDXR      CKCDXR
                 ************************************
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                             *************
SUBROUTINE CKCDXR (RHO,T,X,IWORK,WORK,CDOT,DDOT)

   THIS SUBROUTINE RETURNS THE MOLAR CREATION AND DESTRUCTION
   RATES OF THE SPECIES GIVEN THE MASS DENSITY, TEMPERATURE
   AND MOLE FRACTIONS. REFERENCE EQUATION (II.5.13).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CDOT    - ARRAY OF CHEMICAL MOLAR CREATION RATES FOR THE KK
             SPECIES.
                CGS UNITS - MOLE/(CM**3*SEC).
                DIMENSION CDOT(*) AT LEAST KK.
   DDOT    - ARRAY OF CHEMICAL MOLAR DESTRUCTION RATES FOR THE
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            KK SPECIES.
               CGS UNITS - MOLES/(CM**3*SEC).
               DIMENSION DDOT(*) AT LEAST KK.


CKCDYP      CKCDYP      CKCDYP      CKCDYP      CKCDYP      CKCDYP
               ************************************
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                           *************
SUBROUTINE CKCDYP (P,T,Y,IWORK,WORK,CDOT,DDOT)

   THIS SUBROUTINE RETURNS THE MOLAR CREATION AND DESTRUCTION
   RATES OF THE SPECIES GIVEN MASS DENSITY, TEMPERATURE AND
   MASS FRACTIONS. REFERENCE EQUATION (II.5.13).

 INPUT
   P       - PRESSURE.
               CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
               CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
               CGS UNITS - NONE.
               DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CDOT    - ARRAY OF CHEMICAL MOLAR CREATION RATES FOR THE KK
             SPECIES.
               CGS UNITS - MOLE/(CM**3*SEC).
               DIMENSION CDOT(*) AT LEAST KK.
   DDOT    - ARRAY OF CHEMICAL MOLAR DESTRUCTION RATES FOR THE
             KK SPECIES.
               CGS UNITS - MOLES/(CM**3*SEC).
               DIMENSION DDOT(*) AT LEAST KK.


CKCDYR      CKCDYR      CKCDYR      CKCDYR      CKCDYR      CKCDYR
               ************************************
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                           *************
SUBROUTINE CKCDYR (RHO,T,Y,IWORK,WORK,CDOT,DDOT)

   THIS SUBROUTINE RETURNS THE MOLAR CREATION AND DESTRUCTION
   RATES OF THE SPECIES GIVEN THE MASS DENSITY, TEMPERATURE
   AND MASS FRACTIONS. REFERENCE EQUATION (II.5.13)

 INPUT
   RHO     - MASS DENSITY.
               CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
               CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
               CGS UNITS - NONE.
               DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.
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 OUTPUT
   CDOT    - ARRAY OF CHEMICAL MOLAR CREATION RATES FOR THE KK
             SPECIES.
                CGS UNITS - MOLE/(CM**3*SEC).
                DIMENSION CDOT(*) AT LEAST KK.
   DDOT    - ARRAY OF CHEMICAL MOLAR DESTRUCTION RATES FOR THE
             KK SPECIES.
                CGS UNITS - MOLES/(CM**3*SEC).
                DIMENSION DDOT(*) AT LEAST KK.


CKCHRG       CKCHRG       CKCHRG       CKCHRG       CKCHRG       CKCHRG
                ************************************
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                             *************
SUBROUTINE CKCHRG (IWORK,WORK,KCHARG)

   THIS SUBROUTINE RETURNS THE ELECTRONIC CHARGES OF THE
   SPECIES.

 INPUT
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   KCHARG - ARRAY OF THE CHARGES OF THE  KK  SPECIES.  FOR EXAMPLE
            KCHARG(K)=-2 INDICATES THAT THE K TH SPECIES HAS TWO
            EXCESS ELECTRONS.
                DIMENSION KCHARG(*) AT LEAST KK.


CKCOMP       CKCOMP       CKCOMP       CKCOMP       CKCOMP       CKCOMP
                ************************************
                       *************************
                             *************
SUBROUTINE CKCOMP (LENIH,IH1,IH2,ISAME)

   THIS SUBROUTINE COMPARES TWO HOLLERITH STRINGS TO
   DETERMINE IF THEY ARE THE SAME OR NOT.

 INPUT
   LENIH   - LENGH OF ARRAY OF HOLLERITH CHARACTERS TO BE COMPARED
   IH1     - ARRAY OF A1 HOLLERITH CHARACTERS
                DIMENSION IH1(*) AT LEAST LENIH
   IH2     - ARRAY OF A1 HOLLERITH CHARCTERS
                DIMENSION IH2(*) AT LEAST LENIH

 OUTPUT
   ISAME   - FLAG FOR COMPARISON OF TWO HOLLERITH ARRAYS
             ISAME=1  IH1 IS IDENTICAL TO IH2
             ISAME=0  IH1 IS NOT IDENTICAL TO IH2
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CKCONT      CKCONT      CKCONT      CKCONT      CKCONT      CKCONT
              ************************************
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                            *************
SUBROUTINE CKCONT (K,ROP,IWORK,WORK,CIK)

   THIS SUBROUTINE RETURNS THE CONTRIBUTION OF THE II REACTIONS
   TO THE MOLAR PRODUCTION RATE OF THE K TH SPECIES.

 INPUT
   ROP     - ARRAY OF RATE OF PROGRESS VARIABLES FOR THE II
             REACTIONS.
                CGS UNITS - MOLES/(CM**3*SEC).
                DIMENSION ROP(*) AT LEAST II.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CIK     - ARRAY OF THE CONTRIBUTIONS OF THE II REACTIONS TO
             THE MOLAR PRODUCTION RATE OF THE K TH SPECIES.
                CGS UNITS - MOLE/(CM**3*SEC)
                DIMENSION CIK(*) AT LEAST II.


CKCPBL      CKCPBL      CKCPBL      CKCPBL      CKCPBL      CKCPBL
              ************************************
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                            *************
SUBROUTINE CKCPBL (T,X,IWORK,WORK,CPBML)

   THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN SPECIFIC
   HEAT AT CONSTANT PRESSURE. REFERENCE EQUATION (II.4.20).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CPBML   - MOLAR WEIGHTED MEAN SPECIFIC HEAT AT CONSTANT PRESSURE
             IN MOLAR UNITS.
                CGS UNITS - ERGS/(MOLE*K).
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CKCPBS      CKCPBS      CKCPBS      CKCPBS      CKCPBS      CKCPBS
                ************************************
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                            *************
SUBROUTINE CKCPBS (T,Y,IWORK,WORK,CPBMS)

   THIS SUBROUTINE RETURNS THE MASS WEIGHTED MEAN SPECIFIC
   HEAT AT CONSTANT PRESSURE. REFERENCE EQUATION (II.4.21).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE,
                DIMENSION Y(*) AT LEAST KK,
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CPBMS   - MASS WEIGHTED MEAN SPECIFIC HEAT AT CONSTANT PRESSURE
             IN MASS UNITS.
                CGS UNITS - ERGS/(GM*K).


CKCPML      CKCPML      CKCPML      CKCPML      CKCPML      CKCPML
                ************************************
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                            *************
SUBROUTINE CKCPML (T,IWORK,WORK,CPML)

   THIS SUBROUTINE RETURNS THE SPECIFIC HEATS AT CONSTANT
   PRESSURE IN MOLAR UNITS. REFERENCE EQUATION (II.4.1).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CPML    - ARRAY OF SPECIFIC HEATS AT CONSTANT PRESSURE IN MOLAR
             UNITS FOR THE KK SPECIES.
                CGS UNITS - ERGS/(MOLE*K).
                DIMENSION CPML(*) AT LEAST KK.


CKCPMS      CKCPMS      CKCPMS      CKCPMS      CKCPMS      CKCPMS
                ************************************
                      *************************
                            *************
SUBROUTINE CKCPMS (T,IWORK,WORK,CPMS)

   THIS SUBROUTINE RETURNS THE SPECIFIC HEATS AT CONSTANT
   PRESSURE IN MASS UNITS. REFERENCE EQUATION (II.4.13).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
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```
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CPMS   - ARRAY OF SPECIFIC HEATS AT CONSTANT PRESSURE IN MASS
            UNITS FOR THE KK SPECIES.
               CGS UNITS - ERGS/(GM*K).
               DIMENSION CPMS(*) AT LEAST KK.


CKCPOR      CKCPOR      CKCPOR      CKCPOR      CKCPOR      CKCPOR
               ***************************************
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                           *************
SUBROUTINE CKCPOR (T,IWORK,WORK,CPOR)

   THIS SUBROUTINE RETURNS THE NONDIMENSIONAL SPECIFIC
   HEATS AT CONSTANT PRESSURE. REFERENCE EQUATION
   (II.4.1) OR (II.4.6).

 INPUT
   T      - TEMPERATURE.
               CGS UNITS - K
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CPOR   - ARRAY OF NONDIMENSIONAL SPECIFIC HEATS AT CONSTANT
            PRESSURE FOR THE KK SPECIES.
               CGS UNITS - NONE.
               DIMENSION CPOR(*) AT LEAST KK.


CKCTC       CKCTC       CKCTC       CKCTC       CKCTC       CKCTC
               ***************************************
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                           *************
SUBROUTINE CKCTC (T,C,IWORK,WORK,CDOT,TAU)

   THIS SUBROUTINE RETURNS THE MOLAR CREATION RATES AND
   CHARACTERISTIC DESTRUCTION TIMES OF THE SPECIES GIVEN
   THE TEMPERATURE AND MOLAR CONCENTRATIONS. REFERENCE
   EQUATION (II.5.16).

 INPUT
   T      - TEMPERATURE.
               CGS UNITS - K
   C      - MOLAR CONCENTRATIONS OF THE KK SPECIES.
               CGS UNITS - MOLE/CM**3
               DIMENSION C(*) AT LEAST KK.
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.
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 OUTPUT
   CDOT    - ARRAY OF CHEMICAL MOLAR CREATION RATES FOR THE KK
             SPECIES.
                CGS UNITS - MOLE/(CM**3*SEC).
                DIMENSION CDOT(*) AT LEAST KK.
   TAU     - ARRAY OF CHARACTERISTIC DESTRUCTION TIMES FOR THE
             KK SPECIES.
                CGS UNITS - SEC.
                DIMENSION TAU(*) AT LEAST KK.


CKCTX        CKCTX        CKCTX        CKCTX        CKCTX        CKCTX
                ***************************************
                      ***************************
                            *************
 SUBROUTINE CKCTX (C,IWORK,WORK,X)

    THIS SUBROUTINE RETURNS THE MOLE FRACTIONS GIVEN THE
    MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.3.8).

  INPUT
    C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
    IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
              IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
    WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
              INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

  OUTPUT
    X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.


CKCTXP       CKCTXP       CKCTXP       CKCTXP       CKCTXP       CKCTXP
                ***************************************
                      ***************************
                            *************
 SUBROUTINE CKCTXP (P,T,X,IWORK,WORK,CDOT,TAU)

    THIS SUBROUTINE RETURNS THE MOLAR CREATION RATES AND
    CHARACTERISTIC DESTRUCTION TIMES OF THE SPECIES GIVEN
    THE PRESSURE, TEMPERATURE AND MOLE FRACTIONS. REFERENCE
    EQUATION (II.5.16).

  INPUT
    P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
    T       - TEMPERATURE.
                CGS UNITS - K
    X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
    IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
              IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
    WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
              INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

  OUTPUT
    CDOT    - ARRAY OF CHEMICAL MOLAR CREATION RATES FOR THE KK
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            SPECIES.
               CGS UNITS - MOLE/(CM**3*SEC).
               DIMENSION CDOT(*) AT LEAST KK.
   TAU      - ARRAY OF CHARACTERISTIC DESTRUCTION TIMES FOR THE
            KK SPECIES.
               CGS UNITS - SEC.
               DIMENSION TAU(*) AT LEAST KK.


CKCTXR      CKCTXR      CKCTXR      CKCTXR      CKCTXR      CKCTXR
               ***************************************
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                           *************
SUBROUTINE CKCTXR (RHO,T,X,IWORK,WORK,CDOT,TAU)

   THIS SUBROUTINE RETURNS THE MOLAR CREATION RATES AND
   CHARACTERISTIC DESTRUCTION TIMES OF THE SPECIES GIVEN
   THE MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS. REFERENCE
   EQUATION (II.5.16).

 INPUT
   RHO      - MASS DENSITY.
               CGS UNITS - GM/CM**3.
   T        - TEMPERATURE.
               CGS UNITS - K
   X        - MOLE FRACTIONS OF THE KK SPECIES.
               CGS UNITS - NONE.
               DIMENSION X(*) AT LEAST KK.
   IWORK    - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK     - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CDOT     - ARRAY OF CHEMICAL MOLAR CREATION RATES FOR THE KK
            SPECIES.
               CGS UNITS - MOLE/(CM**3*SEC).
               DIMENSION CDOT(*) AT LEAST KK.
   TAU      - ARRAY OF CHARACTERISTIC DESTRUCTION TIMES FOR THE
            KK SPECIES.
               CGS UNITS - SEC.
               DIMENSION TAU(*) AT LEAST KK.


CKCTY       CKCTY       CKCTY       CKCTY       CKCTY       CKCTY
               ***************************************
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                           *************
SUBROUTINE CKCTY (C,IWORK,WORK,Y)

   THIS SUBROUTINE RETURNS THE MASS FRACTIONS GIVEN THE
   MOLAR CONCENTRATIONS. REFERENCE EQUATION (II.3.7).

 INPUT
   C        - MOLAR CONCENTRATIONS OF THE KK SPECIES.
               CGS UNITS - MOLE/CM**3
               DIMENSION C(*) AT LEAST KK.
   IWORK    - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK     - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.
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 OUTPUT
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.


CKCTYP       CKCTYP       CKCTYP       CKCTYP       CKCTYP       CKCTYP
                ************************************
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                            *************
SUBROUTINE CKCTYP (P,T,Y,IWORK,WORK,CDOT,TAU)

   THIS SUBROUTINE RETURNS THE MOLAR CREATION RATES AND
   CHARACTERISTIC DESTRUCTION TIMES OF THE SPECIES GIVEN
   THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS. REFERENCE
   EQUATION (II.5.16).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CDOT    - ARRAY OF CHEMICAL MOLAR CREATION RATES FOR THE KK
             SPECIES.
                CGS UNITS - MOLE/(CM**3*SEC).
                DIMENSION CDOT(*) AT LEAST KK.
   TAU     - ARRAY OF CHARACTERISTIC DESTRUCTION TIMES FOR THE
             KK SPECIES.
                CGS UNITS - SEC.
                DIMENSION TAU(*) AT LEAST KK.


CKCTYR       CKCTYR       CKCTYR       CKCTYR       CKCTYR       CKCTYR
                ************************************
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                            *************
SUBROUTINE CKCTYR (RHO,T,Y,IWORK,WORK,CDOT,TAU)

   THIS SUBROUTINE RETURNS THE MOLAR CREATION RATES AND
   CHARACTERISTIC DESTRUCTION TIMES OF THE SPECIES GIVEN
   THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS.  REFERENCE
   EQUATION (II.5.16)

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
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                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CDOT    - ARRAY OF CHEMICAL MOLAR CREATION RATES FOR THE KK
             SPECIES.
                CGS UNITS - MOLE/(CM**3*SEC).
                DIMENSION CDOT(*) AT LEAST KK.
   TAU     - ARRAY OF CHARACTERISTIC DESTRUCTION TIMES FOR THE
             KK SPECIES.
                CGS UNITS - SEC.
                DIMENSION TAU(*) AT LEAST KK.


CKCVBL       CKCVBL       CKCVBL       CKCVBL       CKCVBL       CKCVBL
                ************************************
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                            *************
SUBROUTINE CKCVBL (T,X,IWORK,WORK,CVBML)

   THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN SPECIFIC
   HEAT AT CONSTANT VOLUME IN MOLAR UNITS. REFERENCE EQUATION
   (II.4.26).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CVBML   - MOLAR WEIGHTED MEAN SPECIFIC HEAT AT CONSTANT VOLUME
             IN MOLAR UNITS.
                CGS UNITS - ERGS/(MOLE*K).


CKCVBS       CKCVBS       CKCVBS       CKCVBS       CKCVBS       CKCVBS
                ************************************
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                            *************
SUBROUTINE CKCVBS (T,Y,IWORK,WORK,CVBMS)

   THIS SUBROUTINE RETURNS THE MASS WEIGHTED MEAN SPECIFIC HEAT
   AT CONSTANT VOLUME IN MASS UNITS. REFERENCE EQUATION
   (II.4.27).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.
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 OUTPUT
   CVBMS  - MASS WEIGHTED MEAN SPECIFIC HEAT AT CONSTANT VOLUME
            IN MASS UNITS.
               CGS UNITS - ERGS/(GM*K).


CKCVML       CKCVML       CKCVML       CKCVML       CKCVML       CKCVML
                 ************************************
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                             *************
SUBROUTINE CKCVML (T,IWORK,WORK,CVML)

   THIS SUBROUTINE RETURNS THE SPECIFIC HEATS IN CONSTANT
   VOLUME IN MOLAR UNITS. REFERENCE EQUATION (II.4.9).

 INPUT
   T      - TEMPERATURE.
               CGS UNITS - K
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CVML   - ARRAY OF SPECIFIC HEATS AT CONSTANT VOLUME IN MOLAR
            UNITS FOR THE KK SPECIES.
               CGS UNITS - ERGS/(MOLE*K).
               DIMENSION CVML(*) AT LEAST KK.


CKCVMS       CKCVMS       CKCVMS       CKCVMS       CKCVMS       CKCVMS
                 ************************************
                       **************************
                             *************
SUBROUTINE CKCVMS (T,IWORK,WORK,CVMS)

   THIS SUBROUTINE RETURNS THE SPECIFIC HEATS AT CONSTANT
   VOLUME IN MASS UNITS. REFERENCE EQUATION (II.4.16).

 INPUT
   T      - TEMPERATURE.
               CGS UNITS - K
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   CVMS   - ARRAY OF SPECIFIC HEATS AT CONSTANT VOLUME IN MASS
            UNITS FOR THE KK SPECIES.
               CGS UNITS - ERGS/(GM*K).
               DIMENSION CVMS(*) AT LEAST KK.
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CKDAML      CKDAML      CKDAML      CKDAML      CKDAML      CKDAML
              ************************************
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                            *************
SUBROUTINE CKDAML (T,IWORK,WORK,DADTML)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   HELMHOLTZ FREE ENERGIES IN MOLAR UNITS WITH RESPECT TO
   RESPECT TO TEMPERATURE.  REFERENCE EQUATION (II.9.7).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DADTML - ARRAY OF PARTIAL DERIVATIVES OF THE STANDARD STATE
            HELMHOLTZ FREE ENERGY OF THE KK SPECIES IN MOLAR UNITS
            WITH RESPECT TO TEMPERATURE.
               CGS UNITS - ERGS/(MOLE*K).
               DIMENSION DADTML(*) AT LEAST KK.


CKDAMS      CKDAMS      CKDAMS      CKDAMS      CKDAMS      CKDAMS
              ************************************
                     *************************
                            *************
SUBROUTINE CKDAMS (T,IWORK,WORK,DADTMS)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   STANDARD STATE HELMHOLTZ FREE ENERGIES IN MASS UNITS WITH
   RESPECT TO TEMPERATURE.  REFERENCE EQUATION (II.9.14).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DADTMS - ARRAY OF PARTIAL DERIVATIVES OF THE STANDARD STATE
            HELMHOLTZ FREE ENERGY OF THE KK SPECIES IN MASS UNITS
            WITH RESPECT TO TEMPERATURE.
               CGS UNITS - ERGS/(GM*K).
               DIMENSION DADTMS(*) AT LEAST KK.
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CKDCPL      CKDCPL      CKDCPL      CKDCPL      CKDCPL      CKDCPL
            ************************************
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                        *************
SUBROUTINE CKDCPL (T,IWORK,WORK,DCPTML)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   SPECIFIC HEATS AT CONSTANT PRESSURE IN MOLAR UNITS WITH
   RESPECT TO TEMPERATURE.  REFERENCE EQUATION (II.9.1).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCPTML  - ARRAY OF PARTIAL DERIVATIVES OF THE SPECIFIC HEATS
             AT CONSTANT PRESSURE OF THE KK SPECIES IN MOLAR
             UNITS WITH RESPECT TO TEMPERATURE.
                CGS UNITS - ERGS/(MOLE*K**2).
                DIMENSION DCPTML(*) AT LEAST KK.


CKDCPS      CKDCPS      CKDCPS      CKDCPS      CKDCPS      CKDCPS
            ************************************
                  *************************
                        *************
SUBROUTINE CKDCPS (T,IWORK,WORK,DCPTMS)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   SPECIFIC HEATS AT CONSTANT PRESSURE IN MASS UNITS WITH
   RESPECT TO TEMPERATURE.  REFERENCE EQUATION (II.9.3).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE. THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCPTMS  - ARRAY OF PARTIAL DERIVATIVES OF THE SPECIFIC HEATS
             AT CONSTANT PRESSURE OF THE KK SPECIES IN MASS UNITS
             WITH RESPECT TO TEMPERATURE.
                CGS UNITS - ERGS/(GM*K**2).
                DIMENSION DCPTMS(*) AT LEAST KK.
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CKDCPX      CKDCPX      CKDCPX      CKDCPX      CKDCPX      CKDCPX
              ************************************
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                            *************
SUBROUTINE CKDCPX (P,T,X,IWORK,WORK,DCDPTX)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   CONCENTRATIONS WITH RESPECT TO PRESSURE GIVEN PRESSURE,
   TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION (II.8.12).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCDPTX - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR
            CONCENTRATIONS OF THE KK SPECIES WITH RESPECT TO
            PRESSURE.  TEMPERATURE AND MOLE FRACTIONS HELD
            FIXED.
                CGS UNITS - MOLE/(CM*DYNES)
                DIMENSION DCDPTX(*) AT LEAST KK


CKDCPY      CKDCPY      CKDCPY      CKDCPY      CKDCPY      CKDCPY
              ************************************
                     *************************
                            *************
SUBROUTINE CKDCPY (P,T,Y,IWORK,WORK,DCDPTY)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   CONCENTRATIONS WITH RESPECT TO PRESSURE GIVEN PRESSURE,
   TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION (II.8.12).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCDPTY - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR
            CONCENTRATIONS OF THE KK SPECIES WITH RESPECT TO
            PRESSURE.  TEMPERATURE AND MASS FRACTIONS HELD
            FIXED.
                CGS UNITS - MOLE/(CM*DYNES)
                DIMENSION DCDPTY(*) AT LEAST KK
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CKDCRX       CKDCRX       CKDCRX       CKDCRX       CKDCRX       CKDCRX
                 ************************************
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                              *************
SUBROUTINE CKDCRX (RHO,T,X,IWORK,WORK,DCDRTX)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   CONCENTRATIONS WITH RESPECT TO MASS DENSITY GIVEN MASS
   DENSITY, TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION
   (II.8.11).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCDRTX - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR
            CONCENTRATIONS OF THE KK SPECIES WITH RESPECT TO
            MASS DENSITY.  TEMPERATURE AND MOLE FRACTIONS HELD
            FIXED.
                CGS UNITS - MOLE**2/(CM**3*GM)
                DIMENSION DCDRTX(*) AT LEAST KK


CKDCRY       CKDCRY       CKDCRY       CKDCRY       CKDCRY       CKDCRY
                 ************************************
                        **************************
                              *************
SUBROUTINE CKDCRY (RHO,T,Y,IWORK,WORK,DCDRTY)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   CONCENTRATIONS WITH RESPECT TO MASS DENSITY GIVEN MASS
   DENSITY, TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION
   (II.8.10).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCDRTY - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR
            CONCENTRATIONS OF THE KK SPECIES WITH RESPECT TO
            MASS DENSITY.  TEMPERATURE AND MASS FRACTIONS HELD
            FIXED.
                CGS UNITS - MOLE**2/(CM**3*GM)
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```
                DIMENSION DCDRTY(*) AT LEAST KK


CKDCTX       CKDCTX       CKDCTX       CKDCTX       CKDCTX       CKDCTX
                ***********************************
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                            *************
SUBROUTINE CKDCTX (P,T,X,IWORK,WORK,DCDTPX)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   CONCENTRATIONS WITH RESPECT TO TEMPERATURE GIVE THE PRESSURE,
   TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION (II.8.8).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCDTPX - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR
            CONCENTRATIONS OF THE KK SPECIES WITH RESPECT TO
            TEMPERATURE.  PRESSURE AND MOLE FRACTIONS HELD
            FIXED.
                CGS UNITS - MOLE/(CM**3*K).
                DIMENSION DCDTPX(*) AT LEAST KK.


CKDCTY       CKDCTY       CKDCTY       CKDCTY       CKDCTY       CKDCTY
                ***********************************
                      *************************
                            *************
SUBROUTINE CKDCTY (P,T,Y,IWORK,WORK,DCDTPY)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   CONCENTRATIONS WITH RESPECT TO TEMPERATURE GIVEN THE
   PRESSURE, TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION
   (II.8.7).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCDTPY - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR
    .       CONCENTRATIONS OF THE KK SPECIES WITH RESPECT TO
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            TEMPERATURE.  PRESSURE AND MASS FRACTION HELD FIXED.
               CGS UNITS - MOLE/(CM**3*K).
               DIMENSION DCDTPY(*) AT LEAST KK.


CKDCVL      CKDCVL      CKDCVL      CKDCVL      CKDCVL      CKDCVL
               ***************************************
                     *************************
                           *************
SUBROUTINE CKDCVL (T,IWORK,WORK,DCVTML)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   SPECIFIC HEATS AT CONSTANT VOLUME IN MOLAR UNITS WITH RESPECT
   TO TEMPERATURE.  REFERENCE EQUATION (II.9.4).

 INPUT
   T       - TEMPERATURE.
               CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCVTML - ARRAY OF PARTIAL DERIVATIVES OF THE SPECIFIC HEATS
            AT CONSTANT VOLUME OF THE KK SPECIES IN MOLAR
            UNITS WITH RESPECT TO TEMPERATURE.
               CGS UNITS - ERGS/(MOLE*K**2).
               DIMENSION DCVTML(*) AT LEAST KK.


CKDCVS      CKDCVS      CKDCVS      CKDCVS      CKDCVS      CKDCVS
               ***************************************
                     *************************
                           *************
SUBROUTINE CKDCVS (T,IWORK,WORK,DCVTMS)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   SPECIFIC HEATS AT CONSTANT VOLUME IN MASS UNITS WITH RESPECT
   TO TEMPERATURE.  REFERENCE EQUATION (II.9.11).

 INPUT
   T       - TEMPERATURE.
               CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCVTMS - ARRAY OF PARTIAL DERIVATIVES OF THE SPECIFIC HEATS
            AT CONSTANT VOLUME OF THE KK SPECIES IN MASS
            UNITS WITH RESPECT TO TEMPERATURE.
               CGS UNITS - ERGS/(GM*K**2).
               DIMENSION DCVTMS(*) AT LEAST KK.
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CKDCXP      CKDCXP      CKDCXP      CKDCXP      CKDCXP      CKDCXP
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                            *************
SUBROUTINE CKDCXP (P,T,X,KDIM,IWORK,WORK,DCKDXN)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   CONCENTRATIONS WITH RESPECT TO THE MOLE FRACTIONS GIVEN THE
   PRESSURE, TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION
   (II.8.5).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCKDXN - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR
            CONCENTRATIONS OF THE KK SPECIES WITH RESPECT TO THE
            MOLE FRACTIONS OF THE KK SPECIES.  PRESSURE AND
            TEMPERATURE HELD FIXED.  DCKDXN(K,N) IS THE PARTIAL
            DERIVATIVE OF THE MOLAR CONCENTRATION OF SPECIES K
            WITH RESPECT TO THE MOLE FRACTION OF SPECIES N.
               CGS UNITS - MOLE/CM**3.
               DIMENSION DCKDXN(KDIM,*) EXACTLY KDIM FOR THE
               FIRST DIMENSION AND AT LEAST KK FOR THE SECOND.


CKDCXR      CKDCXR      CKDCXR      CKDCXR      CKDCXR      CKDCXR
              ************************************
                     *************************
                            *************
SUBROUTINE CKDCXR (RHO,T,X,KDIM,IWORK,WORK,DCKDXN)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   CONCENTRATIONS WITH RESPECT TO THE MOLE FRACTIONS GIVEN THE
   MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS.  REFERENCE
   EQUATION (II.8.6).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
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                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCKDXN - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR
            CONCENTRATIONS OF THE KK SPECIES WITH RESPECT TO THE
            MOLE FRACTIONS OF THE KK SPECIES.  DENSITY AND
            TEMPERATURE HELD FIXED.  DCKDXN(K,N) IS THE PARTIAL
            DERIVATIVE OF THE MOLAR CONCENTRATION OF SPECIES K
            WITH RESPECT TO THE MOLE FRACTION OF SPECIES N.
               CGS UNITS - MOLE/CM**3.
               DIMENSION DCKDXN(KDIM,*) EXACTLY KDIM FOR THE
               FIRST DIMENSION AND AT LEAST KK FOR THE SECOND.


CKDCYP      CKDCYP      CKDCYP      CKDCYP      CKDCYP      CKDCYP
               ************************************
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                           *************
SUBROUTINE CKDCYP (P,T,Y,KDIM,IWORK,WORK,DCKDYN)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   CONCENTRATIONS WITH RESPECT TO THE MASS FRACTIONS GIVEN THE
   PRESSURE, TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION
   (II.8.3).

 INPUT
   P      - PRESSURE.
               CGS UNITS - DYNES/CM**2.
   T      - TEMPERATURE.
               CGS UNITS - K
   Y      - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
               CGS UNITS - NONE.
               DIMENSION Y(*) AT LEAST KK.
   KDIM   - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
            KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
            NUMBER OF SPECIES, KK.
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCKDYN - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR
            CONCENTRATIONS OF THE KK SPECIES WITH RESPECT TO
            THE MASS FRACTIONS OF THE KK SPECIES.  PRESSURE
            AND TEMPERATURE HELD FIXED.  DCKDYN(K,N) IS THE
            PARTIAL DERIVATIVE OF THE MOLAR CONCENTRATION OF
            SPECIES K WITH RESPECT TO THE MASS FRACTION OF
            SPECIES N.
               CGS UNITS - MOLE/CM**3.
               DIMENSION DCKDYN(KDIM,*) EXACTLY KDIM FOR THE
               FIRST DIMENSION AND AT LEAST KK FOR THE SECOND.
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CKDCYR      CKDCYR      CKDCYR      CKDCYR      CKDCYR      CKDCYR
            ************************************
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                            *************
SUBROUTINE CKDCYR (RHO,T,Y,KDIM,IWORK,WORK,DCKDYN)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   CONCENTRATIONS WITH RESPECT TO THE MASS FRACTIONS GIVEN THE
   MASS DENSITY, TEMPERATURE AND MASS FRACTIONS.  REFERENCE
   EQUATION (II.8.4).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DCKDYN - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR
            CONCENTRATIONS OF THE KK SPECIES WITH RESPECT TO
            THE MASS FRACTIONS OF THE KK SPECIES.  DENSITY
            AND TEMPERATURE HELD FIXED.  DCKDYN(K,N) IS THE
            PARTIAL DERIVATIVE OF THE MOLAR CONCENTRATION OF
            SPECIES K WITH RESPECT TO THE MASS FRACTION OF
            SPECIES N.
                CGS UNITS - MOLE/CM**3.
                DIMENSION DCKDYN(KDIM,*) EXACTLY KDIM FOR THE
                FIRST DIMENSION AND AT LEAST KK FOR THE SECOND.


CKDGML      CKDGML      CKDGML      CKDGML      CKDGML      CKDGML
            ************************************
                    *************************
                            *************
SUBROUTINE CKDGML (T,IWORK,WORK,DGDTML)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE GIBBS
   STATE GIBBS FREE ENERGIES IN MOLAR UNITS WITH RESPECT TO
   TEMPERATURE.  REFERENCE EQUATION (II.9.6).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DGDTML - ARRAY OF PARTIAL DERIVATIVES OF THE STANDARD STATE
            GIBBS FREE ENERGY IN MOLAR UNITS WITH RESPECT TO
            TEMPERATURE.
                CGS UNITS - ERGS/(MOLE*K).
```

DIMENSION DGDTML(*) AT LEAST KK.

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CKDGMS      CKDGMS      CKDGMS      CKDGMS      CKDGMS      CKDGMS
                 ************************************
                       *************************
                             *************
SUBROUTINE CKDGMS (T,IWORK,WORK,DGDTMS)
```

THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE STANDARD STATE GIBBS ENERGIES IN MASS UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.13).

INPUT

T - TEMPERATURE.
CGS UNITS - K

IWORK - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR DETAILS ON THE REQUIRED LENGTH OF IWORK.

WORK - ARRAY OF REAL INTERNAL WORK SPACE. THE WORK ARRAY IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR DETAILS ON THE REQUIRED LENGTH OF WORK.

OUTPUT

DGDTMS - ARRAY OF PARTIAL DERIVATIVES OF THE STANDARD STATE GIBBS FREE ENERGY OF THE KK SPECIES IN MASS UNITS WITH RESPECT TO TEMPERATURE.
CGS UNITS - ERGS/(GM*K).
DIMENSION DGDTMS(*) AT LEAST KK.

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CKDHML      CKDHML      CKDHML      CKDHML      CKDHML      CKDHML
                 ************************************
                       *************************
                             *************
SUBROUTINE CKDHML (T,IWORK,WORK,DHDTML)
```

THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE ENTHALPIES IN MOLAR UNITS WITH RESPECT TO TEMPERATURE. REFERENCE EQUATION (II.9.2).

INPUT

T - TEMPERATURE.
CGS UNITS - K

IWORK - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR DETAILS ON THE REQUIRED LENGTH OF IWORK.

WORK - ARRAY OF REAL INTERNAL WORK SPACE. THE WORK ARRAY IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR DETAILS ON THE REQUIRED LENGTH OF WORK.

OUTPUT

DHDTML - ARRAY OF PARTIAL DERIVATIVES OF THE ENTHALPIES OF THE KK SPECIES IN MOLAR UNITS WITH RESPECT TO TEMPERATURE.
CGS UNITS - ERGS/(MOLE*K).
DIMENSION DHDTML(*) AT LEAST KK.

```
CKDHMS      CKDHMS      CKDHMS      CKDHMS      CKDHMS      CKDHMS
                ************************************
                      *************************
                            *************
SUBROUTINE CKDHMS (T,IWORK,WORK,DHDTMS)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   ENTHALPIES IN MASS UNITS WITH RESPECT TO TEMPERATURE.
   REFERENCE EQUATION (II.9.9).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DHDTMS  - ARRAY OF PARTIAL DERIVATIVES OF THE ENTHALPIES
             OF THE KK SPECIES IN MASS UNITS WITH RESPECT TO
             TEMPERATURE.
                CGS UNITS - ERGS/(GM*K).
                DIMENSION DHDTMS(*) AT LEAST KK.


CKDPDC      CKDPDC      CKDPDC      CKDPDC      CKDPDC      CKDPDC
                ************************************
                      *************************
                            *************
SUBROUTINE CKDPDC (RHO,T,C,IWORK,WORK,DPDC)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE
   PRESSURE WITH RESPECT TO THE MOLAR CONCENTRATIONS
   GIVEN THE MASS DENSITY, TEMPERATURE AND MOLAR CONCENTRATIONS.
   REFERENCE EQUATION (II.7.15).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DPDC    - ARRAY OF PARTIAL DERIVATIVES OF THE PRESSURE
             WITH RESPECT TO THE MOLAR CONCENTRATIONS OF
             THE KK SPECIES.
                CGS UNITS - DYNES*CM/MOLE.
                DIMENSION DPDC(*) AT LEAST KK.
```

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CKDPDX      CKDPDX      CKDPDX      CKDPDX      CKDPDX      CKDPDX
            ************************************
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                            **************
SUBROUTINE CKDPDX (RHO,T,X,IWORK,WORK,DPDX)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   PRESSURE WITH RESPECT TO MOLE FRACTIONS GIVEN MASS DENSITY,
   TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION (II.7.14).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DPDX    - ARRAY OF PARTIAL DERIVATIVES OF THE PRESSURE
             WITH RESPECT TO THE MOLE FRACTIONS OF THE KK
             SPECIES.
                CGS UNITS - DYNES/CM**2.
                DIMENSION DPDX(*) AT LEAST KK.


CKDPDY      CKDPDY      CKDPDY      CKDPDY      CKDPDY      CKDPDY
            ************************************
                    ***************************
                            **************
SUBROUTINE CKDPDY (RHO,T,Y,IWORK,WORK,DPDY)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF PRESSURE
   WITH RESPECT TO THE MASS FRACTIONS GIVEN THE MASS DENSITY,
   TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION (II.7.13).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DPDY    - ARRAY OF PARTIAL DERIVATIVES OF THE PRESSURE
             WITH RESPECT TO THE MASS FRACTIONS OF THE KK
             SPECIES.
                CGS UNITS - DYNES/CM**2.
                DIMENSION DPDY(*) AT LEAST KK.
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CKDPTC      CKDPTC      CKDPTC      CKDPTC      CKDPTC      CKDPTC
            ***************************************
                    ****************************
                            *************
SUBROUTINE CKDPTC (RHO,T,C,IWORK,WORK,DPDT)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE PRESSURE
   WITH RESPECT TO TEMPERATURE GIVEN THE MASS DENSITY, TEMPERATURE
   AND MOLAR CONCENTRATIONS.  REFERENCE EQUATION (II.7.12).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DPDT    - PARTIAL DERIVATIVE OF THE PRESSURE WITH RESPECT
             TO TEMPERATURE.
                CGS UNITS - DYNES/(CM**2*K).


CKDPTX      CKDPTX      CKDPTX      CKDPTX      CKDPTX      CKDPTX
            ***************************************
                    ****************************
                            *************
SUBROUTINE CKDPTX (RHO,T,X,IWORK,WORK,DPDT)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE PESSURE
   WITH RESPECT TO TEMPERATURE GIVEN THE MASS DENSITY, TEMPERATURE
   AND MOLE FRACTIONS.  REFERENCE EQUATION (II.7.11)

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DPDT    - PARTIAL DERIVATIVE OF THE PRESSURE WITH RESPECT
             TO TEMPERATURE.
                CGS UNITS - DYNES/(CM**2*K).
```

```
CKDPTY      CKDPTY      CKDPTY      CKDPTY      CKDPTY      CKDPTY
                ************************************
                      *************************
                            *************
SUBROUTINE CKDPTY (RHO,T,Y,IWORK,WORK,DPDT)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE PRESSURE
   WITH RESPECT TO TEMPERATURE GIVEN THE MASS DENSITY, TEMPERATURE
   AND MASS FRACTIONS.  REFERENCE EQUATION (II.7.10)

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DPDT    - PARTIAL DERIVATIVE OF THE PRESSURE WITH RESPECT
             TO TEMPERATURE.
                CGS UNITS - DYNES/(CM**2*K).


CKDRDC      CKDRDC      CKDRDC      CKDRDC      CKDRDC      CKDRDC
                ************************************
                      *************************
                            *************
SUBROUTINE CKDRDC (P,T,C,IWORK,WORK,DRHODC)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MASS
   DENSITY WITH RESPECT TO THE MOLAR CONCENTRATIONS GIVEN THE
   PRESSURE, TEMPERATURE AND MOLAR CONCENTRATIONS.  REFERENCE
   EQUATION (II.7.9).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DRHODC - ARRAY OF PARTIAL DERIVATIVES OF THE MASS DENSITY
            WITH RESPECT TO THE MOLAR CONCENTRATIONS OF THE
            KK SPECIES.
               CGS UNITS - GM/MOLE.
               DIMENSION DRHODC(*) AT LEAST KK.
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CKDRDX      CKDRDX      CKDRDX      CKDRDX      CKDRDX      CKDRDX
                 ************************************
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                               *************
SUBROUTINE CKDRDX (P,T,X,IWORK,WORK,DRHODX)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MASS
   DENSITY WITH RESPECT TO THE MOLE FRACTIONS GIVEN THE PRESSURE,
   TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION (II.7.8).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DRHODX - ARRAY OF PARTIAL DERIVATIVES OF THE MASS DENSITY
            WITH RESPECT TO THE MOLE FRACTIONS OF THE KK
            SPECIES.
               CGS UNITS - GM/CM**3.
               DIMENSION DRHODX(*) AT LEAST KK.


CKDRDY      CKDRDY      CKDRDY      CKDRDY      CKDRDY      CKDRDY
                 ************************************
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                               *************
SUBROUTINE CKDRDY (P,T,Y,IWORK,WORK,DRHODY)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MASS
   DENSITY WITH RESPECT TO MASS FRACTIONS GIVEN PRESSURE,
   TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION (II.7.7).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DRHODY - ARRAY OF PARTIAL DERIVATIVES OF THE MASS DENSITY
            WITH RESPECT TO THE MASS FRACTIONS OF THE KK
            SPECIES.
               CGS UNITS - GM/CM**3.
               DIMENSION DRHODY(*) AT LEAST KK.
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CKDRTC      CKDRTC      CKDRTC      CKDRTC      CKDRTC      CKDRTC
                 ************************************
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                             *************
SUBROUTINE CKDRTC (P,T,C,IWORK,WORK,DRHODT)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE MASS
   DENSITY WITH RESPECT TO TEMPERATURE GIVEN PRESSURE,
   TEMPERATURE AND MOLAR CONCENTRATION.  REFERENCE EQUATION
   (II.7.6).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DRHODT - PARTIAL DERIVATIVE OF THE MASS DENSITY WITH RESPECT
            TO TEMPERATURE.
                CGS UNITS - GM/(CM**3*K).


CKDRTX      CKDRTX      CKDRTX      CKDRTX      CKDRTX      CKDRTX
                 ************************************
                       *************************
                             *************
SUBROUTINE CKDRTX (P,T,X,IWORK,WORK,DRHODT)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE MASS
   DENSITY WITH RESPECT TO TEMPERATURE GIVEN PRESSURE,
   TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION
   (II.7.5)

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DRHODT - PARTIAL DERIVATIVE OF THE MASS DENSITY WITH RESPECT
            TO TEMPERATURE.
                CGS UNITS - GM/(CM**3*K).
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CKDRTY       CKDRTY       CKDRTY       CKDRTY       CKDRTY       CKDRTY
                 ************************************
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                             *************
SUBROUTINE CKDRTY (P,T,Y,IWORK,WORK,DRHODT)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE MASS
   DENSITY WITH RESPECT TO TEMPERATURE GIVEN THE PRESSURE,
   TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION (II.7.4)

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DRHODT - PARTIAL DERIVATIVE OF THE MASS DENSITY WITH RESPECT
            TO TEMPERATURE.
                CGS UNITS - GM/(CM**3*K).


CKDSML       CKDSML       CKDSML       CKDSML       CKDSML       CKDSML
                 ************************************
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                             *************
SUBROUTINE CKDSML (T,IWORK,WORK,DSDTML)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   STANDARD STATE ENTROPIES IN MOLAR UNITS WITH RESPECT TO
   TEMPERATURE.  REFERENCE EQUATION (II.9.3).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DSDTML - ARRAY OF PARTIAL DERIVATIVES OF THE STANDARD STATE
            ENTROPIES OF THE KK SPECIES IN MOLAR UNITS WITH
            RESPECT TO TEMPERATURE.
                CGS UNITS - ERGS/(MOLE*K**2).
                DIMENSION DSDTML(*) AT LEAST KK.
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CKDSMS      CKDSMS      CKDSMS      CKDSMS      CKDSMS      CKDSMS
                ************************************
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                            *************
SUBROUTINE CKDSMS (T,IWORK,WORK,DSDTMS)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   STANDARD STATE ENTROPIES IN MASS UNITS WITH RESPECT TO
   TEMPERATURE.  REFERENCE EQUATION (II.9.10).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DSDTMS - ARRAY OF PARTIAL DERIVATIVES OF THE STANDARD STATE
            ENTROPIES OF THE KK SPECIES IN MASS UNITS WITH RESPECT
            TO TEMPERATURE.
                CGS UNITS - ERGS/(GM*K**2).
                DIMENSION DSDTMS(*) AT LEAST KK.


CKDTC       CKDTC       CKDTC       CKDTC       CKDTC       CKDTC
                ************************************
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                            *************
SUBROUTINE CKDTC (T,C,IWORK,WORK,DWDTC)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO TEMPERATURE
   GIVEN THE TEMPERATURE AND MOLAR CONCENTRATIONS.  REFERENCE
   EQUATION (II.10.1).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDTC  - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO TEMPERATURE.
            MOLAR CONCENTRATIONS HELD FIXED.
                CGS UNITS - MOLE/(CM**3*SEC*K).
                DIMENSION DWDTC(*) AT LEAST KK.
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CKDTXP      CKDTXP      CKDTXP      CKDTXP      CKDTXP      CKDTXP
                ************************************
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                            *************
SUBROUTINE CKDTXP (P,T,X,IWORK,WORK,DWDTPX)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO TEMPERATURE
   GIVEN THE PRESSURE AND MOLE FRACTIONS.  REFERENCE EQUATION
   (II.10.1).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDTPX - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR
            PRODUCTION RATES OF THE KK SPECIES WITH RESPECT
            TO TEMPERATURE.  PRESSURE AND MOLE FRACTIONS HELD
            FIXED.
                CGS UNITS - MOLE/(CM**3*SEC*K).
                DIMENSION DWDTPX(*) AT LEAST KK.


CKDTXR      CKDTXR      CKDTXR      CKDTXR      CKDTXR      CKDTXR
                ************************************
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                            *************
SUBROUTINE CKDTXR (RHO,T,X,IWORK,WORK,DWDTRX)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO TEMPERATURE
   GIVEN THE MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS.
   REFERENCE EQUATION (II.10.1).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDTRX - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT OT TEMPERATURE.
            DENSITY AND MOLE FRACTION HELD FIXED.
                CGS UNITS - MOLE/(CM**3*SEC*K).
                DIMENSION DWDTRX(*) AT LEAST KK.
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CKDTYP      CKDTYP      CKDTYP      CKDTYP      CKDTYP      CKDTYP
                ************************************
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                            *************
SUBROUTINE CKDTYP (P,T,Y,IWORK,WORK,DWDTPY)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO TEMPERATURE
   GIVEN THE PRESSURE, TEMPERATURE AND MASS FRACTIONS.
   REFERENCE EQUATION (II.10.1).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDTPY - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR
            PRODUCTION RATES OF THE KK SPECIES WITH RESPECT
            TO TEMPERATURE.  PRESSURE AND MASS FRACTIONS HELD
            FIXED.
                CGS UNITS - MOLE/(CM**3*SEC*K).
                DIMENSION DWDTPY(*) AT LEAST KK.


CKDTYR      CKDTYR      CKDTYR      CKDTYR      CKDTYR      CKDTYR
                ************************************
                      *************************
                            *************
SUBROUTINE CKDTYR (RHO,T,Y,IWORK,WORK,DWDTRY)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO TEMPERATURE
   GIVEN THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS.
   REFERENCE EQUATION (II.10.1).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDTRY - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR
            PRODUCTION RATES OF THE KK SPECIES WITH RESPECT
            TO TEMPERATURE.  DENSITY AND MASS FRACTIONS HELD
            FIXED.
                CGS UNITS - MOLE/(CM**3*SEC*K).
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                DIMENSION DWDTRY(*) AT LEAST KK.


CKDUML       CKDUML       CKDUML       CKDUML       CKDUML       CKDUML
                ************************************
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                            *************
SUBROUTINE CKDUML (T,IWORK,WORK,DUDTML)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   INTERNAL ENERGIES IN MOLAR UNITS WITH RESPECT TO TEMPERATURE.
   REFERENCE EQUATION (II.9.5).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DUDTML - ARRAY OF PARTIAL DERIVATIVES OF THE INTERNAL ENERGIES
            OF THE KK SPECIES IN MOLAR UNITS WITH RESPECT TO
            TEMPERATURE.
                CGS UNITS - ERGS/(MOLE*K).
                DIMENSION DUDTML(*) AT LEAST KK.


CKDUMS       CKDUMS       CKDUMS       CKDUMS       CKDUMS       CKDUMS
                ************************************
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                            *************
SUBROUTINE CKDUMS (T,IWORK,WORK,DUDTMS)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   INTERNAL ENERGIES IN MASS UNITS WITH RESPECT TO TEMPERATURE.
   REFERENCE EQUATION (II.9.12).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DUDTMS - ARRAY OF PARTIAL DERIVATIVES OF THE INTERNAL ENERGIES
            OF THE KK SPECIES IN MASS UNITS WITH RESPECT TO
            TEMPERATURE.
                CGS UNITS - ERGS/(GM*K).
                DIMENSION DUDTMS(*) AT LEAST KK.
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CKDWBC      CKDWBC      CKDWBC      CKDWBC      CKDWBC      CKDWBC
            ************************************
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                            *************
SUBROUTINE CKDWBC (C,IWORK,WORK,DWBDC)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   MEAN MOLECULAR WEIGHT WITH RESPECT TO THE MOLAR
   CONCENTRATIONS GIVEN THE MOLAR CONCENTRATIONS.  REFERENCE
   EQUATION (II.7.3).

 INPUT
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWBDC   - ARRAY OF PARTIAL DERIVATIVES OF THE MEAN MOLECULAR
             WEIGHT WITH RESPECT TO THE MOLAR CONCENTRATIONS
             OF THE KK SPECIES.
                DIMENSION DWBDC(*) AT LEAST KK.
                CGS UNITS - GM*CM**3/MOLE**2.


CKDWBX      CKDWBX      CKDWBX      CKDWBX      CKDWBX      CKDWBX
            ************************************
                    *************************
                            *************
SUBROUTINE CKDWBX (X,IWORK,WORK,DWBDX)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE
   MEAN MOLECULAR WEIGHT WITH RESPECT TO THE MOLE FRACTIONS
   GIVEN THE MOLE FRACTIONS.  REFERENCE EQUATION (II.7.2).

 INPUT
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWBDX   - ARRAY OF PARTIAL DERIVATIVES OF THE MEAN MOLECULAR
             WEIGHT WITH RESPECT TO THE MOLE FRACTIONS OF THE
             KK SPECIES.
                CGS UNITS - GM/MOLE.
                DIMENSION DWBDX(*) AT LEAST KK.
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CKDWBY      CKDWBY      CKDWBY      CKDWBY      CKDWBY      CKDWBY
            ************************************
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                            ***********
SUBROUTINE CKDWBY (Y,IWORK,WORK,DWBDY)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVE OF THE
   MEAN MOLECULAR WEIGHT WITH RESPECT TO THE MASS FRACTIONS
   GIVEN THE MASS FRACTIONS.  REFERENCE EQUATION (II.7.1).

 INPUT
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWBDY   - ARRAY OF PARTIAL DERIVATIVES OF THE MEAN MOLECULAR
             WEIGHT WITH RESPECT TO THE MASS FRACTIONS OF THE
             KK SPECIES.
                CGS UNITS - GM/MOLE.
                DIMENSION DWBDY(*) AT LEAST KK.


CKDWC       CKDWC       CKDWC       CKDWC       CKDWC       CKDWC
            ************************************
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                            *************
SUBROUTINE CKDWC (T,C,KDIM,IWORK,WORK,DWDCT)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO MOLAR
   CONCENTRATIONS GIVEN THE TEMPERATURE AND MOLAR CONCENTRATIONS.
   REFERENCE EQUATION (II.10.25).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDCT   - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR
             PRODUCTION RATES OF THE KK SPECIES WITH RESPECT TO
             THE MOLAR CONCENTRATIONS OF THE KK SPECIES.
             TEMPERATURE HELD FIXED.  DWDCT(K,N) IS THE PARTIAL
             DERIVATIVE OF THE MOLAR PRODUCTION RATE FOR SPECIES
             K WITH RESPECT TO THE MOLAR CONCENTRATION OF SPECIES
             N.
                CGS UNITS - 1/SEC.
                DIMENSION DWDCT(KDIM,*) EXACTLY KDIM FOR THE
                FIRST DIMENSION AND AT LEAST KK FOR THE SECOND.
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CKDWPX       CKDWPX       CKDWPX       CKDWPX       CKDWPX       CKDWPX
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                              *************
SUBROUTINE CKDWPX (P,T,X,IWORK,WORK,DWDPTX)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO PRESSURE
   GIVEN THE PRESSURE, TEMPERATURE AND MOLE FRACTIONS.
   REFERENCE EQUATION (II.10.32).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDPTX - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO PRESSURE.
            TEMPERATURE AND MOLE FRACTIONS HELD FIXED.
                CGS UNITS - MOLE/(CM*SEC*DYNES).
                DIMENSION DWDPTX(*) AT LEAST KK.


CKDWPY       CKDWPY       CKDWPY       CKDWPY       CKDWPY       CKDWPY
                 ****************************************
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                              *************
SUBROUTINE CKDWPY (P,T,Y,IWORK,WORK,DWDPTY)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO PRESSURE
   GIVEN THE PRESSURE, TEMPERATURE AND MASS FRACTIONS.
   REFERENCE EQUATION (II.10.32).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDPTY - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO PRESSURE.
            TEMPERATURE AND MASS FRACTIONS HELD FIXED.
                CGS UNITS - MOLE/(CM*SEC*DYNES).
                DIMENSION DWDPTY(*) AT LEAST KK.
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CKDWRX      CKDWRX      CKDWRX      CKDWRX      CKDWRX      CKDWRX
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                            *************
SUBROUTINE CKDWRX (RHO,T,X,IWORK,WORK,DWDRTX)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE MASS
   DENSITY GIVEN THE MASS DENSITY, TEMPERATURE AND MOLE
   FRACTIONS.  REFERENCE EQUATION (II.10.38).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDRTX - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO DENSITY.
            TEMPERATURE AND MOLE FRACTIONS HELD FIXED.
                CGS UNITS - MOLE/(SEC*GM).
                DIMENSION DWDRTX(*) AT LEAST KK.


CKDWRY      CKDWRY      CKDWRY      CKDWRY      CKDWRY      CKDWRY
                ************************************
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                            *************
SUBROUTINE CKDWRY (RHO,T,Y,IWORK,WORK,DWDRTY)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE MASS
   DENSITY GIVEN THE MASS DENSITY, TEMPERATURE AND MASS
   FRACTIONS. REFERENCE EQUATION (II.10.38).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDRTY - ARRAY OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO DENSITY.
            TEMPERATURE AND MASS FRACTIONS HELD FIXED.
                CGS UNITS - MOLE/(SEC*GM).
                DIMENSION DWDRTY(*) AT LEAST KK.
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CKDWXP      CKDWXP      CKDWXP      CKDWXP      CKDWXP      CKDWXP
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SUBROUTINE CKDWXP (P,T,X,KDIM,IWORK,WORK,DWDXPT)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO MOLE FRACTIONS
   GIVEN THE PRESSURE, TEMPERATURE AND MOLE FRACTIONS.  REFERENCE
   EQUATION (II.10.19).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDXPT  - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR
             PRODUCTION RATES OF THE KK SPECIES WITH RESPECT TO
             THE MOLE FRACTIONS OF THE KK SPECIES.  PRESSURE
             AND TEMPERATURE HELD FIXED.  DWDXPT(K,N) IS THE
             PARTIAL DERIVATIVE OF THE MOLAR PRODUCTION RATE FOR
             SPECIES K WITH RESPECT TO THE MOLE FRACTION OF
             SPECIES N.
                CGS UNITS - MOLE/(CM**3*SEC).
                DIMENSION DWDXPT(KDIM,*) EXACTLY KDIM FOR THE
                FIRST DIMENSION AND AT LEAST KK FOR THE SECOND.


CKDWXR      CKDWXR      CKDWXR      CKDWXR      CKDWXR      CKDWXR
              ************************************
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                            *************
SUBROUTINE CKDWXR (RHO,T,X,KDIM,IWORK,WORK,DWDXRT)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO MOLE FRACTIONS
   GIVEN THE MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS.
   REFERENCE EQUATION (II.10.19).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
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            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDXRT - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR
            PRODUCTION RATES OF THE KK SPECIES WITH RESPECT TO
            THE MOLE FRACTIONS OF THE KK SPECIES.  DENSITY AND
            TEMPERATURE HELD FIXED.  DWDXRT(K,N) IS THE PARTIAL
            DERIVATIVE OF THE MOLAR PRODUCTION RATE OF SPECIES
            K WITH RESPECT TO THE MOLE FRACTION OF SPECIES N.
               CGS UNITS - MOLE/(CM**3*SEC).
               DIMENSION DWDXRT(KDIM,*) EXACTLY KDIM FOR THE
               FIRST DIMENSION AND AT LEAST KK FOR THE SECOND.


CKDWYP       CKDWYP       CKDWYP       CKDWYP       CKDWYP       CKDWYP
               ************************************
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                             *************
SUBROUTINE CKDWYP (P,T,Y,KDIM,IWORK,WORK,DWDYPT)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE MASS
   FRACTIONS GIVEN THE PRESSURE, TEMPERATURE AND MASS FRACTION.
   REFERENCE EQUATION (II.10.13).

 INPUT
   P      - PRESSURE.
               CGS UNITS - DYNES/CM**2.
   T      - TEMPERATURE.
               CGS UNITS - K
   Y      - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
               CGS UNITS - NONE.
               DIMENSION Y(*) AT LEAST KK.
   KDIM   - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
            KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
            NUMBER OF SPECIES, KK.
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDYPT - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO THE MASS
            FRACTIONS OF THE KK SPECIES. PRESSURE AND TEMPERATURE
            FIXED. DWDYPT(K,N) IS THE PARTIAL DERIVATIVE OF THE
            MOLAR PRODUCTION RATE FOR SPECIES K WITH RESPECT TO
            THE MASS FRACTION OF SPECIES N.
               CGS UNITS - MOLES/(CM**3 SEC)
               DIMENSION DWDYPT(KDIM,*) EXACTLY KDIM FOR THE
               FIRST DIMENSION AND AT LEAST KK FOR THE SECOND.
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CKDWYR      CKDWYR      CKDWYR      CKDWYR      CKDWYR      CKDWYR
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SUBROUTINE CKDWYR (RHO,T,Y,KDIM,IWORK,WORK,DWDYRT)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE MASS
   FRACTIONS GIVEN THE MASS DENSITY, TEMPERATURE AND MASS
   FRACTIONS.  REFERENCE EQUATION (II.10.13).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
           - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWDYRT - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR
            PRODUCTION RATES OF THE KK SPECIES WITH RESPECT TO
            THE MASS FRACTIONS OF THE KK SPECIES.  DENSITY AND
            TEMPERATURE HELD FIXED.  DWDYRT(K,N) IS THE PARTIAL
            DERIVATIVE OF THE MOLAR PRODUCTION RATE FOR SPECIES
            K WITH RESPECT TO THE MASS FRACTION OF SPECIES N.
               CGS UNITS - MOLE/(CM**3*SEC).
               DIMENSION DWDYRT(KDIM,*) EXACTLY KDIM FOR THE FIRST
               DIMENSION AND AT LEAST KK FOR THE SECOND.


CKDXDY      CKDXDY      CKDXDY      CKDXDY      CKDXDY      CKDXDY
                ************************************
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                            *************
SUBROUTINE CKDXDY (Y,KDIM,IWORK,WORK,DXKDYN)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLE
   FRACTIONS WITH RESPECT TO THE MASS FRACTIONS GIVEN THE MASS
   FRACTIONS.  REFERENCE EQUATION (II.8.2).

 INPUT
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DXKDYN - MATRIX OF PARTIAL DERIVATIVES OF THE MOLE FRACTIONS
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            OF THE KK SPECIES WITH RESPECT TO THE MASS FRACTIONS
            OF THE KK SPECIES.  DXKDYN(K,N) IS THE PARTIAL
            DERIVATIVE OF THE MOLE FRACTION OF SPECIES K WITH
            RESPECT TO THE MASS FRACTION OF SPECIES N.
               CGS UNITS - NONE.
               DIMENSION DXKDYN(KDIM,*) EXACTLY KDIM FOR THE
               FIRST DIMENSION AND AT LEAST KK FOR THE SECOND.


CKDYDX      CKDYDX      CKDYDX      CKDYDX      CKDYDX      CKDYDX
               ***************************************
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                           *************
SUBROUTINE CKDYDX (X,KDIM,IWORK,WORK,DYKDXN)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MASS
   FRACTIONS WITH RESPECT TO THE MOLE FRACTIONS GIVEN THE MOLE
   FRACTIONS.  REFERENCE EQUATION (II.8.1).

 INPUT
   X       - MOLE FRACTIONS OF THE KK SPECIES.
               CGS UNITS - NONE.
               DIMENSION X(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DYKDXN - MATRIX OF PARTIAL DERIVATIVES OF THE MASS
            FRACTIONS OF THE KK SPECIES WITH RESPECT TO THE
            MOLE FRACTIONS OF THE KK SPECIES.  DYKDXN(K,N) IS
            THE PARTIAL DERIVATIVE OF THE MASS FRACTION OF
            SPECIES K WITH RESPECT TO THE MOLE FRACTION OF
            SPECIES N.
               CGS UNITS - NONE.
               DIMENSION DYKDXN(KDIM,*) EXACTLY KDIM FOR THE
               FIRST DIMENSION AND AT LEAST KK FOR THE SECOND.


CKEQC       CKEQC       CKEQC       CKEQC       CKEQC       CKEQC
               ***************************************
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                           *************
SUBROUTINE CKEQC (T,C,IWORK,WORK,EQKC)

   THIS SUBROUTINE RETURNS THE EQUILIBRIUM CONSTANTS OF THE
   REACTIONS GIVEN TEMPERATURE, AND MOLAR CONCENTRATIONS.
   REFERENCE EQUATION (II.5.7).

 INPUT
   T       - TEMPERATURE.
               CGS UNITS - K
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
               CGS UNITS - MOLE/CM**3
               DIMENSION C(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
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                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   EQKC    - ARRAY OF EQUILIBRIUM CONSTANTS IN CONCENTRATION UNITS
             FOR THE II REACTIONS.
                CGS UNITS - (MOLE/CM**3)**SOME POWER
                DIMENSION EQKC(*) AT LEAST II.


CKEQXP      CKEQXP      CKEQXP      CKEQXP      CKEQXP      CKEQXP
                ************************************
                      *************************
                            *************
SUBROUTINE CKEQXP (P,T,X,IWORK,WORK,EQKC)

   THIS SUBROUTINE RETURNS THE EQUILIBRIUM CONSTANTS FOR THE
   REACTIONS GIVEN PRESSURE, TEMPERATURE AND MOLE FRACTIONS.
   REFERENCE EQUATION (II.5.7).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   EQKC    - ARRAY OF EQUILIBRIUM CONSTANTS IN CONCENTRATION UNITS
             FOR THE II REACTIONS.
                CGS UNITS - (MOLE/CM**3)**SOME POWER
                DIMENSION EQKC(*) AT LEAST II.


CKEQXR      CKEQXR      CKEQXR      CKEQXR      CKEQXR      CKEQXR
                ************************************
                      *************************
                            *************
SUBROUTINE CKEQXR (RHO,T,X,IWORK,WORK,EQKC)

   THIS SUBROUTINE RETURNS THE EQUILIBRIUM CONSTANTS OF THE
   REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS.
   REFERENCE EQUATION (II.5.7).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.
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 OUTPUT
   EQKC    - ARRAY OF EQUILIBRIUM CONSTANTS IN CONCENTRATION UNITS
             FOR THE II REACTIONS.
                CGS UNITS - (MOLE/CM**3)**SOME POWER
                DIMENSION EQKC(*) AT LEAST II.


CKEQYP       CKEQYP       CKEQYP       CKEQYP       CKEQYP       CKEQYP
                ************************************
                      *************************
                            *************
SUBROUTINE CKEQYP (P,T,Y,IWORK,WORK,EQKC)

   THIS SUBROUTINE RETURNS THE EQUILIBRIUM CONSTANTS FOR THE
   REACTIONS GIVEN PRESSURE, TEMPERATURE AND MASS FRACTIONS.
   REFERENCE EQUATION (II.5.7).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   EQKC    - ARRAY OF EQUILIBRIUM CONSTANTS IN CONCENTRATION UNITS
             FOR THE II REACTIONS.
                CGS UNITS - (MOLE/CM**3)**SOME POWER
                DIMENSION EQKC(*) AT LEAST II.


CKEQYR       CKEQYR       CKEQYR       CKEQYR       CKEQYR       CKEQYR
                ************************************
                      *************************
                            *************
SUBROUTINE CKEQYR (RHO,T,Y,IWORK,WORK,EQKC)

   THIS SUBROUTINE RETURNS THE EQUILIBRIUM CONSTANTS OF THE
   REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MASS FRACTIONS.
   REFERENCE EQUATION (II.5.7).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   EQKC    - ARRAY OF EQUILIBRIUM CONSTANTS IN CONCENTRATION UNITS
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            FOR THE II REACTIONS.
               CGS UNITS - (MOLE/CM**3)**SOME POWER
               DIMENSION EQKC(*) AT LEAST II.


CKGBML      CKGBML      CKGBML      CKGBML      CKGBML      CKGBML
               ************************************
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                           *************
SUBROUTINE CKGBML (T,X,IWORK,WORK,GBML)

   THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN STANDARD
   STATE GIBBS FREE ENERGY OF THE MIXTURE IN MOLAR UNITS.
   REFERENCE EQUATION (II.4.30).

 INPUT
   T       - TEMPERATURE.
               CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
               CGS UNITS - NONE.
               DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   GBML    - MOLAR WEIGHTED MEAN STANDARD STATE GIBBS FREE ENERGY
             IN MOLAR UNITS.
               CGS UNITS - ERGS/MOLE.


CKGBMS      CKGBMS      CKGBMS      CKGBMS      CKGBMS      CKGBMS
               ************************************
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                           *************
SUBROUTINE CKGBMS (T,Y,IWORK,WORK,GBMS)

   THIS SUBROUTINE RETURNS THE MASS WEIGHTED MEAN STANDARD
   STATE GIBBS FREE ENERGY OF THE MIXTURE IN MASS UNITS. REFERENCE
   EQUATION (II.4.31).

 INPUT
   T       - TEMPERATURE.
               CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
               CGS UNITS - NONE.
               DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   GBMS    - MASS WEIGHTED MEAN STANDARD STATE GIBBS FREE ENERGY IN
             MASS UNITS.
               CGS UNITS - ERGS/GM.
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CKGML        CKGML        CKGML        CKGML        CKGML        CKGML
                ************************************
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                            *************
SUBROUTINE CKGML (T,IWORK,WORK,GML)

   THIS SUBROUTINE RETURNS THE STANDARD STATE GIBBS FREE ENERGIES
   IN MOLAR UNITS. REFERENCE EQUATION (II.4.11).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   GML     - ARRAY OF STANDARD STATE GIBBS FREE ENERGIES IN MOLAR
             UNITS FOR THE KK SPECIES.
                CGS UNITS - ERGS/MOLE.
                DIMENSION GML(*) AT LEAST KK.


CKGMS        CKGMS        CKGMS        CKGMS        CKGMS        CKGMS
                ************************************
                      *************************
                            *************
SUBROUTINE CKGMS (T,IWORK,WORK,GMS)

   THIS SUBROUTINE RETURNS THE STANDARD STATE GIBBS FREE ENERGIES
   IN MASS UNITS. REFERENCE EQUATION (II.4.18).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   GMS     - ARRAY OF STANDARD STATE GIBBS FREE ENERGIES IN MASS
             UNITS FOR THE KK SPECIES.
                CGS UNITS - ERGS/GM.
                DIMENSION GMS(*) AT LEAST KK.


CKHBML       CKHBML       CKHBML       CKHBML       CKHBML       CKHBML
                ************************************
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                            *************
SUBROUTINE CKHBML (T,X,IWORK,WORK,HBML)

   THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN ENTHALPY
   OF THE MIXTURE IN MOLAR UNITS. REFERENCE EQUATION (II.4.22).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
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                DIMENSION X(*) AT LEAST KK.
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   HBML   - MOLAR WEIGHTED MEAN ENTHALPY IN MOLAR UNITS.
                CGS UNITS - ERGS/MOLE.


CKHBMS       CKHBMS       CKHBMS       CKHBMS       CKHBMS       CKHBMS
                ************************************
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                                *************
SUBROUTINE CKHBMS (T,Y,IWORK,WORK,HBMS)

   THIS SUBROUTINE RETURNS THE MASS WEIGHTED MEAN ENTHALPY
   OF THE MIXTURE IN MASS UNITS. REFERENCE EQUATION (II 4.23).

 INPUT
   T      - TEMPERATURE.
                CGS UNITS - K
   Y      - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   HBMS   - MASS WEIGHTED MEAN ENTHALPY IN MASS UNITS.
                CGS UNITS - ERGS/GM.


CKHML        CKHML        CKHML        CKHML        CKHML        CKHML
                ************************************
                        *************************
                                *************
SUBROUTINE CKHML (T,IWORK,WORK,HML)

   THIS SUBROUTINE RETURNS THE ENTHALPIES IN MOLAR UNITS.
   REFERENCE EQUATION (II.4.3).

 INPUT
   T      - TEMPERATURE.
                CGS UNITS - K
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   HML    - ARRAY OF ENTHALPIES IN MOLAR UNITS FOR THE KK SPECIES.
                CGS UNITS - ERGS/MOLE.
                DIMENSION HML(*) AT LEAST KK.
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CKHMS        CKHMS        CKHMS        CKHMS        CKHMS        CKHMS
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SUBROUTINE CKHMS (T,IWORK,WORK,HMS)

   THIS SUBROUTINE RETURNS THE ENTHALPIES IN MASS UNITS.
   REFERENCE EQUATION (II.4.14).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   HMS     - ARRAY OF ENTHALPIES IN MASS UNITS FOR THE KK SPECIES.
                CGS UNITS - ERGS/GM.
                DIMENSION HMS(*) AT LEAST KK.


CKHORT       CKHORT       CKHORT       CKHORT       CKHORT       CKHORT
                ************************************
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                                *************
SUBROUTINE CKHORT (T,IWORK,WORK,HORT)

   THIS SUBROUTINE RETURNS THE NONDIMENSIONAL ENTHALPIES.
   REFERENCE EQUATION (II.4.3) OR (II.4.7).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   HORT    - ARRAY OF NONDIMENSIONAL ENTHALPIES FOR THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION HORT(*) AT LEAST KK.


CKINDX       CKINDX       CKINDX       CKINDX       CKINDX       CKINDX
                ************************************
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                                *************
SUBROUTINE CKINDX (IWORK,WORK,MM,KK,II,LENEL,LENSYM,NFIT)

   THIS SUBROUTINE RETURNS A GROUP OF INDICES DEFINING THE
   SIZE OF THE PARTICULAR REACTION MECHANISM.

 INPUT
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
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                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   MM     - TOTAL NUMBER OF ELEMENTS IN MECHANISM.
   KK     - TOTAL NUMBER OF SPECIES IN MECHANISM.
   II     - TOTAL NUMBER OF REACTIONS IN MECHANISM.
   LENEL  - TOTAL NUMBER OF A1 HOLLERITH CHARACTERS IN THE
            ELEMENT NAMES.
   LENSYM - TOTAL NUMBER OF A1 HOLLERITH CHARACTERS IN THE
            SPECIES NAMES.
   NFIT   - NUMBER OF COEFFICIENTS IN FITS TO THERMODYNAMIC
            DATA FOR ONE TEMPERATURE RANGE.  NFIT = NUMBER OF
            COEFFICIENTS IN POLYNOMIAL FITS TO CP/R  +  2.


CKINIT      CKINIT      CKINIT      CKINIT      CKINIT      CKINIT
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                            *************
SUBROUTINE CKINIT (LENIWK,LENWK,LINK,LOUT,IWORK,WORK)

   THIS SUBROUTINE SERVES TO READ THE LINKING FILE AND
   CREATE THE INTERNAL WORK ARRAYS, IWORK AND WORK.
   CKINIT MUST BE CALLED BEFORE ANY OTHER CHEMKIN SUBROUTINE
   IS CALLED.  THE WORK ARRAYS MUST THEN BE MADE AVAILABLE
   AS INPUT TO THE OTHER CHEMKIN SUBROUTINES.

 INPUT
   LENIWK - ACTUAL DIMENSION OF THE INTEGER WORK ARRAY, IWORK.
            THE MINIMUM LENGTH OF IWORK(*) IS COMPUTED FROM THE
            FOLLOWING FORMULA.
               LENIWK = MM*(LENEL+KK) + KK*(LENSYM+2) +
                        II*(2*MAXSP+MAXTB+4) + 1
                 WHERE-
                   MM = NUMBER OF ELEMENTS IN MECHANISM.
                   KK = NUMBER OF SPECIES IN MECHANISM.
                   II = NUMBER OF REACTIONS IN MECHANISM.
                   LENEL = NUMBER OF A1 HOLLERITH SYMBOLS IN THE
                       ELEMENT NAMES.  DEFAULT IS LENEL=2 UNLESS
                       THE INTERPRETER IS CHANGED.
                   LENSYM = NUMBER OF A1 HOLLERITH SYMBOLS IN THE
                       SPECIES NAMES.  DEFAULT IS LENSYM=10 UNLESS
                       THE INTERPRETER IS CHANGED.
                   MAXSP = MAXIMUM NUMBER OF SPECIES ALLOWED IN
                       ONE REACTION.  DEFAULT IS MAXSP=6 UNLESS
                       THE INTERPRETER IS CHANGED.
                   MAXTB = MAXIMUM NUMBER OF ENHANCED THIRD BODIES
                       ALLOWED IN ONE REACTION.  DEFAULT IS
                       MAXTB=6 UNLESS THE INTERPRETER IS CHANGED.
            IF NO CHANGES ARE MADE IN THE INTERPRETER THE FORMULA
            FOR LENIWK IS-
               LENIWK = MM*(2+KK) + KK*(12) + II*(22) + 1
   LENWK  - ACTUAL DIMENSION OF THE REAL WORK ARRAY, WORK.
            THE MINIMUM LENGTH OF  WORK(*) IS COMPUTED FROM THE
            FOLLOWING FORMULA.
               LENWK =  MM + KK*(NCP2T2+8) + II*(MAXTB+4) + 3
                 WHERE-
                   NCP2T2 = THE NUMBER OF COEFFICIENTS IN THE FITS
                       TO THE THERMODYNAMIC PROPERTIES TIMES 2.
                       THE DEFAULT IS NCP2T2=14 UNLESS THE FORM
                       OF THE THERMODYNAMIC DATA BASE IS CHANGED
                       IN THE INTERPRETER.
            IF NO CHANGES ARE MADE IN THE INTERPRETER THE FORMULA
            FOR LENWK IS-
               LENWK = MM + KK*(22) + II*(10) + 3
   LINK   - LOGICAL FILE NUMBER FOR THE LINKING FILE
   LOUT   - OUTPUT FILE FOR PRINTED ERROR MESSAGES.

 OUTPUT
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE STARTING
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            ADDRESSES FOR THE IWORK SPACE ARE STORED
            IN COMMON/CKSTRT/.  SEE APPENDIX A FOR THE DETAILS.
               DIMENSION IWORK(*) AT LEAST LENIWK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE STARTING
            ADDRESSES FOR THE WORK SPACE ARE STORED
            IN COMMON/CKSTRT/.  SEE APPENDIX A FOR THE DETAILS.
               DIMENSION WORK(*) AT LEAST LENWK.


CKITR        CKITR        CKITR        CKITR        CKITR        CKITR
                ***************************************
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                            **************
SUBROUTINE CKITR (IWORK,WORK,ITHB,IREV)

   THIS SUBROUTINE RETURNS A SET OF FLAGS INDICATING WHETHER
   THE REACTIONS ARE REVERSIBLE OR WHETHER THEY CONTAIN
   ARBITRARY THIRD BODIES.

 INPUT
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   ITHB   - ARRAY OF FLAGS REGARDING THREE BODY REACTIONS.
            ITHB(I)= -1  REACTION I IS NOT A THREE BODY REACTION
                         WITH M FOR THE THIRD BODY.
            ITHB(I)=  0  REACTION I IS A THREE BODY REACTION WITH
                         M AS THE THIRD BODY, BUT WITH NO ENHANCED
                         THIRD BODY EFFICIENCIES.
            ITHB(I)=  N  REACTION I IS A THREE BODY REACTION WITH
                         M AS THE THIRD BODY, AND IN ADDITION
                         THERE ARE N SPECIES WITH ENHANCED THIRD
                         BODY EFFICIENCIES.
               DIMENSION ITHB(*) AT LEAST II


   IREV   - ARRAY OF FLAGS REGARDING THE REVERSIBILITY AND THE
            NUMBER OF STOICHIOMETRIC COEFFICIENTS OF THE II
            REACTIONS.
            IREV(I)=+N REACTION I IS REVERSIBLE AND IT HAS N
                       NON-ZERO STOICHIOMETRIC COEFFICIENTS.
            IREV(I)=-N REACTION I IS IRREVERSIBLE AND IT HAS N
                       NON-ZERO STOICHIOMETRIC COEFFICIENTS.
               DIMENSION IREV(*) AT LEAST II


CKMMWC       CKMMWC       CKMMWC       CKMMWC       CKMMWC       CKMMWC
                ***************************************
                      ***************************
                            **************
SUBROUTINE CKMMWC (C,IWORK,WORK,WTM)

   THIS SUBROUTINE RETURNS THE MEAN MOLECULAR WEIGHT OF THE
   GAS MIXTURE GIVEN THE MOLAR CONCENTRATIONS. REFERENCE
   EQUATION (II.2.5).

 INPUT
   C      - MOLAR CONCENTRATIONS OF THE KK SPECIES.
               CGS UNITS - MOLE/CM**3
               DIMENSION C(*) AT LEAST KK.
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
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                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   WTM     - MEAN MOLECULAR WEIGHT OF THE SPECIES MIXTURE.
                CGS UNITS - GM/MOLE.


CKMMWX       CKMMWX       CKMMWX       CKMMWX       CKMMWX       CKMMWX
                ************************************
                      *************************
                            *************
SUBROUTINE CKMMWX (X,IWORK,WORK,WTM)

   THIS SUBROUTINE RETURNS THE MEAN MOLECULAR WEIGHT OF THE
   GAS MIXTURE GIVEN THE MOLE FRACTIONS. REFERENCE EQUATION
   (II.2.4).

 INPUT
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   WTM     - MEAN MOLECULAR WEIGHT OF THE SPECIES MIXTURE.
                CGS UNITS - GM/MOLE.


CKMMWY       CKMMWY       CKMMWY       CKMMWY       CKMMWY       CKMMWY
                ************************************
                      *************************
                            *************
SUBROUTINE CKMMWY (Y,IWORK,WORK,WTM)

   THIS SUBROUTINE RETURNS THE MEAN MOLECULAR WEIGHT OF THE
   GAS MIXTURE GIVEN THE MASS FRACTIONS. REFERENCE EQUATION
   (II.2.3)

 INPUT
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   WTM     - MEAN MOLECULAR WEIGHT OF THE SPECIES MIXTURE.
                CGS UNITS - GM/MOLE.
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CKNCF        CKNCF        CKNCF        CKNCF        CKNCF        CKNCF
                ************************************
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                                ***************
SUBROUTINE CKNCF (MDIM,IWORK,WORK,NCF)

   THIS SUBROUTINE RETURNS THE ELEMENTAL COMPOSITION OF THE
   SPECIES.

 INPUT
   MDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             MDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF ELEMENTS, MM.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   NCF     - MATRIX GIVING THE ELEMENTAL MAKEUP OF EACH SPECIES.
             NCF(M,K) IS NUMBER OF ATOMS OF THE M TH ELEMENT IN
             THE K TH SPECIES.
                DIMENSION NCF(MDIM,*) EXACTLY MDIM FOR THE FIRST
                DIMENSION AND AT LEAST KK, THE TOTAL NUMBER OF
                SPECIES, FOR THE SECOND.  MDIM MUST BE AT LEAST MM,
                THE TOTAL NUMBER OF ELEMENTS IN THE PROBLEM.


CKNU         CKNU         CKNU         CKNU         CKNU         CKNU
                ************************************
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                                *************
SUBROUTINE CKNU (KDIM,IWORK,WORK,NUKI)

   THIS SUBROUTINE RETURNS THE STOICHIOMETRIC COEFFICIENTS
   OF THE REACTION MECHANISM. REFERENCE EQUATIONS (II.5.1)
   AND (II.5.3).

 INPUT
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   NUKI    - MATRIX OF STOICHIOMETRIC COEFFICIENTS FOR THE KK
             SPECIES IN THE II REACTIONS.  NUKI(K,I) IS THE
             STOICHIOMETRIC COEFFICIENT OF SPECIES K IN REACTION I.
                DIMENSION NUKI(KDIM,*) EXACTLY KDIM FOR THE FIRST
                DIMENSION AND AT LEAST II FOR THE SECOND.
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CKPC          CKPC          CKPC          CKPC          CKPC          CKPC
              ***************************************
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                              *************
SUBROUTINE CKPC (RHO,T,C,IWORK,WORK,P)

   THIS SUBROUTINE RETURNS THE PRESSURE OF THE GAS MIXTURE
   GIVEN THE MASS DENSITY, TEMPERATURE AND MOLAR CONCENTRATIONS.
   REFERENCE EQUATION (II.2.1).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.


CKPHAZ        CKPHAZ        CKPHAZ        CKPHAZ        CKPHAZ        CKPHAZ
              ***************************************
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                              *************
SUBROUTINE CKPHAZ (IWORK,WORK,KPHASE)

   THIS SUBROUTINE RETURNS A SET OF FLAGS INDICATING THE
   PHASE OF EACH SPECIES.

 INPUT
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   KPHASE  - ARRAY OF FLAGS INDICATING THE PHASE OF THE KK SPECIES.
             KPHASE(K)=-1  THE K TH SPECIES IS SOLID
             KPHASE(K)= 0  THE K TH SPECIES IS GASEOUS
             KPHASE(K)=+1  THE K TH SPECIES IS LIQUID
                DIMENSION KPHASE(*) AT LEAST KK
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CKPX          CKPX          CKPX          CKPX          CKPX          CKPX
                ************************************
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                            *************
SUBROUTINE CKPX (RHO,T,X,IWORK,WORK,P)

   THIS SUBROUTINE RETURNS THE PRESSURE OF THE GAS MIXTURE
   GIVEN THE MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS.
   REFERENCE EQUATION (II.2.1).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.


CKPY          CKPY          CKPY          CKPY          CKPY          CKPY
                ************************************
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                            *************
SUBROUTINE CKPY (RHO,T,Y,IWORK,WORK,P)

   THIS SUBROUTINE RETURNS THE PRESSURE OF THE GAS MIXTURE
   GIVEN THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS.
   REFERENCE EQUATION (II.2.10).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
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CKQC          CKQC          CKQC          CKQC          CKQC          CKQC
                 ************************************
                       *************************
                             *************
SUBROUTINE CKQC (T,C,IWORK,WORK,ROP)

   THIS SUBROUTINE RETURNS THE RATE OF PROGRESS VARIABLES FOR
   THE REACTIONS GIVEN TEMPERATURE AND MOLAR CONCENTRATIONS.
   REFERENCE EQUATIONS (II.5.4) AND (II.5.11).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   ROP     - ARRAY OF RATE OF PROGRESS VARIABLES FOR THE II
             REACTIONS.
                CGS UNITS - MOLES/(CM**3*SEC).
                DIMENSION ROP(*) AT LEAST II.


CKQXP         CKQXP         CKQXP         CKQXP         CKQXP         CKQXP
                 ************************************
                       *************************
                             *************
SUBROUTINE CKQXP (P,T,X,IWORK,WORK,ROP)

   THIS SUBROUTINE RETURNS THE RATE OF PROGRESS VARIABLES FOR
   THE REACTIONS GIVEN PRESSURE, TEMPERATURE AND MOLE FRACTIONS.
   REFERENCE EQUATIONS (II.5.4) AND (II.5.11).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   ROP     - ARRAY OF RATE OF PROGRESS VARIABLES FOR THE II
             REACTIONS.
                CGS UNITS - MOLES/(CM**3*SEC).
                DIMENSION ROP(*) AT LEAST II.
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CKQXR        CKQXR        CKQXR        CKQXR        CKQXR        CKQXR
                 ************************************
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                             *************
SUBROUTINE CKQXR (RHO,T,X,IWORK,WORK,ROP)

   THIS SUBROUTINE RETURNS THE RATE OF PROGRESS VARIABLES FOR
   THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MOLE
   FRACTIONS.  REFERENCE EQUATIONS (II.5.4) AND (II.5.11).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   ROP     - ARRAY OF RATE OF PROGRESS VARIABLES FOR THE II
             REACTIONS.
                CGS UNITS - MOLES/(CM**3*SEC).
                DIMENSION ROP(*) AT LEAST II.


CKQYP        CKQYP        CKQYP        CKQYP        CKQYP        CKQYP
                 ************************************
                       *************************
                             *************
SUBROUTINE CKQYP (P,T,Y,IWORK,WORK,ROP)

   THIS SUBROUTINE RETURNS THE RATE OF PROGRESS VARIABLES FOR
   THE REACTIONS GIVEN PRESSURE, TEMPERATURE AND MASS FRACTIONS.
   REFERENCE EQUATIONS (II.5.4) AND (II.5.11).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   ROP     - ARRAY OF RATE OF PROGRESS VARIABLES FOR THE II
             REACTIONS.
                CGS UNITS - MOLES/(CM**3*SEC).
                DIMENSION ROP(*) AT LEAST II.
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CKQYR        CKQYR        CKQYR        CKQYR        CKQYR        CKQYR
                 ************************************
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                             *************
SUBROUTINE CKQYR (RHO,T,Y,IWORK,WORK,ROP)

   THIS SUBROUTINE RETURNS THE RATE OF PROGRESS VARIABLES FOR
   THE REACTIONS GIVEN MASS DENSITY, TEMPERATURE AND MASS
   FRACTIONS.  REFERENCE EQUATIONS (II.5.4) AND (II.5.11).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   ROP     - ARRAY OF RATE OF PROGRESS VARIABLES FOR THE II
             REACTIONS.
                CGS UNITS - MOLES/(CM**3*SEC).
                DIMENSION ROP(*) AT LEAST II.


CKRHOC       CKRHOC       CKRHOC       CKRHOC       CKRHOC       CKRHOC
                 ************************************
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                             *************
SUBROUTINE CKRHOC (P,T,C,IWORK,WORK,RHO)

   THIS SUBROUTINE RETURNS THE MASS DENSITY OF THE GAS MIXTURE
   GIVEN THE PRESSURE, TEMPERATURE AND MOLAR CONCENTRATIONS.
   REFERENCE EQUATION (II.2.3).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
```

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CKRHOX       CKRHOX       CKRHOX       CKRHOX       CKRHOX       CKRHOX
                 ************************************
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                             *************
SUBROUTINE CKRHOX (P,T,X,IWORK,WORK,RHO)

   THIS SUBROUTINE RETURNS THE MASS DENSITY OF THE GAS MIXTURE
   GIVEN THE PRESSURE, TEMPERATURE AND MOLE FRACTIONS.
   REFERENCE EQUATION (II.2.2).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.


CKRHOY       CKRHOY       CKRHOY       CKRHOY       CKRHOY       CKRHOY
                 ************************************
                       **************************
                             *************
SUBROUTINE CKRHOY (P,T,Y,IWORK,WORK,RHO)

   THIS SUBROUTINE RETURNS THE MASS DENSITY OF THE GAS MIXTURE
   GIVEN THE PRESSURE, TEMPERATURE AND MASS FRACTIONS.
   REFERENCE EQUATION (II.2.2).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
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CKRP        CKRP        CKRP        CKRP        CKRP        CKRP
            ***************************************
                    *************************
                            *************
SUBROUTINE CKRP (IWORK,WORK,RU,RUC,PA)

   THIS SUBROUTINE RETURNS UNIVERSAL GAS CONSTANTS AND THE
   PRESSURE OF ONE STANDARD ATMOSPHERE.

 INPUT
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS CN THE REQUIRED LENGTH OF WORK.

 OUTPUT
   RU     - UNIVERSAL GAS CONSTANT.
               CGS UNITS - 8.314E7 ERGS/(MOLE*K)
   RUC    - UNIVERSAL GAS CONSTANT USED ONLY IN CONJUCTION WITH
            ACTIVATION ENERGY.
               PREFERRED UNITS - 1.987 CAL/(MOLE*K).
   PA     - PRESSURE OF ONE STANDARD ATMOSPHERE.
               CGS UNITS - 1.01325E6 DYNES/CM**2


CKSAC       CKSAC       CKSAC       CKSAC       CKSAC       CKSAC
            ***************************************
                    *************************
                            *************
SUBROUTINE CKSAC (T,C,KDIM,IWORK,WORK,DWKDAI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE PRE-
   EXPONENTIAL CONSTANTS OF THE REACTIONS GIVEN TEMPERATURE AND
   MOLAR CONCENTRATIONS.  REFERENCE EQUATION (II.11.3).

 INPUT
   T      - TEMPERATURE.
               CGS UNITS - K
   C      - MOLAR CONCENTRATIONS OF THE KK SPECIES.
               CGS UNITS - MOLE/CM**3
               DIMENSION C(*) AT LEAST KK.
   KDIM   - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
            KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
            NUMBER OF SPECIES, KK.
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS CN THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDAI - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO THE PRE-
            EXPONENTIAL CONSTANTS OF THE II REACTIONS.  DWKDAI
            (K,I) IS THE PARTIAL DERIVATIVE OF THE MOLAR
            PRODUCTION RATE OF SPECIES K WITH RESPECT TO THE
            PRE-EXPONENTIAL CONSTANT OF REACTION I.
               CGS UNITS - DEPENDS ON REACTION
               DIMENSION DWKDAI(KDIM,*) EXACTLY DKIM FOR THE
               FIRST DIMENSION AND AT LEAST II FOR THE SECOND.
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CKSAXP      CKSAXP      CKSAXP      CKSAXP      CKSAXP      CKSAXP
                ************************************
                      **************************
                            *************
SUBROUTINE CKSAXP (P,T,X,KDIM,IWORK,WORK,DWKDAI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE PRE-
   EXPONENTIAL CONSTANTS OF THE REACTIONS GIVEN PRESSURE,
   TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION (II.11.3).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDAI  - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
             RATES OF THE KK SPECIES WITH RESPECT TO THE PRE-
             EXPONENTIAL CONSTANTS OF THE II REACTIONS.  DWKDAI
             (K,I) IS THE PARTIAL DERIVATIVE OF THE MOLAR
             PRODUCTION RATE OF SPECIES K WITH RESPECT TO THE
             PRE-EXPONENTIAL CONSTANT OF REACTION I.
                CGS UNITS - DEPENDS ON REACTION
                DIMENSION DWKDAI(KDIM,*) EXACTLY DKIM FOR THE
                FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSAXR      CKSAXR      CKSAXR      CKSAXR      CKSAXR      CKSAXR
                ************************************
                      **************************
                            *************
SUBROUTINE CKSAXR (RHO,T,X,KDIM,IWORK,WORK,DWKDAI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE PRE-
   EXPONENTIAL CONSTANTS OF THE REACTIONS GIVEN MASS DENSITY,
   TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION (II.11.3).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
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                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDAI - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO THE PRE-
            EXPONENTIAL CONSTANTS OF THE II REACTIONS.  DWKDAI
            (K,I) IS THE PARTIAL DERIVATIVE OF THE MOLAR
            PRODUCTION RATE OF SPECIES K WITH RESPECT TO THE
            PRE-EXPONENTIAL CONSTANT OF REACTION I.
                CGS UNITS - DEPENDS ON REACTION
                DIMENSION DWKDAI(KDIM,*) EXACTLY DKIM FOR THE
                FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSAYP      CKSAYP      CKSAYP      CKSAYP      CKSAYP      CKSAYP
                ************************************
                        *************************
                                *************
SUBROUTINE CKSAYP (P,T,Y,KDIM,IWORK,WORK,DWKDAI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE PRE-
   EXPONENTIAL CONSTANTS OF THE REACTIONS GIVEN PRESSURE,
   TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION (II.11.3).

 INPUT
   P      - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T      - TEMPERATURE.
                CGS UNITS - K
   Y      - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   KDIM   - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
            KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
            NUMBER OF SPECIES, KK.
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDAI - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO THE PRE-
            EXPONENTIAL CONSTANTS OF THE II REACTIONS.  DWKDAI
            (K,I) IS THE PARTIAL DERIVATIVE OF THE MOLAR
            PRODUCTION RATE OF SPECIES K WITH RESPECT TO THE
            PRE-EXPONENTIAL CONSTANT OF REACTION I.
                CGS UNITS - DEPENDS ON REACTION
                DIMENSION DWKDAI(KDIM,*) EXACTLY DKIM FOR THE
                FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSAYR      CKSAYR      CKSAYR      CKSAYR      CKSAYR      CKSAYR
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                                *************
SUBROUTINE CKSAYR (RHO,T,Y,KDIM,IWORK,WORK,DWKDAI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE PRE-
   EXPONENTIAL CONSTANTS OF THE REACTIONS GIVEN MASS DENSITY,
   TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION (II.11.3).

 INPUT
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   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDAI - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO THE PRE-
            EXPONENTIAL CONSTANTS OF THE II REACTIONS.  DWKDAI
            (K,I) IS THE PARTIAL DERIVATIVE OF THE MOLAR
            PRODUCTION RATE OF SPECIES K WITH RESPECT TO THE
            PRE-EXPONENTIAL CONSTANT OF REACTION I.
                CGS UNITS - DEPENDS ON REACTION
                DIMENSION DWKDAI(KDIM,*) EXACTLY DKIM FOR THE
                FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSBC        CKSBC        CKSBC        CKSBC        CKSBC        CKSBC
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                            *************
SUBROUTINE CKSBC (T,C,KDIM,IWORK,WORK,DWKDBI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   TEMPERATURE EXPONENTS OF THE REACTIONS GIVEN TEMPERATURE
   AND MOLAR CONCENTRATIONS.  REFERENCE EQUATION (II.11.4).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDBI - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO THE
            TEMPERATURE EXPONENT IN THE RATE CONSTANTS OF THE II
            REACTIONS.  DWKDBI(K,I) IS THE PARTIAL DERIVATIVE
            OF THE PRODUCTION RATE OF SPECIES K WITH RESPECT
            TO THE TEMPERATURE EXPONENT OF REACTION I.
                CGS UNITS - DEPENDS ON REACTION
                DIMENSION DWKDBI(KDIM,*) EXACTLY KDIM FOR THE
                FIRST DIMENSION AND AT LEAST II FOR THE SECOND.
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CKSBML      CKSBML      CKSBML      CKSBML      CKSBML      CKSBML
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SUBROUTINE CKSBML (T,X,IWORK,WORK,SBML)

   THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN STANDARD STATE
   ENTROPY OF THE MIXTURE IN MOLAR UNITS. REFERENCE EQ. (II.4.24)

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   SBML    - MOLAR WEIGHTED MEAN STANDARD STATE ENTROPY IN MOLAR
             UNITS.
                CGS UNITS - ERGS/(MOLE*K).


CKSBMS      CKSBMS      CKSBMS      CKSBMS      CKSBMS      CKSBMS
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                            *************
SUBROUTINE CKSBMS (T,Y,IWORK,WORK,SBMS)

   THIS SUBROUTINE RETURNS THE MASS WEIGHTED MEAN STANDARD STATE
   ENTROPY OF THE MIXTURE IN MASS UNITS. REFERENCE EQ. (II.4.25)

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   SBMS    - MASS WEIGHTED MEAN STANDARD STATE ENTROPY IN MASS
             UNITS.
                CGS UNITS - ERGS/(GM*K).
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CKSBXP      CKSBXP      CKSBXP      CKSBXP      CKSBXP      CKSBXP
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SUBROUTINE CKSBXP (P,T,X,KDIM,IWORK,WORK,DWKDBI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   TEMPERATURE EXPONENTS OF THE REACTIONS GIVEN PRESSURE,
   TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION (II.11.4).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDBI - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO THE
            TEMPERATURE EXPONENT IN THE RATE CONSTANTS OF THE II
            REACTIONS.  DWKDBI(K,I) IS THE PARTIAL DERIVATIVE
            OF THE PRODUCTION RATE OF SPECIES K WITH RESPECT
            TO THE TEMPERATURE EXPONENT OF REACTION I.
                CGS UNITS - DEPENDS ON REACTION
                DIMENSION DWKDBI(KDIM,*) EXACTLY KDIM FOR THE
                FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSBXR      CKSBXR      CKSBXR      CKSBXR      CKSBXR      CKSBXR
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                             *************
SUBROUTINE CKSBXR (RHO,T,X,KDIM,IWORK,WORK,DWKDBI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   TEMPERATURE EXPONENTS OF THE REACTIONS GIVEN MASS DENSITY,
   TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION (II.11.4).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
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                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDBI - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO THE
            TEMPERATURE EXPONENT IN THE RATE CONSTANT OF THE II
            REACTIONS.  DWKDBI(K,I) IS THE PARTIAL DERIVATIVE
            OF THE PRODUCTION RATE OF SPECIES K WITH RESPECT
            TO THE TEMPERATURE EXPONENT OF REACTION I.
               CGS UNITS - DEPENDS ON REACTION
               DIMENSION DWKDBI(KDIM,*) EXACTLY KDIM FOR THE
               FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSBYP      CKSBYP      CKSBYP      CKSBYP      CKSBYP      CKSBYP
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                           *************
SUBROUTINE CKSBYP (P,T,Y,KDIM,IWORK,WORK,DWKDBI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   TEMPERATURE EXPONENTS OF THE REACTIONS GIVEN MASS DENSITY,
   TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION (II.11.4).

 INPUT
   P      - PRESSURE.
               CGS UNITS - DYNES/CM**2.
   T      - TEMPERATURE.
               CGS UNITS - K
   Y      - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
               CGS UNITS - NONE.
               DIMENSION Y(*) AT LEAST KK.
   KDIM   - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
            KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
            NUMBER OF SPECIES, KK.
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDBI - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO THE
            TEMPERATURE EXPONENT IN THE RATE CONSTANTS OF THE II
            REACTIONS.  DWKDBI(K,I) IS THE PARTIAL DERIVATIVE
            OF THE PRODUCTION RATE OF SPECIES K WITH RESPECT
            TO THE TEMPERATURE EXPONENT OF REACTION I.
               CGS UNITS - DEPENDS ON REACTION
               DIMENSION DWKDBI(KDIM,*) EXACTLY KDIM FOR THE
               FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSBYR      CKSBYR      CKSBYR      CKSBYR      CKSBYR      CKSBYR
               ****************************************
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                           *************
SUBROUTINE CKSBYR (RHO,T,Y,KDIM,IWORK,WORK,DWKDBI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   TEMPERATURE EXPONENTS OF THE REACTIONS GIVEN MASS DENSITY,
   TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION (II.11.4)

 INPUT
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   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDBI  - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
             RATES OF THE KK SPECIES WITH RESPECT TO THE
             TEMPERATURE EXPONENT IN THE RATE CONSTANTS OF THE II
             REACTIONS.  DWKDBI(K,I) IS THE PARTIAL DERIVATIVE
             OF THE PRODUCTION RATE OF SPECIES K WITH RESPECT
             TO THE TEMPERATURE EXPONENT OF REACTION I.
                CGS UNITS - DEPENDS ON REACTION
                DIMENSION DWKDBI(KDIM,*) EXACTLY KDIM FOR THE
                FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSEC        CKSEC        CKSEC        CKSEC        CKSEC        CKSEC
                ****************************************
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                                *************
SUBROUTINE CKSEC (T,C,KDIM,IWORK,WORK,DWKDEI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   ACTIVATION ENERGY OF THE REACTIONS GIVEN TEMPERATURE AND
   MOLAR CONCENTRATIONS.  REFERENCE EQUATION (II.11.5).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDEI  - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
             RATES OF THE KK SPECIES WITH RESPECT TO THE
             ACTIVATION ENERGIES OF THE II REACTIONS.  DWKDEI(K,I)
             IS THE PARTIAL DERIVATIVE OF THE PRODUCTION
             RATE OF SPECIES K WITH RESPECT TO THE ACTIVATION
             ENERGY OF REACTION I.
                CGS UNITS - DEPENDS ON REACTION
                DIMENSION DWKDEI(KDIM,*) EXACTLY KDIM FOR THE
                FIRST DIMENSION AND AT LEAST II FOR THE SECOND.
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CKSEXP      CKSEXP      CKSEXP      CKSEXP      CKSEXP      CKSEXP
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SUBROUTINE CKSEXP (P,T,X,KDIM,IWORK,WORK,DWKDEI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   ACTIVATION ENERGY OF THE REACTIONS GIVEN PRESSURE, TEMPERATURE
   AND MOLE FRACTIONS.  REFERENCE EQUATION (II.11.5).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDEI  - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
             RATES OF THE KK SPECIES WITH RESPECT TO THE
             ACTIVATION ENERGIES OF THE II REACTIONS.  DWKDEI(K,I)
             IS THE PARTIAL DERIVATIVE OF THE PRODUCTION
             RATE OF SPECIES K WITH RESPECT TO THE ACTIVATION
             ENERGY OF REACTION I.
                CGS UNITS - DEPENDS ON REACTION
                DIMENSION DWKDEI(KDIM,*) EXACTLY KDIM FOR THE
                FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSEXR      CKSEXR      CKSEXR      CKSEXR      CKSEXR      CKSEXR
                ************************************
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                            **************
SUBROUTINE CKSEXR (RHO,T,X,KDIM,IWORK,WORK,DWKDEI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   ACTIVATION ENERGY OF THE REACTIONS GIVEN MASS DENSITY
   TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION (II.11.5).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
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                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDEI - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO THE
            ACTIVATION ENERGIES OF THE II REACTIONS.  DWKDEI(K,I)
            IS THE PARTIAL DERIVATIVE OF THE PRODUCTION
            RATE OF SPECIES K WITH RESPECT TO THE ACTIVATION
            ENERGY OF REACTION I.
               CGS UNITS - DEPENDS ON REACTION
               DIMENSION DWKDEI(KDIM,*) EXACTLY KDIM FOR THE
               FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSEYP      CKSEYP      CKSEYP      CKSEYP      CKSEYP      CKSEYP
               ***************************************
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                           *************
SUBROUTINE CKSEYP (P,T,Y,KDIM,IWORK,WORK,DWKDEI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   ACTIVATION ENERGY OF THE REACTIONS GIVEN PRESSURE, TEMPERATURE
   AND MASS FRACTIONS.  REFERENCE EQUATION (II.11.5).

 INPUT
   P       - PRESSURE.
               CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
               CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
               CGS UNITS - NONE.
               DIMENSION Y(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDEI - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO THE
            ACTIVATION ENERGIES OF THE II REACTIONS.  DWKDEI(K,I)
            IS THE PARTIAL DERIVATIVE OF THE PRODUCTION
            RATE OF SPECIES K WITH RESPECT TO THE ACTIVATION
            ENERGY OF REACTION I.
               CGS UNITS - DEPENDS ON REACTION
               DIMENSION DWKDEI(KDIM,*) EXACTLY KDIM FOR THE
               FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSEYR      CKSEYR      CKSEYR      CKSEYR      CKSEYR      CKSEYR
               ***************************************
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                           *************
SUBROUTINE CKSEYR (RHO,T,Y,KDIM,IWORK,WORK,DWKDEI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE MOLAR
   PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   ACTIVATION ENERGY OF THE REACTIONS GIVEN MASS DENSITY,
   TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION (II.11.5).

 INPUT
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   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS -- NONE.
                DIMENSION Y(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDEI  - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
             RATES OF THE KK SPECIES WITH RESPECT TO THE
             ACTIVATION ENERGIES OF THE II REACTIONS.  DWKDEI(K,I)
             IS THE PARTIAL DERIVATIVE OF THE PRODUCTION
             RATE OF SPECIES K WITH RESPECT TO THE ACTIVATION
             ENERGY OF REACTION I.
                CGS UNITS - DEPENDS ON REACTION
                DIMENSION DWKDEI(KDIM,*) EXACTLY KDIM FOR THE
                FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSKC        CKSKC        CKSKC        CKSKC        CKSKC        CKSKC
                ************************************
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                            *************
SUBROUTINE CKSKC (T,C,KDIM,IWORK,WORK,DWKDKI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   FORWARD RATE CONSTANTS OF THE REACTIONS GIVEN TEMPERATURE
   AND MOLAR CONCENTRATIONS.  REFERENCE EQUATION (II.11.2).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDKI  - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
             RATES OF THE KK SPECIES WITH RESPECT TO THE FORWARD
             RATE CONSTANTS OF THE II REACTIONS.  DWKDKI(K,I)
             THE PARTIAL DERIVATIVE OF THE PRODUCTION RATE OF
             SPECIES K WITH RESPECT TO THE FORWARD RATE CONSTANT
             OF REACTION I.
                CGS UNITS - DEPENDS ON REACTION
                DIMENSION DWKDKI(DKIM,*) EXACTLY KDIM FOR THE
                FIRST DIMENSION AND AT LEAST II FOR THE SECOND.
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CKSKXP      CKSKXP      CKSKXP      CKSKXP      CKSKXP      CKSKXP
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SUBROUTINE CKSKXP (P,T,X,KDIM,IWORK,WORK,DWKDKI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   FORWARD RATE CONSTANTS OF THE REACTIONS GIVEN PRESSURE,
   TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION (II.11.2).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDKI  - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
             RATES OF THE KK SPECIES WITH RESPECT TO THE FORWARD
             RATE CONSTANTS OF THE II REACTIONS.  DWKDKI(K,I)
             THE PARTIAL DERIVATIVE OF THE PRODUCTION RATE OF
             SPECIES K WITH RESPECT TO THE FORWARD RATE CONSTANT
             OF REACTION I.
                CGS UNITS - DEPENDS ON REACTION
                DIMENSION DWKDKI(KDIM,*) EXACTLY KDIM FOR THE
                FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSKXR      CKSKXR      CKSKXR      CKSKXR      CKSKXR      CKSKXR
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                            *************
SUBROUTINE CKSKXR (RHO,T,X,KDIM,IWORK,WORK,DWKDKI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   FORWARD RATE CONSTANTS OF THE REACTIONS GIVEN MASS DENSITY,
   TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION (II.11.2).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
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                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDKI - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO THE FORWARD
            RATE CONSTANTS OF THE II REACTIONS.  DWKDKI(K,I)
            THE PARTIAL DERIVATIVE OF THE PRODUCTION RATE OF
            SPECIES K WITH RESPECT TO THE FORWARD RATE CONSTANT
            OF REACTION I.
               CGS UNITS - DEPENDS ON REACTION
               DIMENSION DWKDKI(DKIM,*) EXACTLY KDIM FOR THE
               FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSKYP      CKSKYP      CKSKYP      CKSKYP      CKSKYP      CKSKYP
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SUBROUTINE CKSKYP (P,T,Y,KDIM,IWORK,WORK,DWKDKI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   FORWARD RATE CONSTANTS OF THE REACTIONS GIVEN PRESSURE,
   TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION (II.11.2).

 INPUT
   P      - PRESSURE.
               CGS UNITS - DYNES/CM**2.
   T      - TEMPERATURE.
               CGS UNITS - K
   Y      - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
               CGS UNITS - NONE.
               DIMENSION Y(*) AT LEAST KK.
   KDIM   - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
            KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
            NUMBER OF SPECIES, KK.
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDKI - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
            RATES OF THE KK SPECIES WITH RESPECT TO THE FORWARD
            RATE CONSTANTS OF THE II REACTIONS.  DWKDKI(K,I)
            THE PARTIAL DERIVATIVE OF THE PRODUCTION RATE OF
            SPECIES K WITH RESPECT TO THE FORWARD RATE CONSTANT
            OF REACTION I.
               CGS UNITS - DEPENDS ON REACTION
               DIMENSION DWKDKI(DKIM,*) EXACTLY KDIM FOR THE
               FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSKYR      CKSKYR      CKSKYR      CKSKYR      CKSKYR      CKSKYR
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                            *************
SUBROUTINE CKSKYR (RHO,T,Y,KDIM,IWORK,WORK,DWKDKI)

   THIS SUBROUTINE RETURNS THE PARTIAL DERIVATIVES OF THE
   MOLAR PRODUCTION RATES OF THE SPECIES WITH RESPECT TO THE
   FORWARD RATE CONSTANTS OF THE REACTIONS GIVEN MASS DENSITY,
   TEMPERATURE AND MASS FRACTIONS.  REFERENCE EQUATION (II.11.2).

 INPUT
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   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   DWKDKI  - MATRIX OF PARTIAL DERIVATIVES OF THE MOLAR PRODUCTION
             RATES OF THE KK SPECIES WITH RESPECT TO THE FORWARD
             RATE CONSTANTS OF THE II REACTIONS.  DWKDKI(K,I)
             THE PARTIAL DERIVATIVE OF THE PRODUCTION RATE OF
             SPECIES K WITH RESPECT TO THE FORWARD RATE CONSTANT
             OF REACTION I.
                CGS UNITS - DEPENDS ON REACTION
                DIMENSION DWKDKI(DKIM,*) EXACTLY KDIM FOR THE
                FIRST DIMENSION AND AT LEAST II FOR THE SECOND.


CKSML        CKSML        CKSML        CKSML        CKSML        CKSML
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                            *************
SUBROUTINE CKSML (T,IWORK,WORK,SML)

   THIS SUBROUTINE RETURNS THE STANDARD STATE ENTROPIES IN MOLAR
   UNITS.  REFERENCE EQUATION (II.4.5).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   SML     - ARRAY OF STANDARD STATE ENTROPIES IN MOLAR UNITS FOR
             THE KK SPECIES.
                CGS UNITS - ERGS/(MOLE*K).
                DIMENSION SML(*) AT LEAST KK.
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CKSMS        CKSMS        CKSMS        CKSMS        CKSMS        CKSMS
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SUBROUTINE CKSMS (T,IWORK,WORK,SMS)

   THIS SUBROUTINE RETURNS THE STANDARD STATE ENTROPIES IN MASS
   UNITS.  REFERENCE EQUATION (II.4.15).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   SMS     - ARRAY OF STANDARD STATE ENTROPIES IN MASS UNITS FOR
             THE KK SPECIES.
                CGS UNITS - ERGS/(GM*K).
                DIMENSION SMS(*) AT LEAST KK.


CKSOR        CKSOR        CKSOR        CKSOR        CKSOR        CKSOR
                 ************************************
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                             *************
SUBROUTINE CKSOR (T,IWORK,WORK,SOR)

   THIS SUBROUTINE RETURNS THE NONDIMENSIONAL ENTROPIES.
   REFERENCE EQUATION (II.4.5) OR (II.4.8).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   SOR     - ARRAY OF NONDIMENSIONAL ENTROPIES FOR THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION SOR(*) AT LEAST KK.


CKSYME       CKSYME       CKSYME       CKSYME       CKSYME       CKSYME
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SUBROUTINE CKSYME (LMDIM,IWORK,WORK,MHOL)

   THIS SUBROUTINE RETURNS THE HOLLERITH SYMBOLS
   FOR THE ELEMENT NAMES.

 INPUT
   LMDIM   - ACTUAL FIRST DIMENSION OF MATRIX OF ELEMENT HOLLERITH
             CHARACTERS.  LMDIM MUST BE AT LEAST LENEL, THE TOTAL
             NUMBER OF HOLLERITH CHARACTERS FOR THE ELEMENT NAMES.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
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                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   MHOL    - MATRIX OF A1 HOLLERITH SYSMBOLS FOR THE ELEMENT NAMES.
             MHOL(L,M) IS THE L TH A1 HOLLERITH CHARACTER FOR THE
             M TH  ELEMENT.  THERE ARE LENEL CHARACTERS FOR EACH
             ELEMENT.
                DIMENSION MHOL(LMDIM,*) EXACTLY LMDIM FOR THE FIRST
                DIMENSION AND AT LEAST MM FOR THE SECOND. LMDIM
                MUST BE AT LEAST LENEL.


CKSYMR       CKSYMR       CKSYMR       CKSYMR       CKSYMR       CKSYMR
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SUBROUTINE CKSYMR (I,LENIHL,IWORK,WORK,LT,IHOL)

   THIS SUBROUTINE RETURNS AN A1 HOLLERITH ARRAY WHICH
   DESCRIBES THE I TH REACTION.

 INPUT
   I       - REACTION INDEX
   LENIHL  - LENGTH OF THE A1 HOLLERITH ARRAY PROVIDED FOR THE
             HOLLERITH DESCRIPTIONS OF THE REACTIONS.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   LT      - ACTUAL NUMBER OF A1 HOLLERITH CHARACTERS IN THE
             REACTION DESCRIPTION.  LT WILL ALWAYS BE LESS THAN
             OR EQUAL TO LENIHL.
   IHOL    - ARRAY OF A1 HOLLERITH CHARACTERS DESCRIBING
             THE I TH  REACTION.
                DIMENSION IHOL(*) AT LEAST LENIHL.


CKSYMS       CKSYMS       CKSYMS       CKSYMS       CKSYMS       CKSYMS
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                            *************
SUBROUTINE CKSYMS (LKDIM,IWORK,WORK,KHOL)

   THIS SUBROUTINE RETURNS THE HOLLERITH SYMBOLS
   FOR THE SPECIES NAMES.

 INPUT
   LKDIM   - ACTUAL FIRST DIMENSION OF MATRIX OF SPECIES HOLLERITH
             CHARACTERS.  LKDIM MUST BE AT LEAST LENSYM, THE TOTAL
             NUMBER OF HOLLERITH CHARACTER FOR THE SPECIES NAMES.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.
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 OUTPUT
   KHOL    - MATRIX OF A1 HOLLERITH SYMBOLS FOR THE SPECIES NAMES.
             KHOL(L,K) IS THE L TH A1 HOLLERITH CHARACTER FOR THE
             KK SPECIES.  THERE ARE LENSYM CHARACTERS FOR EACH
             SPECIES.
                DIMENSION KHOL(LKDIM,*) EXACTLY LKDIM FOR THE FIRST
                DIMENSION AND AT LEAST KK FOR THE SECOND. LKDIM
                MUST BE AT LEAST LENSYM.


CKTHB        CKTHB        CKTHB        CKTHB        CKTHB        CKTHB
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SUBROUTINE CKTHB (KDIM,IWORK,WORK,AKI)

   THIS SUBROUTINE RETURNS MATRIX OF ENHANCED THIRD BODY
   COEFFICIENTS, REFERENCE EQUATION (II.5.11).

 INPUT
   KDIM    - ACTUAL FIRST DIMENSION OF TWO DIMENSIONAL ARRAY.
             KDIM MUST BE GREATER THAN OR EQUAL TO THE TOTAL
             NUMBER OF SPECIES, KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   AKI     - MATRIX OF ENHANCED THIRD BODY EFFICIENCIES OF THE KK
             SPECIES IN THE II REACTIONS. AKI(K,I) IS THE ENHANCED
             EFFICIENCY OF THE K TH SPECIES IN THE I TH REACTION.
                DIMENSION AKI(KDIM,*) EXACTLY KDIM FOR THE FIRST
                DIMENSION AND AT LEAST II FOR THE SECOND.


CKUBML       CKUBML       CKUBML       CKUBML       CKUBML       CKUBML
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                            *************
SUBROUTINE CKUBML (T,X,IWORK,WORK,UBML)

   THIS SUBROUTINE RETURNS THE MOLAR WEIGHTED MEAN INTERNAL
   ENERGY OF THE MIXTURE IN MOLAR UNITS. REFERENCE EQUATION
   (II.4.28).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   UBML    - MOLAR WEIGHTED MEAN INTERNAL ENERGY IN MOLAR UNITS.
                CGS UNITS - ERGS/MOLE.
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CKUBMS      CKUBMS      CKUBMS      CKUBMS      CKUBMS      CKUBMS
                ************************************
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                            *************
SUBROUTINE CKUBMS (T,Y,IWORK,WORK,UBMS)

   THIS SUBROUTINE RETURNS THE MASS WEIGHTED MEAN INTERNAL
   ENERGY OF THE MIXTURE IN MASS UNITS. REFERENCE EQUATION
   (II.4.29).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   UBMS    - MASS WEIGHTED MEAN INTERNAL ENERGY IN MASS UNITS.
                CGS UNITS - ERGS/GM.


CKUML       CKUML       CKUML       CKUML       CKUML       CKUML
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SUBROUTINE CKUML (T,IWORK,WORK,UML)

   THIS SUBROUTINE RETURNS THE INTERNAL ENERGIES IN MOLAR
   UNITS. REFERENCE EQUATION (II.4.10).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   UML     - ARRAY OF INTERNAL ENERGIES IN MOLAR UNITS FOR THE
             KK SPECIES.
                CGS UNITS - ERGS/MOLE.
                DIMENSION UML(*) AT LEAST KK.


CKUMS       CKUMS       CKUMS       CKUMS       CKUMS       CKUMS
                ************************************
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                            *************
SUBROUTINE CKUMS (T,IWORK,WORK,UMS)

   THIS SUBROUTINE RETURNS THE INTERNAL ENERGIES IN MASS
   UNITS. REFERENCE EQUATION (II.4.17).

 INPUT
   T       - TEMPERATURE.
                CGS UNITS - K
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   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   UMS    - ARRAY OF INTERNAL ENERGIES IN MASS UNITS FOR THE
            KK SPECIES.
               CGS UNITS - ERGS/GM.
               DIMENSION UMS(*) AT LEAST KK.


CKUNIT       CKUNIT       CKUNIT       CKUNIT       CKUNIT       CKUNIT
               ************************************
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                           *************
SUBROUTINE CKUNIT (RU,RUC,PA,IWORK,WORK)

   THIS SUBROUTINE IS USED TO CHANGE UNITS IN THE CODE.
   CARE MUST BE TAKEN TO MAKE SURE THAT IF THE UNITS ARE
   CHANGED THEY ARE CONSISTENT.

 INPUT
   RU     - UNIVERSAL GAS CONSTANT.
               CGS UNITS - 8.314E7 ERGS/(MOLE*K)
   RUC    - UNIVERSAL GAS CONSTANT USED ONLY IN CONJUCTION WITH
            ACTIVATION ENERGY.
               PREFERRED UNITS - 1.987 CAL/(MOLE*K).
   PA     - PRESSURE OF ONE STANDARD ATMOSPHERE.
               CGS UNITS - 1.01325E6 DYNES/CM**2
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.


CKWC         CKWC         CKWC         CKWC         CKWC         CKWC
               ************************************
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SUBROUTINE CKWC (T,C,IWORK,WORK,WDOT)

   THIS SUBROUTINE RETURNS THE MOLAR PRODUCTION RATES OF THE
   SPECIES GIVEN THE TEMPERATURE AND MOLAR CONCENTRATIONS.
   REFERENCE EQUATION (11.5.2.)

 INPUT
   T      - TEMPERATURE.
               CGS UNITS - K
   C      - MOLAR CONCENTRATIONS OF THE KK SPECIES.
               CGS UNITS - MOLE/CM**3
               DIMENSION C(*) AT LEAST KK.
   IWORK  - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
            IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK   - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
            INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
               DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
               DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
```

```
   WDOT    - ARRAY OF CHEMICAL MOLAR PRODUCTION RATES FOR THE KK
             SPECIES.
                CGS UNITS - MOLES/(CM**3*SEC).
                DIMENSION WDOT(*) AT LEAST KK.


CKWL         CKWL         CKWL         CKWL         CKWL         CKWL
                ***************************************
                      ***************************
                            *************
SUBROUTINE CKWL (IWORK,WORK,WL)

   THIS SUBROUTINE RETURNS A SET OF FLAGS PROVIDING INFORMATION
   ON THE WAVE LENGTH OF PHOTON RADIATION.

 INPUT
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   WL      - ARRAY OF RADIATION WAVELENGTH INFORMATION FOR THE II
             REACTIONS.
             WL(I)= 0.   REACTION I DOES NOT HAVE RADIATION AS
                         EITHER A REACTANT R PRODUCT
             WL(I)=-A    REACTION I HAS RADIATION OF WAVELENGTH A
                         AS A REACTANT
             WL(I)=+A    REACTION I HAS RADIATION OF WAVELENGTH A
                         AS A PRODUCT
             IF A = 1.0 THEN NO WAVELENGTH INFORMATION WAS GIVEN.
                DIMENSION WL(*) AT LEAST II
                UNITS -  ANGSTROMS


CKWT         CKWT         CKWT         CKWT         CKWT         CKWT
                ***************************************
                      ***************************
                            *************
SUBROUTINE CKWT (IWORK,WORK,WT)

   THIS SUBROUTINE RETURNS THE MOLECULAR WEIGHTS OF THE SPECIES.

 INPUT
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   WT      - ARRAY OF MOLECULAR WEIGHT FOR THE KK SPECIES.
                CGS UNITS - GM/MOLE.
                DIMENSION WT(*) AT LEAST KK.
```

```
CKWXP        CKWXP        CKWXP        CKWXP        CKWXP        CKWXP
                 ************************************
                       *************************
                             *************
SUBROUTINE CKWXP (P,T,X,IWORK,WORK,WDOT)

   THIS SUBROUTINE RETURNS THE MOLAR PRODUCTION RATES OF THE
   SPECIES GIVEN THE PRESSURE, TEMPERATURE AND MOLE FRACTIONS.
   REFERENCE EQUATION (II.5.2).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   WDOT    - ARRAY OF CHEMICAL MOLAR PRODUCTION RATES FOR THE KK
             SPECIES.
                CGS UNITS - MOLES/(CM**3*SEC).
                DIMENSION WDOT(*) AT LEAST KK.


CKWXR        CKWXR        CKWXR        CKWXR        CKWXR        CKWXR
                 ************************************
                       *************************
                             *************
SUBROUTINE CKWXR (RHO,T,X,IWORK,WORK,WDOT)

   THIS SUBROUTINE RETURNS THE MOLAR PRODUCTION RATES OF THE
   SPECIES GIVEN THE MASS DENSITY, TEMPERATURE AND MOLE
   FRACTIONS. REFERENCE EQUATION (II.5.2).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   WDOT    - ARRAY OF CHEMICAL MOLAR PRODUCTION RATES FOR THE KK
             SPECIES.
                CGS UNITS - MOLES/(CM**3*SEC).
                DIMENSION WDOT(*) AT LEAST KK.
```

```
CKWYP        CKWYP        CKWYP        CKWYP        CKWYP        CKWYP
                 ************************************
                       *************************
                             *************
SUBROUTINE CKWYP (P,T,Y,IWORK,WORK,WDOT)

   THIS SUBROUTINE RETURNS THE MOLAR PRODUCTION RATES
   OF THE SPECIES GIVEN THE PRESSURE, TEMPERATURE AND MASS
   FRACTIONS. REFERENCE EQUATION (II.5.2).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   WDOT    - ARRAY OF CHEMICAL MOLAR PRODUCTION RATES FOR THE KK
             SPECIES.
                CGS UNITS - MOLES/(CM**3*SEC).
                DIMENSION WDOT(*) AT LEAST KK.


CKWYR        CKWYR        CKWYP        CKWYR        CKWYR        CKWYR
                 ************************************
                       *************************
                             *************
SUBROUTINE CKWYR (RHO,T,Y,IWORK,WORK,WDOT)

   THIS SUBROUTINE RETURNS THE MOLAR PRODUCTION RATES OF THE
   SPECIES GIVEN THE MASS DENSITY, TEMPERATURE AND MASS
   FRACTIONS. REFERENCE EQUATION (II.5.2).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   WDOT    - ARRAY OF CHEMICAL MOLAR PRODUCTION RATES FOR THE KK
             SPECIES.
                CGS UNITS - MOLES/(CM**3*SEC).
                DIMENSION WDOT(*) AT LEAST KK.
```

```
CKXTCP      CKXTCP      CKXTCP      CKXTCP      CKXTCP      CKXTCP
            ************************************
                    **************************
                            *************
SUBROUTINE CKXTCP (P,T,X,IWORK,WORK,C)

   THIS SUBROUTINE RETURNS THE MOLAR CONCENTRATIONS GIVEN THE
   PRESSURE, TEMPERATURE AND MOLE FRACTIONS.  REFERENCE EQUATION
   (II.3.5)

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.


CKXTCR      CKXTCR      CKXTCR      CKXTCR      CKXTCR      CKXTCR
            ************************************
                    **************************
                            *************
SUBROUTINE CKXTCR (RHO,T,X,IWORK,WORK,C)

   THIS SUBROUTINE RETURNS THE MOLAR CONCENTRATIONS GIVEN
   THE MASS DENSITY, TEMPERATURE AND MOLE FRACTIONS.
   REFERENCE EQUATION (II.3.6).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
```

```
CKXTY        CKXTY        CKXTY        CKXTY        CKXTY        CKXTY
                 ************************************
                       *************************
                             *************
SUBROUTINE CKXTY (X,IWORK,WORK,Y)

   THIS SUBROUTINE RETURNS THE MASS FRACTIONS GIVEN THE
   MOLE FRACTIONS. REFERENCE EQUATION (II.3.4).

 INPUT
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.


CKYTCP       CKYTCP       CKYTCP       CKYTCP       CKYTCP       CKYTCP
                 ************************************
                       *************************
                             *************
SUBROUTINE CKYTCP (P,T,Y,IWORK,WORK,C)

   THIS SUBROUTINE RETURNS THE MOLAR CONCENTRATIONS GIVEN
   THE PRESSURE, TEMPERATURE AND MASS FRACTIONS. REFERENCE
   EQUATION (II.3.2).

 INPUT
   P       - PRESSURE.
                CGS UNITS - DYNES/CM**2.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.
```

```
CKYTCR       CKYTCR       CKYTCR       CKYTCR       CKYTCR       CKYTCR
                 ****************************************
                        ***************************
                               *************
SUBROUTINE CKYTCR (RHO,T,Y,IWORK,WORK,C)

   THIS SUBROUTINE RETURNS THE MOLAR CONCENTRATIONS GIVEN
   THE MASS DENSITY, TEMPERATURE AND MASS FRACTIONS.
   REFERENCE EQUATION (II.3.3).

 INPUT
   RHO     - MASS DENSITY.
                CGS UNITS - GM/CM**3.
   T       - TEMPERATURE.
                CGS UNITS - K
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   C       - MOLAR CONCENTRATIONS OF THE KK SPECIES.
                CGS UNITS - MOLE/CM**3
                DIMENSION C(*) AT LEAST KK.


CKYTX        CKYTX        CKYTX        CKYTX        CKYTX        CKYTX
                 ****************************************
                        ***************************
                               *************
SUBROUTINE CKYTX (Y,IWORK,WORK,X)

   THIS SUBROUTINE RETURNS THE MOLE FRACTIONS GIVEN THE
   MASS FRACTIONS. REFERENCE EQUATION (II.3.1).

 INPUT
   Y       - ARRAY OF MASS FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION Y(*) AT LEAST KK.
   IWORK   - ARRAY OF INTEGER INTERNAL WORK SPACE. THE IWORK ARRAY
             IS INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION IWORK(*) AT LEAST LENIWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF IWORK.
   WORK    - ARRAY OF REAL INTERNAL WORK SPACE.  THE WORK ARRAY IS
             INITIALIZED BY THE CALL TO SUBROUTINE CKINIT.
                DIMENSION WORK(*) AT LEAST LENWK. SEE CKINIT FOR
                DETAILS ON THE REQUIRED LENGTH OF WORK.

 OUTPUT
   X       - MOLE FRACTIONS OF THE KK SPECIES.
                CGS UNITS - NONE.
                DIMENSION X(*) AT LEAST KK.
```

VII. Sample Problem

Before using CHEMKIN on a problem, the user must: 1) define a system of governing equations, 2) define a reaction mechanism, and 3) choose a solution method. In this sample problem we will solve the equations describing constant pressure combustion for a hydrogen-air reaction mechanism. The governing energy and mass conservation equations are:

$$\frac{dT}{dt} = -\frac{1}{\rho \bar{c}_p} \sum_{k=1}^{K} h_k \dot{\omega}_k W_k$$

$$\frac{dY_k}{dt} = \frac{\dot{\omega}_k W_k}{\rho} \qquad k = 1....K$$

where T is temperature and Y_k are the mass fractions of the K species involved. The independent variable, t, is time. Other variables are: ρ, mass density, $\bar{c}_p$, mass weighted mean specific heat at constant pressure, h_k, the specific enthalpies of the species, $\dot{\omega}_k$, the molar production rates of the species, and W_k, the molecular weights of the species.

The governing system of ordinary differential equations forms an initial value problem. Solution of the equations will be via the code LSODE[6] written by Alan Hindmarsh. We find this code to be highly reliable for the solution of very wide range of stiff initial value problems.

The FORTRAN code for solution of the sample problem is given below in Section 3. After initializing CHEMKIN, the code reads the initial mass fractions from input. It then repeatedly calls subroutine LSODE to obtain the solution at uniform print intervals. The governing equation formulation is found in SUBROUTINE FUN which is called by LSODE.

The following sections present in chronological order the input required and the output produced by the codes. The last section lists a brief description of the call sequence for LSODE. This is needed to understand the sample problem coding. The Thermodynamic Data for the problem are taken from the Data Base given in Appendix B.

1. Input to INTERPRETER

```
ELEMENTS
  H   O   N
END
SPECIES
  H2  O2  N2  H  O  N  OH  HO2  H2O  NO
END
REACTIONS
H2+O2=2OH                                          1.7E13     0.000    47780.
H2+OH=H2O+H                                        5.2E13     0.000     6500.
H+O2=OH+O                                         1.22E17    -0.907    16620.
O+H2=OH+H                                          1.8E10     1.000     8826.
H+O2+M=HO2+M                                       2.0E15     0.000     -870.
   H2O / 20./
OH+HO2=H2O+O2                                      1.2E13     0.000        0.
H+HO2=2OH                                          6.0E13     0.000        0.
O+HO2=O2+OH                                        1.0E13     0.000        0.
2OH=O+H2O                                          1.7E06     2.030    -1190.
H2+M=2H+M                                         2.23E12     0.500    92600.
  H2O/5/
O2+M=2O+M                                         1.85E11     0.500    95560.
H+OH+M=H2O+M                                       7.5E23    -2.600        0.
  H2O/20.0/
H+HO2=H2+O2                                        1.3E13     0.000        0.
O+N2=NO+N                                          1.4E14     0.000    75800.
N+O2=NO+O                                          6.4E09     1.000     6280.
OH+N=NO+H                                          4.0E13     0.000        0.
END
```

2. Output from INTERPRETER

OUTPUT FROM INTERPRETER

ELEMENTS CONSIDERED

	ELEMENTS	ATOMIC WEIGHT
1.	H	1.01
2.	O	16.0
3.	N	14.0

SPECIES CONSIDERED

	SPECIES	PHASE	CHARGE	MOLECULAR WEIGHT	LOW TEMP	HIGH TEMP	MID TEMP	ELEMENT COUNT H	O	N
1.	H2	G	0	2.01594	300.00	5000.00	1000.00	2	0	0
2.	O2	G	0	31.9988	300.00	5000.00	1000.00	0	2	0
3.	N2	G	0	28.0134	300.00	5000.00	1000.00	0	0	2
4.	H	G	0	1.00797	300.00	5000.00	1000.00	1	0	0
5.	O	G	0	15.9994	300.00	5000.00	1000.00	0	1	0
6.	N	G	0	14.0067	300.00	5000.00	1000.00	0	0	1
7.	OH	G	0	17.0074	300.00	5000.00	1000.00	1	1	0
8.	HO2	G	0	33.0068	300.00	5000.00	1000.00	1	2	0
9.	H2O	G	0	18.0153	300.00	5000.00	1000.00	2	1	0
10.	NO	G	0	30.0061	300.00	5000.00	1000.00	0	1	1

REACTIONS CONSIDERED

		PRE EXP	TEMP EXP	ACT ENG
1.	H2+O2=2OH	.170E+14	0.	47780.
2.	H2+OH=H2O+H	.520E+14	0.	6500.0
3.	H+O2=OH+O	.122E+18	-.90700	16620.
4.	O+H2=OH+H	.180E+11	1.0000	8826.0
5.	H+O2+M=HO2+M	.200E+16	0.	-870.00
	H2O ENHANCED BY 2.000E+01			
6.	OH+HO2=H2O+O2	.120E+14	0.	0.
7.	H+HO2=2OH	.600E+14	0.	0.
8.	O+HO2=O2+OH	.100E+14	0.	0.
9.	2OH=O+H2O	.170E+07	2.0300	-1190.0
10.	H2+M=2H+M	.223E+13	.50000	92600.
	H2O ENHANCED BY 5.000E+00			
11.	O2+M=2O+M	.185E+12	.50000	95560.
12.	H+OH+M=H2O+M	.750E+24	-2.6000	0.
	H2O ENHANCED BY 2.000E+01			
13.	H+HO2=H2+O2	.130E+14	0.	0.
14.	O+N2=NO+N	.140E+15	0.	75800.
15.	N+O2=NO+O	.640E+10	1.0000	6280.0
16.	OH+N=NO+H	.400E+14	0.	0.

3. User's FORTRAN Code

```
      PROGRAM CKSAMP(INPUT,OUTPUT,TAPE95,TAPE6=OUTPUT,TAPE5=INPUT)
      DIMENSION Y(10),Z(11),KSYM(10,10),ISYMR(10),ELWRK(242),IELWRK(31)
      COMMON/WRK/IWORK(510),WORK(386)
      COMMON/PARAM/KK,P,RU,WT(10)
      EXTERNAL FUN
      DATA LIW,LRW/31,242/
      DATA LENWK,LENIWK/386,510/
      DATA NK,NLMAX/5,55/
      DATA LOUT,LINK/6,95/
C
C        THE INDEPENDENT VARIABLE IN THIS PROBLEM IS TIME.
C      THE DEPENDENT VARIABLES IN THIS PROBLEM ARE TEMPERATURE,T AND
C      MASS FRACTION,Y(K).  HOWEVER THE ODE SOLVER IS DESIGNED TO SOLVE
C      SYSTEMS OF THE FORM  DZ/DX = F(X,Z) .  THEREFORE THE DEPENDENT
C      VARIABLES MUST BE PUT INTO A SINGLE VECTOR Z.  WE HAVE DEFINED
C                  X=TIME
C                  Z(1)=T
C                  Z(K+1)=Y(K)
C
C
C         INITIALIZE CHEMKIN
C
      CALL CKINIT(LENIWK,LENWK,LINK,LOUT,IWORK,WORK)
C
C         OBTAIN INFORMATION ON SPECIES AND REACTIONS FROM CHEMKIN
C
      CALL CKINDX(IWORK,WORK,MM,KK,II,LENEL,LENSYM,NFIT)
      CALL CKSYMS(LENSYM,IWORK,WORK,KSYM)
      CALL CKRP(IWORK,WORK,RU,RUC,PATM)
      CALL CKWT(IWORK,WORK,WT)
C
C         INITIALIZE ALL MASS FRACTIONS, Y(K), TO ZERO
C
      DO 10 K=1,KK
      Y(K)=0.0
   10 CONTINUE
C
C         READ NON-ZERO INITIAL MASS FRACTIONS FROM INPUT
C
      DO 20 L=1,KK
      READ(5,7500)(ISYMR(M),M=1,LENSYM),YIN
      IF(ISYMR(1).EQ.1H ) GO TO 25
C         LOOK FOR A SPECIES MATCH
      DO 15 K=1,KK
C        COMPARE INPUT SPECIES NAMES WITH THOSE IN CHEMKIN
      CALL CKCOMP(LENSYM,KSYM(1,K),ISYMR,ISAME)
      IF(ISAME.EQ.1)GO TO 17
   15 CONTINUE
      PRINT 7700
      CALL EXIT
C
C         SPECIES MATCH FOUND, SET INITAL MASS FRACTION
   17 CONTINUE
      Y(K)=YIN
   20 CONTINUE
   25 CONTINUE
C
C         SET PRESSURE,P, AND INITIAL TEMPERATURE,T.
C
      T=1000.
      P=1.0*PATM
C
C         SET INITIAL TIME,FINAL TIME, AND PRINT INTERVAL
      T1=0.
      T2=1.E-2
      DT=1.E-3
```

```
C
C          SET THE INTEGRATION CONTROL PARAMETERS FOR LSODE
C
      NEQ=KK+1
      MF=22
      ITOL=1
      IOPT=0
      RTOL=1.E-4
      ITASK=1
      ATOL=1.E-15
      ISTATE=1
C
C          SET INITIAL CONDITIONS INTO THE Z VECTOR
C
      Z(1)=T
      DO 100 K=1,KK
      Z(K+1)=Y(K)
  100 CONTINUE
      TT1=T1
      TT2=T1
      NLINES=NLMAX+1
C
C          INTEGRATICN LOOP
C
  250 CONTINUE
      IF(NLINES.LT.NLMAX)GO TO 270
C
C          PRINT PAGE HEADING
C
      NLINES=0
      WRITE(6,7003)
      DO 200 K1=1,KK,NK
      K2=K1+NK-1
      IF(K2.GT.KK)K2=KK
      IF(K1.GT.1)GO TO 180
      WRITE(6,7100) ((KSYM(L,K),L=1,LENSYM),K=K1,K2)
      NLINES=NLINES+1
      GO TO 200
  180 CONTINUE
      WRITE(6,7110) ((KSYM(L,K),L=1,LENSYM),K=K1,K2)
      NLINES=NLINES+1
  200 CONTINUE
C
C          PRINT THE SOLUTION
C
  270 CONTINUE
      DO 300 K1=1,KK,NK
      K2=K1+NK-1
      IF(K2.GT.KK)K2=KK
      IF(K1.GT.1)GO TO 280
      WRITE(6,7105)TT1,T,(Y(K),K=K1,K2)
      NLINES=NLINES+1
      GO TO 300
  280 CONTINUE
      WRITE(6,7115)(Y(K),K=K1,K2)
      NLINES=NLINES+1
  300 CONTINUE
C
C          CALL THE DIFFERENTIAL EQUATION SOLVER
C
      TT2=TT2+DT
      CALL LSODE(FUN,NEQ,Z,TT1,TT2,ITOL,RTOL,ATOL,ITASK,ISTATE,IOPT,ELWR
     1K,LRW,IELWRK,LIW,JAC,MF)
      T=Z(1)
      DO 400 K=1,KK
      Y(K)=Z(K+1)
  400 CONTINUE
      IF(TT1.LT.T2)GO TO 250
      CALL EXIT
C
```

```
C         FORMATS
C
 7003 FORMAT(1H1)
 7100 FORMAT(3X,6HT(SEC),6X,6HTMP(K),6X,5(1X,10A1))
 7105 FORMAT(12E11.3)
 7110 FORMAT(27X,5(1X,10A1))
 7115 FORMAT(22X,10E11.3)
 7500 FORMAT(10A1,E10.0)
 7700 FORMAT(10X,50HINITIAL MASS FRACTION GIVEN FOR AN UNKNOWN SPECIES)
      END


      SUBROUTINE FUN(N,TIME,Z,ZP)
      DIMENSION Z(N),ZP(N)
      COMMON/WRK/IWORK(510),WORK(386)
      COMMON/PARAM/KK,P,RU,WT(10)
      COMMON/DUM/WDOT(10),H(10)
C
C          VARIABLES IN Z ARE
C               Z(1)=T
C               Z(K+1)=Y(K)
C
C               CALL CHEMKIN SUBROUTINES
C
      CALL CKRHOY(P,Z(1),Z(2),IWORK,WORK,RHO)
      CALL CKCPBS(Z(1),Z(2),IWORK,WORK,CPB)
      CALL CKWYP(P,Z(1),Z(2),IWORK,WORK,WDOT)
      CALL CKHMS(Z(1),IWORK,WORK,H)
C
C               FORM GOVERNING EQUATION
C
      SUM=0.
      DO 100 K=1,KK
      SUM=SUM+H(K)*WDOT(K)*WT(K)
  100 CONTINUE
      ZP(1)=-SUM/(RHO*CPB)
      DO 200 K=1,KK
      ZP(K+1)=WDOT(K)*WT(K)/RHO
  200 CONTINUE
      RETURN
      END
```

4. Input to FORTRAN Code

H2	0.0283
O2	0.226
N2	0.7457

5. Output from FORTRAN Code

T(SEC)	TMP(K)	H2 N	O2 OH	N2 HO2	H H2O	O NO
0.	.100E+04	.283E-01	.226E+00	.746E+00	0.	0.
		0.	0.	0.	0.	0.
.100E-02	.269E+04	.297E-02	.177E-01	.745E+00	.434E-03	.266E-02
		.297E-06	.149E-01	.379E-05	.215E+00	.204E-02
.200E-02	.269E+04	.299E-02	.169E-01	.744E+00	.429E-03	.256E-02
		.428E-06	.146E-01	.361E-05	.215E+00	.422E-02
.300E-02	.268E+04	.301E-02	.164E-01	.743E+00	.427E-03	.249E-02
		.513E-06	.144E-01	.351E-05	.214E+00	.577E-02
.400E-02	.268E+04	.303E-02	.160E-01	.743E+00	.426E-03	.245E-02
		.567E-06	.143E-01	.344E-05	.214E+00	.680E-02
.500E-02	.268E+04	.304E-02	.158E-01	.742E+00	.425E-03	.243E-02
		.600E-06	.142E-01	.340E-05	.214E+00	.746E-02
.600E-02	.268E+04	.304E-02	.156E-01	.742E+00	.424E-03	.241E-02
		.620E-06	.142E-01	.337E-05	.214E+00	.787E-02
.700E-02	.268E+04	.305E-02	.155E-01	.742E+00	.424E-03	.240E-02
		.632E-06	.141E-01	.335E-05	.214E+00	.813E-02
.800E-02	.268E+04	.305E-02	.155E-01	.742E+00	.424E-03	.239E-02
		.639E-06	.141E-01	.334E-05	.214E+00	.828E-02
.900E-02	.268E+04	.305E-02	.155E-01	.742E+00	.424E-03	.239E-02
		.644E-06	.141E-01	.334E-05	.214E+00	.838E-02

6. Comments on Use of LSODE

```
      SUBROUTINE LSODE (F, NEQ, Y, T, TOUT, ITOL, RTOL, ATOL, ITASK,
     1             ISTATE, IOPT, RWORK, LRW, IWORK, LIW, JAC, MF)
      EXTERNAL F, JAC
      INTEGER NEQ, ITOL, ITASK, ISTATE, IOPT, LRW, IWORK, LIW, MF
      REAL Y, T, TOUT, RTOL, ATOL, RWORK
      DIMENSION NEQ(1), Y(1), RTOL(1), ATOL(1), RWORK(LRW), IWORK(LIW)
C-----------------------------------------------------------------------
C THIS IS THE JANUARY 21, 1980 VERSION OF
C LSODE.. LIVERMORE SOLVER FOR ORDINARY DIFFERENTIAL EQUATIONS.
C THIS VERSION IS IN SINGLE PRECISION.
C
C LSODE SOLVES THE INITIAL VALUE PROBLEM FOR STIFF OR NONSTIFF
C SYSTEMS OF FIRST ORDER ODE-S,
C     DY/DT = F(T,Y) ,  OR, IN COMPONENT FORM,
C     DY(I)/DT = F(I) = F(I,T,Y(1),Y(2),...,Y(NEQ)) (I = 1,...,NEQ).
C LSODE IS A PACKAGE BASED ON THE GEAR AND GEARB PACKAGES, AND ON THE
C OCTOBER 23, 1978 VERSION OF THE TENTATIVE ODEPACK USER INTERFACE
C STANDARD, WITH MINOR MODIFICATIONS.
C AUTHOR AND CONTACT.. ALAN C. HINDMARSH,
C                      MATHEMATICS AND STATISTICS SECTION, L-300
C                      LAWRENCE LIVERMORE LABORATORY
C                      LIVERMORE, CA 94550.
C-----------------------------------------------------------------------
C SUMMARY OF USAGE.
C
C COMMUNICATION BETWEEN THE USER AND THE LSODE PACKAGE, FOR NORMAL
C SITUATIONS, IS SUMMARIZED BELOW.  SEE THE FULL DESCRIPTION FOR
C DETAILS, INCLUDING OPTIONAL COMMUNICATION, NONSTANDARD OPTIONS,
C AND INSTRUCTIONS FOR SPECIAL SITUATIONS.  SEE ALSO THE EXAMPLE
C PROBLEM (WITH PROGRAM AND OUTPUT) FOLLOWING THIS SUMMARY.
C
C A. FIRST PROVIDE A SUBROUTINE OF THE FORM..
C                SUBROUTINE F (NEQ, T, Y, YDOT)
C                DIMENSION Y(NEQ), YDOT(NEQ)
C WHICH SUPPLIES THE VECTOR FUNCTION F BY LOADING YDOT(I) WITH F(I).
C
C B. NEXT DETERMINE (OR GUESS) WHETHER OR NOT THE PROBLEM IS STIFF.
C STIFFNESS OCCURS WHEN THE JACOBIAN MATRIX DF/DY HAS AN EIGENVALUE
C WHOSE REAL PART IS NEGATIVE AND LARGE IN MAGNITUDE, COMPARED TO THE
C RECIPROCAL OF THE T SPAN OF INTEREST.  IF THE PROBLEM IS NONSTIFF,
C USE A METHOD FLAG MF = 10.  IF IT IS STIFF, THERE ARE FOUR STANDARD
C CHOICES FOR MF, AND LSODE REQUIRES THE JACOBIAN MATRIX IN SOME FORM.
C THIS MATRIX IS REGARDED EITHER AS FULL (MF = 21 OR 22),
C OR BANDED (MF = 24 OR 25).  IN THE BANDED CASE, LSODE REQUIRES TWO
C HALF-BANDWIDTH PARAMETERS ML AND MU.  THESE ARE, RESPECTIVELY, THE
C WIDTHS OF THE LOWER AND UPPER PARTS OF THE BAND, EXCLUDING THE MAIN
C DIAGONAL.  THUS THE BAND CONSISTS OF THE LOCATIONS (I,J) WITH
C I-ML .LE. J .LE. I+MU, AND THE FULL BANDWIDTH IS ML+MU+1.
C
C C. IF THE PROBLEM IS STIFF, YOU ARE ENCOURAGED TO SUPPLY THE JACOBIAN
C DIRECTLY (MF = 21 OR 24), BUT IF THIS IS NOT FEASIBLE, LSODE WILL
C COMPUTE IT INTERNALLY BY DIFFERENCE QUOTIENTS (MF = 22 OR 25).
C IF YOU ARE SUPPLYING THE JACOBIAN, PROVIDE A SUBROUTINE OF THE FORM..
C                SUBROUTINE JAC (NEQ, T, Y, ML, MU, PD, NROWPD)
C                DIMENSION Y(NEQ), PD(NROWPD,NEQ)
C WHICH SUPPLIES DF/DY BY LOADING PD AS FOLLOWS..
C     FOR A FULL JACOBIAN (MF = 21), LOAD PD(I,J) WITH DF(I)/DY(J),
C THE PARTIAL DERIVATIVE OF F(I) WITH RESPECT TO Y(J).  (IGNORE THE
C ML AND MU ARGUMENTS IN THIS CASE.)
C     FOR A BANDED JACOBIAN (MF = 24), LOAD PD(I-J+MU+1,J) WITH
C DF(I)/DY(J), I.E. LOAD THE DIAGONAL LINES OF DF/DY INTO THE ROWS OF
C PD FROM THE TOP DOWN.
C     IN EITHER CASE, ONLY NONZERO ELEMENTS NEED BE LOADED.
C
```

```
C D. WRITE A MAIN PROGRAM WHICH CALLS SUBROUTINE LSODE ONCE FOR
C EACH POINT AT WHICH ANSWERS ARE DESIRED.  THIS SHOULD ALSO PROVIDE
C FOR POSSIBLE USE OF LOGICAL UNIT 3 FOR OUTPUT OF ERROR MESSAGES
C BY LSODE.  ON THE FIRST CALL TO LSODE, SUPPLY ARGUMENTS AS FOLLOWS..
C F      = NAME OF SUBROUTINE FOR RIGHT-HAND SIDE VECTOR F.
C          THIS NAME MUST BE DECLARED EXTERNAL IN CALLING PROGRAM.
C NEQ    = NUMBER OF FIRST ORDER ODE-S.
C Y      = ARRAY OF INITIAL VALUES, OF LENGTH NEQ.
C T      = THE INITIAL VALUE OF THE INDEPENDENT VARIABLE.
C TOUT   = FIRST POINT WHERE OUTPUT IS DESIRED (.NE. T).
C ITOL   = 1 OR 2 ACCORDING AS ATOL (BELOW) IS A SCALAR OR ARRAY.
C RTOL   = RELATIVE TOLERANCE PARAMETER (SCALAR).
C ATOL   = ABSOLUTE TOLERANCE PARAMETER (SCALAR OR ARRAY).
C          THE LOCAL ERROR IN Y(I) WILL BE CONTROLLED SO AS TO BE
C          ROUGHLY LESS THAN  RTOL*ABS(Y(I)) + ATOL  IF ITOL = 1,
C          OR  RTOL*ABS(Y(I)) + ATOL(I)  IF ITOL = 2.
C ITASK  = 1 FOR NORMAL COMPUTATION OF OUTPUT VALUES OF Y AT T = TOUT.
C ISTATE = INTEGER FLAG (INPUT AND OUTPUT).  SET ISTATE = 1.
C IOPT   = 0 TO INDICATE NO OPTIONAL INPUTS USED.
C RWORK  = REAL WORK ARRAY OF LENGTH AT LEAST..
C             20 + 16*NEQ                      FOR MF = 10,
C             22 +  9*NEQ + NEQ**2             FOR MF = 21 OR 22,
C             22 + 10*NEQ + (2*ML + MU)*NEQ    FOR MF = 24 OR 25.
C LRW    = DECLARED LENGTH OF RWORK (IN USER-S DIMENSION).
C IWORK  = INTEGER WORK ARRAY OF LENGTH AT LEAST..
C             20        FOR MF = 10,
C             20 + NEQ  FOR MF = 21, 22, 24, OR 25.
C          IF MF = 24 OR 25, INPUT IN IWORK(1),IWORK(2) THE LOWER
C          AND UPPER HALF-BANDWIDTHS ML,MU.
C LIW    = DECLARED LENGTH OF IWORK (IN USER-S DIMENSION).
C JAC    = NAME OF SUBROUTINE FOR JACOBIAN MATRIX (MF = 21 OR 24).
C          IF USED, THIS NAME MUST BE DECLARED EXTERNAL IN CALLING
C          PROGRAM.  IF NOT USED, PASS A DUMMY NAME.
C MF     = METHOD FLAG.  STANDARD VALUES ARE..
C          10 FOR NONSTIFF (ADAMS) METHOD, NO JACOBIAN USED.
C          21 FOR STIFF (BDF) METHOD, USER-SUPPLIED FULL JACOBIAN.
C          22 FOR STIFF METHOD, INTERNALLY GENERATED FULL JACOBIAN.
C          24 FOR STIFF METHOD, USER-SUPPLIED BANDED JACOBIAN.
C          25 FOR STIFF METHOD, INTERNALLY GENERATED BANDED JACOBIAN.
C
C E. THE OUTPUT FROM THE FIRST CALL (OR ANY CALL) IS..
C      Y = ARRAY OF COMPUTED VALUES OF Y(T) VECTOR.
C      T = CORRESPONDING VALUE OF INDEPENDENT VARIABLE (NORMALLY TOUT).
C ISTATE = 2  IF LSODE WAS SUCCESSFUL, NEGATIVE OTHERWISE.
C          -1 MEANS EXCESS WORK DONE ON THIS CALL (PERHAPS WRONG MF).
C          -2 MEANS EXCESS ACCURACY REQUESTED (TOLERANCES TOO SMALL).
C          -3 MEANS ILLEGAL INPUT DETECTED (SEE PRINTED MESSAGE).
C          -4 MEANS REPEATED ERROR TEST FAILURES (CHECK ALL INPUTS).
C          -5 MEANS REPEATED CONVERGENCE FAILURES (PERHAPS BAD JACOBIAN
C             SUPPLIED OR WRONG CHOICE OF MF OR TOLERANCES).
C          -6 MEANS ERROR WEIGHT BECAME ZERO DURING PROBLEM. (SOLUTION
C             COMPONENT I VANISHED, AND ATOL OR ATOL(I) = 0.)
C
C F. TO CONTINUE THE INTEGRATION AFTER A SUCCESSFUL RETURN, SIMPLY
C RESET TOUT AND CALL LSODE AGAIN.  NO OTHER PARAMETERS NEED BE RESET.
C
```

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APPENDIX A. STORAGE ALLOCATION IN THE WORK ARRAYS

THE WORK ARRAYS CONTAIN ALL THE PERTINENT INFORMATION ABOUT THE SPECIES AND THE REACTION MECHANISM. THEY ALSO CONTAIN SOME WORK SPACE WHICH IS NEEDED BY VARIOUS ROUTINES FOR INTERNAL MANIPULATIONS. IF A USER WISHES TO MODIFY A CHEMKIN SUBROUTINE OR TO WRITE NEW ROUTINES, HE WILL PROBABLY WANT TO USE THE WORK ARRAYS DIRECTLY. THE STARTING ADDRESSES FOR INFORMATION STORED IN THE WORK ARRAYS ARE FOUND IN THE LABELED COMMON BLOCK, COMMON/CKSTRT/, AND ARE EXPLAINED BELOW.

```
      COMMON /CKSTRT/ NMM,NKK,NII,NMAXSP,NMAXTB,NLENEL,NLNSYM,NTHCF,
     1                NCP1,NCP2,NCP2T2,  IMH,IKH,INC,IPH,ICH,INU,INK,
     2                INS,ITB,IRV,INN,INT,  NAW,NWT,NWL,NTL,NTH,NTM,
     3                NAA,NAI,NRA,NRB,NRE,NRU,NRC,NPA,NK1,NK2,NK3,NK4
```

****

INDEX CONSTANTS.

- NMM - NUMBER OF ELEMENTS
- NKK - NUMBER OF SPECIES
- NII - NUMBER OF REACTIONS
- NMAXSP - MAXIMUM NUMBER OF SPECIES IN ANY ONE REACTION. UNLESS CHANGED IN THE INTERPRETER NMAXSP=6.
- NMAXTB - MAXIMUM NUMBER OF ENHANCED THIRD BODY EFFICIENCIES ALLOWED IN ANY ONE REACTION. UNLESS CHANGED IN THE INTERPRETER NMAXTB=6.
- NLENEL - NUMBER OF A1 HOLLERITH SYMBOLS IN THE ELEMENT NAMES. UNLESS CHANGED IN THE INTERPRETER NLENEL=2.
- NLNSYM - NUMBER OF A1 HOLLERITH SYMBOLS IN TEH SPECIES NAMES. UNLESS CHANGED IN THE INTERPRETER NLNSYM=10.
- NTHCF - NUMBER OF POLYNOMIAL COEFFICIENTS TO FITS OF CP/R. UNLESS THE THERMODYNAMIC DATA BASE IS CHANGED, AND THE INTERPRETER IS CHANGED NTCHF=5.
- NCP1 - NTHCF + 1
- NCP2 - NTHCF + 2
- NCP2T2 - 2*(NCP2). TOTAL NUMBER OF THERMODYNAMIC FIT COEFFICIENTS FOR BOTH TEMPERATURE RANGES. UNLESS CHANGED NCP2T2=14.

STARTING ADDRESSES FOR THE INTEGER WORK SPACE, IWORK.

- IMH - IWORK(IMH+(M-1)*NLENEL+L-1) IS THE LTH A1 HOLLERITH CHARACTER FOR THE MTH ELEMENT
- IKH - IWORK(IKH+(K-1)*NLNSYM+L-1) IS THE LTH A1 HOLLERITH CHARACTER FOR THE KTH SPECIES.
- INC - IWORK(INC+(K-1)*NMM+M-1) IS THE NUMBER OF ATOMS OF ELEMENT M IN SPECIES K.
- IPH - STARTING ADDRESS OF THE ARRAY OF FLAGS INDICATING THE PHASE OF EACH SPECIES.
  IWORK(IPH+K-1)=-1 SPECIES K IS SOLID
  = 0 SPECIES K IS GAS
  =+1 SPECIES K IS LIQUID

```
ICH     - STARTING ADDRESS OF THE ARRAY OF THE ELECTRONIC CHARGE
          OF EACH SPECIES.
          FOR EXAMPLE,
          IWORK(ICH+K-1)=-2 MEANS THAT SPECIES K HAS TWO EXCESS
          ELECTRONS.
INU     - STARTING ADDRESS OF THE MATRIX OF NON-ZERO
          STOICHIOMETRIC COEFFICIENTS OF THE REACTIONS.
          IWORK(INU+(I-1)*NMAXSP+L-1) IS
          THE LTH STOICHIOMETRIC COEFFICIENT IN REACTION
          I.  THE SPECIES NUMBERS OF THESE COEFFICIENTS
          ARE STORED BEGINNING AT INK.
INK     - STARTING ADDRESS OF THE MATRIX OF SPECIES
          NUMBERS OF THE NON-ZERO STOICHIOMETRIC
          COEFFICIENTS OF THE REACTIONS.
          IWORK(INK+(I-1)*NMAXSP+L-1) IS THE
          SPECIES NUMBER OF THE LTH NON-ZERO
          STOICHIOMETRIC COEFFICIENT IN REACTION I.
INS     - IWORK(INS+I-1) IS THE SUMMATION OF
          STOICHIOMETRIC COEFFICIENTS IN REACTION I.
          (SEE, FOR EXAMPLE, EQ(II.5.7)).
ITB     - STARTING ADDRESS OF AN ARRAY OF FLAGS
          CONCERNING THIRD BODIES IN THE REACTIONS
          IWORK(ITB+I-1)=-1 REACTION I DOES NOT
                            CONTAIN M AS A THIRD BODY
                        = 0 REACTION I CONTAINS M AS A THIRD
                            BODY BUT NO ENHANCED THIRD
                            BODY EFFICIENCIES ARE GIVEN
                        = N REACTION I CONTAINS M AS A THIRD
                            BODY AND N ENHANCED THIRD BODY
                            EFFICIENCIES ARE GIVEN
IRV - STARTING ADDRESS OF FLAGS CONCERNING THE
          REVERSIBILITY OF THE REACTIONS.
          IWORK(IRV+I-1)=+N REACTION I IS REVERSIBLE AND
                            CONTAINS N NON-ZERO STOICHIOMETRIC
                            COEFFICIENTS.
                        =-N REACTION I IS IRREVERSIBLE AND
                            CONTAINS N NON-ZERO STOICHIOMETRIC
                            COEFFICIENTS.
INN     - IWORK(INN+I-1) IS THE NUMBER OF REACTANT SPECIES IN
          REACTION I (I.E.,NUMBER OF NEGATIVE
          STOICHIOMETRIC COEFFICIENTS).
INT     - STARTING ADDRESS OF THE MATRIX OF SPECIES
          NUMBERS CORRESPONDING TO THE ENHANCED THIRD
          BODY EFFICIENCY FACTORS WHICH ARE STORED
          AT WORK(NAI).
          IWORK(INT+(I-1)*NMAXTB+L-1) IS THE
          SPECIES NUMBER OF THE LTH ENHANCED THIRD
          BODY EFFICIENCY FACTOR.

STARTING ADDRESSES FOR THE REAL WORK SPACE, WORK.

NAW     - WORK(NAW+M-1) IS THE ATOMIC WEIGHT OF ELEMENT M
NWT     - WORK(NWT+K-1) IS THE MOLECULAR WEIGHT OF SPECIES K
NWL     - STARTING ADDRESS OF THE WAVELENGTH INFORMATION
          FOR THE REACTIONS.
          WORK(NWL+I-1) = 0. REACTION I DOES NOT CONTAIN AN HV
                        =-A. REACTION I CONTAINS RADIATION
                             OF WAVELENGTH A AS A REACTANT.
                        =+A. REACTION I CONTAINS RADIATION OF
                             WAVELENGTH A AS A PRODUCT.
          IF A=1.0 NO WAVELENGTH INFORMATION WAS GIVEN.
NTL     - WORK(NTL+K-1) IS THE LOWER TEMPERATURE
          BOUND FOR THE THERMODYNAMIC FITS TO SPECIES K.
NTH     - WORK(NTH+K-1) IS THE UPPER TEMPERATURE
          BOUND FOR THERMODYNAMIC FITS TO SPECIES K.
NTK     - WORK(NTH+K-1) IS THE COMMON TEMPERATURE FOR
          THE THERMODYNAMIC FITS TO SPECIES K.
```

```
NAA     - STARTING ADDRESS FOR THE THREE DEMENSIONAL ARRAY
          OF COEFFICIENT FOR THE FITS TO THE THERMODYNAMIC
          PROPERTIES,A(N,L,K)
          A(N,L,K)=WORK(NAA+(L-1)*NCP2+(K-1)*NCP2T2+N-1)
          WHERE
          FOR N=1,NTHCF A(N,L,K)REPRESENT THE POLYNOMIAL
          COEFFICIENTS IN THE FITS TO CP/R FOR SPECIES K.
          A(NCP1,L,K)=FORMATICN ENTHALPY FOR SPECIES K
          A(NCP2,L,K)=FORMATION ENTROPY FOR SPECIES K
          L=1 IS FOR THE LOW TEMPERATURE RANGE.
          L=2 IS FOR THE HIGH TEMPERATURE RANGE.
NAI     - STARTING ADDRESS OF THE MATRIX OF ENHANCED
          THIRD BODY EFFICEIENCY FACTORS.  THE CORRESPONDING
          SPECIES NUMBERS ARE STORED AT IWORK(INT).
          WORK(NAI+(I-1)*NMAXTB+L-1) IS THE ENHANCED
          EFFICIENCY FACTOR FOR THE LTH ENHANCED EFFICIENCY
          FACTOR IN REACTION I.
NRA     - WORK(NRA+I-1) IS THE ARRHENIUS PRE-EXPONENTIAL
          FACTOR IN THE RATE CONSTANT OF REACTION I.
NRB     - WORK(NRB+I-1)IS THE ARRHENIUS TEMPERATURE
          EXPONENT IN THE RATE CONSTANT OF REACTION I.
NRE     - WORK(NRE+I-1) IS THE ACTIVATION ENERGY OF REACTION I.
NRU     - WORK(NRU)IS THE UNIVERSAL GAS CONSTANT.
NRC     - WORK(NRC)IS THE UNIVERSAL GAS CONSTANT IN UNITS
          CONSISTENT WITH THE INPUT VALUES FOR THE
          ACTIVATION ENERGIES.
NPA     - WORK(NPA) IS THE VALUE OF THE PRESSURE OF ONE
          ATMOSPHERE.
NK1,NK2- STARTING ADDRESSES OF ARRAYS OF INTERNAL WORK
NK3,NK4        SPACE OF LENGTH NKK.

*************************************************************
```

APPENDIX B. A THERMODYNAMIC DATA BASE FOR SOME TYPICAL COMBUSTION PROBLEMS

The data base listed here is one that we find to be useful for certain combustion problems. This data base is a subset of the one given in the NASA Equilibrium code,[3] and the cards were taken directly from that code.

Although it is possible to use an arbitrarily large data base, the execution time required by the INTERPRETER increases with the length of the data base. Therefore, it will be to the users advantage to create a data base which includes only species which are likely to appear in his class of problems.

```
THERMO
   300.000  1000.000  5000.000
AR                  L 5/66AR  100  000  000  0G   300.000  5000.000              1
 0.25000000E 01 0.              0.              0.              0.               2
-0.74537502E 03 0.43660006E 01 0.25000000E 01 0.               0.               3
 0.             0.              -0.74537498E 03 0.43660006E 01                   4
AR+                 L12/66AR  1E  -100  000  0G   300.000  5000.000              1
 0.28420672E 01-0.87648603E-04-0.26463209E-07 0.12240311E-10-0.11885139E-14       2
 0.18272563E 06 0.36720201E 01 0.24857001E 01-0.55682660E-03 0.33194849E-05       3
-0.39236795E-08 0.14143279E-11 0.18290215E 06 0.58880154E 01                      4
C(S)                J 3/61C   10   00   00   0S   300.000  5000.000              1
 0.13604942E 01 0.19182237E-02-0.84040389E-06 0.16448707E-09-0.11672670E-13       2
-0.65713870E 03-0.80070207E 01-0.44778053E 00 0.53691002E-02-0.39775571E-06       3
-0.40459298E-08 0.21134939E-11-0.94280688E 02 0.16840791E 01  2.                 4
C                   J 3/61C   100  000  000  0G   300.000  5000.000              1
 0.25810663E 01-0.14696202E-03 0.74388084E-07-0.79481079E-11 0.58900977E-16       2
 0.85216294E 05 0.43128879E 01 0.25328705E 01-0.15887641E-03 0.30682082E-06       3
-0.26770064E-09 0.87488827E-13 0.85240422E 05 0.46062374E 01                      4
C+                  L12/66C   1E  -100  000  0G   300.000  5000.000              1
 0.25118274E 01-0.17359784E-04 0.95042676E-08-0.22188518E-11 0.18621892E-15       2
 0.21667721E 06 0.42861298E 01 0.25953840E 01-0.40686645E-03 0.68923669E-06       3
-0.52664878E-09 0.15083377E-12 0.21666281E 06 0.38957298E 01                      4
C-                  J 9/65C   1E   100  000  0G   300.000  5000.000              1
 0.24470591E 01 0.11286428E-03-0.78591462E-07 0.19778614E-10-0.11105555E-14       2
 0.69972969E 05 0.42356992E 01 0.24925640E 01 0.53[illegible]3068E-04-0.13307994E-06  3
 0.13951379E-09-0.52150992E-13 0.69955757E 05 0.39811657E 01                      4
CH                  J12/67C   1H   10   00   0G   300.000  5000.000              1
 0.22673116E 01 0.22043000E-02-0.62250191E-06 0.69689940E-10-0.21274952E-14       2
 0.70836037E 05 0.87889352E 01 0.35632752E 01-0.20031372E-03-0.401298[illegible]2E-06  3
 0.18226922E-08-0.86768311E-12 0.70405506E 05 0.17628023E 01                      4
CH+                 J12/71C   1H   1E  -1   0G   300.000  5000.000              1
 0.27466401E+01 0.15496991E-02-0.52858324E-06 0.86132075E-10-0.50909775E-14       2
 0.19483672E+06 0.46994695E+01 0.35601593E+01-0.22478101E-03-0.26341623E-06       3
 0.16716214E-08-0.89478626E-12 0.19460363E+06 0.41570213E+00                      4
CH2                 J12/72C   1H   2    0    0G   300.000  5000.000              1
 0.27525479E+01 0.39782047E-02-0.14921731E-05 0.25956899E-09-0.17110673E-13       2
 0.45547759E+05 0.66534799E+01 0.35883347E+01 0.21724137E-02-0.13323408E-05       3
 0.19469445E-08-0.89431394E-12 0.45315188E+05 0.22627869E+01                      4
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CH2O                J 5/61C   1H   2O   1O   0G   300.000  5000.000                1
 0.28364249E 01 0.68605298E-02-0.26882647E-05 0.47971258E-09-0.32118406E-13 2
-0.15236031E 05 0.78531169E 01 0.37963783E 01-0.25701785E-02 0.18548815E-04 3
-0.17869177E-07 0.55504451E-11-0.15088947E 05 0.47548163E 01                4
CH3                 J 6/69C   1H   3O   0O   0G   300.000  5000.000                1
 0.28400327E 01 0.60869086E-02-0.21740338E-05 0.36042576E-09-0.22725300E-13 2
 0.16449813E 05 0.55056751E 01 0.34666350E 01 0.38301845E-02 0.10116802E-05 3
-0.18859236E-08 0.66803182E-12 0.16313104E 05 0.24172192E 01                4
CH4                 J 3/61C   1H   4O   0O   0G   300.000  5000.000                1
 0.15027072E 01 0.10416798E-01-0.39181522E-05 0.67777899E-09-0.44283706E-13 2
-0.99787078E 04 0.10707143E 02 0.38261932E 01-0.39794581E-02 0.24558340E-04 3
-0.22732926E-07 0.69626957E-11-0.10144950E 05 0.86690073E 00                4
CN                  J 6/69C   1N   1O   0O   0G   300.000  5000.000                1
 0.36036285E 01 0.33644390E-03 0.10028933E-06-0.16318166E-10-0.36286722E-15 2
 0.51159833E 05 0.35454505E 01 0.37386307E 01-0.19239224E-02 0.47055189E-05 3
-0.31113000E-08 0.61675318E-12 0.51270927E 05 0.34490218E 01                4
CN+                 J12/70C   1N   1E  -1O   0G   300.000  5000.000                1
 0.36522919E+01 0.81427579E-03-0.20853348E-06 0.29073604E-10-0.17865094E-14 2
 0.21560182E+06 0.43916910E+01 0.36175018E+01-0.20179550E-02 0.79359855E-05 3
-0.77300616E-08 0.24798477E-11 0.21578134E+06 0.53579527E+01                4
CN-                 J12/70C   1N   1E   1O   0G   300.000  5000.000                1
 0.29471725E+01 0.14988427E-02-0.57579547E-06 0.10177789E-09-0.67478503E-14 2
 0.63644338E+04 0.63743952E+01 0.37034310E+01-0.14896426E-02 0.31864701E-05 3
-0.14831305E-08 0.48121663E-13 0.62335826E+04 0.27722843E+01                4
CNN                 J 6/66C   1N   2O   0O   0G   300.000  5000.000                1
 0.48209077E 01 0.24790014E-02-0.94644109E-06 0.16548764E-09-0.10899129E-13 2
 0.68685948E 05-0.48484039E 00 0.35077779E 01 0.72023958E-02-0.75574589E-05 3
 0.42979217E-08-0.94257935E-12 0.68994281E 05 0.60234964E 01                4
CN2                 J12/70C   1N   2O   0O   0G   300.000  5000.000                1
 0.55626268E+01 0.20860606E-02-0.88123724E-06 0.16505783E-09-0.11366697E-13 2
 0.54897907E+05-0.55989355E+01 0.32524003E+01 0.70010737E-02-0.22653599E-05 3
-0.28939808E-08 0.18270077E-11 0.55609085E+05 0.66966778E+01                4
CO                  J 9/65C   1O   1O   0O   0G   300.000  5000.000                1
 0.29840696E 01 0.14891390E-02-0.57899684E-06 0.10364577E-09-0.69353550E-14 2
-0.14245228E 05 0.63479156E 01 0.37100928E 01-0.16190964E-02 0.36923594E-05 3
-0.20319674E-08 0.23953344E-12-0.14356310E 05 0.29555351E 01                4
COS                 J 3/61C   1O   1S   1O   0G   300.000  5000.000                1
 0.52392000E 01 0.24100584E-02-0.96064522E-06 0.17778347E-09-0.12235704E-13 2
-0.18480455E 05-0.30910517E 01 0.24625321E 01 0.11947992E-01-0.13794370E-04 3
 0.80707736E-08-0.18327653E-11-0.17803987E 05 0.10792556E 02                4
CO2                 J 9/65C   1O   2O   0O   0G   300.000  5000.000                1
 0.44608041E 01 0.30981719E-02-0.12392571E-05 0.22741325E-09-0.15525954E-13 2
-0.48961442E 05-0.98635982E 00 0.24007797E 01 0.87350957E-02-0.66070878E-05 3
 0.20021861E-08 0.63274039E-15-0.48377527E 05 0.96951457E 01                4
CO2-                J12/66C   1O   2E   1O   0G   300.000  5000.000                1
 0.45454640E 01 0.26054316E-02-0.10928732E-05 0.20454421E-09-0.14184542E-13 2
-0.54761968E 05 0.18317369E 01 0.24743737E 01 0.16913805E-02 0.73533603E-05 3
-0.99554255E-08 0.36846719E-11-0.54249049E 05 0.83834329E 01                4
CS                  J12/62C   1S   1O   0O   0G   300.000  5000.000                1
 0.36942533E 01 0.89086274E-03-0.36600044E-06 0.68778176E-10-0.47810000E-14 2
 0.26452213E 05 0.38176082E 01 0.33093030E 01 0.28164439E-04 0.44317874E-05 3
-0.55253895E-08 0.20392468E-11 0.26658986E 05 0.62942707E 01                4
CS2                 J 6/61C   1S   2O   0O   0G   300.000  5000.000                1
 0.59867719E 01 0.16394436E-02-0.68384845E-06 0.12836890E-09-0.89167448E-14 2
 0.12043850E 05-0.63998223E 01 0.32144238E 01 0.10443846E-01-0.11042989E-04 3
 0.52967662E-08-0.83022695E-12 0.12745874E 05 0.76185765E 01                4
C2                  J12/69C   2O   0O   0O   0G   300.000  5000.000                1
 0.40435359E 01 0.20573654E-03 0.10907575E-06-0.36427874E-10 0.34127865E-14 2
 0.99709486E 05 0.12775158E 01 0.74518140E 01-0.10144686E-01 0.85879735E-05 3
 0.87321100E-09-0.24429792E-11 0.98911989E 05-0.15846678E 02                4
C2-                 J12/69C   2E   1O   0O   0G   300.000  5000.000                1
 0.36926257E 01 0.41576040E-03 0.11654211E-07 0.23755880E-11-0.14585314E-14 2
 0.52118953E 05 0.22470173E 01 0.37342914E 01-0.22034649E-02 0.68417833E-05 3
-0.58120827E-08 0.16604296E-11 0.52281427E 05 0.27860423E 01                4
C2H                 J 3/67C   2H   1O   0O   0G   300.000  5000.000                1
 0.44207650E 01 0.22119303E-02-0.59294945E-06 0.94195775E-10-0.68527594E-14 2
 0.55835444E 05-0.11588093E 01 0.26499400E 01 0.84919515E-02-0.98165375E-05 3
 0.65373629E-08-0.17356273E-11 0.56275751E 05 0.76898609E 01                4
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C2H2                J 3/61C   2H   200  000  0G   300.000  5000.000                1
 0.45751083E 01 0.51238358E-02-0.17452354E-05 0.28673065E-09-0.17951426E-13    2
 0.25607428E 05-0.35737940E 01 0.14102768E 01 0.19057275E-01-0.24501390E-04    3
 0.16390872E-07-0.41345447E-11 0.26188208E 05 0.11393827E 02                   4
C2H4                J 9/65C   2H   400  000  0G   300.000  5000.000                1
 0.34552152E 01 0.11491803E-01-0.43651750E-05 0.76155095E-09-0.50123200E-13    2
 0.44773119E 04 0.26987959E 01 0.14256821E 01 0.11383140E-01 0.79890006E-05    3
-0.16253679E-07 0.67491256E-11 0.53370755E 04 0.14621819E 02                   4
C2H6                L 5/72C   2H   6    0    0G   300.000  1500.000                1
 0.21555281E+01 0.14779861E-01 0.23352804E-05-0.64146428E-08 0.19036925E-11    2
-0.11524517E+05 0.10776316E+02 0.21415788E+01 0.10529720E-01 0.18730274E-04    3
-0.26691187E-07 0.10049332E-10-0.11410486E+05 0.11647757E+02                   4
C2N                 J 3/67C   2N   100  000  0G   300.000  5000.000                1
 0.61931308E 01 0.14327539E-02-0.61255161E-06 0.11578707E-09-0.80401339E-14    2
 0.64818372E 05-0.84132298E 01 0.32670394E 01 0.98211307E-02-0.83284733E-05    3
 0.17650559E-08 0.59632768E-12 0.65589057E 05 0.65682304E 01                   4
C2N2                J 3/61C   2N   200  000  0G   300.000  5000.000                1
 0.65968935E 01 0.38694131E-02-0.15516161E-05 0.28141546E-09-0.19069442E-13    2
 0.34883726E 05-0.10001801E 02 0.39141782E 01 0.14011008E-01-0.17404350E-04    3
 0.12012779E-07-0.33565772E-11 0.35514550E 05 0.32384353E 01                   4
C2O                 J 9/66C   2O   100  000  0G   300.000  5000.000                1
 0.48990313E 01 0.28430384E-02-0.10209669E-05 0.16112165E-09-0.95542914E-14    2
 0.32800545E 05-0.91382280E 00 0.35364815E 01 0.69543872E-02-0.53071374E-05    3
 0.17030470E-08-0.14108072E-13 0.33151572E 05 0.60172370E 01                   4
C3                  J12/69C   3O   00   00   0G   300.000  5000.000                1
 0.36815361E 01 0.24165236E-02-0.84348112E-06 0.14508198E-09-0.95697300E-14    2
 0.97413955E 05 0.68377802E 01 0.57408464E 01-0.84281238E-02 0.18620198E-04    3
-0.14510529E-07 0.39676977E-11 0.97157524E 05-0.23837376E 01                   4
C3O2                J 6/68C   3O   2O   00   0G   300.000  5000.000                1
 0.81435964E 01 0.54395018E-02-0.22192869E-05 0.40778627E-09-0.27915974E-13    2
-0.14230013E 05-0.15456769E 02 0.37161005E 01 0.19872164E-01-0.20935751E-04    3
 0.11750112E-07-0.26589416E-11-0.13089402E 05 0.69298412E 01                   4
C4                  J12/69C   4O   00   00   0G   300.000  5000.000                1
 0.65602101E 01 0.40985234E-02-0.17000471E-05 0.31615228E-09-0.21842144E-13    2
 0.11430434E 06-0.11820311E 02 0.18432021E 01 0.19343592E-01-0.20627502E-04    3
 0.10822626E-07-0.21289203E-11 0.11550276E 06 0.12006898E 02                   4
C5                  J12/69C   5O   00   00   0G   300.000  5000.000                1
 0.82067016E 01 0.54889888E-02-0.22694876E-05 0.42073365E-09-0.28981924E-13    2
 0.11463647E 06-0.20246108E 02 0.11012446E 01 0.29513421E-01-0.33754342E-04    3
 0.19056534E-07-0.40989018E-11 0.11637970E 06 0.15360193E 02                   4
CS(S)               J 6/68CS  1O   00   00   0S   300.000   301.550                1
 0.              0.              0.              0.              0.            2
 0.              0.              0.31827762E 01-0.48706905E-02 0.18869579E-04    3
 0.89561402E-07-0.24031942E-09-0.96298877E 03-0.75956980E 01                   4
CS(L)               J 6/68CS  1O   00   00   0L   301.550  1500.000                1
 0.33149045E 01 0.82267349E-03-0.45641826E-06-0.95936037E-11 0.55471632E-13    2
-0.70109826E 03-0.78759204E 01 0.47696835E 01-0.49137505E-02 0.84861109E-05    3
-0.64184384E-08 0.18034315E-11-0.10158892E 04-0.14960727E 02                   4
CS                  J 6/68CS  1O   00   00   0G   300.000  5000.000                1
 0.18710101E 01 0.14068071E-02-0.10638222E-05 0.30583738E-09-0.19977219E-13    2
 0.86814554E 04 0.10235611E 02 0.24999466E 01 0.10382792E-05-0.38771191E-08    3
 0.49283910E-11-0.19810542E-14 0.84737829E 04 0.68627707E 01                   4
CS+                 J12/70CS  1E  -1O   00   0G   300.000  5000.000                1
 0.25038682E+01-0.75238859E-05 0.47346482E-08-0.11801810E-11 0.10117554E-15    2
 0.54405152E+05 0.61482962E+01 0.25050509E+01-0.35642646E-04 0.88202967E-07    3
-0.91546770E-10 0.33935528E-13 0.54406031E+05 0.61481749E+01                   4
CSO                 J12/68CS  1O   1O   00   0G   300.000  5000.000                1
 0.44660282E 01 0.11563232E-03-0.59989187E-08 0.13176699E-12 0.57639745E-16    2
 0.61950309E 04 0.52013854E 01 0.39857419E 01 0.21279251E-02-0.32170255E-05    3
 0.22764295E-08-0.59721976E-12 0.62898940E 04 0.75028593E 01                   4
CSOH(S)             J 6/71CS  1O   1H   1O   0S   300.000   493.000                1
 0.              0.              0.              0.              0.            2
 0.              0.              0.22668003E+02-0.79510644E-01-0.98326877E-05    3
 0.59683261E-06-0.72318251E-09-0.54096409E+05-0.96902538E+02                   4
CSOH(S)             J 6/71CS  1O   1H   1O   0S   493.000   588.000                1
 0.              0.              0.              0.              0.            2
 0.              0.              0.94903885E+01 0.20378267E-02-0.37207076E-05    3
-0.24725999E-09 0.59676361E-11-0.52297614E+05-0.41264492E+02                   4
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CSOH(L)             J 6/71CS  10   1H   10   0L   588.000  5000.000                1
 0.98129747E+01 0.              0.              0.              0.                  2
-0.51757654E+05-0.41664444E+02 0.98129747E+01 0.              0.                  3
 0.             0.             -0.51757654E+05-0.41664444E+02                      4
CSOH                J 6/71CS  10   1H   10   0G   300.000  5000.000                1
 0.57005649E+01 0.11820384E-02-0.31939094E-06 0.38642917E-10-0.16635636E-14        2
-0.32919205E+05-0.21318639E+01 0.45486003E+01 0.79612333E-02-0.13326497E-04        3
 0.10314234E-07-0.28973777E-11-0.32810890E+05 0.28487160E+01                       4
CSOH+               J12/71CS  10   1H   1E  -1G   300.000  5000.000                1
 0.57292563E+01 0.11571324E-02-0.31044431E-06 0.37096291E-10-0.15509463E-14        2
 0.51626483E+05-0.58964043E+00 0.48487158E+01 0.68908346E-02-0.11839328E-04        3
 0.94335372E-08-0.27222685E-11 0.51678167E+05 0.30716903E+01                       4
CS2                 J 6/68CS  20   00   00   0G   300.000  5000.000                1
 0.46411470E 01 0.10844908E-03 0.10701307E-08 0.55978765E-10-0.77877416E-14        2
 0.11367604E 05 0.76209601E 01 0.45116580E 01 0.17392705E-03 0.36388656E-06        3
-0.41459947E-09 0.16398515E-12 0.11426704E 05 0.83824693E 01                       4
CS2O                J12/68CS  20   10   00   0G   300.000  5000.000                1
 0.68979467E 01 0.10165098E-03-0.38062062E-07 0.61466393E-11-0.35758216E-15        2
-0.13169989E 05-0.11790802E 01 0.57553639E 01 0.49116073E-02-0.77072518E-05        3
 0.54156957E-08-0.14080898E-11-0.12946829E 05 0.42869913E 01                       4
CS2O2H2             J 6/71CS  20   2H   20   0G   300.000  5000.000                1
 0.95809362E+01 0.53260509E-02-0.18780545E-05 0.30925925E-09-0.19429533E-13        2
-0.86025839E+05-0.13227758E+02 0.75228191E+01 0.79078372E-02 0.35430299E-05        3
-0.10456328E-07 0.43014032E-11-0.85338412E+05-0.19197968E+01                       4
E                   L02/67E   10   00   00   0G   300.000  5000.000                1
 0.25000000E 01 0.              0.              0.              0.                  2
-0.74537496E 03-0.11734026E 02 0.25000000E 01 0.              0.                  3
 0.             0.             -0.74537500E 03-0.11734026E 02                      4
H                   J 9/65H   100  000  000  0G   300.000  5000.000                1
 0.25000000E 01 0.              0.              0.              0.                  2
 0.25471627E 05-0.46011763E 00 0.25000000E 01 0.              0.                  3
 0.             0.              0.25471627E 05-0.46011762E 00                      4
H+                  J 6/66H   1E  -100  000  0G   300.000  5000.000                1
 0.25000000E 01 0.              0.              0.              0.                  2
 0.18403344E 06-0.11538620E 01 0.25000000E 01 0.              0.                  3
 0.             0.              0.18403344E 06-0.11538621E 01                      4
H-                  J 9/65H   1E   100  000  0G   300.000  5000.000                1
 0.25000000E 01 0.              0.              0.              0.                  2
 0.15961045E 05-0.11524488E 01 0.25000000E 01 0.              0.                  3
 0.             0.              0.15961045E 05-0.11524486E 01                      4
HCN                 L12/69H   1C   1N   10   0G   300.000  5000.000                1
 0.37068121E 01 0.33382803E-02-0.11913320E-05 0.19992917E-09-0.12826452E-13        2
 0.14962636E 05 0.20794904E 01 0.24513556E 01 0.87208371E-02-0.10094203E-04        3
 0.67255698E-08-0.17626959E-11 0.15213002E 05 0.80830085E 01                       4
HCO                 J12/70H   1C   10   10   0G   300.000  5000.000                1
 0.34738348E+01 0.34370227E-02-0.13632664E-05 0.24928645E-09-0.17044331E-13        2
 0.39594005E+04 0.60453340E+01 0.38840192E+01-0.82974448E-03 0.77900609E-05        3
-0.70616962E-08 0.19971730E-11 0.40563860E+04 0.48354133E+01                       4
HCO+                J12/70H   1C   10   1E  -1G   300.000  5000.000                1
 0.37411880E+01 0.33441517E-02-0.12397121E-05 0.21189388E-09-0.13704150E-13        2
 0.98884078E+05 0.20654768E+01 0.24739736E+01 0.86715590E-02-0.10031500E-04        3
 0.67170527E-08-0.17872674E-11 0.99146608E+05 0.81625751E+01                       4
HNCO                J12/70H   1N   1C   10   1G   300.000  5000.000                1
 0.51300390E+01 0.43551371E-02-0.16269022E-05 0.28035605E-09-0.18276037E-13        2
-0.14101787E+05-0.22010995E+01 0.23722164E+01 0.13664040E-01-0.13323158E-04        3
 0.64475457E-08-0.10402894E-11-0.13437059E+05 0.11588263E+02                       4
HNO                 J 3/63H   1N   10   10   0G   300.000  5000.000                1
 0.35548619E 01 0.32713182E-02-0.12734071E-05 0.22602046E-09-0.15064827E-13        2
 0.10693734E 05 0.51684901E 01 0.37412008E 01-0.20067061E-03 0.75409300E-05        3
-0.79105713E-08 0.25928389E-11 0.10817845E 05 0.50063473E 01                       4
HNO2                J 6/63H   1N   10   2    0G   300.000  5000.000                1
 0.55144941E+01 0.41394403E-02-0.15878702E-05 0.27977639E-09-0.18584209E-13        2
-0.11276885E+05-0.31425253E+01 0.25098874E+01 0.12171605E-01-0.78618375E-05        3
 0.35351571E-09 0.11540858E-11-0.10450008E+05 0.12399634E+02                       4
HNO3                J 6/63H   1N   10   3    0G   300.000  5000.000                1
 0.70591100E+01 0.56769446E-02-0.22348863E-05 0.40155529E-09-0.27080510E-13        2
-0.18920009E+05-0.10778285E+02 0.14377135E+01 0.20903552E-01-0.14574553E-04        3
 0.11972023E-08 0.19117285E-11-0.17385368E+05 0.18246253E+02                       4
```

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HO2                 J 3/64H   1O   2OO  OOO  OG   300.000  5000.000                1
 0.37866280E 01 0.27885404E-02-0.10168708E-05 0.17183946E-09-0.11021852E-13     2
 0.11888500E 04 0.48147611E 01 0.35094850E 01 0.11499670E-02 0.58784259E-05     3
-0.77795519E-08 0.29607883E-11 0.13803331E 04 0.68276325E 01                    4
H2                  J 3/61H   2O   OO   OO   OG   300.000  5000.000                1
 0.31003901E 01 0.51119464E-03 0.52644210E-07-0.34909973E-10 0.36945345E-14     2
-0.87738042E 03-0.19629421E 01 0.30574451E 01 0.26765200E-02-0.58099162E-05     3
 0.55210391E-08-0.18122739E-11-0.98890474E 03-0.22997056E 01                    4
H2O(S)              L11/65H   2O   1OO  OOO  OS   200.000   273.150                1
 0.              0.              0.              0.              0.             2
 0.              0.             -0.39269330E-01 0.16920420E-01 0.              3
 0.              0.             -0.35949581E 05 0.56933784E 00                  4
H2O(L)              L11/65H   2O   1OO  OOO  OL   273.150   1000.0                1
 0.              0.              0.              0.              0.             2
 0.              0.              0.12712782E 02-0.17662790E-01-0.22556661E-04   3
 0.20820908E-06-0.24078614E-09-0.37483200E 05-0.59115305E 02                    4
H2O                 J 3/61H   2O   1OO  OOO  OG   300.000  5000.000                1
 0.27167633E 01 0.29451374E-02-0.80224374E-06 0.10226682E-09-0.48472145E-14     2
-0.29905826E 05 0.66305671E 01 0.40701275E 01-0.11084499E-02 0.41521180E-05     3
-0.29637404E-08 0.80702103E-12-0.30279722E 05-0.32270046E 00                    4
H2O2                L 2/69H   2O   2O   OO   OG   300.000  5000.000                1
 0.45731667E 01 0.43361363E-02-0.14746888E-05 0.23489037E-09-0.14316536E-13     2
-0.18006961E 05 0.50113696E 00 0.33887536E 01 0.65692260E-02-0.14850126E-06     3
-0.46258055E-08 0.24715147E-11-0.17663147E 05 0.67853631E 01                    4
H2S                 J12/65H   2S   1OO  OOO  OG   300.000  5000.000                1
 0.28479103E 01 0.38415990E-02-0.14099367E-05 0.24278754E-09-0.15783283E-13     2
-0.34469788E 04 0.74781412E 01 0.38811293E 01-0.13211856E-03 0.36517726E-05     3
-0.21820445E-08 0.28783779E-12-0.36350917E 04 0.25161511E 01                    4
HE                  L 5/66HE  1OO  OOO  OOO  OG   300.000  5000.000                1
 0.25000000E 01 0.              0.              0.              0.              2
-0.74537498E 03 0.91534888E 00 0.25000000E 01 0.              0.              3
 0.              0.             -0.74537498E 03 0.91534884E 00                  4
HE+                 L12/66HE  1E  -1OO  OOO  OG   300.000  5000.000                1
 0.25000000E 01 0.              0.              0.              0.              2
 0.28534266E 06 0.16084045E 01 0.25000000E 01 0.              0.              3
 0.              0.             0.28534266E 06 0.16084046E 01                   4
N                   J 3/61N   1OO  OOO  OOO  OG   300.000  5000.000                1
 0.24502682E+01 0.10661458E-03-0.74653373E-07 0.18796524E-10-0.10259839E-14     2
 0.56116040E 05 0.44487581E 01 0.25030714E 01-0.21800181E-04 0.54205287E-07     3
-0.56475602E-10 0.20999044E-13 0.56098904E 05 0.41675664E 01                    4
NH                  J12/71N   1H   1    0    OG   300.000  5000.000                1
 0.27789900E+01 0.13266349E-02-0.41101218E-06 0.69414505E-10-0.44536190E-14     2
 0.44567973E+05 0.57593434E+01 0.34938318E+01 0.24529034E-03-0.12578521E-05     3
 0.22011922E-08-0.92288834E-12 0.44326826E+05 0.18451723E+01                    4
NH2                 J12/65N   1H   2OO  OOO  OG   300.000  5000.000                1
 0.25769524E 01 0.35896090E-02-0.12276328E-05 0.19549576E-09-0.11873401E-13     2
 0.19335912E 05 0.79074890E 01 0.40385791E 01-0.10098163E-02 0.40120903E-05     3
-0.23085312E-08 0.39022887E-12 0.18973010E 05 0.52464285E 00                    4
NH3                 J 9/65N   1H   3OO  OOO  OG   300.000  5000.000                1
 0.24165177E 01 0.61871211E-02-0.21785136E-05 0.37599090E-09-0.24448856E-13     2
-0.64747177E 04 0.77043482E 01 0.35912768E 01 0.49388668E-03 0.83449322E-05     3
-0.83833385E-08 0.27299092E-11-0.66717143E 04 0.22520966E 01                    4
NO                  J 6/63N   1O   1OO  OOO  OG   300.000  5000.000                1
 0.31890000E 01 0.13382281E-02-0.52899318E-06 0.95919332E-10-0.64847932E-14     2
 0.98283290E 04 0.67458126E 01 0.40459521E 01-0.34181783E-02 0.79819190E-05     3
-0.61139316E-08 0.15919076E-11 0.97453934E 04 0.29974988E 01                    4
NO+                 J 6/66N   1O   1E  -1OO  OG   300.000  5000.000                1
 0.28885488E 01 0.15217119E-02-0.57531241E-06 0.10051081E-09-0.66044294E-14     2
 0.11819245E 06 0.70027197E 01 0.36685056E 01-0.11544580E-02 0.21755608E-05     3
-0.48227472E-09-0.27847906E-12 0.11803369E 06 0.31779324E 01                    4
NO2                 J 9/64N   1O   2OO  OOO  OG   300.000  5000.000                1
 0.46240771E 01 0.25260332E-02-0.10609498E-05 0.19879239E-09-0.13799384E-13     2
 0.22899900E 04 0.13324138E 01 0.34589236E 01 0.20647064E-02 0.66866067E-05     3
-0.95556725E-08 0.36195881E-11 0.28152265E 04 0.83116983E 01                    4
NO2-                J 6/72N   1O   2E   1    OG   300.000  5000.000                1
 0.50160903E+01 0.21884463E-02-0.94586144E-06 0.17939789E-09-0.12052428E-13     2
-0.26200160E+05-0.12861447E+01 0.24818036E+01 0.49398681E-02 0.28557293E-05     3
-0.78905297E-08 0.35391483E-11-0.25501540E+05 0.99161680E+01                    4
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NO3                 J12/64N   10   3    0    0G   300.000  5000.000                1
 0.72033289E+01 0.30908791E-02-0.13329045E-05 0.25461601E-09-0.17939047E-13        2
 0.58244016E+04-0.12608119E+02 0.76867377E+00 0.21281075E-01-0.16980256E-04        3
 0.22963836E-08 0.19321041E-11 0.75292921E+04 0.20406284E+02                       4
N2O                 J12/64N   20   100  000  0G   300.000  5000.000                1
 0.47306679E 01 0.28258267E-02-0.11558115E-05 0.21263683E-09-0.14564087E-13        2
 0.81617682E 04-0.17151073E 01 0.26189196E 01 0.86439616E-02-0.68110624E-05        3
 0.22275877E-08-0.80650330E-13 0.87590123E 04 0.92266952E 01                       4
N2H4                J12/65N   2H   400  000  0G   300.000  5000.000                1
 0.50947770E 01 0.93296138E-02-0.33626986E-05 0.56308304E-09-0.35859661E-13        2
 0.92996644E 04-0.35950952E 01 0.79803836E 00 0.21788097E-01-0.13456754E-04        3
-0.12698753E-09 0.25865213E-11 0.10379887E 05 0.18248696E 02                       4
N2                  J 9/65N   20   00   00   0G   300.000  5000.000                1
 0.28963194E 01 0.15154866E-02-0.57235277E-06 0.99807393E-10-0.65223555E-14        2
-0.90586184E 03 0.61615148E 01 0.36748261E 01-0.12081500E-02 0.23240102E-05        3
-0.63217559E-09-0.22577253E-12-0.10611588E 04 0.23580424E 01                       4
N2O+                J12/70N   20   1E  -10   0G   300.000  5000.000                1
 0.53926946E+01 0.22337196E-02-0.93548832E-06 0.17466166E-09-0.12059043E-13        2
 0.15847633E+06-0.36920186E+01 0.34273064E+01 0.63787690E-02-0.22585149E-05        3
-0.20421800E-08 0.13481477E-11 0.15909237E+06 0.67997616E+01                       4
N2O4                J 9/64N   20   400  000  0G   300.000  5000.000                1
 0.10506637E 02 0.58723267E-02-0.24766296E-05 0.46556024E-09-0.32402082E-13        2
-0.28609096E 04-0.26252230E 02 0.36662865E 01 0.23491748E-01-0.16007297E-04        3
 0.11845939E-08 0.20001618E-11-0.90631797E 03 0.93973337E 01                       4
N3                  J12/70N   30   00   00   0G   300.000  5000.000                1
 0.51996828E+01 0.24335678E-02-0.10192340E-05 0.19062350E-09-0.13212412E-13        2
 0.47963131E+05-0.35547759E+01 0.30624389E+01 0.73590658E-02-0.38229374E-05        3
-0.71824202E-09 0.91110236E-12 0.48614547E+05 0.77570129E+01                       4
O                   J 6/62O   100  000  000  0G   300.000  5000.000                1
 0.25420596E 01-0.27550619E-04-0.31028033E-08 0.45510674E-11-0.43680515E-15        2
 0.29230803E 05 0.49203080E 01 0.29464287E 01-0.16381665E-02 0.24210316E-05        3
-0.16028432E-08 0.38906964E-12 0.29147644E 05 0.29639949E 01                       4
O+                  L12/66O   1E  -100  000  0G   300.000  5000.000                1
 0.25060486E 01-0.14464249E-04 0.12446049E-07-0.46858472E-11 0.65548873E-15        2
 0.18794700E 06 0.43479741E 01 0.24984794E 01 0.11410972E-04-0.29761395E-07        3
 0.32246539E-10-0.12375517E-13 0.18794908E 06 0.43864355E 01                       4
O-                  J 6/65O   1E   100  000  0G   300.000  5000.000                1
 0.25437173E 01-0.53258700E-04 0.25119617E-07-0.51851466E-11 0.39011542E-15        2
 0.11480516E 05 0.45202538E 01 0.28115796E 01-0.11905697E-02 0.18710553E-05        3
-0.13479178E-08 0.36663554E-12 0.11428431E 05 0.32402859E 01                       4
OH                  J12/70O   1H   10   00   0G   300.000  5000.000                1
 0.29131230E+01 0.95418248E-03-0.19084325E-06 0.12730795E-10 0.24803941E-15        2
 0.39647060E+04 0.54288735E+01 0.38365518E+01-0.10702014E-02 0.94849757E-06        3
 0.20843575E-09-0.23384265E-12 0.36715807E+04 0.49805456E+00                       4
OH+                 J12/70O   1H   1E  -10   0G   300.000  5000.000                1
 0.27381495E+01 0.14613173E-02-0.46950536E-06 0.73663560E-10-0.41410922E-14        2
 0.15761683E+06 0.61343811E+01 0.35365969E+01-0.47029254E-04-0.62344259E-06        3
 0.17601461E-08-0.82678699E-12 0.15736677E+06 0.18477172E+01                       4
OH-                 J12/70O   1H   1E   10   0G   300.000  5000.000                1
 0.28881148E+01 0.96560229E-03-0.19659254E-06 0.14053802E-10 0.12080617E-15        2
-0.18086455E+05 0.41896259E+01 0.34621427E+01 0.40525802E-03-0.13516992E-05        3
 0.17899459E-08-0.63434810E-12-0.18312355E+05 0.92893220E+00                       4
O2                  J 9/65O   20   00   00   0G   300.000  5000.000                1
 0.36219535E 01 0.73618264E-03-0.19652228E-06 0.36201558E-10-0.28945627E-14        2
-0.12019825E 04 0.36150960E 01 0.36255985E 01-0.18782184E-02 0.70554544E-05        3
-0.67635137E-08 0.21555993E-11-0.10475226E 04 0.43052778E 01                       4
O2-                 J12/66O   2E   100  000  0G   300.000  5000.000                1
 0.38147234E 01 0.77444546E-03-0.30677649E-06 0.56618118E-10-0.36229492E-14        2
-0.69910087E 04 0.29587995E 01 0.31440525E 01 0.12127972E-02 0.23812161E-05        3
-0.40914092E-08 0.16885304E-11-0.67369752E 04 0.67688687E 01                       4
O3                  J 6/61O   30   00   00   0G   300.000  5000.000                1
 0.54665239E+01 0.17326031E-02-0.72204889E-06 0.13721660E-09-0.96233828E-14        2
 0.15214096E+05-0.34712616E+01 0.24660617E+01 0.91703209E-02-0.49698480E-05        3
-0.20634230E-08 0.20015595E-11 0.16059556E+05 0.12172130E+02                       4
S(S)                J12/65S   10   00   00   0S   300.000   388.360                1
 0.              0.              0.              0.              0.                2
 0.              0.             -0.50637025E 01 0.28819353E-02-0.21330205E-04     3
 0.84787862E-06-0.17344967E-08 0.71482629E 03 0.28714074E 02                       4
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S(L)                J12/65S   10   00   00   0L   388.360  2000.000                1
 0.36036672E 01 0.99033405E-03-0.10114410E-05 0.40536327E-09-0.56679135E-13    2
-0.84538383E 03-0.16344708E 02-0.12706310E 02 0.90725216E-01-0.16951786E-03    3
 0.13070637E-06-0.35276150E-10 0.12346069E 04 0.56210160E 02                   4
S                   J 6/71S   10   00   00   0G   300.000  5000.000                1
 0.29093331E+01-0.55587281E-03 0.27836947E-06-0.50194768E-10 0.31254639E-14    2
 0.32531543E+05 0.37928327E+01 0.29270078E+01 0.21982555E-03-0.23808853E-05    3
 0.29034821E-08-0.10846692E-11 0.32491577E+05 0.35120600E+01                   4
S+                  L12/66S   1E  -100  000  0G   300.000  5000.000                1
 0.24118653E 01 0.22103303E-03-0.18939564E-06 0.61886675E-10-0.53887720E-14    2
 0.15375732E 06 0.58861130E 01 0.25088214E 01-0.62478561E-04 0.15513305E-06    3
-0.16148749E-09 0.60012108E-13 0.15373003E 06 0.53857186E 01                   4
SH                  J 6/67S   1H   100  000  0G   300.000  5000.000                1
 0.30371382E 01 0.12752466E-02-0.42314345E-06 0.67719668E-10-0.40934312E-14    2
 0.16545437E 05 0.60722981E 01 0.44098953E 01-0.22063747E-02 0.13171081E-05    3
 0.16467179E-08-0.12144787E-11 0.16180734E 05-0.10226129E 01                   4
SN                  J 6/61S   1N   100  000  0G   300.000  5000.000                1
 0.38493976E 01 0.72756788E-03-0.29370203E-06 0.55013628E-10-0.38123551E-14    2
 0.30459962E 05 0.44179139E 01 0.39422971E 01-0.20035515E-02 0.73534644E-05    3
-0.75168560E-08 0.25591098E-11 0.30563949E 05 0.45669484E 01                   4
SO                  J 6/71S   10   10   00   0G   300.000  5000.000                1
 0.40039062E+01 0.29471359E-03 0.63481159E-07-0.28687405E-10 0.25022781E-14    2
-0.72238721E+03 0.35413673E+01 0.31258711E+01 0.13512854E-02 0.21503879E-05    3
-0.39964434E-08 0.17048142E-11-0.41679715E+03 0.84036007E+01                   4
SO2                 J 6/61S   10   200  000  0G   300.000  5000.000                1
 0.52451364E 01 0.19704204E-02-0.80375769E-06 0.15149969E-09-0.10558004E-13    2
-0.37558227E 05-0.10873524E 01 0.32665338E 01 0.53237902E-02 0.68437552E-06    3
-0.52810047E-08 0.25590454E-11-0.36908148E 05 0.96513476E 01                   4
SO3                 J 9/65S   10   300  000  0G   300.000  5000.000                1
 0.70757376E 01 0.31763387E-02-0.13535760E-05 0.25630912E-09-0.17936044E-13    2
-0.50211376E 05-0.11200793E 02 0.25780385E 01 0.14556335E-01-0.91764173E-05    3
-0.79203022E-09 0.19709473E-11-0.48931753E 05 0.12251863E 02                   4
S2                  J12/65S   200  000  000  0G   300.000  5000.000                1
 0.42051134E 01 0.35309150E-03-0.13543069E-06 0.25245375E-10-0.17357488E-14    2
 0.14182908E 05 0.32094717E 01 0.28724248E 01 0.50434461E-02-0.62055277E-05    3
 0.33097022E-08-0.57376109E-12 0.14487076E 05 0.98082405E 01                   4
END
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