COLLISIONAL RADIATIVE MODELS FOR HYDROGEN ATOMS AND FOR HYDROGEN MOLECULES IN A TOKAMAK PLASMA

BY

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Abstract

A collisional radiative model is applied to study the ionization, recombination, and energy loss rates of an optically thin hydrogen plasma in a Tokamak thermonuclear fusion reactor. The effective ionization and recombination coefficients are found to be increasing functions of electron density, the increase being bigger when the temprature is low. The rate of radiative energy loss is significant only in low density plasmas; and the estimate that has been used by most plasma modelers is pretty big that it cannot be applied for dense plasmas.

Edge plasma cooling due to the interaction of recycling neutral particles near diverter targets with the scrape off layer is an important effect to reduce the heat load on Tokamak vessel components. The relevant atomic data for hydrogenic atoms are well established, whereas the data base for molecules is less complete. Collisional radiative processes are considered to study the effects of hydrogen molecules in the edge plasma boundary. Effective dissociation and dissociative ionization rate coefficients are calculated. Rate coefficients for the production of neutral atoms from hydrogen molecules are also evaluated. Finally the rate of electron energy loss per dissociation of molecules into atoms and/or ions is calculated. The rate of this energy loss is significant and the dissociation of the molecules may account for the missing heating power in the divertor region.

Contents

Introduction

Nearly 90 per cent of the world's energy needs come from fossil fuels. Long-term reliance on this energy source, however, is acknowledged to be a dangerous strategy despite the large reserves of coal available in the world. The use of fossil fuel exacerbates pollution and acid rain and heightens the risk of global warming by adding CO_2 to the atmosphere. Society will be served best if energy production uses environmentally attractive methods that do not involve the combustion of fuels.

The present revival of plasma physics is primarily due to experimental attempts to produce thermonuclear fusion reactions. The elementary process that results in the release of thermonuclear energy on a macroscopic scale is the fusion, up on their collision, of two light nuclei into a heavier nucleus. Such two reactions that have sufficient cross sections to be of interest are:

(1). $2_H + 3_H \rightarrow 4_{He} + n + 17.6\ Mev$

(2). $2_H + 2_H \rightarrow 3_{He} + n + 3.2\ Mev$

Such light nuclei fuse together if they have sufficient energy to overcome the coulomb repulsion between them. Of all the methods that can be used to produce such energetic nuclei, the use of fully ionized high temprature plasma holds the best promise. A vacuum Tokamak vessel is prepared and deutrium and tritium atoms are filled in. Electric current is then applied to raise the temprature and energy of the atoms. As the temprature is raised these atoms start to be ionized and plasma is produced. Since ohmic heating of the plasma particles is not sufficient to produce nuclei of the required energy, it is supplemented by injection of neutral energetic particles. Therefore it is necessary to know the rates of ionization of the atoms and recombination of the ions in a wide range of

temprature.

Briefly the following are the fundamental demands in the design of the thermonuclear fusion reactor:

1 Ionized plasma formed by deutrium/tritium nuclei and electrons.

2 A device which permits the plasma to be heated above the ignition temprature (10^7 to 10^9 kelvins)

3 The particle density must be relatively small; otherwise the kinetic pressure p = nKT would exceed the magnetic pressure that confines the plasma.

4 High purity of the plasma. As the energy loss due to braking of radiation of plasma increases with the square of the charge of elements that have a higher atomic number, every thermonuclear reactor needs an ultrahigh - vacuum pump which permits the thorough evacuation of the working space before it is filled with deutrium or tritium.

5 The magnetic vessel. No material used for the vessel containing the plasma can stand the enormous tempratures that are required for controlled nuclear fussion. The plasma must therefore be insulated from the vessel in order to prevent it from being contaminated by materials evaporating from the walls. An approach suitable under terrestial conditions in the insulation by means of a magnetic field in the vacuum.

6 Using the magentohydrodynamic principle for converting the energy released in the thermonuclear reaction in to electric power. Heated by the thermonuclear energy released in the reaction, the plasma expands and cuts across the force lines of the magnetic field confining it.

While energy is being supplied to increase the energy of the plasma particles, some part of the input energy is lost mainly due to radiation. This is

because an atom initially in the ground state may be excited to higher levels followed by radiative decay before it is ionized by electronic collision. Therefore the thermonuclear reactor requires a device which permits the plasma to be heated above a temprature at which thermonuclear energy is released at a rate at least capable of balancing the losses. On reaching this temprature the heating device is disconnected and the reaction will continue spontaneously. It is important to know the rate of energy loss in order to supply a suitable amount of energy and reach this required temprature.

The importance of understanding the effects of electronic collisions with molecular hydrogen in plasmas has been pointed out, e.g. by Janev et al./1/ and Harrison /2/. Hydrogenic ions escaping from a magnetically confined plasma are neutralized at the wall and some of these particles are scattered back into the confined plasma. The remaining particles which are not scattered back are, unless pumped, re-emitted as thermal hydrogen molecules.

These molecules are primarily subjected to electronic collisions. These inelastic collisions may lead to different states of the post collision particles. For example, a molecule may be excited to higher quantum energy levels and then radiatively decay to lower levels emitting a photon with energy equal to the energy difference of the two levels. In this case, because the plasma is transparent to most of the emitted radiation, the molecules act as energy sink for the electrons in the plasma. If a molecule is excited to the continuum of the excited states, it gets dissociated into two hydrogen atoms. These may be in the ground or excited atomic states. The energy of the incident electron is again reduced when separating the two atoms apart and some fraction of the energy is taken as kinetic energy by the atoms. Furthermore, electronic collision with molecular hydrogen may lead to the formation of molecular ion followed by dissociation into hydrogen atoms and/or ions. This chain of reactions will reduce the energy of the electrons. Ions produced by this process also reduce the temperature of the plasma by equilibriating via coulomb collisions with background plasma ions.

The density and the temperature of electrons in the edge plasma boundary are often high enough to activate the above processes in the near target surface region, and therefore the molecules do not usually penetrate deep into the plasma. For typical electron densities of 10^{12} — 10^{14} cm^3 ,we can limit ourselves to the temperature range between 1 eV and 100 eV. One of our goals is to collect the rates of all relevant channels and to construct a collisional radiative model for the break-up of hydrogen molecules in the edge plasma.

The steps of preparation of this paper are as follows. First the basic principles and fundamental demands of thermonuclear fusion reactor are explained. The fuel of the reactor is in the plasma state. Therefore two basic plasma models called Local Thermal Equilibrium (LTE) and corona models that can be used to study some properties of plasmas under specific conditions are roughly reviewed in the first chapter. The second chapter is devoted to the formulation, calculation and interpretation of effective ionization, recombination and energy loss rates of hydrogen plasma in a wide range of temperatures and densities. A collisional radiative model for studying the effects of the dissociation of molecular hydrogen is developed in chapter 3 and the results are discussed. Finally the important results are summarized and the fortran computer programmes that are used to calculate and plot all the results of this work are given in appendices A and B.

$$\frac{n_E(p)}{n_E(q)} = \frac{p^2}{q^2} \exp\left(\frac{\Delta E}{KT}\right), \qquad (1.2)$$

ΔE being the energy gap between the two levels p and q.

And the Saha equation is written as:

$$n_E(p) = p^2 \left(\frac{h^2}{2\pi mKT}\right)^{\frac{3}{2}} \exp\left\{\frac{\chi(p)}{KT}\right\} n_i n_e, \qquad (1.3)$$

where $n_\varepsilon(p)$ is the population density of the various levels designated by this quantum number p, $\chi(p)$. is the ionization potential energy of level p, and n_e and n_i are electron and ion densities. Equations 1.1, 1.2, and 1.3 describe the state of an electron in LTE model plasma.

Consider a hydrogen atom in an excited quantum level p. It may radiatively decay into a lower level q with some transition probability A(p,q). It may also be de-excited to a lower level q due to electronic collision the rate of which is given by

Collisional transition rate = ne n(p) C(p,q) (1.4)

transition/unit volume/unit time where C(p,q) is defined as the de-excitation rate coefficient from p to q time.

It has been pointed out by Wilson (3) and Griem (4) that one reason why the LTE model should not apply to a plasma is that at a sufficiently low density the probability of a radiative transition becomes comparable with or even exceeds the probability of the corresponding collisional transition. Since in an optically thin plasma the emission of a photon is a process that is not balanced by its inverse, the population distribution among the levels departs from that predicted by the Boltzmann and Saha equations.

For radiative decay rates to cause less than ten per cent departures from LTE, for instance, the collisional rates must be at least about ten times the radiative rates. Thus, for all levels p and q:

$$n_e\, n(p)\, c(p,q) \geq 10\, n(p)\, A(p,q) \qquad (1.5)$$

Consideration of the collisional de-excitation and spontaneous radiative decay probabilities shows that this criterion is not satisfied for a wide range of plasma parameters, and it particularly fails in low density plasma.

1.2 Steady-state corona model

In order to explain some features of the spectrum of the solar corona an atomic model was proposed (5) which is found useful in studying low-density laboratory plasmas.

Unlike in the LTE model in which each collision process is balanced by its inverse collision process, in the corona model the balance is between collisional ionization (and excitation) and radiative recombination (and spontaneous decay). Again the plasma is assumed to be optically thin.

In the LTE model when the plasma density was lowered radiative processes begin to compete with collisions that influence population densities. Suppose the plasma density is further lowered until only the strongest collision processes are left with any influence. Consider the processes of collisional ionization and three-body recombination which, because they are inverse processes, must take place at equal rates in LTE. For an atom n(p) in state p :

$$e + n(p) \rightleftarrows n_i + e + e$$

Thus the ionization rate is proportional to n_e and the recombination rate to this level to $(n_e)^2$. Positive ions may also recombine with electrons by a radiative process,

$$e + n_i \rightarrow n(p) + h\nu$$

where $h\nu$ represents the radiated photon.

The rate of this process is proportional to n_e so that it is more important at a sufficiently low density than three-body recombination. Thus, the ionization equilibrium is a balance between radiative recombination and ionization by electron collision. This clearly refers to plasma of much lower density than in the LTE model. Unlike the LTE model, the quantitative interpretation of the corona model depends on cross sectional atomic data.

Assuming a change in the plasma parameters that takes place sufficiently slowly so that the population densities take up their new steady state values at each instant, the equations which describe the steady state corona may be written with the following considerations:

(a) It is assumed that the electrons of the plasma have a Maxwellian velocity distribution in which case equation (1.1) applies to the free electrons. It is not necessary to make any specific assumption about the velocity distribution of the heavy particles, except that their mean energy should be of the same order or less than that of the electrons so that other possible collisions excluding those involving electrons are not important.

(b) Compared with the ground level only negligible numbers of ions are assumed to result from excited levels. Thus the ionization and recombination balance equation may be given as :

At the limiting value of n_e there are as many collisional transitions out of level p as radiative decays which causes a 50 per cent deviation of the line intensity predictions of the corona model. Because with an increasing quantum level the probability of spontaneous decay decreases whereas that of collisional excitation increases. There is always some value of p for which the criterion is not satisfied no matter how low the density may be.

CHAPTER II

Collisional Radiative Model for Hydrogen Atoms

A collisional radiative model was introduced by Bates et al (6) in order to overcome some of the restrictions imposed on the corona model by the possibility of stepwise collision processes. The essential difference between the collisional radiative model and the corona model is that the collisional radiative model takes electron collision processes involving excited levels into account.

2.1 Formulation of the collisional radiative model

The collisional radiative model is based on the following assumptions:

(1) The free electrons have a Maxwellian velocity distribution given by equation 1.1.

(2) Ionization occurs from any bound level due to electron collision and is partially balanced by three-body recombination into any level. This is represented by:

$H(p) + e \rightleftarrows H^+ + e + e$

where H(p) represents hydrogen atom in quantum level p,
H^+ is a corresponding ion, and
e is an electron. Reaction rate coefficients S(p) and $\alpha(p)$ for the ionization and three-body recombination processes respectively are defined to give:

(a) Ionization, $S(p)\, n_e\, n(p)\ cm^{-3}s^{-1}$

(b) Three-body recombination, $\alpha(p) ne^2 n_i\ cm^{-3}s^{-1}$,

where n(p) is the number density of atoms in quantum state p and n_i is the number density of ions;

(3) Transition between any pair of bound levels is induced by electron collision. This process is represented by $H(p) + e \rightleftarrows H(q) + e$, where the rate of each process, excitation or de-excitation according to whether q > p or q < p respectively, is given by $C(p,q)n_e n(p)$ transitions / cm^3 / Sec where C(p,q) is defined as the corresponding reaction rate coefficient.

(4) Radiation is emitted when an electron in an upper bound level makes a spontaneous transition to a lower level and when a free electron makes a transition into a bound level. These radiative processes are represented by

$H(p) \rightarrow H(q) + h\nu$, $q < p$, and

$H^+ + e \rightarrow H(p) + h\nu$

The corresponding rates of these processes are given by:

(a) Spontaneous decay ; $A(p,q)n(p)$ cm^{-3} s^{-1}
where A(p,q) is defined as spontaneous radiative decay probability;

(b) Radiative recombination, $\beta(p)n_e n_i\ cm^{-3}s^{-1}$,
where $\beta(p)$ is defined as radiative recombination coefficient to p ;

(5) The plasma is assumed to be optically thin so that all emitted radiation escapes from the plasma without being reabsorbed.

Using the above assumptions, the set of equations that describes the rates at which the bound atomic levels are populated or depopulated is written as:

$$\frac{d}{dt}n(p) = -\left\{\sum_{q \neq p} C(p,q)n_e + \sum_{q<p} A(p,q) + S(p)n_e\right\} n(p)$$

$$+ \sum_{q \neq p} \{ C(q,p)n_e + A(q,p) \}\, n(q)$$

$$+ \{ \alpha(p) n_e + \beta(p) \} n_e n_i \qquad (2.1)$$

The summations in equation 2.1 go over all possible values of q within the limits indicated. Nevertheless, we can avoid dealing with impossibly large summations and an equally large number of differential equations. Because with increasing quantum number the level spacing becomes smaller and the probability of collisional processes become greater while at the same time the probability of radiative process becomes smaller, we can, to any desired degree of accuracy, always find some level above which the effect of the radiative process may be neglected. Therefore the levels above this level can be assumed to be in local thermal equilibrium where their population distribution is given by the Saha equation (1.3).

However, because of the effects of the confining magnetic field, the upper lying levels are mixed to the continuum states, and Janev /1 / suggested the highest bound level to be 26 for a magnetic field of 2T. Therefore equation 2.1 reduces to 26 differential equations.

Furthermore, the rates at which excited states are produced and destroyed by collisional and radiative processes are much faster than the rates at which the number densities of the free electrons and ions change as the plasma decays. Consideration of relaxation times for the population densities of the bound levels to exchange with each other and with the continuum of free electrons shows that these rates are some orders of magnitude larger than those associated with the ground level. For the excited levels the relaxation times are the lifetimes for spontaneous radiative decay or are shorter. Compared to the relaxation time for the ground level population these others may be regarded as instantaneous. By their nature atomic lifetimes are the minimum resolving time of any spectroscopic measurement. Thus we can seek quasi-steady state solutions for the set of equations 2.1 by setting the derivatives zero except for the ground level. Then the set of differential equations reduces to a set of simultaneous equations and one rate equation.

It is convenient to define a reduced population density

$$\rho(p) = \frac{n(p)}{n_E(p)}, \tag{2.2}$$

Where $n_E(p)$ is the number density of hydrogen atoms in level p in Saha equilibrium at temperature T.

We write $n_E(P) = Z(p) n_e n_i$, (2.3)

where

$$Z(p) = p^2 \left[\frac{(h)^2}{2\pi m KT}\right]^{3/2} \exp\left(\frac{x(p)}{KT}\right) \tag{2.4}$$

Then equation 2.1 with the derivative set to zero is written for $\rho(p)$, p>1 :

$$0 = -\left[\sum_{q \neq p} C(p,q) n_e + \sum_{q<p} A(p,q) + S(p) n_e\right] \rho(p) + \sum_{q \neq p} [c(q,p) n_e$$

$$+ A(q,p)] \frac{Z(q)}{Z(p)} \rho(q) + \frac{1}{Z(p)} [\alpha(p) n_e + \beta(p)] \tag{2.5}$$

Now applying the principle of detailed balancing, $C(p,q)n_E(p) = C(q,p)n_E(q)$ and $S(p)n_e n_E(p) = \alpha(p) n_e^2 n_i$. Followingly we express the electronic impact de-excitation and three-body recombination rate coefficients interms of excitation and ionization rate coefficients respectively as

$$c(q,p) = \frac{Z(p)}{Z(q)} c(p,q) \tag{2.6}$$

and

$$\alpha(p) = Z(p)S(p) \tag{2.7}$$

Substituting expressions 2.6 and 2.7 in to 2.5 and rearranging:

$$0 = -\left\{\sum_{q \neq p} c(p,q)n_e + \sum_{q<p} A(p,q) + S(p)n_e\right\}\rho(p)$$

$$+ \sum_{q \neq p,1} \left\{c(p,q)n_e + A(q,p)\frac{Z(q)}{Z(p)}\right\}\rho(q)$$

$$+ c(p,1)n_e n(1) + \left\{S(p)n_e + \frac{1}{Z(P)}\beta(p)\right\} \tag{2.8}$$

The set of equation given by 2.8 can be written in a matrix form:

$$\begin{pmatrix} W_{22} & W_{23} & \cdots & W_{2s} \\ W_{32} & W_{33} & \cdots & W_{3s} \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ W_{s2} & W_{3s} & \cdots & W_{ss} \end{pmatrix} \begin{pmatrix} \rho(2) \\ \rho(3) \\ \cdot \\ \cdot \\ \cdot \\ \rho(s) \end{pmatrix} = \begin{pmatrix} b_{20} \\ b_{30} \\ \cdot \\ \cdot \\ \cdot \\ b_{s0} \end{pmatrix} + \begin{pmatrix} b_{21} \\ b_{31} \\ \cdot \\ \cdot \\ \cdot \\ b_{s1} \end{pmatrix} \rho(1) \tag{2.9}$$

where

$$W_{pp} = \left\{ \sum_{q \neq p} c(p,q) n_e + \sum_{q<p} A(p,q) + S(p) n_e \right\}, \tag{2.10}$$

$$W_{pq} = - \sum_{q \neq p,1} \left\{ c(p,q) n_e + A(q,p) \frac{Z(q)}{Z(p)} \right\}, P \neq q, \tag{2.11}$$

$$b_{p0} = S(p) n_e + \frac{1}{Z(p)} \beta(p) \tag{2.12}$$

$$b_{p1} = c(p,1) n_e \tag{2.13}$$

Following eqn. 2.9 we can write the solution for $\rho(p)$ in the form

$$\rho(p) = r_0(p) + r_1(p) \rho(1), p > 1 \tag{2.14}$$

where $r_0(p) = W^{-1} b_{p0}$, and (2.15)

$$r_1(p) = W^{-1} b_{p1}, \tag{2.16}$$

W is the square matrix in equation 2.9.

We can then write equation 2.1 for the ground (p=1) level :

$$\frac{d}{dt} n(1) = - \left\{ \sum_{q \neq 1} [c(1,q) + S(1) - c(1,q) r_1(q) - - \frac{A9q,1) Z(q)}{n_e \quad Z(1)} r_1(q)] n_e n(1) \right\}$$

$$+ \left\{ \sum_{q \neq 1} c(1,q) n_e Z(1) r_0(q) + A(q,1) Z(q) r_0(q) + Z(1) S(1) n_e + \beta(1) \right\} n_e n_i \tag{2.17}$$

This can be written as :

$$\frac{d}{dt} n(1) = -S n_e n(1) + \alpha n_e n_i, \tag{2.18}$$

where S is referred to as collisional radiative ionization coefficient and α as collisional radiative recombination coefficient given by:

$$S = \sum_{q \neq 1} \left\{ c(1,q) + s(1) - c(1,q) r_1(q) - \frac{A(q,1)}{n_e} \frac{Z(q)}{Z(1)} r_1(q) \right\} \tag{2.19}$$

$$\alpha = \sum_{q \neq 1} \left\{ c(1,q) n_e Z(1) r_0(q) + A(q,1) Z(q) r_0(q) \right\} + Z(1) S(1) n_e + \beta(1) \tag{2.20}$$

2.2 Atomic data

The excitation, ionization and radiative recombination rate coefficients are taken from ref. /7 /.

2.2.1. Electron impact excitation rate coefficients

The electron impact excitation rate coefficient from a lower level p to a higher level q is given by the approximate formula

$$c(p,q) = \left(\frac{8KT}{\pi m}\right)^{1/2} \frac{2p^2}{x} \pi a_0^2 y^2 \, Apq \, [(\frac{1}{y} + \frac{1}{2})E_{1(y)}$$

$$- (\frac{1}{z} + \frac{1}{2}E_1(z)\,] + (Bpq - Apq \ln \frac{2p^2}{x})\left\{\frac{1}{y}E_2(y) - \frac{1}{Z}E_2(Z)\right\} \quad (2.21)$$

where $X = \frac{Epq}{x(p)} = 1 - (\frac{p}{q})^2$

a_0 is the bohr radius

$$y = \frac{Epq}{KT}$$

$$E_i(Z) = \int_1^\infty e^{-Zt} t^{-i} dt \qquad (i = 0,1,2,...)$$

with $E_{i+1}(Z) = \frac{1}{i}[e^{-Z} - ZE_i(Z)] \quad (i = 1,2,...)$

$$Apq = \frac{2p^2}{x} fpq$$

with $fpq = \frac{32}{3\sqrt{3}\pi} \frac{p}{q^3} x^{-3} g(p,x)$

$Z = r_{pq} + E_{pq} / KT$

with $r_{pq} = r_p x$;
$r_1 = 0.45$,
$r_p = 1.94p^{-1.57}$, $p \geq 2$

$$Bpq = \frac{4p^2}{q^3}x^{-2}\left(1 + \frac{4}{3}x^{-1} + b_p x^{-2}\right)$$

with $b_1 = -0.602$

$$b_p = \frac{1}{p}(4.0 - 18.63p^{-1} - 36.24p^{-2} - 28.09p^{-3}),\ p \geq 2$$

$$g(p,x) = g_0(p) + g_1(p)x^{-1} + g_2(p)x^{-2}$$

with

	p = 1	p = 2	p ≥ 3
$g_0(p)$	1.1330	1.0785	$0.9935 + 0.2328\ p^{-1} - 0.1296\ p^{-2}$
$g_1(p)$	-0.4059	-0.2319	$-p^{-1}(0.6282 - 0.5598\ p^{-1} - 0.5299\ p^{-2})$
$g_2(p)$	0.07014	0.02947	$p^{-2}(0.3887 - 1.181\ p^{-1} - 1.470\ p^{-2})$

2.2.2. Ionization rate coefficients

The ionization rate coefficient from level p is

$$S(p) = \left(\frac{8KT}{\pi}m\right)^{\frac{1}{2}} 2p^2\pi a_0^2 y_p \left\{A_p\left[\frac{1}{y_p}E_1(y_p) - \frac{1}{Z_p}E_1(Z_p)\right]\right.$$

$$+ (b_p - A_p ln(2)p^2) \left\{\xi(y_p) - \xi(Z_p)\right\} \quad (2.22)$$

where $y_p = \frac{x(p)}{KT}$, x(p) = ionization energy of level p

$$Zp = \text{Ip} + \frac{x(p)}{KT}$$

$$\xi(t) = E_0(t) - 2E_1(t) + E_2(t)$$

2.2.3. Radiative recombination rate coefficients

The radiative recombination rate coefficient to level p is

$$\beta(p) = D(\frac{x(p)}{KT})^{\frac{3}{2}} \exp(\frac{x(p)}{KT}) \sum_{i=0}^{2} g_i(n) E_{i+1}(\frac{x(p)}{KT}) \quad (2.23)$$

where D = 5.197 X 10^{-14} cm^3 s^{-1}

2.2.4. Spontaneous radiative decay probabilities

The spontaneous radiative decay probabilities for transitions involving lower levels are taken from the table of ref. /1/. For higher lying levels approximate formula is taken from ref. /1/.

$$A(p,q) = \frac{1}{qp^5 X_{pq}} g(q, x_{qp}) \quad (2.24)$$

Where $X_{qp} = 1 - (\frac{q}{p})^2$

2.3 Results and Discussion

The most important result is that at high densities, the ionization and recombination rates are increased due to multistep collisions. The atom can first be excited from the ground to a higher state. Then it can be more easily ionized

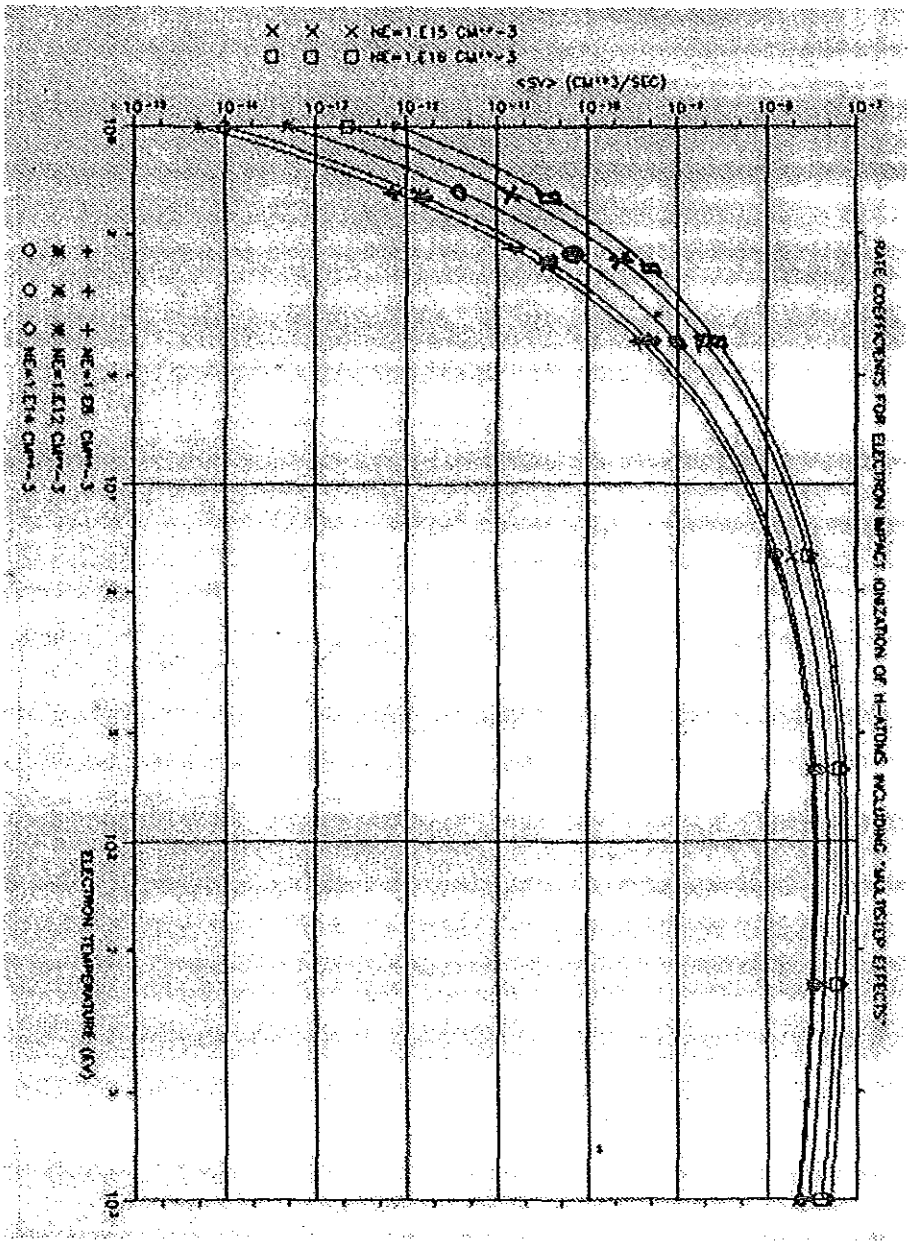

Figure 1.

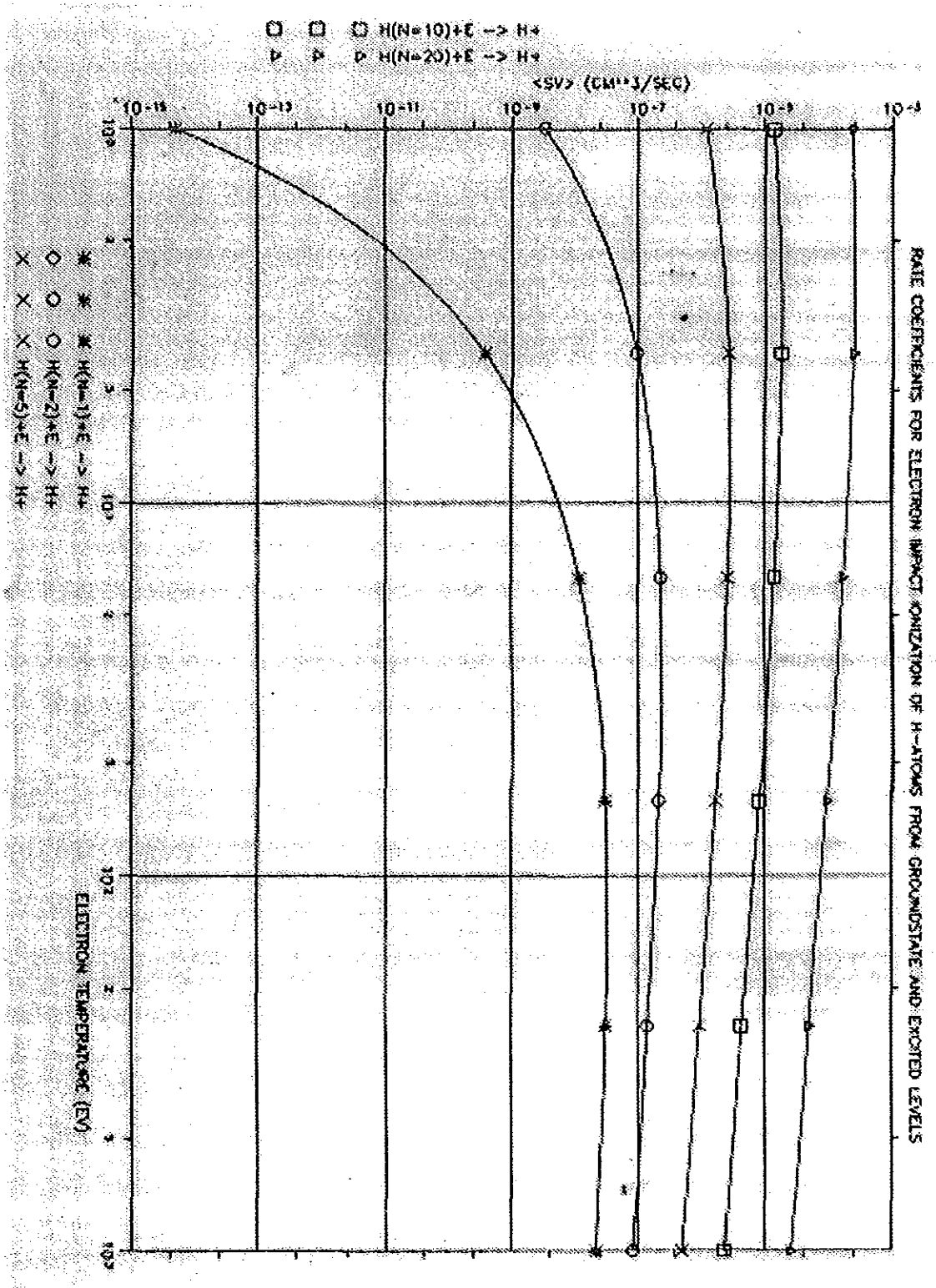
RATE COEFFICIENTS FOR ELECTRON IMPACT IONIZATION OF H-ATOMS FROM GROUNDSTATE AND EXCITED LEVELS
<SV> (CM**3/SEC)
ELECTRON TEMPERATURE (EV)
H(N=10)+E --> H+
H(N=20)+E --> H+
H(N=1)+E --> H+
H(N=2)+E --> H+
H(N=5)+E --> H+

Figure 2.

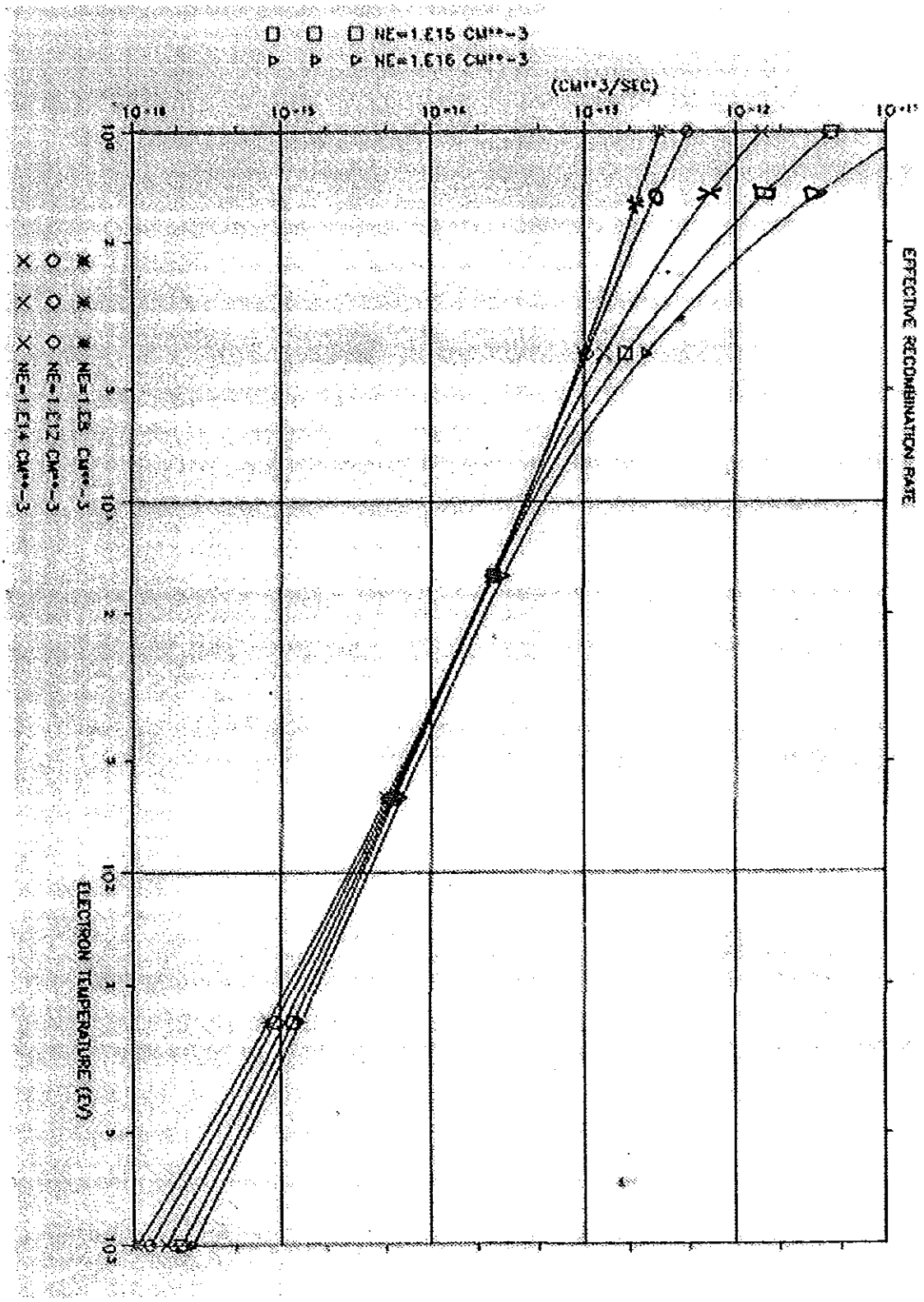
NE=1.E15 CM**-3
NE=1.E16 CM**-3
(CM**3/SEC)
EFFECTIVE RECOMBINATION RATE
ELECTRON TEMPERATURE (EV)
NE=1.E13 CM**-3
NE=1.E12 CM**-3
NE=1.E14 CM**-3

Figure 3.

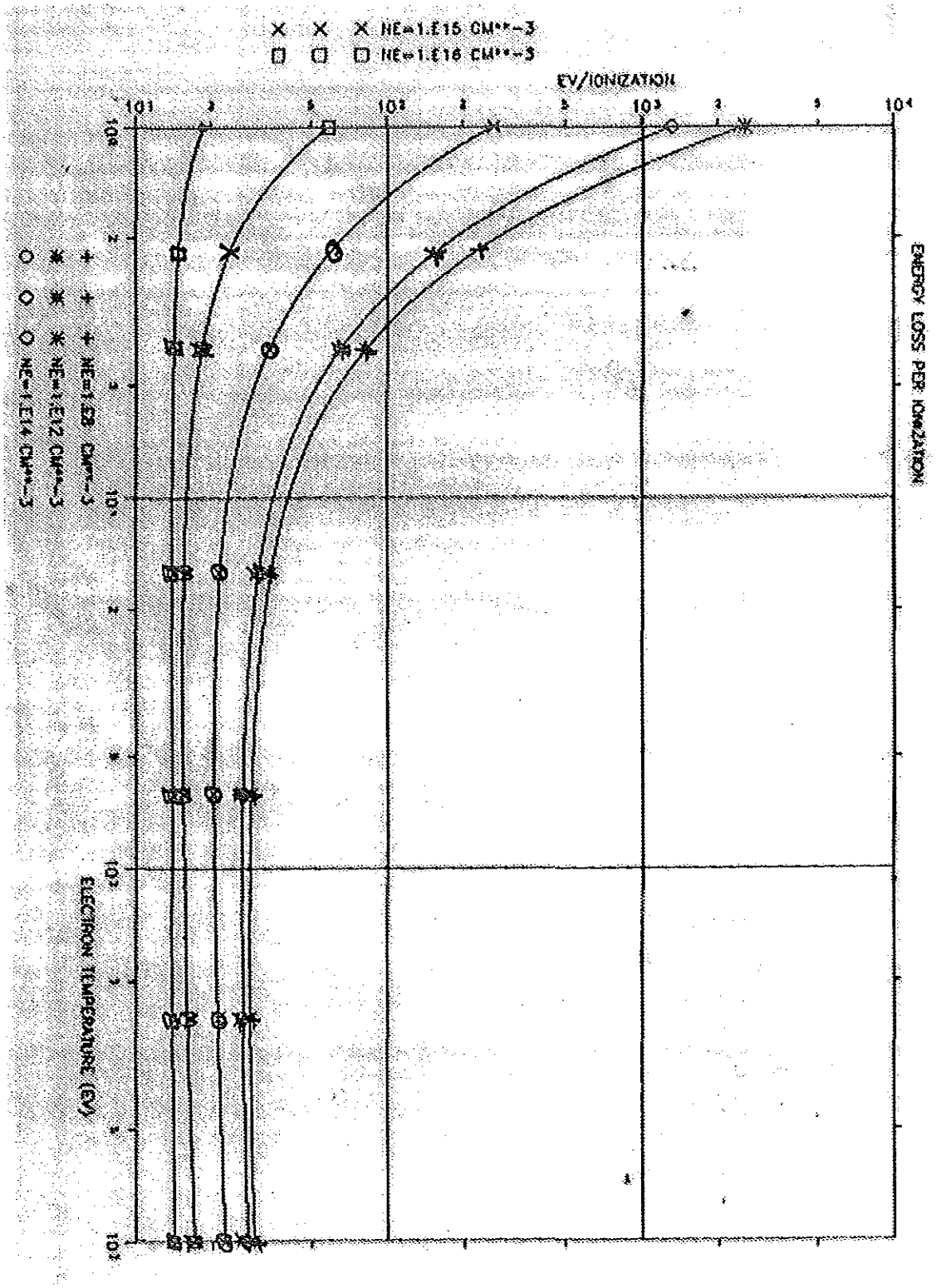
NE=1.E15 CM**-3
NE=1.E16 CM**-3
EV/IONIZATION
ENERGY LOSS PER IONIZATION
NE=1.E13 CM**-3
NE=1.E12 CM**-3
NE=1.E14 CM**-3
ELECTRON TEMPERATURE (EV)

Figure 4.

from the excited level since the electron binding energy is smaller. As the density increases, three-body recombination followed by collisional de-excitation can also become important.

Figure 1 shows the effective ionization rate for a family of densities and that the ionization rate increases with density for a fixed energy. Figure 2 shows the rate coefficients for ionization from different levels, which clearly shows the increase of the coefficient with the increase of quantum level.

The effective recombination rate as a function of temprature for a family densities is shown in figure 3. The rate at low temprature (~ 1 - 10 ev) significantly increases with density. However, this result is probably not useful since the rate is still too small to effect edge plasmas significantly. Recombination takes place primarily when the plasma hits the wall. Part of the increase in the recombination rate is due to three-body recombination effects.

Hydrogen line radiation can be an important energy loss mechanism. Figure 4 shows the energy loss due to radiation from radiative decay and ionization per ionization:

$$\frac{\sum_{p>q} A_{pq} n(p)(E_p - E_q) + S(p) n_e n(p)\ 13.6 \quad (ev.)}{\sum_p S(p) n(p) n_e}$$

The typical value used by plasma modulers is about 40 ev which is a good estimate for higher temperature and densities of 10^{13} cm^{-3}. At higher densities the multistep processes interfere with the radiative losses by ionizing the excited states before they can radiatively decay and the energy loss per ionization is simply the ionization energy 13.6 ev.

For electrons with energies much greater than 13.6 ev, there is little difference, at most a factor of 2, between the electron excitation and ionization rates. Thus multistep processes involving excited states are relativeley unimportant. Electrons with energies between 10.2 ev, the excitation energy for the first excited level n being 2, and 13.6 ev, the ground state ionization potential, can excite or ionize only those states with $n > 2$. The ratio of such particles can become very large at low temperature and there be many excitations per ionization. Once the electron gets excited to $n = 2$ level, then the transition to $n = 3$ takes only 1.89 ev and 3.4 ev to $n = \infty$. For $T \sim 1 - 5$ ev there are plenty of electrons with such energies. Thus we expect the biggest effects to occur when the temprature is 5 - 6 ev, that is where the increase in the radiation rates become large.

Chapter 3

Collisional Radiative Model for Hydrogen Molecules

3.1. Molecular physics of H_2 molecule

The physics of collisional radiative processes involving H_2 molecules is much more complicated than for isolated atoms. The complexity is partly reduced because of the much smaller mass of the electrons compared to the mass of the nuclei while the forces acting on them are comparable. The electronic states can therefore be determined at each value of the internuclear separation by assuming the nuclei as fixed; and the electronic and nuclear motions can be treated independently. The energy of the electrons is then a function of the nuclear positions which determine the nuclear motion.

There are three important contributions to the total energy of molecules. The first is eletronic energy which is associated with the orbit of the electrons around the nuclei. For the lowest levels, this energy is in the order of few electron volts and the spectral lines that result from transitions between these levels are observed in the ultra violet and visible regions. The second contribution stems from the internal vibrations of the nuclei about their equilibrium separation position. Vibrational energies are roughly two orders of magnitude smaller than electronic energies. Therefore, vibrational transitions at fixed electronic state yield photons in the infrared region. The third component is rotational energy that comes due to the rotation of the entire system of nuclei. Rotational energies are again two orders of magnitude less than vibrational energies. Transitions between rotational levels at fixed electronic and vibrational level can therefore be observed only in the far infrared and microwave regions.

In contrast to atoms in which the Hamiltonian has a spherical symmetry, the internuclear axis of a diatomic molecule takes a particular direction in space, and hence the Hamiltonian has only axial symmetry. If this axis is lies along the z-axis, then the Hamiltonian of a diatomic molecule commutes only with the z component L_z of the total angular momentum. Therefore only the projection of the total angular momentum along the internuclear axis is considered while the x and y components are not important. By analogy with the spectroscopic notation S, P, D, F, etc., used for atoms, code letters Σ,Π,Δ,Φetc.,. are associated with the respective magnitudes 0, 1, 2, 3,etc., of the projection of the total angular momentum along the internuclear axis. Lower case letters $\sigma,\pi,\delta,\varphi$etc., are used in dealing with individual electrons in the same way as small letters s, p, d, f, etc., are used for individual atomic electrons.

The electronic Hamiltonian of a diatomic molecule is invariant under reflection in all planes containing the internuclear axis. For electronic states for which the projection of the total angular momentum along the internuclear axis is nonzero, reflection about such a plane converts the wave function into another one with opposite projection of angular momentum. This gives rise to a double degeneracy, each value of energy corresponding to two states which differ by the direction of angular momentum along the internuclear axis. On the other hand the Σ states, for which the projection is zero, are non degenerate so that these states can only be multiplied by a constant in reflection about a plane containing the molecular axis. For a complete specification of Σ states of diatomic molecules, Σ^+ states for which the wave function is unchanged upon the reflection are distinguish from Σ^- states for which it changes sign.

For homonuclear diatomic molecules like H_2 there is a center of symmetry at the mid point of the nuclei. Choosing this point as the origin of coordinates, the Hamiltonian is invariant under the inversion of all electronic coordinates along it. The electronic states are split into two sets according to wether the wave functions change sign with this inversion or not. Those states which do not

change sign are called gerade states and are denoted by a subscript g, while those which change sign are called ungerade states and are denoted by a subscript u.

Denoting by $\vec{S}$ the resultant of the electronic spins,with a multiplicity quantity 2S + 1 which gives the degeneracy associated with S, is called the multiciplicity of the state and is written as a left superscript. For H_2 molecule, in which there are two electrons, the two electronic spins can be either antiparallel (S = 0) with multiplicity equal to one or parallel (S = 1) with multiplicity equal to three. The former are called singlet states and the later is triplet states.

The various singlet electronic states are distinguished by upper case letters A, B, C,etc., while the triplet states are labelled by lower case letters a, b, c, etc., X is often used for the ground electronic state. Hydrogen has no an A state. For instance, the ground electronic state of hydrogen molecule is represented by $X1\Sigma^+_g(1s\sigma)^2$. Thus, it is a singlet, even with reflection about a plane containing the molecular axis and with inversion about the center of symmetry, and with no projection of the total angular momentum along the molecular axis. $(1s\sigma)^2$ designates the molecular orbitals of each electron in the united atom configuration. In the notations, unless it is stated, one electron is assumed to be in the $1s\sigma$ orbital and only the orbital for the excited electron is listed. Similarly, the next electronic state in the potential energy diagram of H_2 which is a triplet is represented by $b\ 3\Sigma^+_u 2s\sigma$ where one of the electrons is in excited orbital $2s\sigma$. Some important electronic potential energy curves of H_2 and H^+_2 are shown in Figure 5

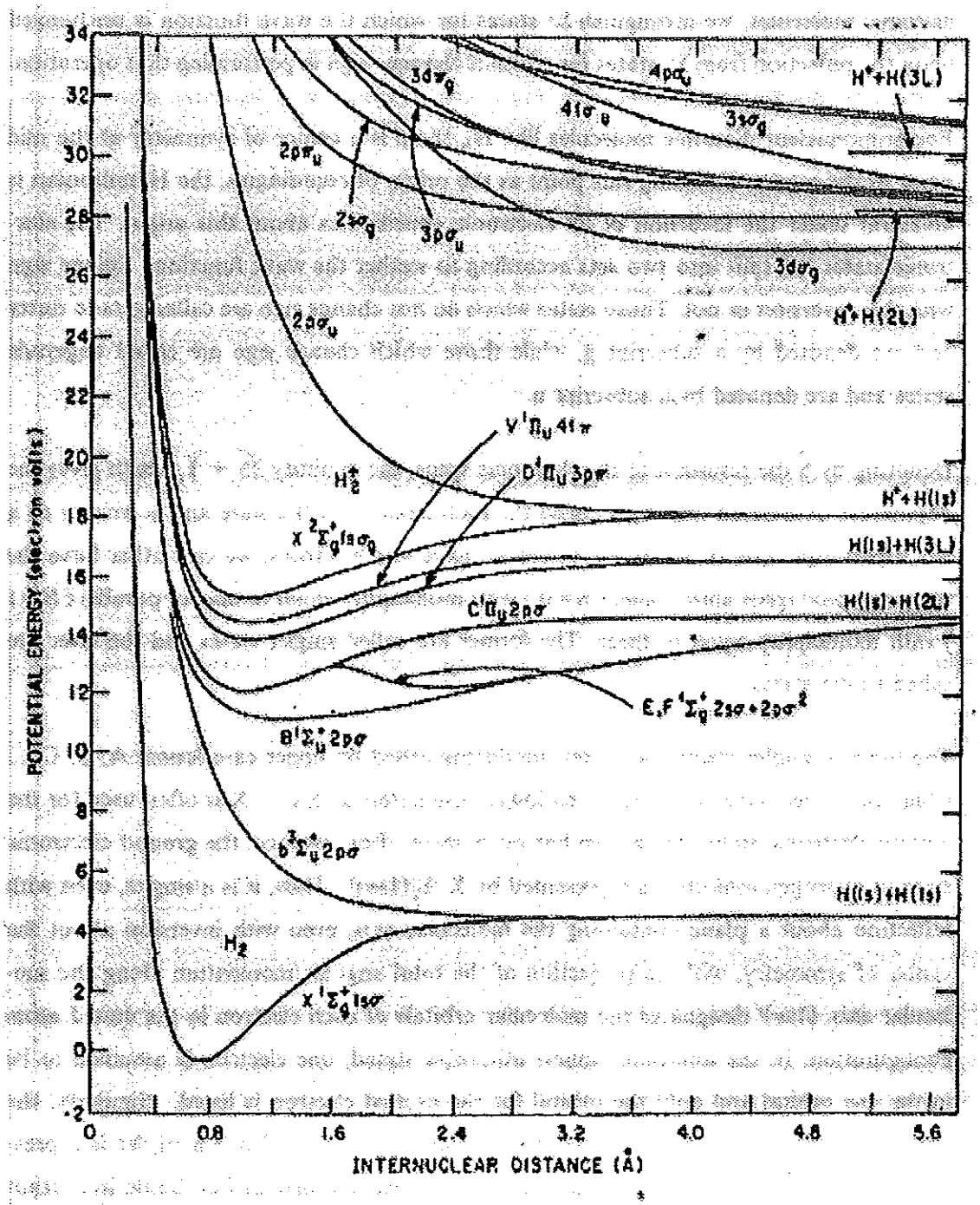

Fig.5: Electronic potential energy curves of H_2 and H_2^+

3.2. Rate equation

To facilitate presentation, we label the electronic states considered by numbers: $X\ \Sigma^+_g \rightarrow 1$, $B\ \Sigma^+_u \rightarrow 2$, $C\ \Pi_u \rightarrow 3$, $E,F\ \Sigma^+_g$ 4, group of triplet states that dissociate into ground state atoms ($b\ \Sigma^+_u$, $a\ \Sigma^+_g$, $e\ \Pi_u$)$\rightarrow 5$, the group of electronic states with one electron in the ground and the other in excited orbital of the united atom configuration ($1s\sigma_g$, $nl\lambda$) ($n\geq 3$) $\rightarrow 6$, the group of autodissociative states that give atoms both in the first excited state ($2p\sigma_u$ $nl\lambda$) $\rightarrow 7$, and the state that dissociates into one ground and another second excited state ($2p\sigma_u$ $3l\lambda$)$\rightarrow 8$, where the notations are as discussed in the last section. The relevant molecular processes are presented below:

(a) Electron impact excitation(q > p) or de-excitation(q < p) from electronic state p to q:

$$H_2\,(p) + e \rightarrow H_2\,(q) + e,$$

the corresponding rate coefficient is denoted by C(p,q).

(b) Electron impact dissociative excitation into two atoms from state p through state q and its inverse three-body recombination:

$$H_2(p) + e \underset{\rightarrow}{\leftarrow} H_2(q) + e \rightarrow H + H + e,$$

the corresponding rate coefficients are denoted by D(p,q) and $\alpha_1(q,p)$ respectively.

(c) Electron impact ionization of state p and its inverse three body recombination:

$$H_2(p) + e^{-}_{\rightarrow} H_2^{+} + e + e,$$

the corresponding rate coefficients are denoted by S(p) and $\alpha(p)$ respectively.

(d) Electron impact dissociative ionization of state p into $H + H^+$ through the states of molecular ion H_2^{**} and its inverse three-body recombination

$$H_2(p) + e^{-}_{\rightarrow} H_2^{+} + e + e \rightarrow H + H^{+} + e + e,$$

the corresponding rate coefficients are denoted by $S'(p)$ and $\alpha'(p)$ respectively.

(e) Electron impact radiative recombination into state p with emission of a photon:

$$H_2^{+}(p) + e \rightarrow H_2(p) + h\mu,$$

the corresponding rate coefficient is denoted by $\beta(p)$.

(f) Spontaneous radiative decay of state p to the bound vibrational levels of a lower state q:

$$H_2(p) \rightarrow H_2(q) + e,$$

the corresponding transition probability is denoted by $A'(p,q)$.

(g) Spontaneous radiative decay of p to the dissociation continuum of a lower state q:

$$H_2(p) \rightarrow H_2(q) + e \rightarrow H + H,$$

the corresponding transition probability is denoted by $A''(p,q)$.

Note that $A(p,q) = A'(p,q) + A''(p,q)$.

Then the rate equation for the population density $n_{H_2}(p)$ of electronic state p is written:

$$\frac{d}{dt} n_{H_2}(p) = -\left\{\sum_{q\neq p}^{4} C(p,q)n_e + \sum_{q=5\neq p}^{8} D(p,q)n_e \right.$$

$$+ \left[[S(p) + S'(p)]n_e + \sum_{q<p} [A'(p,q) + A''(p,q)]\right] n_{H_2}(p)$$

$$+ \sum_{q\neq p} \left\{C(q,p)n_e + A'(q,p)\right\} n_{H_2}(p) + \left\{\alpha(p) + \beta(p)\right\} n_e n_{H_2^+}$$

$$+ \left\{\sum_{q} \alpha_1(q,p)n_H + \alpha'(p)n_{H^+}\right\} n_e n_H \qquad (3.1)$$

where $n_{H_2^+}$, n_H and n_{H^+} are molecular ion, atomic and atomic ion number densities respectively. This is a general system of rate equations in which many of the coefficients are not established. We simplify it with the following assumptions .

The triplet electronic state b Σ_u^+ is repulsive and its excitation simultaneously results in dissociation into two ground state hydrogen atoms in $\approx 10^{-14}$ sec. /9/ (see the dissociation limit in fig. 5). Direct excitation of this state accounts for

about 50% /10,11/ of the total dissociation through b Σ_u^+ into H(1s) + H(1s). It's excitation cross section is taken as dissociation cross section.

The triplets a Σ_u^+ and c Σ_u^+ radiatively decay to bΣ_u^+ very fas /12-14/. Therefore, effectively, they contribute to the dissociation of H_2 into two ground state atoms. These two triplet states account for about 20% and 16% respectively /9/ of the total dissociation through b Σ_u^+. The excitation rates of these states are taken as dissociation rates together with b Σ_u^+. Small contributions of about 6% and 5% come from cascades of e Σ_u^+ and dΠ_u respectively; but these are not included in this work.

The singlet states B Σ_u^+ and CΠ_u. have many bound vibrational levels, and molecular transitions to these states form a major part of electronic impact excitation from the ground state. These states radiatively decay to the bound vibrational levels and the dissociation continuum of the ground state giving rise to the well known Lyman and Werner bands. These emissions were first experimentally measured in ref. /15/. The parts that decay into the continuum contribute to the dissociation into two ground state atoms.

Excitation of the E, F Σ_g^+ state is followed by fast cascade to B Σ_u^+ /16,17/, which on the other hand decays to the ground state.

Excitations of the groups of electronic states $H_2(1s\sigma_g, nl\lambda)$ $(n\geq 3)$, $H_2(2p\sigma_u, nl\lambda)$ and $H_2(2p\sigma_u, 3l\lambda)$ /18,19/ are assumed to lead to dissociation producing H(1s)+H(2s), H(2p)+H(2s) and H(1s)+H(3l) atoms respectively, where the notations are as discussed in the last section. The potential energy curves of these states are shallow and more displaced to larger internuclear separation. Excitation of these states therefore leads to the dissociation continuum in accordance to the Franck-Condon principle /20/. Their excitation cross sections are effectively taken as dissociation cross sections. It is çalculated in ref./17/ that about 70% of

$D\Pi_u$ and 3% of $B''\ \Sigma_u^+$ states result in radiative decay to the ground state rather than dissociation. However, since the excitation cross sections of these individual states are very small /21/, it should not have serious effect.

Thus electronic states that have dissociation limits up to principal quantum number n = 3 are considered. The uncovered electronic states which may lead to more excited atoms ($n \geq 3$) have much smaller cross sections /13,17,22-26/ and should not have much effect.

Transitions yielding H($n \geq 3$) are indeed by one or more orders of magnitude less than those yielding H(n = 3). This rapid fall off in the excitation cross sections with increasing principal quantum number of the molecular orbitals is consistent with the fact that the oscillator strength varies as the inverse cube of the principal quantum number /27/.

The ground state molecules are assumed to be in the ground vibrational level, and the excitation cross sections and energies used are taken with respect to this level. It is shown in ref. /28/ that generally the excitation treshold energy decreases and the cross section increases with increasing vibrational level of the initial electronic state. However, the excitation cross sections of the excited vibrational levels from the lowest level strongly decrease with increasing vibrational level with maximum values of about $5\ X\ 10^{-17} cm^2$ ($v = 0 \rightarrow 1$), $4\ X\ 10^{-19} cm^2$ ($v = 0 \rightarrow 3$), $5\ X\ 10^{-20} cm^2$ ($v = 0 \rightarrow 6$), /21,29/ for the ground electronic state. Followingly, the corresponding reaction rates are very small at higher temperatures ($\geq$ 10 eV) . The excitation of the vibrational levels of the ground state are indeed important only at low temperatures in the study of magnetic multicusp discharges /28,30/. Moreover, spontaneous radiative decay of the higher electronic states to the bound levels of the ground state is assumed to lead to the lowest vibrational level.

The lifetimes of excited molecules which either radiatively decay or dissociate are very small. For instance, we obtained the mean lifetimes of $B\,\Sigma_u^+$ and $C\,\Pi_u$ by averaging the lifetime of each vibrational level of these states given by Stephens and Dalgarno /26/ over the corresponding relative excitation cross sections given by Ajello et al. /12/ to be 8.467 X 10^{-10} sec. and 8.842 X 10^{-10} sec. respectively. Their spontaneous radiative decay probabilities are then 1.181 X 10^9 sec^{-1} and 1.131 X 10^9 sec^{-1} respectively . The dissociation times of the repulsive and autodissociative states are also much smaller. We have already mentioned that $b\,\Sigma_u^+$ dissociates in $\approx 10^{-14}$ sec. /9/. The autodissociative states also dissociate in less than 10^{-11} sec. /32,33,17/. Therefore the probability of electron collision with excited molecules is small. Partly based on this fact, and because of the lack of molecular data, electronic collisions with excited molecules are neglected. Therefore all rate coeffficients associated with electron collisions with excited molecules are set equal to zero.

In the same way as we have obtained the above lifetimes of $B\,\Sigma_u^+$ and $C\,\Pi_u$ we have calculated their respective spontaneous transition probabilities to the bound vibrational levels of the ground state to be 9.143 X 10^8 sec^{-1} and 1.121 X 10^9 sec^{-1} , and to the continuum to be 2.700 X 10^8 sec^{-1} and 1.031 X 10^7 sec^{-1} respectively. From these transition probabilities we obtain the fraction of molecules that dissociate through transition to the continuum to those that decay to the bound levels of the ground state to be 29.5% and 0.919% for $B\,\Sigma_u^+$ and $C\,\Pi_u$ respectively.

Three body recombination effects that necessarily involve a simultaneous collision of two atoms (and/or) ions and an electron are assumed to be negligible and the associated rate coefficients are set to zero.

Moreover, three body and radiative recombinations of H_2^+ are neglected and the corresponding rate coefficients are set to zero. This assumption is based on the fact that electron collision with molecular ions would rather lead to excited

molecular ions followed by dissociation, and there is no data available for this process.

Since the excitation and radiative decay of the bound excited molecular states occur within a time of the order of their lifetimes, their population density reaches equilibrium very fast and the derivatives in the right hand side of eqn.(1) can be set to zero for p > 1 compared to the rate of change of the population of the ground state.

Then, the rate equations reduce to:

$$C(1,2)n_e n_{H_2}(1) + A(4,2)n_{H_2}(4) - A(2,1)n_{H_2}(2) = 0, \text{ for } p = 2 \qquad (3.2)$$

$$C(1,3)n_e n_{H_2}(1) - A(3,1)n_{H_2}(3) = 0, \text{ for } p = 3 \qquad (3.3)$$

$$C(1,4)n_e n_{H_2}(1) - A(4,2)n_{H_2}(4) = 0, \text{ for } p = 4 \qquad (3.4)$$

and for the ground state

$$\frac{d}{dt}n_{H_2}(1) = -\left\{\sum_{q=3}^{4} C(1,q) + \sum_{q=5}^{8} D(1,q) + S(1) + S'(1)\right\} n_e n_{H_2}(1)$$

$$+ \sum_{q=2}^{3} A'(q,1)n_{H_2}(q) \qquad (3.5)$$

Substituting the expressions for n sub $H_2(2), n_{H_2}(3)$ and $n_{H_2}(4)$ from eqns.(2-4) into eqn.(5), we obtain

$$\frac{d}{dt}n_{H_2}(1) = -\left\{\frac{A''(2,1)}{A(2,1)}[C(1,2) + C(1,4)] + \frac{A''(3,1)}{A(3,1)}C(1,3) + \sum_{q=5}^{8} D(1,q) + S(1) + S'(1)\right\} n_e n_{H_2}(1) \quad \textbf{(3.6)}$$

These rate cefficients are shown in fig.6.

Using the values of spontaneous radiative decay probabilities given above, we obtain

$$\frac{d}{dt}n_{H_2}(1) = -\{0.229[C(1,2) + C(1,4)] + 0.00912C(1,3) + \sum_{q=5}^{8} C(1,q) + S(1) + S'(1)\} \quad \textbf{(3.7)}$$

Note that the first three terms give the rate of spontaneous transition of the excited states to the continuum of the ground state.

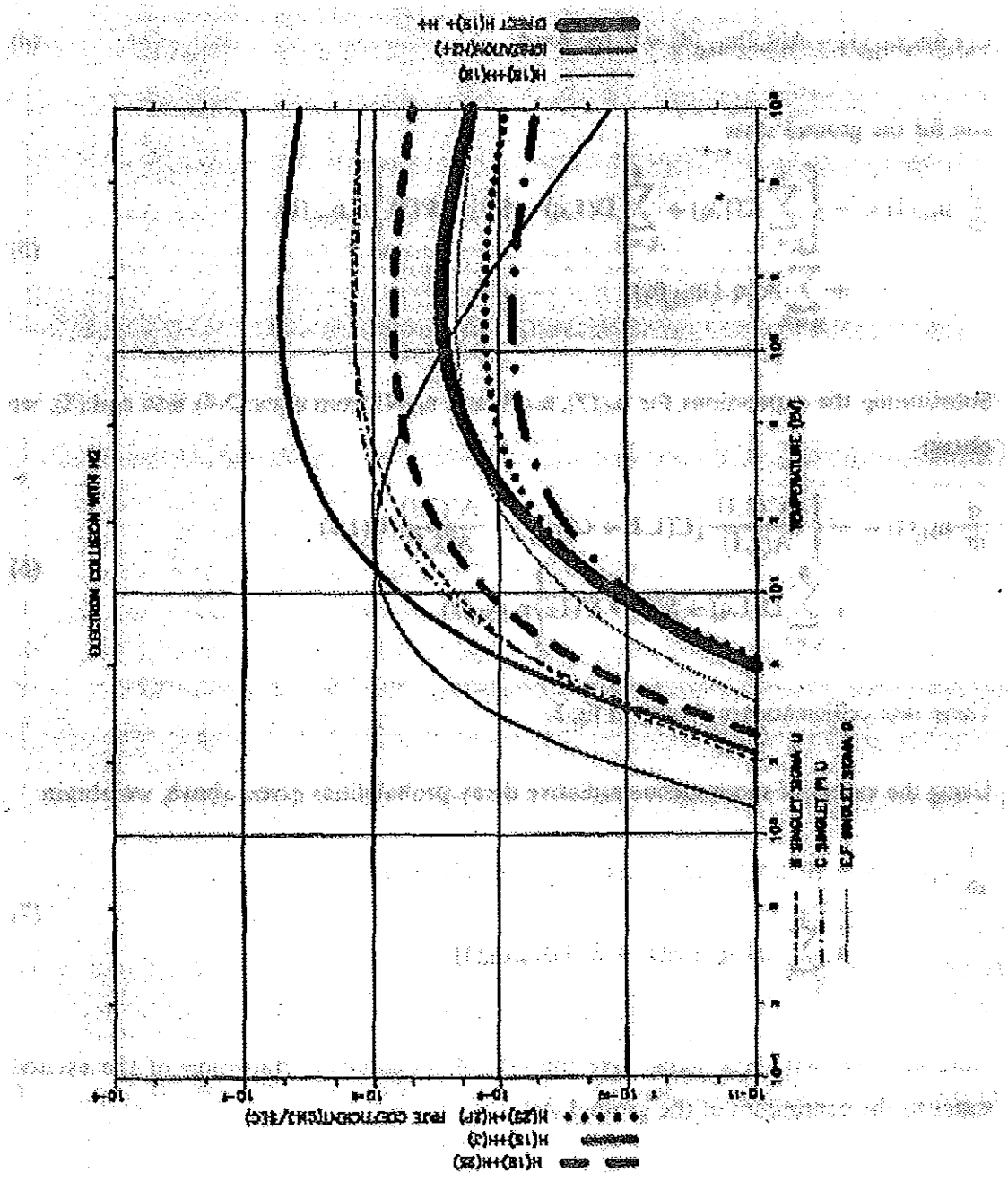

Fig6: Electron impact excitation rate coefficients of electronic states of H_2 from the ground state

Now consider the molecular ions produced upon electronic collisions with neutral hydrogen molecules. Since the minima of the ground electronic state potential curves of H_2 and H_2^+ are displaced from each other, all available vibrational levels of H_2^+ are populated. The vibrational levels of H_2^+ have very long lifetimes ($\approx 10^6$ *sec.*) /34/. Therefore, the molecular ions suffer further electronic collisions and the following products are possible /35/:

(a) $e + H_2^+(v) \rightarrow e + H^+ + H^+ + e$

(b) $e + H_2^+(v) \rightarrow e + H_2^+(2p\sigma_u) \rightarrow e + H^+ + H(1)$

(c) $e + H_2^+(v) \rightarrow e + H_2^+(2p\sigma_u) \rightarrow e + H^+ + H(2)$

(d) $e + H_2^+(v) \rightarrow H(1) + H(n),\ n \geq 2$

H_2 (v = 0-9) accounts for 97.8% /30/ of the whole vibrational distribution of $H_2^+(v)$ and the higher levels (v > 9) are not considered.

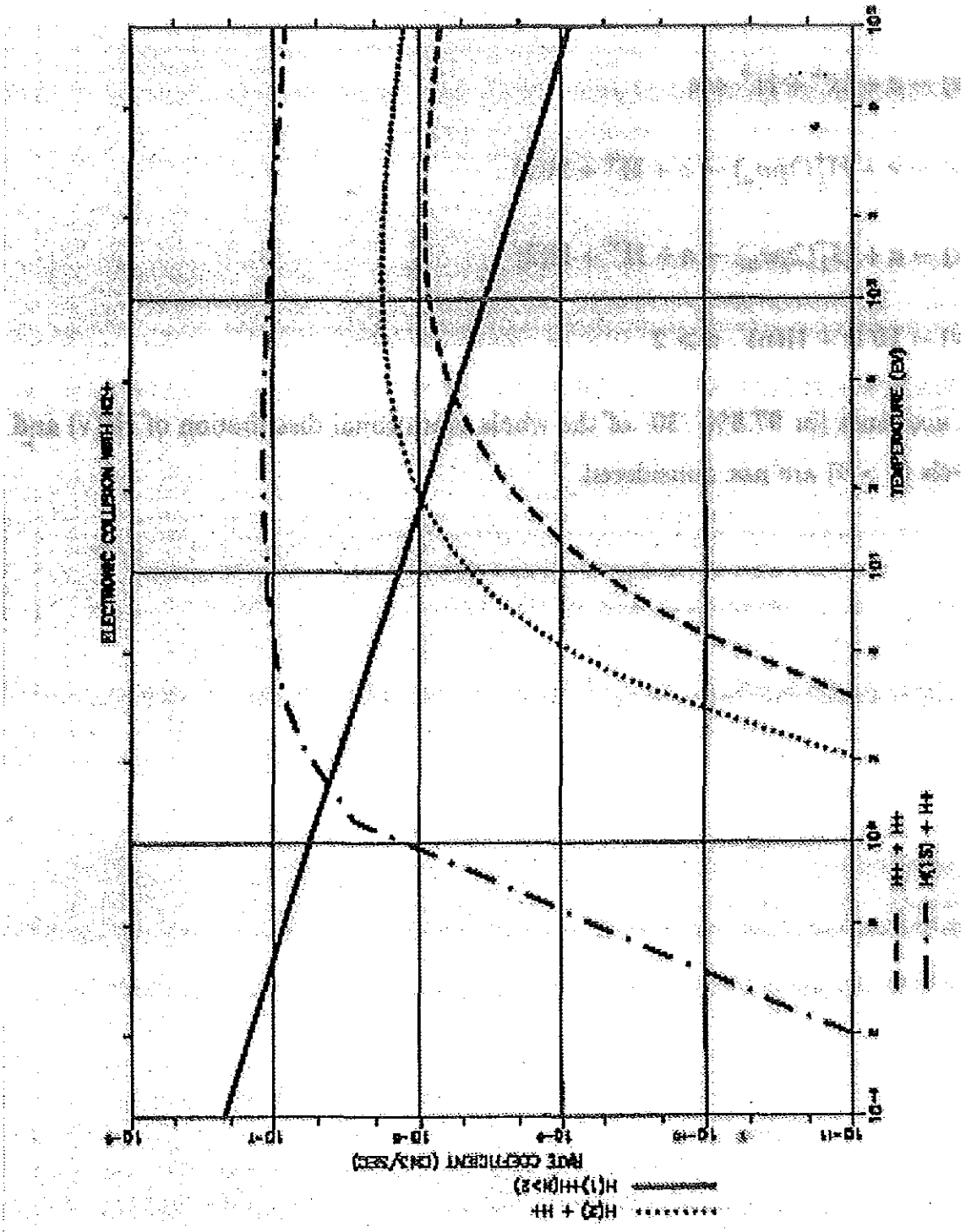

Fig.7: Electron impact dissociative excitation rate coefficients of H_2^+

Denote the reaction rate coefficient of reactions (a) - (d) shown in fig.7 by C_a , C_b , C_c and C_d. The sum of these rate coefficients is much bigger than the ionization rate S(1) of H_2 into H_2^+ so that the molecular ions produced dissociate through channels (a) - (d) very fast. The reaction rate coefficients for the formation of $H^+ + H^+$, $H^+ + H(1)$, $H^+ + H(2)$ and $H(1) + H(n)(n \geq 2)$ from H_2 through (a) - (d) which we denote by R_a , R_b , R_c and R_d respectively are then:

$$R_1 = \frac{C_1}{C_a + C_b + C_c + C_d} S(1) \quad (1 = a, b, c, d) \tag{3.8}$$

where (a) - (d) are assumed to be the only channels of electronic collisions with hydrogen molecular ions. The rate coefficients for the formation of H(1) + H(n) in reaction (d) which we denote by R_{dn} are then obtained using the relative rates given in ref. /30/

$$R_{d2} = 0.10\ R_d\ ,\ R_{d3} = 0.45\ R_d\ ,\ R_{d4} = 0.22\ R_d\ ,\ R_{d5} = 0.12\ R_d$$

$$R_{d6} = 0.069\ R_d\ ,\ R_{d7} = 0.041\ R_d$$

since R_{dn} (n = 2-6) is 95.9% of R_d , the coefficient for the formation of H(1) + H(n $\geq$ 7) R_{dn} ($n \geq 7$) is simply taken to be the coefficient for n = 7.

The rate equation (eqn.(3.1)) can then be written as

$$\frac{d}{dt} n_{H_1} = -[0.229[C(1,2) + C(1,4)] + 0.00912C(1,3) + \sum_{q=5}^{8} D(1,q) + S(1) + R_a + R_b + R_c + \sum_{n=2}^{7} R_{dn}] n_e n_{H_1}(1) \tag{3.9}$$

3.3 Rate coefficients for electron collisions with H_2 molecules and its molecular ion.

The cross section corresponding to the different reactions are obtained from ref. /35/. Since these cross sections are available in the form of graphs, the transformation of the data in to numbers is made using a Tektronix Graphics Tablet.

Since σ varies over many orders of magnitude, the polynomial fitting is made for lnσ in terms of ln E:

$$\ln\sigma = \sum_{n=0}^{8} a_n (lnE)^n$$

The reaction rate coefficients are then obtained by multiplying each σ by velocity of the electron v and averaging over a Maxwellian distribution:

$$< \sigma V > = 2\sqrt{\frac{2}{m\pi}} \frac{1}{(KT)^{\frac{3}{2}}} \int_{E_{th}}^{\infty} \sigma(E)\, E \exp(\frac{-E}{KT})\, dE$$

where E_{th} is the threshold electron energy for the corresponding reaction.

Again an eight order polynomial fitting is made for ln < σV > in terms of ln T :

$$\ln < \sigma V > = \sum_{n=0}^{8} b_n (lnT)^n$$

The values of b_n are given below and the curves are shown in fig. 2 and 3.

Reaction 1 : Excitation of B singlet sigma U

Coefficients

b_0 = -3.081902926338 E + 01

b_1 = 1.038866780735 E + 01

b_2 = -4.259768348687 E + 00

b_3 = 1.181228673120 E + 00

b_4 = -2.277513907465 E - 01

b_5 = 2.900576728856 E - 02

b_6 = -2.287591474628 E - 03

b_7 = 1.004346442778 E - 04

b_8 = -1.869930069131 E - 06

T_{min} = 2.00 E + 00 ev, $< \sigma V > (T_{min})$ = 9.88 E - 12

Reaction 2 : Excitation of C singlet pi U

Coefficients

b_0 = -3.348199796300 E + 01

b_1 = 1.371702271009 E + 01

b_2 = -5.922607900694 E + 00

b_3 = 1.709719148860 E + 00

b_4 = -3.505232830275 E - 01

b_5 = 4.834376067841 E - 02

b_6 = -4.131406425550 E - 03

b_7 = 1.948388368131 E - 04

b_8 = -3.854278715563 E - 06

T_{min} = 2.00 E + 00 ev, $< \sigma V > (T_{min})$ = 3.59 E - 12

Reaction 3 : Excitation of E,F singlet sigma g

Coefficients

b_0 = -3.646589741675 E + 01

b_1 = 1.430361969329 E + 01

b_2 = -6.074430521073 E + 00

b_3 = 1.677305768580 E + 00

b_4 = -3.128705597349 E - 01

b_5 = 3.8054247304473 E - 02

b_6 = -2.860085821803 E - 03

b_7 = 1.199641410078 E - 04

b_8 = -2.142231851104 E - 06

T_{min} = 2.00 E + 00 ev, $< \sigma V > (T_{min})$ = 5.27 E - 12

Reaction 4 : Dossociative excitation through the triplets a, b, c of H_2

Coefficients

b_0 = -2.787217511174 E + 01

b_1 = 1.052252660075 E + 01

b_2 = -4.973212347860 E + 00

b_3 = 1.451198183114 E + 00

b_4 = -3.062790554644 E - 01

b_5 = 4.433379509258 E - 02

b_6 = -4.096344172875 E - 03

b_7 = 2.159670289222 E - 04

b_8 = -4.928545325189 E - 06

T_{min} = 1.26 E + 00 ev, $< \sigma V > (T_{min})$ = 3.25 E - 12

Reaction 5: Dissociative excitation in to H(1s) + H(2s) through a group of dissociative states of H_2

Coefficients

b_0 = -3.454175591367 E + 01

b_1 = 1.412655911280 E + 01

b_2 = -6.004466156761 E + 00

b_3 = 1.589476697488 E + 00

b_4 = -2.775796909649 E - 01

b_5 = 3.152736888124 E - 02

b_6 = -2.229578042005 E - 03

b_7 = 8.890114963166 E - 05

b_8 = -1.523912962346 E - 06

T_{min} = 2.51 E + 00 ev, $< \sigma V > (T_{min})$ = 7.88 E - 12

Reaction 6: Dissociative excitation in to H(2p) + H(2s) through a group of autodissociative states of H_2

Coefficients

b_0 = -4.794288960529 E + 01

b_1 = 2.629649351119 E + 01

b2 = -1.151117702256 E + 01

b_3 = 2.991954880790 E + 00

b_4 = -4.949305181578 E - 01

b_5 = 5.236320848415 E - 02

b_6 = -3.433774290547 E - 03

b_7 = 1.272097387363 E - 04

b_8 = -2.036079507592 E - 06

T_{min} = 5.01 E + 00 ev, $< \sigma V >$ (T_{min}) = 4.09 E - 12

Reaction 7: Ionization of H2 in to H_2^+

Coefficients

b_0 = -3.568640293666 E + 01

b_1 = 1.733468989961 E + 01

b_2 = -7.767466989961 E + 00

b_3 = 2.211579405415 E + 00

b_4 = -4.169840174384 E - 01

b_5 = 5.088289820867 E - 02

b_6 = -3.832737518325 E - 03

b_7 = 1.612863120371 E - 04

b_8 = -2.893391904431 E - 06

T_{min} = 2.00 E + 00 ev, $< \sigma V >$ (T_{min}) = 2.34 E - 12

Reaction 8: Dissociative excitation in to H(1s) + H^+ through direct excitation of the continuum states of H_2^+

Coefficients

b_0 = -3.834597006782 E + 01

b_1 = 1.426322356722 E + 01

b_2 = -5.826468569506 E + 00

b_3 = 1.727940947913 E + 00

b_4 = -3.598120866343 E - 01

b_5 = 4.822199350494 E - 02

b_6 = -3.909402993006 E - 03

b_7 = 1.738776657690 E - 04

b_8 = -3.252844486351 E - 06

T_{min} = 3.98 E + 00 ev, $< \sigma V >$ (T_{min}) = 1.00 E - 12

Reaction 9: Dissociation into $H^+ + H^+$ due to electron collision with H_2^+

Coefficients

b_0 = -3.746192301092 E + 01

b_1 = 1.559355031108 E + 01

b_2 = -6.693238367093 E + 00

b_3 = 1.981700292134 E + 00

b_4 = -4.044820889297 E - 01

b_5 = 5.352391623039 E - 02

b_6 = -4.317451841436 E - 03

b7 = 1.918499873454 E - 04

b8 = -3.591779705491 E - 06

Reaction 10: Dissociation into H(1s) + H^+ due to electron collision with H_2^+

Coefficients:

b_0 = -1.781416067709 E + 01

b_1 = 2.277799785711 E + 00

b_2 = -1.266868411626 E + 00

b_3 = 4.296170447419 E + 01

b_4 = -9.609908013189 E - 02

b_5 = 1.387958040699 E - 02

b_6 = -1.231349039470 E - 03

b_7 = 6.042383126281 E - 05

b_8 = -1.247521040900 E - 06

Reaction 11: Dissociation into H(2) + H^+ due to electron collision with H_2^+

Coefficients:

b_0 = -3.408905929046 E + 01

b_1 = 1.573560727511 E + 01

b_2 = -6.992177456733 E + 00

b_3 = 1.852216261706 E + 00

b_4 = -3.130312806531 E - 01

b_5 = 3.383704123189 E - 02

b_6 = -2.265770525273 E - 03

b_7 = 8.565603779673 E - 05

b_8 = -1.398131377085 E - 06

Reaction 12: Dissociation into H(1) + H(n ≥ 2) due to electron collision with H_2^+

Coefficients:

b_0 = -1.670435653561 E + 01

b_1 = -6.035644995682 E - 01

b_2 = -1.942745783445 E - 08

b_3 = -2.005652284492 E - 07

b_4 = 2.962996104431 E - 08

b_5 = 2.134293274971 E - 08

b_6 = -6.353973401838 E - 09

b_7 = 6.152557460831 E - 10

b_8 = -2.025361858319 E - 11

3.4. Results and discussion

The rate coefficients and mean energy losses and gains of individual reactions that are used in the calculations are taken from Janev et al /35/.

Eqn.(3.9) can be written as

$$\frac{d}{dt}n_{H_2}(1) = -(D_{H+H} + D_{H+H'} + D_{H'+H'})n_e n_{H_2}(1) \qquad (3.13)$$

where D_{H+H}, $D_{H+H'}$ and $D_{H'+H'}$ are effective rate coefficients for the dissociation of :f. H_2 into two neutral atoms, atom and ion, and two ions respectively given by

$$D_{H+H} = 0.229[C(1,2) + C(1,4)] + 0.00912C(1,3) + \sum_{q=5}^{8} C(1,q) + R_d \qquad (3.14)$$

$$D_{H+H'} = S'(1) + R_b + R_c \qquad (3.15)$$

$$D_{H'+H'} = R_a \qquad (3.16)$$

These effective rate coefficients are shown in fig.(8).

The rate coefficients for the production of individual hydrogen atoms in the various quantum levels are:

For H(1),

2 {0.229 (C(1,2)+C(1,4)) + 0.00912 C(1,3) + C(1,5) } + C(1,6) +
C(1,8) + S' (1) + R_b + R_d

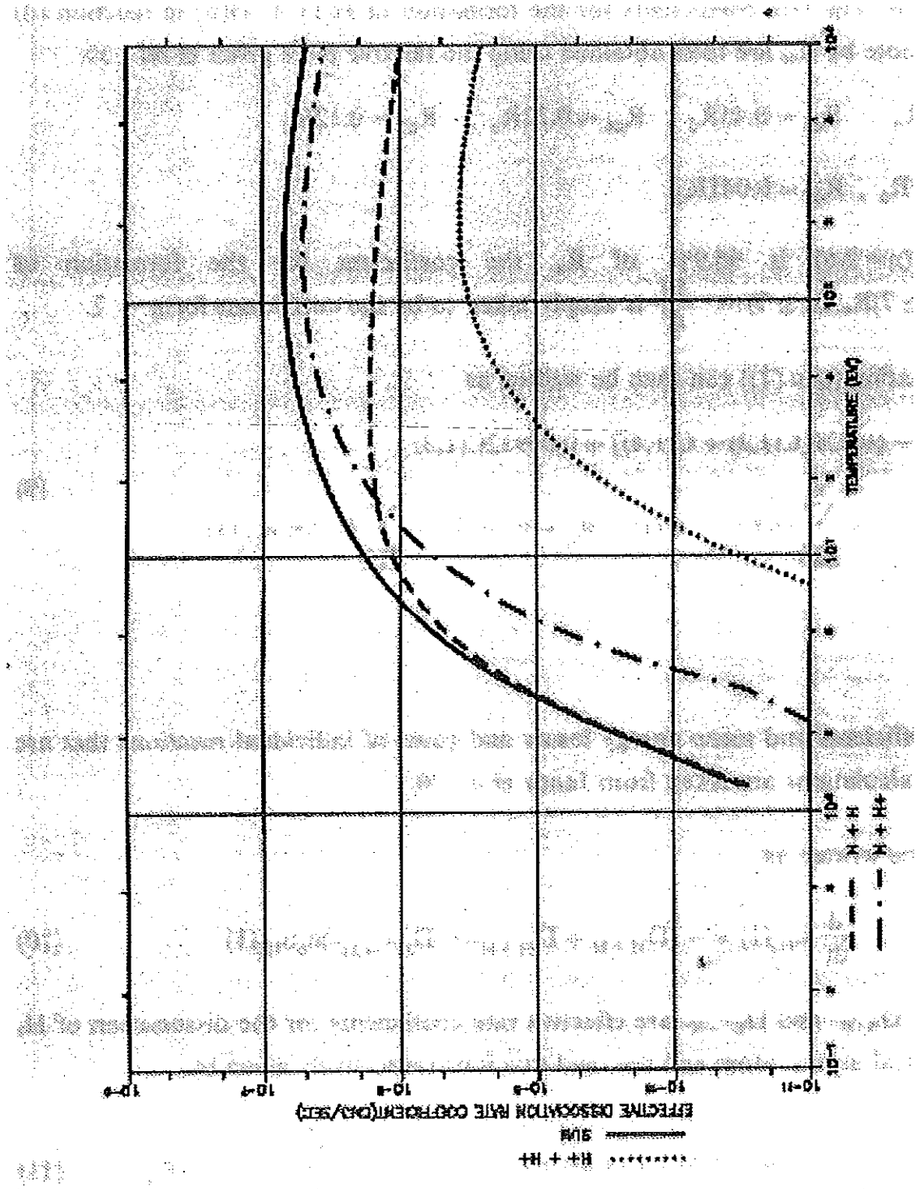

Fig. 8 Effective dissociation rate coefficients

For H(2),

$2C(1,7) + C(1,6) + R_c + R_{d2}$

For H(3),

$C(1,8) + R_{d3}$

For H ($n \geq 4$) , the rate coefficients are simply R_{dn} . See Fig.(9).

These coefficients can for instance be introduced as source terms in a collisional radiative model for hydrogen atom.

Fig.9: Rates of production of neutral atoms

The rates of average electronic energy loss (ΔE^-) and average atomic and ionic energy gain (ΔE^+) per dissociation of H_2 into a pair of atoms (and/or) ions are

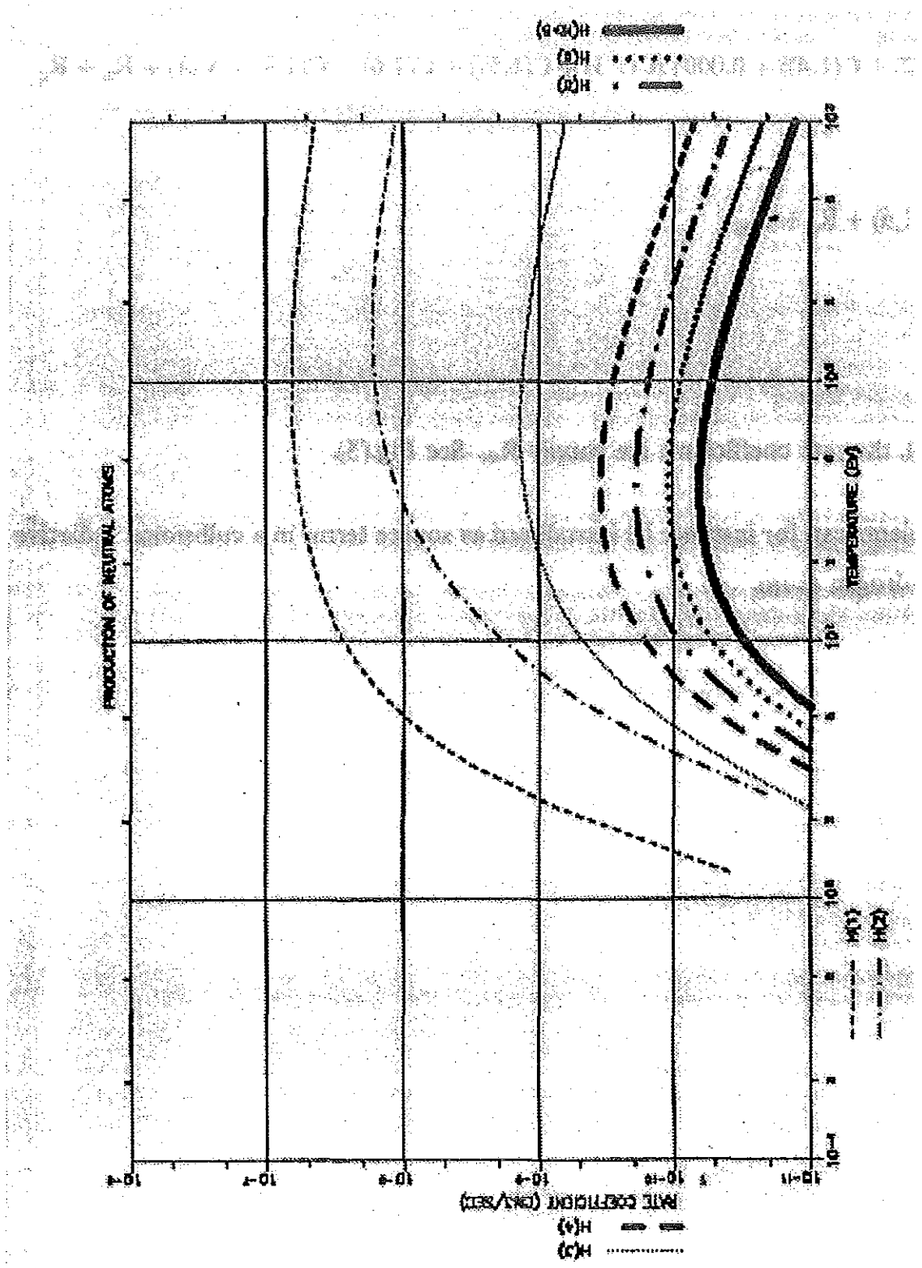

Fig. 9: Rates of production of neutral atoms

$$\frac{\Delta E^{\pm}}{dissociation} = \frac{\sum_{q=2}^{8} C(1,q)\Delta_q^{\pm} + S(1)\Delta E_s^{-} + S'(1)\Delta E_{s'}^{\pm} + \sum_{1=a,b,c} R_1 \Delta E_1^{\pm}}{D_{H+H} + D_{H+H'} + D_{H'+H'}} \qquad (3.17)$$

ΔE_q^- is mean electronic energy transferred in exciting a neutral molecule from the ground to electronic state q and ΔE_q^+ is mean energy taken by the product atoms or ions. Since excitations of $B\Sigma^+_u$, $C\Pi_u$ and $E,F\,\Sigma^+_g$ are followed by radiation, $\Delta E_q^+ = 0$ for q = 2, 3 and 4; and

$\Delta E_2^- = 12.1eV$, $\Delta E_3^- = 12.4eV$, $\Delta E_4^- = 12.7eV$, $\Delta E_5^- = 10eV$

$\Delta E_6^- = 15.3eV$, $\Delta E_7^- = 34.6eV$, $\Delta E_8^- = 21.5eV$

$\Delta E_5^+ = 6.0eV$, $\Delta E_6^+ = 0.6eV$, $\Delta E_7^+ = 9.7eV$, $\Delta E_8^+ = 5.0eV$

ΔE_s^-, is average ionization energy, $\Delta E_s^- = 15.4$. eV. $\Delta E_{s'}^-$ is average electronic energy loss in the direct dissociative ionization, $\Delta E_{s'}^- = 33.6$ eV. The corresponding atomic and atomic ion energy gain is $\Delta E_{s'}^+ = 15.6$ eV. These values depend on the energy of the incident elctron; but the net energy loss is 18 eV.

The mean energy losses and gains in reactions (a) - (c) are

$\Delta E_a^- = 15.5eV$, $\Delta E_b^- = 10.5eV$, $\Delta E_c^- = 17.5eV$

$\Delta E_a^+ = 0.8eV$, $\Delta E_b^+ = 8.6eV$, $\Delta E_c^+ = 3.0eV$

In reaction (d) an electron combines with a molecular ion and two neutral atoms are formed, one in the ground state and the other excited. This reaction has maximum cross section at very low energy and it can be undertaken by the slowest electrons. The energy loss and gain in this reaction are not considered separately. However the net energy loss is $\frac{Ry}{n^2}$ /35/ where Ry is the Rydberg energy and n is the principal quantum number of the excited atom.

Thus the rate of net energy loss per dissociation is

$$(\Delta E^- - \Delta E^+) + \frac{\sum_{n=2}^{7} R_{dn} \frac{Ry}{n^2}}{D_{H+H} + D_{H+H'} + D_{H'+H'}} \qquad (3.15)$$

See fig.10

Fig.10: Rate of energy loss per dissociation

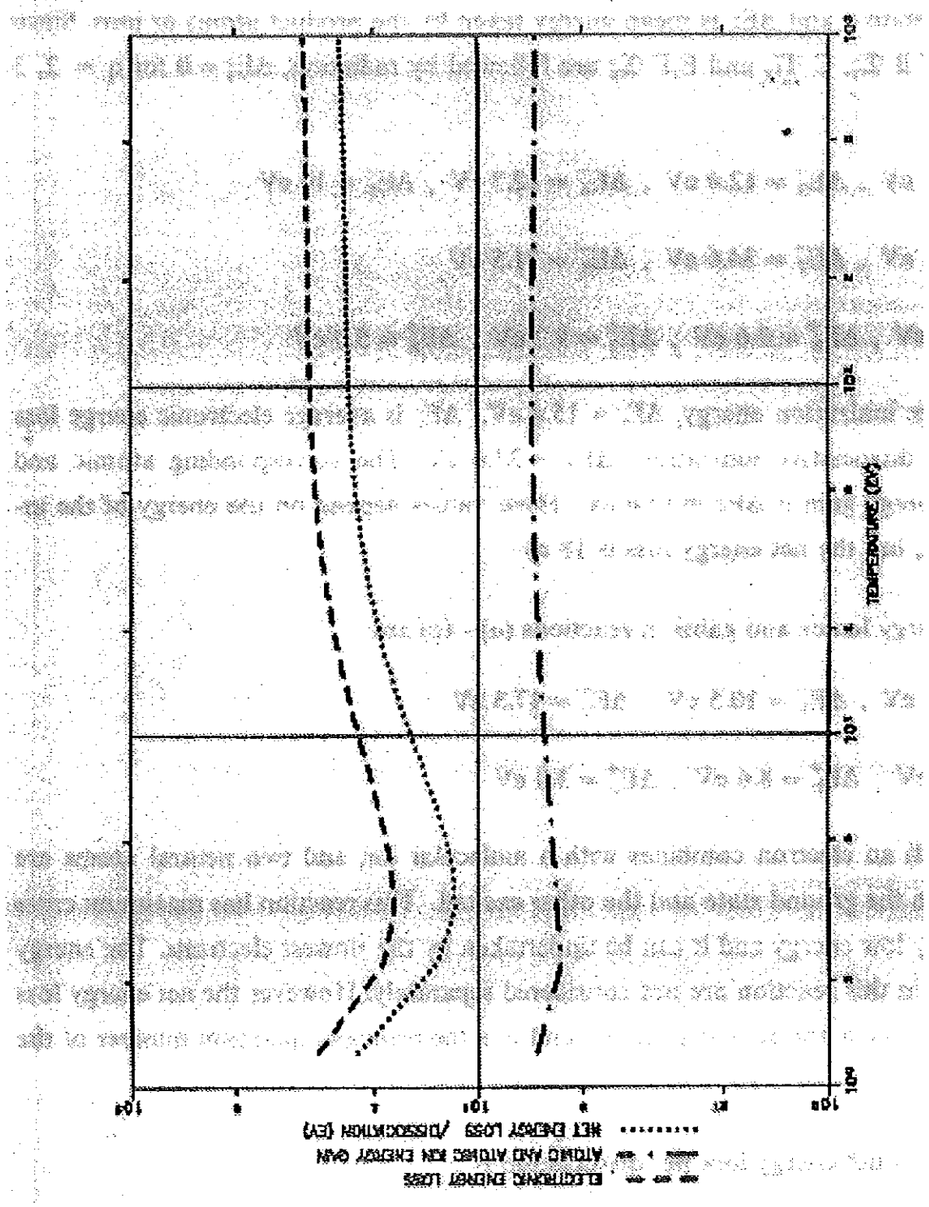

Fig. 6: Rate of energy loss per dissociation

Briefly, the effective dissociation and dissociative ionization rate coefficients in fig. 8 show the extent of production of new pair of atoms or(and) atomic ions from hydrogen molecules. We see that the production of two neutral atoms is dominant at lower temperature while that of one atom and another atomic ion is more significant after the ionization limit of the molecules is reached. This is because the electronic states that dissociate into two atoms are excited at comparatively smaller impact energies. Dissociative ionization into two atomic ions is small; it is indeed by about two orders of magnitude less for a wide range of temperature. Therefore it is not much importrant in the edge plasma where the temperature is low.

The rate coefficients for the production of individual atoms in the various principal quantum levels, shown in fig. 9 can be introduced as production terms in a collisional radiative model for hydrogen atoms. Thus the rate equations for collisional radiative processes of H_2 molecules and H atoms are coupled to each other. A detailed analysis of the subject should therefore solve the coupled equations of the two models simultaneously.

The net energy loss rate in fig. 10 shows the average energy loss through radiation and excitation of the dissociative states whenever a pair of atoms (and/or) is produced. It should be more accurate than the electronic energy loss and atomic(and ionic) energy gain, since it does not depend on the energy of the incident electron while the later do. This energy loss rate can very significantly contribute to the cooling down of the plasma particularly in dense plasmas.

Electron collision with excited molecules is neglected based on the fact that all excited molecules have very short lifetimes. We could not however check the effects of its inclusion because of the lack of molecular data for such process. Neverthless we expect that it would slightly change our calculations and could particularly have more effect in dense plasmas.

The power lost due to electron collisions with H_2 molecules available in the divertor region is estimated by

$$D\, n_e n_{H_2}\, (1)\, \Delta E\, V$$

where D is effective rate coefficient of dissociation, ΔE is the net energy lost per dissociation, and V is the volume of the divertor.

Experimental measurements show that less than 20 - 30 per cent of the heating power in beam heated discharges reaches the neutralizer plates in the divertor /1/. In beam heated discharges the power may be as high as 5 - 6 MW. Now we discuss the possibility that the dissociation of hydrogen molecules can account for the missing power.

The average energy loss per dissociation is about 27 ev for a large temperature range. For effective dissociation rate of 10^{-8} cm^3 s^{-1} order (see fig.6), 10^{13} cm^{-3} electron density and the same order of molecular density, and 10^2 cm^3 divertor volume (which is about the volume of the neutralizing divertor) the molecules account for the missing power.

SUMMARY

The ionization and recombination rate coefficients of a plasma are effectively functions of the density of the plasma electrons which induce the ionization reactions. This dependence on electron density is because of the possibility of ionization through multistep excitations which are more significant in low temperature plasmas where the energy of the free electrons is not enough to ionize atoms directly from the ground state/

The energy of electrons lost to ionize the atoms and due to radiation can not be avoided in optically thin laboratory plasmas. This is because optical radiation has long path length so that the photons emitted escape from the plasma before reabsorption in small size laboratory plasmas. This energy loss rate per ionization is bigger in low density plasmas because an atom excited to a higher quantum level is more probable to decay radiatively to lower levels than to be ionized through further electron collisions. The corresponding power loss can be estimated by multiplying this loss rate by the rate of ionization and the volume of the plasma.

The hydrogen molecules produced in the wall of the Tokamak vessel play a role of plasma cooling. This cooling has both positive and negative effects. The positive effect is the thermal equilibration of the scrape off plasma. This reduces the potential of the plasma boundary particles to escape from the magnetic confinement thus minimizing the heat load on plasma vessel components, The negative effect is the reduction of the total energy content of the plasma which is spent in the dissociation of the molecules. This energy loss rate may account for the missing heating power in the diverter region. The rates of productions of atoms and ions from the dissociation of the molecules have to be introduced as source terms in the collisional radiative model for hydrogen atoms for a better

treatment of the problem; and the two collisional radiative models for hydrogen atoms and for hydrogen molecules are not practically independent.

Appendix A

Fortran Programme for the collisional radiative model for hydrogen atoms

This Fortran programme computes effective ionization, recombination and energy loss rates in the collisional radiative model for hydrogen atoms. It displays all the figures shown in chapter 2.

```
      PROGRAM HATOM
      PARAMETER (NDISK=26)
      COMMON /CANGE/
     R XMULT(NDISK),AJM2(NDISK),
     R C(NDISK,NDISK),R(NDISK,NDISK),SGP(NDISK),
     R S,CF,F,DF,CFGG2,RFGG2,EREDUC
C
      DIMENSION DN(NDISK),XTE(101),YP(101),CRVTE(5,101),DNE(5),
     .          CRVTB(5,101),CRVEI(5,101),XP(6)
      CHARACTER*48 TX1(14),TX2(14),TX3(14),TX4(14)
      DATA TX1/'#H(N=1)+E -> H+                                 ',
     .         '              ELECTRON TEMPERATURE (EV)         ',
     .         '#H(N=2)+E -> H+                                 ',
     .         '                                                ',
     .         '#H(N=5)+E -> H+                                 ',
     .         '                                                ',
     .         '#H(N=10)+E -> H+                                ',
     .         '#H(N=20)+E -> H+                                ',
     .         '                                <SV> (CM**3/SEC)',
     .       3*'                                                ',
     .         'RATE COEFFICIENTS FOR ELECTRON IMPACT IONIZATION',
     .         ' OF H-ATOMS FROM GROUNDSTATE AND EXCITED LEVELS '/
      DATA TX2/'#NE=1.E8 -CM**-3                                ',
     .         '              ELECTRON TEMPERATURE (EV)         ',
     .         '#NE=1.E12 CM**-3                                ',
     .         '                                                ',
     .         '#NE=1.E14 CM**-3                                ',
     .         '                                                ',
     .         '#NE=1.E15 CM**-3                                ',
     .         '#NE=1.E16 CM**-3                                ',
     .         '                                <SV> (CM**3/SEC)',
     .       3*'                                                ',
     .         'RATE COEFFICIENTS FOR ELECTRON IMPACT IONIZATION',
     .         ' OF H-ATOMS INCLUDING "MULTISTEP EFFECTS"       '/
     DATA TX3/'#NE=1.E8  CM**-3                                 ',
     .         '              ELECTRON TEMPERATURE (EV)         ',
     .         '#NE=1.E12 CM**-3                                ',
     .         '                                                ',
     .         '#NE=1.E14 CM**-3                                ',
     .         '                                                ',
     .         '#NE=1.E15 CM**-3                                ',
     .         '#NE=1.E16 CM**-3                                ',
     .         '                                   EV/IONIZATION',
     .       3*'                                                ',
     .         'ENERGY LOSS PER IONIZATION                      ',
     .         '                                                '/
     DATA TX4/'#NE=1.E8  CM**-3                                 ',
     .         '              ELECTRON TEMPERATURE (EV)         ',
     .         '#NE=1.E12 CM**-3                                ',
     .         '                                                ',
```

```
     .         '#NE=1.E14 CM**-3                                    ',
     .         '                                                    ',
     .         '#NE=1.E15 CM**-3                                    ',
     .         '#NE=1.E16 CM**-3                                    ',
     .         '                                        (CM**3/SEC) ',
     .       3*'                                                    ',
     .         'EFFECTIVE RECOMBINATION RATE                        ',
     .         '                                                    '/
      DATA DNE/1.E8,1.E12,1.E14,1.E15,1.E16/
      EIONH=13.6
C
      N=101
      TEEND=ALOG10(1000.)
      DTE=TEEND/FLOAT(N-1)
      DO 1 J=1,N
1     XTE(J)=10.**((J-1)*DTE)
C
      DN(1)=1.
      DENEIN=1.
      FAC=0.
c     FAC=1.
      DO 10 I=1,5
        DO 20 J=1,N
          CALL ANGE(NDISK,XTE(J),DNE(I),DNE(I),DN,FAC,1)
          IF (I.EQ.1.AND.J.LE.10) WRITE (6,'(1X,A4/(1X,1P,5E12.4))')
     .                                  ' DN ',(DN(II),II=1,NDISK)
          CRVTE(1,J)=C(1,1)*CFGG2*DENEIN
          CRVTE(2,J)=C(2,2)*CFGG2*DENEIN
          CRVTE(3,J)=C(5,5)*CFGG2*DENEIN
          CRVTE(4,J)=C(10,10)*CFGG2*DENEIN
          CRVTE(5,J)=C(20,20)*CFGG2*DENEIN
          PC=0.
          DO 15 NP=1,NDISK
15          PC=PC+DN(NP)
C
          PC=1.
          IF (FAC.EQ.1) GOTO 25
          CADD=0.
          DO 16 NP=1,NDISK
16          CADD=CADD+DN(NP)/PC*C(NP,NP)*CFGG2
          CRVTB(I,J)=CADD*DENEIN
          CRVEI(I,J)=0.
          DO 17 ID1=2,NDISK
          DO 17 ID2=1,ID1-1
            CRVEI(I,J)=CRVEI(I,J)+RFGG2*R(ID1,ID2)*DN(ID1)/PC*
     .                 (1./ID2**2-1./ID1**2)
17        CONTINUE
          CRVEI(I,J)=CRVEI(I,J)*EIONH/(CRVTB(I,J)*DNE(I))+EIONH
C
          GOTO 20
```

```
C
25        CONTINUE
          DNEF=DNE(I)/F
          CADD=1./SGP(1)*(R(1,1)+DNEF*C(1,1))
C         WRITE (6,*) 'CADD ',CADD
          DO 27 ID1=2,NDISK
            RH=DN(ID1)*SGP(ID1)/DNEF/DNE(I)
C           WRITE (6,*) I,J,ID1,DN(ID1),RHO
27          CADD=CADD+1./SGP(ID1)*(R(ID1,ID1)+DNEF*C(ID1,ID1))*(1.-RH)
          CRVTB(I,J)=CADD*CFGG2*DENEIN*DENEIN
          TJ=XTE(J)
C         WRITE (6,*) 'I,J,DNE(I),TJ,R ',I,J,DNE(I),TJ,CRVTB(I,J)
20      CONTINUE
C


C  PLOT IONISATION RATES OF GROUND AND EXCITED STATES
                NEND=N/5
          IF (I.EQ.1) THEN
          CALL GRSTRT (35,8)
          CALL GRSCLC (1.,2.,39.5,28.7)
C          DO 30 J=1,N
C            ZLN=ALOG(XTE(J))
C30          CRVTE(1,J)=CIO(ZLN)
C  SYMBOL:
          DO 40 K=1,5
            II=0
            DO 41 J=1,N,NIND
              II=II+1
              XP(II)=XTE(J)
41            YP(II)=CRVTE(K,J)
            CALL KURVEF (XP,YP,II,K+1)
40        CONTINUE
C  CURVE:
          DO 43 K=1,5
            DO 42 J=1,N
              YP(J)=CRVTE(K,J)
42          CALL KURVEF (XTE,YP,N,16)
43        CONTINUE
          CALL GRBLD (30.,20.,-101,-101,666.,666.,666.,666.,10)
          CALL GRLGND (TX1)
        ENDIF
10    CONTINUE
C
C  PLOT EFFECTIVE IONISATION RATES AND ENERGY LOSS
C  SYMBOL
      DO 50 K=1,5
      II=0
      DO 55 J=1,N,NIND
      II=II+1


65
```

```
      XP(II)=XTE(J)
55    YP(II)=CRVTB(K,J)
      CALL KURVEF (XP,YP,II,K+1)
50    CONTINUE
C
C  LINES
      DO 51 K=1,5
      DO 56 J=1,N
56    YP(J)=CRVTB(K,J)
      CALL KURVEF (XTE,YP,N,16)
51    CONTINUE
      YMIN=666.
      YMAX=666.
      IF (FAC.EQ.1.) THEN
        YMIN=1.E-16
        YMAX=1.E-11
      ENDIF
      CALL GRBLD (30.,20.,-101,-101,666.,666.,YMIN,YMAX,10)
      IF (FAC.EQ.0.) CALL GRLGND (TX2)
      IF (FAC.EQ.1.) CALL GRLGND (TX4)
C
C  ENERGY LOSS:
IF (FAC.EQ.1) GOTO 100
C  SYMBOL
      DO 60 K=1,5
      II=0
      DO 65 J=1,N,NIND
      II=II+1
      XP(II)=XTE(J)
65    YP(II)=CRVEI(K,J)
      CALL KURVEF (XP,YP,II,K+1)
60    CONTINUE
C  LINIES
      DO 61 K=1,5
      DO 66 J=1,N
66    YP(J)=CRVEI(K,J)
      CALL KURVEF (XTE,YP,N,16)
61    CONTINUE
      CALL GRBLD (30.,20.,-101,-101,666.,666.,1.E1,1.E4,10)
      CALL GRLGND (TX3)
100   CALL GREND
      STOP
      END
FUNCTION CIO(AL)
C   MAXWELLIAN RATES, AL=LN(KT), FIT FROM JANEV ET AL
      DIMENSION CFION(9)
C   E + H --> H+ + 2E
      DATA CFION
     ./-3.271397E+01,1.353656E+01,-5.739329E 00,1.563155E 00,
     . -2.877056E-01,3.482560E-02,-2.631976E-03,1.119544E-04,


66
```

```
     . -2.039150E-06/
      EXPO=CFION(9)
      DO 10 II=1,8
      , IF8=9-II
        EXPO=EXPO*AL+CFION(IF8)
10    CONTINUE
      CIO=EXP(EXPO)
      RETURN
      END
C
C*DK ANGE
      SUBROUTINE ANGE (NP,TE,DE,DI,DN,FAC,NMACH)
C INPUT
C  NP   = NUMBER OF DISCRETE LEVELS
C  TE   = ELECTRON TEMP.(EV)
C  DE   = ELECTRON DENSITY (1/CM**3)
C  DI   = ION DENSITY, HYDROGEN (1/CM**3)
C  DN(1) = DENSITY OF NEUTRAL HYDROGEN, GROUND STATE (1/CM**3)
C  FAC = 0.  ONLY COPPLING TO CONTINUUM
C  FAC = 0.5 WITH   - " -
C  FAC = 1.  NO     - " -
C OUTPUT
C  DN(2) -- DN(NP) : DENSITY OF EXCITED LEVELS
      PARAMETER (NDISK=26)
      COMMON /CANGE/
     R XMULT(NDISK),AJM2(NDISK),
     R C(NDISK,NDISK),R(NDISK,NDISK),SGP(NDISK),
     R S,CF,F,DF,CFGG2,RFGG2,EREDUC
C
      DIMENSION DN(NDISK),DELTA(NDISK),EPS(NDISK),
     .          DELT(NDISK,NDISK),A(NDISK,NDISK+2),
     .          B(NDISK,2),WKAREA(NDISK*NDISK+3*NDISK)
      IF (NP.GT.NDISK) THEN
        WRITE (6,*) 'TOO MANY LEVELS REQUIRED IN SUBR. ANGE'
        WRITE (6,*) 'STORAGE ONLY PROFIDED FOR NP<=NDISK'
        CALL EXIT
      ENDIF
C
      FACNM    = 1./(FAC*FAC+(1.-FAC)*(1.-FAC))
      CF       = 2.1285E-8
      F        = 3.69855E17
      DF       = 1./F
      ALF      = 2.44166E-6
      RFGG2    = 2.*F*CF
      CFGG2    = 2.*CF
      CF2      = CFGG2
      DNPP2    = 1./FLOAT((NP+1)**2)
      EREDUC   = 13.6*(1.-DNPP2)
      S        = EREDUC/TE
      AS       = ALF*SQRT(S**3)
```

```
C
      CALL CRAIE (NP)
C  MAHN-WELGE 3.6.A, I=1
      S11       = S*(1.-DNPP2)
      EXPM      = EXP(-S11)
      SGP(1)    = EXPM/AS
DO 1.   M = 2,NP
      S1          = 0.
      S2          = 0.
      DO 37    K = 1,NP
   37 DELTA(K)   = 0.
      I           = M
      I1          = I-1
      P           = I
      DP          = 1./P
      P2          = P*P
      DP2         = DP*DP
      SP          = S*DP2
      SP1         = SP*(1.-P2*DNPP2)
      EXPM        = EXP(-SP1)
C  MAHN-WELGE 3.6.A, I>1
      SGP(I)      = DP2*EXPM/AS
DO 35   K = 1,I1
      Q           = K
      DQ          = 1./Q
      Q2          = Q*Q
      DQ2         = DQ*DQ
      SR          = SP*(1.-P2*DQ2)
      EXPM        = EXP(-SR)
      S1          = S1+Q2*DP2*EXPM*C(K,I)
      S2          = S2+R(I,K)
35    DELTA(K)    = CF2*DE*C(K,I)
S2          = S2*F
      I1          = I+1
      S4          = 0.
      DO 36    K = I1,NP
      Q           = K
      DQ          = 1./Q
      Q2          = Q*Q
      DQ2         = DQ*DQ
      SQ          = S*DQ2
      SR          = SQ*(1.-Q2*DP2)
      EXPM        = EXP(-SR)
C  MAHN-WELGE 3.6.B
      SQP         = P2*DQ2*EXPM
      S4          = S4+C(I,K)
   36 DELTA(K)    = +CF2*(DE*SQP*C(I,K)+F*R(K,I))
C
   34 DELTA(I)    = -CF2*(DE*(S1+S4+C(I,I))+S2)
   EPS(I)      = CF2*DE*DI*(DE*DF*C(I,I)+R(I,I))/SGP(I)
```

```
      DO 1     N = 1,NP
    1 DELT(M,N) = DELTA(N)
      NPM=NP-1
      DO 2 M=1,NPM
        M1=M+1
        DO 3 N=1,NPM
          N1=N+1
    3     A(M,N)=DELT(M1,N1)
        B(M,1)=-(1.-FAC)*DELT(M1,1)*DN(1)-FAC*EPS(M1)
        B(M,1)=B(M,1)*FACNM
    2   A(M,NP)=B(M,1)
C   SOLVE LINEAR EQUATION  AND RETURN RESULT
      IDGT=5
        CALL LEQT2F (A,1,NPM,NDISK,B,IDGT,WKAREA,IER)
      DO 4 N = 1,NPM
      4   DN(N+1)     = B(N,1)
        RETURN
      END
C*DK CRAIE
      SUBROUTINE CRAIE (NP)
      PARAMETER (NDISK=26)
      COMMON /CANGE/
     R XMULT(NDISK),AJM2(NDISK),
     R C(NDISK,NDISK),R(NDISK,NDISK),SGP(NDISK),
     R S,CF,F,DF,CFGG2,RFGG2,EREDUC
      REAL MMDEI
      DIMENSION G(3),E(7)
C
      DO 30    I = 1,NP
      I1         = I+1
      P          = I
      P2         = P*P
      P3         = P2*P
      P4         = P3*P
      DP         = 1./P
      DP2        = DP*DP
      DP3        = DP2*DP
      DP5        = DP3*DP2
      SP         = S*DP2
      IF (I-2) 40,41,42
   40 G(1)       = 1.133
      G(2)       = -0.4059
      G(3)       = 0.07014
      RI         = 0.45
      BI         = -0.603
      GO TO 43
   41 G(1)       = 1.0785
      G(2)       = -0.2319
      G(3)       = 0.02947
      RI         = 1.94*DP**(1.57)
```

```
      BI        = (4.-18.63*DP+36.24*DP2-28.09*DP3)*DP
      GO TO 43
   42 G(1)      = 0.9935+0.2328*DP-0.1296*DP2
      G(2)      = -(0.6282-0.5598*DP+0.5299*DP2)*DP
      G(3)      = (0.3847-1.181*DP+1.47*DP2)*DP2
      RI        = 1.94*DP**(1.57)
      BI        = (4.-18.63*DP+36.24*DP2-28.09*DP3)*DP
   43 PM2       = (NP+1)**2
      XP1       = (1.-P2/PM2)
      DX1       = 1./XP1
      DX2       = DX1*DX1
      SP1       = XP1*SP
      DS1       = 1./SP1
      ZP1       = XP1*(RI+SP)
      DZ1       = 1./ZP1
C
C  SET ARRAY E(7)
C
      EXPMX     = EXP(-ZP1)
      E(1)      = EXPMX/ZP1
      XX        = ZP1
C**   E(2)      = MMDEI(2,XX,IER)
      E(2)      = E1(XX)
      E(3)      = EXPMX-ZP1*E(2)
      EXPMX     = EXP(-SP1)
      E(4)      = EXPMX/SP1
      XX        = SP1
C**   E(5)      = MMDEI(2,XX,IER)
      E(5)      = E1(XX)
      E(6)      = EXPMX-SP1*E(5)
      E(7)      = (EXPMX-SP1*E(6))/2.
   RS         = G(1)*E(5)+G(2)*E(6)+G(3)*E(7)
      R(I,I)    = RS*0.5*DP5*DX1
C  AP1=G(1)*DX1**3/3+G(2)*DX1**4/4+G(3)*DX1**5/5
      AP1       = AP1*1.96*P
      EZZ       = E(1)-2.*E(2)+E(3)
      EZS       = E(4)-2.*E(5)+E(6)
      BP1       = (3.+2.*DX1+BI*DX2)*2./3.*P2*DX1
      C(I,I)=(AP1*(E(5)*DS1-E(2)*DZ1)+(BP1-AP1*ALOG(2.*P2*DX1))*
     .       (EZS-EZZ))*P*SQRT(SP1**3*DX1)
C
   DO 38   J = I1,NP
      DQ        = 1./FLOAT(J)
      DQ2       = DQ*DQ
      DQ3       = DQ2*DQ
      DQ5       = DQ3*DQ2
      XR        = 1.-P2*DQ2
      DXR       = 1./XR
      DX2       = DXR*DXR
      DX4       = DX2*DX2


70
```

```
      SR        = SP*XR
      DSR       = 1./SR
      ZR        = SR+RI*XR
      DZR       = 1./ZR
      GS        = G(1)+G(2)*DXR+G(3)*DX2
      R(J,I)    = GS*DP*DQ5*DXR
C
      AR        = 3.92*P3*DQ3*DX4*GS
      BR        = 4.*P4*DQ3*DX2*(1.+4./3.*DXR+BI*DX2)
      EXPMX     = EXP(-SR)
      XX        = SR
C**   E(1)      = MMDEI(2,XX,IER)
      E(1)      = E1(XX)
      E(2)      = EXPMX-SR*E(1)
      EXPMX     = EXP(-ZR)
      XX        = ZR
C**   E(3)      = MMDEI(2,XX,IER)
      E(3)      = E1(XX)
      E(4)      = EXPMX-ZR*E(3)
      ASW       = SR*SR*SR
      C(I,J)    = P*SQRT(ASW*DXR)*(AR*(E(1)*(0.5+DSR)-E(3)*(0.5+DZR))
     .           +(BR-AR*ALOG(2.*P2*DXR))*(E(2)*DSR-E(4)*DZR))
   38 CONTINUE
30 CONTINUE
      RETURN
      END
*DK EIRMAT
      REAL FUNCTION MMDEI (IOPT,S,IER)
      X=S
      Y=ABS(X)
      Z=0.25D+0*Y
      IF(Z-1.0D0)11,11,12
   11
VALUE=((((((((((((((((((-.483702D-8*Z+.2685377D-7)*Z-.11703642D-
     1
6)*Z+.585911692D-6)*Z-.2843937873D-5)*Z+.1284394756D-4)*Z-.547380
     1
648948D-4)*Z+.21992775413732D-3)*Z-.8290046678016D-3)*Z+.00291878
     1
85699858)*Z-.0095523774824170)*Z+.028895941356815)*Z-.08026651003
     1 2735)*Z+.20317460364863)*Z-.46439909294939)*Z+.948148
     1 1480886)*Z-1.706666666669
     1
)*Z+2.6666666666702)*Z-3.5555555555546)*Z+3.999999999999
     1 4)*Z-3.9999999999996)*Z+.57721566490143+ALOG(Y)
      VALUE=-VALUE
      GO TO 13
   12 Z=1.0D0/Z
      VALUE=((((((((((((((((((-.77769007188383D-3*Z+.84295295893998D-2
```

```
     1
)*Z-.04272827083185)*Z+.13473041266261)*Z-.29671551148)*Z+.486188
     1
06480858)*Z-.61743468824936)*Z+.62656052544291)*Z-.52203502518727
     1 )*Z+.36771959879483)*Z-.22727998629908)*Z+.12965447884319)*Z
     1 -.72886262704894D-1)*Z+.043418637381012)*Z-.29244589614262D-1
     1 )*Z+.23433749581188D-1)*Z-.023437317333964)*Z+.03124999448124
     1 )*Z-.062499999910765)*Z+.24999999999935)*Z-.20933859981036D-14
      VALUE=VALUE*EXP(-Y)
   13 VAL=VALUE
      MMDEI=VAL
      RETURN
      END
C   IMSL ROUTINE NAME   - UERTST
C
C-----------------------------------------------------------------------
-
C
C   COMPUTER            - IBM/SINGLE
C
C   LATEST REVISION     - JANUARY 1, 1978
C
C   PURPOSE             - PRINT A MESSAGE REFLECTING AN ERROR CONDITION
C
C   USAGE               - CALL UERTST (IER,NAME)
C
C   ARGUMENTS    IER    - ERROR PARAMETER. (INPUT)
C                            IER = I+J WHERE
C                              I = 128 IMPLIES TERMINAL ERROR,
C                              I =  64 IMPLIES WARNING WITH FIX, AND
C                              I =  32 IMPLIES WARNING.
C                              J = ERROR CODE RELEVANT TO CALLING
C                                  ROUTINE.
C                NAME   - A SIX CHARACTER LITERAL STRING GIVING THE
C                            NAME OF THE CALLING ROUTINE. (INPUT)
C
C   PRECISION/HARDWARE  - SINGLE/ALL
C
C   REQD. IMSL ROUTINES - UGETIO
C
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                            CONVENTIONS IS AVAILABLE IN THE MANUAL
C                            INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C   REMARKS      THE ERROR MESSAGE PRODUCED BY UERTST IS WRITTEN
C                ONTO THE STANDARD OUTPUT UNIT. THE OUTPUT UNIT
C                NUMBER CAN BE DETERMINED BY CALLING UGETIO AS
C                FOLLOWS..   CALL UGETIO(1,NIN,NOUT).
C                THE OUTPUT UNIT NUMBER CAN BE CHANGED BY CALLING
C                UGETIO AS FOLLOWS..
```

```
C                               NIN = 0
C                               NOUT = NEW OUTPUT UNIT NUMBER
C                               CALL UGETIO(3,NIN,NOUT)
C                     SEE THE UGETIO DOCUMENT FOR MORE DETAILS.
C
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C
C   WARRANTY              - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN
C                           APPLIED TO THIS CODE. NO OTHER WARRANTY,
C                           EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C-----------------------------------------------------------------------
-
C
      SUBROUTINE UERTST (IER,NAME)
C                                     SPECIFICATIONS FOR ARGUMENTS
      INTEGER             IER
      CHARACTER*6 NAME
C                                     SPECIFICATIONS FOR LOCAL VARIABLES
      CHARACTER*6 NAMSET,NAMEQ
      CHARACTER*1 IEQ
      DATA                NAMSET/'UERSET'/
      DATA                NAMEQ/'      '/
C                                     FIRST EXECUTABLE STATEMENT
      DATA                LEVEL/4/,IEQDF/0/,IEQ/'='/
      IF (IER.GT.999) GO TO 25
      IF (IER.LT.-32) GO TO 55
      IF (IER.LE.128) GO TO 5
      IF (LEVEL.LT.1) GO TO 30
C                                     PRINT TERMINAL MESSAGE
      CALL UGETIO(1,NIN,IOUNIT)
      IF (IEQDF.EQ.1) WRITE(IOUNIT,35) IER,NAMEQ,IEQ,NAME
      IF (IEQDF.EQ.0) WRITE(IOUNIT,35) IER,NAME
      GO TO 30
    5 IF (IER.LE.64) GO TO 10
      IF (LEVEL.LT.2) GO TO 30
C                                     PRINT WARNING WITH FIX MESSAGE
      CALL UGETIO(1,NIN,IOUNIT)
      IF (IEQDF.EQ.1) WRITE(IOUNIT,40) IER,NAMEQ,IEQ,NAME
      IF (IEQDF.EQ.0) WRITE(IOUNIT,40) IER,NAME
      GO TO 30
   10 IF (IER.LE.32) GO TO 15
C                                     PRINT WARNING MESSAGE
      IF (LEVEL.LT.3) GO TO 30
      CALL UGETIO(1,NIN,IOUNIT)
      IF (IEQDF.EQ.1) WRITE(IOUNIT,45) IER,NAMEQ,IEQ,NAME
      IF (IEQDF.EQ.0) WRITE(IOUNIT,45) IER,NAME
      GO TO 30
   15 CONTINUE
C                                     CHECK FOR UERSET CALL
```

```
      IF (NAME.NE.NAMSET) GO TO 25
      LEVOLD = LEVEL
      LEVEL = IER
      IER = LEVOLD
      IF (LEVEL.LT.0) LEVEL = 4
      IF (LEVEL.GT.4) LEVEL = 4
      GO TO 30
   25 CONTINUE
      IF (LEVEL.LT.4) GO TO 30
C                                  PRINT NON-DEFINED MESSAGE
      CALL UGETIO(1,NIN,IOUNIT)
      IF (IEQDF.EQ.1) WRITE(IOUNIT,50) IER,NAMEQ,IEQ,NAME
      IF (IEQDF.EQ.0) WRITE(IOUNIT,50) IER,NAME
   30 IEQDF = 0
      RETURN
   35 FORMAT(19H *** TERMINAL ERROR,10X,7H(IER = ,I3,
     1       20H) FROM IMSL ROUTINE ,A6,A1,A6)
   40 FORMAT(36H *** WARNING WITH FIX ERROR  (IER = ,I3,
     1       20H) FROM IMSL ROUTINE ,A6,A1,A6)
   45 FORMAT(18H *** WARNING ERROR,11X,7H(IER = ,I3,
     1       20H) FROM IMSL ROUTINE ,A6,A1,A6)
   50 FORMAT(20H *** UNDEFINED ERROR,9X,7H(IER = ,I5,
     1       20H) FROM IMSL ROUTINE ,A6,A1,A6)
C                                  SAVE P FOR P = R CASE
C                                    P IS THE PAGE NAME
C                                    R IS THE ROUTINE NAME
   55 IEQDF = 1
      NAMEQ = NAME
   65 RETURN
      END
C   IMSL ROUTINE NAME   - UGETIO
C
C-----------------------------------------------------------------------
-
C
C   COMPUTER            - IBM/SINGLE
C
C   LATEST REVISION     - JANUARY 1, 1978
C
C   PURPOSE             - TO RETRIEVE CURRENT VALUES AND TO SET NEW
C                           VALUES FOR INPUT AND OUTPUT UNIT
C                           IDENTIFIERS.
C
C   USAGE               - CALL UGETIO(IOPT,NIN,NOUT)
C
C   ARGUMENTS    IOPT   - OPTION PARAMETER. (INPUT)
C                           IF IOPT=1, THE CURRENT INPUT AND OUTPUT
C                           UNIT IDENTIFIER VALUES ARE RETURNED IN NIN
C                           AND NOUT, RESPECTIVELY.
C                           IF IOPT=2 (3) THE INTERNAL VALUE OF
```

```
C                           NIN (NOUT) IS RESET FOR SUBSEQUENT USE.
C                NIN     - INPUT UNIT IDENTIFIER.
C                            OUTPUT IF IOPT=1, INPUT IF IOPT=2.
C                NOUT    - OUTPUT UNIT IDENTIFIER.
C                            OUTPUT IF IOPT=1, INPUT IF IOPT=3.
C
C   PRECISION/HARDWARE   - SINGLE/ALL
C
C   REQD. IMSL ROUTINES - NONE REQUIRED
C
C   NOTATION             - INFORMATION ON SPECIAL NOTATION AND
C                            CONVENTIONS IS AVAILABLE IN THE MANUAL
C                            INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C   REMARKS      EACH IMSL ROUTINE THAT PERFORMS INPUT AND/OR OUTPUT
C                OPERATIONS CALLS UGETIO TO OBTAIN THE CURRENT UNIT
C                IDENTIFIER VALUES. IF UGETIO IS CALLED WITH IOPT=2 OR
3
C                NEW UNIT IDENTIFIER VALUES ARE ESTABLISHED. SUBSEQUENT
C                INPUT/OUTPUT IS PERFORMED ON THE NEW UNITS.
C
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C   WARRANTY             - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN
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C                            EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C-----------------------------------------------------------------------
-
C
      SUBROUTINE UGETIO(IOPT,NIN,NOUT)
C                                  SPECIFICATIONS FOR ARGUMENTS
      INTEGER             IOPT,NIN,NOUT
C                                  SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER             NIND,NOUTD
      DATA                NIND/5/,NOUTD/6/
C                                  FIRST EXECUTABLE STATEMENT
      IF (IOPT.EQ.3) GO TO 10
      IF (IOPT.EQ.2) GO TO 5
      IF (IOPT.NE.1) GO TO 9005
      NIN = NIND
      NOUT = NOUTD
      GO TO 9005
    5 NIND = NIN
      GO TO 9005
   10 NOUTD = NOUT
 9005 RETURN
      END
C   IMSL ROUTINE NAME   - LEQT2F
C
```

```
C-----------------------------------------------------------------------
-
C
C   COMPUTER            - IBM/SINGLE
C
C   LATEST REVISION     - JANUARY 1, 1978
C
C   PURPOSE             - LINEAR EQUATION SOLUTION - FULL STORAGE
C                           MODE - HIGH ACCURACY SOLUTION
C
C   USAGE               - CALL LEQT2F (A,M,N,IA,B,IDGT,WKAREA,IER)
C
C   ARGUMENTS    A      - INPUT MATRIX OF DIMENSION N BY N CONTAINING
C                           THE COEFFICIENT MATRIX OF THE EQUATION
C                           AX = B.
C                M      - NUMBER OF RIGHT-HAND SIDES. (INPUT)
C                N      - ORDER OF A AND NUMBER OF ROWS IN B. (INPUT)
C                IA     - ROW DIMENSION OF A AND B EXACTLY AS SPECIFIED
C                           IN THE DIMENSION STATEMENT IN THE CALLING
C                           PROGRAM. (INPUT)
C                B      - INPUT MATRIX OF DIMENSION N BY M CONTAINING
C                           THE RIGHT-HAND SIDES OF THE EQUATION AX =
B.
C                         ON OUTPUT, THE N BY M MATRIX OF SOLUTIONS
C                           REPLACES B.
C                IDGT   - INPUT OPTION.
C                         IF IDGT IS GREATER THAN 0, THE ELEMENTS OF
C                           A AND B ARE ASSUMED TO BE CORRECT TO IDGT
C                           DECIMAL DIGITS AND THE ROUTINE PERFORMS
C                           AN ACCURACY TEST.
C                         IF IDGT EQUALS 0, THE ACCURACY TEST IS
C                           BYPASSED.
C                         ON OUTPUT, IDGT CONTAINS THE APPROXIMATE
C                           NUMBER OF DIGITS IN THE ANSWER WHICH
C                           WERE UNCHANGED AFTER IMPROVEMENT.
C               WKAREA - WORK AREA OF DIMENSION GREATER THAN OR EQUAL
C                           TO N**2+3N.
C                IER    - ERROR PARAMETER. (OUTPUT)
C                         WARNING ERROR
C                           IER = 34 INDICATES THAT THE ACCURACY TEST
C                             FAILED. THE COMPUTED SOLUTION MAY BE IN
C                             ERROR BY MORE THAN CAN BE ACCOUNTED FOR
C                             BY THE UNCERTAINTY OF THE DATA. THIS
C                             WARNING CAN BE PRODUCED ONLY IF IDGT IS
C                             GREATER THAN 0 ON INPUT. (SEE THE
C                             CHAPTER L PRELUDE FOR FURTHER
DISCUSSION.)
C                         TERMINAL ERROR
C                           IER = 129 INDICATES THAT THE MATRIX IS
C                             ALGORITHMICALLY SINGULAR. (SEE THE
```

```
C                          CHAPTER L PRELUDE).
C                        IER = 131 INDICATES THAT THE MATRIX IS TOO
C                          ILL-CONDITIONED FOR ITERATIVE IMPROVEMENT
C                          TO BE EFFECTIVE.
C
C   PRECISION/HARDWARE   - SINGLE AND DOUBLE/H32
C                        - SINGLE/H36,H48,H60
C
C   REQD. IMSL ROUTINES - SINGLE/LUDATF,LUELMF,LUREFF,UERTST,UGETIO
C                        - DOUBLE/LUDATF,LUELMF,LUREFF,UERTST,UGETIO,
C                            VXADD,VXMUL,VXSTO
C
C   NOTATION             - INFORMATION ON SPECIAL NOTATION AND
C                            CONVENTIONS IS AVAILABLE IN THE MANUAL
C                            INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
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C
C-----------------------------------------------------------------------
-
C
      SUBROUTINE LEQT2F (A,M,N,IA,B,IDGT,WKAREA,IER)
C
      DIMENSION          A(IA,*),B(IA,*),WKAREA(*)
C                                FIRST EXECUTABLE STATEMENT
C                                INITIALIZE IER
      IER=0
      JER=0
      J = N*N+1
      K = J+N
      MM = K+N
      KK = 0
      MM1 = MM-1
      JJ=1
      DO 5 L=1,N
         DO 5 I=1,N
            WKAREA(JJ)=A(I,L)
            JJ=JJ+1
    5 CONTINUE
C                                DECOMPOSE A
      CALL LUDATF (WKAREA(1),A,N,N,IDGT,D1,D2,WKAREA(J),WKAREA(K),
     1   WA,IER)
      IF (IER.GT.128) GO TO 25
      IF (IDGT .EQ. 0 .OR. IER .NE. 0) KK = 1
      DO 15 I = 1,M
C                                PERFORMS THE ELIMINATION PART OF
```

```
C                                  AX = B
      CALL LUELMF (A,B(1,I),WKAREA(J),N,N,WKAREA(MM))
C                                  REFINEMENT OF SOLUTION TO AX = B
      IF (KK .NE. 0)
     *   CALL LUREFF (WKAREA(1),B(1,I),A,WKAREA(J),N,N,WKAREA(MM),IDGT,
     *               WKAREA(K),WKAREA(K),JER)
      DO 10 II=1,N
         B(II,I) = WKAREA(MM1+II)
   10 CONTINUE
      IF (JER.NE.0) GO TO 20
   15 CONTINUE
      GO TO 25
   20 IER = 131
   25 JJ=1
      DO 30 J = 1,N
         DO 30 I = 1,N
            A(I,J)=WKAREA(JJ)
            JJ=JJ+1
   30 CONTINUE
      IF (IER .EQ. 0) GO TO 9005
 9000 CONTINUE
      CALL UERTST (IER,6HLEQT2F)
 9005 RETURN
      END
C   IMSL ROUTINE NAME   - LUREFF
C
C-----------------------------------------------------------------------
-
C
C   COMPUTER            - IBM/SINGLE
C
C   LATEST REVISION     - JANUARY 1, 1978
C
C   PURPOSE             - REFINEMENT OF SOLUTION TO LINEAR EQUATIONS -
C                           FULL STORAGE MODE
C
C   USAGE               - CALL LUREFF (A,B,UL,IPVT,N,IA,X,IDGT,RES,DX,
C                           IER)
C
C   ARGUMENTS    A      - THE COEFFICIENT MATRIX, AX=B, WHERE A
C                           IS N X N. (INPUT)
C                B      - THE RIGHT HAND SIDE, A VECTOR OF SIZE N.
C                           (INPUT)
C                UL     - A GIVEN N X N MATRIX, UL IS THE LU
C                           DECOMPOSITION OF A AS SUPPLIED BY IMSL
C                           ROUTINE LUDATF. (INPUT)
C                IPVT   - A GIVEN VECTOR OF PIVOT INDICES OF SIZE N AS
C                           SUPPLIED BY IMSL ROUTINE LUDATF. (INPUT)
C                N      - ORDER OF A AND UL, AND ALSO THE LENGTH OF
C                           B, IPVT, X, RES, AND DX. (INPUT)
```

```
C               IA      - ROW DIMENSION OF A AND UL EXACTLY AS
C                           SPECIFIED IN THE DIMENSION STATEMENT IN THE
C                           CALLING PROGRAM. (INPUT)
C               X       - AN INPUT VECTOR OF SIZE N, X IS AN ESTIMATE
C                           TO THE SOLUTION OF AX=B. ON OUTPUT, THE
C                           IMPROVED RESULT OVERWRITES THE INPUT VECTOR
C                           X.
C               IDGT    - APPROXIMATE NUMBER OF DIGITS IN THE ANSWER
C                           WHICH WERE UNCHANGED AFTER IMPROVEMENT.
C                           (OUTPUT)
C               RES     - THE RESIDUAL VECTOR OF SIZE N, USED AS A WORK
C                           VECTOR.
C               DX      - A WORK VECTOR OF SIZE N.
C               IER     - ERROR PARAMETER. (OUTPUT)
C                         TERMINAL ERROR
C                           IER=129 INDICATES ITERATIVE IMPROVEMENT
C                             FAILED. MATRIX IS TOO ILL CONDITIONED.
C
C   PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32
C                       - SINGLE/H36,H48,H60
C
C   REQD. IMSL ROUTINES - SINGLE/LUELMF,UERTST,UGETIO
C                       - DOUBLE/LUELMF,UERTST,UGETIO,VXADD,VXMUL,
C                           VXSTO
C
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                           CONVENTIONS IS AVAILABLE IN THE MANUAL
C                           INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
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C                           APPLIED TO THIS CODE. NO OTHER WARRANTY,
C                           EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C-----------------------------------------------------------------------
-
C
      SUBROUTINE LUREFF (A,B,UL,IPVT,N,IA,X,IDGT,RES,DX,IER)
C
      DIMENSION
A(IA,*),UL(IA,*),B(*),X(*),RES(*),DX(*),IPVT(*)
      DOUBLE PRECISION   SUM
      DATA               ITMAX/50/,ZERO/0.0/
C                                  FIRST EXECUTABLE STATEMENT
      IER= 0
      XNORM = ZERO
      DO 10 I=1,N
         XNORM = AMAX1(XNORM,ABS(X(I)))
   10 CONTINUE
```

```
      IF (XNORM .NE. ZERO) GO TO 20
      IDGT = 50
      GO TO 9005
   20 DO 45 ITER=1,ITMAX
         DO 30 I=1,N
            SUM = DBLE(B(I))
            DO 25 J=1,N
               SUM = SUM - DBLE(A(I,J)) * DBLE(X(J))
   25       CONTINUE
            RES(I) = SUM
   30    CONTINUE
         CALL LUELMF (UL,RES,IPVT,N,IA,DX)
         DXNORM = ZERO
         XNORM = ZERO
         DO 35 I=1,N
            X(I) = X(I) + DX(I)
            DXNORM = AMAX1(DXNORM,ABS(DX(I)))
            XNORM = AMAX1(XNORM,ABS(X(I)))
   35    CONTINUE
         IF (ITER .NE. 1) GO TO 40
         IDGT = 50
         IF (DXNORM .NE. ZERO) IDGT = IFIX(-ALOG10(DXNORM/XNORM))
   40    IF (XNORM+DXNORM .EQ. XNORM) GO TO 9005
   45 CONTINUE
C                                    ITERATION DID NOT CONVERGE
      IER = 129
 9000 CONTINUE
      CALL UERTST(IER,6HLUREFF)
 9005 RETURN
      END
 9005 RETURN
      END
C   IMSL ROUTINE NAME   - IQHSCU
C
C-----------------------------------------------------------------------
-
C
C   COMPUTER            - IBM/SINGLE
C
C   LATEST REVISION     - JANUARY 1, 1978
C
C   PURPOSE             - ONE-DIMENSIONAL QUASI-CUBIC HERMITE
C                           INTERPOLATION
C
C   USAGE               - CALL IQHSCU (X,Y,NX,C,IC,IER)
C
C   ARGUMENTS    X      - VECTOR OF LENGTH NX CONTAINING THE ABSCISSAE
C                           OF THE NX DATA POINTS (X(I),Y(I)) I=1,...,
C                           NX. (INPUT) X MUST BE ORDERED SO THAT
C                           X(I) .LT. X(I+1).
C                Y      - VECTOR OF LENGTH NX CONTAINING THE ORDINATES
C                           (OR FUNCTION VALUES) OF THE NX DATA POINTS.
```

```
C                          (INPUT)
C                NX      - NUMBER OF ELEMENTS IN X AND Y. (INPUT) NX
C                          MUST BE .GE. 4.
C                C       - SPLINE COEFFICIENTS. (OUTPUT) C IS AN NX BY
C                          3 MATRIX. THE VALUE OF THE SPLINE
C                          APPROXIMATION AT T IS
C                          S(T) = ((C(I,3)*D+C(I,2))*D+C(I,1))*D+Y(I)
C                          WHERE X(I) .LE. T .LT. X(I+1) AND
C                          D = T-X(I).
C                IC      - ROW DIMENSION OF MATRIX C EXACTLY AS
C                          SPECIFIED IN THE DIMENSION STATEMENT
C                          IN THE CALLING PROGRAM. (INPUT)
C                IER     - ERROR PARAMETER. (OUTPUT)
C                          TERMINAL ERROR
C                            IER = 129, IC IS LESS THAN NX.
C                            IER = 130, NX IS LESS THAN 4.
C                            IER = 131, INPUT ABSCISSAE ARE NOT ORDERED
C                              SO THAT X(1) .LT. X(2) ... .LT. X(NX).
C
C   PRECISION/HARDWARE   - SINGLE AND DOUBLE/H32
C                        - SINGLE/H36,H48,H60
C
C   REQD. IMSL ROUTINES - UERTST,UGETIO
C
C   NOTATION             - INFORMATION ON SPECIAL NOTATION AND
C                            CONVENTIONS IS AVAILABLE IN THE MANUAL
C                            INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C   REMARKS      THE COEFFICIENTS OF THE INTERPOLATING POLYNOMIAL
C                ARE CONTAINED IN THE FIRST NX-1 ROWS OF THE MATRIX C.
C                THE ONE REMAINING ROW OF THE MATRIX C IS USED AS A
C                WORK STORAGE AREA.
C
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C                            APPLIED TO THIS CODE. NO OTHER WARRANTY,
C                            EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C-----------------------------------------------------------------------
-
C
      SUBROUTINE IQHSCU (X,Y,NX,C,IC,IER)
C                                SPECIFICATIONS FOR ARGUMENTS
      INTEGER             NX,IC,IER
      REAL                X(NX),Y(NX),C(IC,3)
C                                SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER             I,NO
      REAL                T1,T2,B,RM1,RM2,RM3,RM4,HALF,ONE,ZERO
      DATA                HALF/0.50/,ONE/1.0/,ZERO/0.0/
```

```
C                                     FIRST EXECUTABLE STATEMENT
      IF (IC .GE. NX) GO TO 5
C                                     TERMINAL - IC LESS THAN NX
      IER = 129
      GO TO 9000
    5 IF (NX .GT. 3) GO TO 10
C                                     TERMINAL - TOO FEW DATA POINTS
      IER = 130
      GO TO 9000
   10 DO 15 I=2,NX
         IF (X(I) .GT. X(I-1)) GO TO 15
C                                     TERMINAL - X NOT MONOTONE INCREASING
         IER = 131
         GO TO 9000
   15 CONTINUE
      IER = 0
      RM3 = (Y(2)-Y(1))/(X(2)-X(1))
      T1 = RM3-(Y(2)-Y(3))/(X(2)-X(3))
      RM2 = RM3+T1
      RM1 = RM2+T1
C                                     NOW GET THE SLOPES
      N0 = NX-2
      DO 40 I=1,NX
         IF (I .GT. N0) GO TO 20
         RM4 = (Y(I+2)-Y(I+1))/(X(I+2)-X(I+1))
         GO TO 25
   20    RM4 = RM3-RM2+RM3
   25    T1 = ABS(RM4-RM3)
         T2 = ABS(RM2-RM1)
         B = T1+T2
         IF (B .NE. ZERO) GO TO 30
C                                  IF DENOMINATOR IS ZERO, GET AVERAGE
         C(I,1) = HALF*(RM2+RM3)
         GO TO 35
   30    C(I,1) = (T1*RM2+T2*RM3)/B
   35    RM1 = RM2
         RM2 = RM3
         RM3 = RM4
   40 CONTINUE
      N0 = NX-1
C                                   COMPUTE THE COEFFICIENTS FOR THE
C                                     NX-1 INTERVALS
      DO 45 I=1,N0
         T1 = ONE/(X(I+1)-X(I))
         T2 = (Y(I+1)-Y(I))*T1
         B = (C(I,1)+C(I+1,1)-T2-T2)*T1
         C(I,3) = B*T1
         C(I,2) = -B+(T2-C(I,1))*T1
   45 CONTINUE
 9000 CONTINUE
```

```
      IF (IER .NE. 0) CALL UERTST(IER,6HIQHSCU)
 9005 RETURN
      END
C   IMSL ROUTINE NAME   - LUDATF
C
C-----------------------------------------------------------------------
-
C
C   COMPUTER            - IBM/SINGLE
C
C   LATEST REVISION     - JANUARY 1, 1978
C
C   PURPOSE             - L-U DECOMPOSITION BY THE CROUT ALGORITHM
C                           WITH OPTIONAL ACCURACY TEST.
C
C   USAGE               - CALL LUDATF (A,LU,N,IA,IDGT,D1,D2,IPVT,
C                           EQUIL,WA,IER)
C
C   ARGUMENTS    A      - INPUT MATRIX OF DIMENSION N BY N CONTAINING
C                           THE MATRIX TO BE DECOMPOSED.
C                LU     - REAL OUTPUT MATRIX OF DIMENSION N BY N
C                           CONTAINING THE L-U DECOMPOSITION OF A
C                           ROWWISE PERMUTATION OF THE INPUT MATRIX.
C                           FOR A DESCRIPTION OF THE FORMAT OF LU, SEE
C                           EXAMPLE.
C                N      - INPUT SCALAR CONTAINING THE ORDER OF THE
C                           MATRIX A.
C                IA     - INPUT SCALAR CONTAINING THE ROW DIMENSION OF
C                           MATRICES A AND LU EXACTLY AS SPECIFIED IN
C                           THE CALLING PROGRAM.
C                IDGT   - INPUT OPTION.
C                           IF IDGT IS GREATER THAN ZERO, THE NON-ZERO
C                           ELEMENTS OF A ARE ASSUMED TO BE CORRECT TO
C                           IDGT DECIMAL PLACES.  LUDATF PERFORMS AN
C                           ACCURACY TEST TO DETERMINE IF THE COMPUTED
C                           DECOMPOSITION IS THE EXACT DECOMPOSITION
C                           OF A MATRIX WHICH DIFFERS FROM THE GIVEN
C                           ONE BY LESS THAN ITS UNCERTAINTY.
C                         IF IDGT IS EQUAL TO ZERO, THE ACCURACY TEST
C                           IS BYPASSED.
C                D1     - OUTPUT SCALAR CONTAINING ONE OF THE TWO
C                           COMPONENTS OF THE DETERMINANT. SEE
C                           DESCRIPTION OF PARAMETER D2, BELOW.
C                D2     - OUTPUT SCALAR CONTAINING ONE OF THE
C                           TWO COMPONENTS OF THE DETERMINANT. THE
C                           DETERMINANT MAY BE EVALUATED AS
(D1)(2**D2).
C                IPVT   - OUTPUT VECTOR OF LENGTH N CONTAINING THE
C                           PERMUTATION INDICES. SEE DOCUMENT
C                           (ALGORITHM).
```

```
C                EQUIL  - OUTPUT VECTOR OF LENGTH N CONTAINING
C                         RECIPROCALS OF THE ABSOLUTE VALUES OF
C                         THE LARGEST (IN ABSOLUTE VALUE) ELEMENT
C                         IN EACH ROW.
C                WA     - ACCURACY TEST PARAMETER, OUTPUT ONLY IF
C                         IDGT IS GREATER THAN ZERO.
C                         SEE ELEMENT DOCUMENTATION FOR DETAILS.
C                IER    - ERROR PARAMETER. (OUTPUT)
C                         TERMINAL ERROR
C                           IER = 129 INDICATES THAT MATRIX A IS
C                             ALGORITHMICALLY SINGULAR. (SEE THE
C                             CHAPTER L PRELUDE).
C                         WARNING ERROR
C                           IER = 34 INDICATES THAT THE ACCURACY TEST
C                             FAILED.  THE COMPUTED SOLUTION MAY BE IN
C                             ERROR BY MORE THAN CAN BE ACCOUNTED FOR
C                             BY THE UNCERTAINTY OF THE DATA.  THIS
C                             WARNING CAN BE PRODUCED ONLY IF IDGT IS
C                             GREATER THAN 0 ON INPUT.  SEE CHAPTER L
C                             PRELUDE FOR FURTHER DISCUSSION.
C
C   PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32
C                       - SINGLE/H36,H48,H60
C
C   REQD. IMSL ROUTINES - UERTST,UGETIO
C
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                           CONVENTIONS IS AVAILABLE IN THE MANUAL
C                           INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C   REMARKS      A TEST FOR SINGULARITY IS MADE AT TWO LEVELS:
C                1.  A ROW OF THE ORIGINAL MATRIX A IS NULL.
C                2.  A COLUMN BECOMES NULL IN THE FACTORIZATION
PROCESS.
C
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C   WARRANTY            - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN
C                           APPLIED TO THIS CODE. NO OTHER WARRANTY,
C                           EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C-----------------------------------------------------------------------
-
C
      SUBROUTINE LUDATF (A,LU,N,IA,IDGT,D1,D2,IPVT,EQUIL,WA,IER)
C
      DIMENSION          A(IA,*),LU(IA,*),IPVT(*),EQUIL(*)
      REAL               LU
      DATA               ZERO,ONE,FOUR,SIXTN,SIXTH/0.0,1.,4.,16.,.0625/
C                                  FIRST EXECUTABLE STATEMENT
```

```
C                                  INITIALIZATION
      IER = 0
      RN = N
      WREL = ZERO
      D1 = ONE
      D2 = ZERO
      BIGA = ZERO
      DO 10 I=1,N
         BIG = ZERO
         DO 5 J=1,N
            P = A(I,J)
            LU(I,J) = P
            P = ABS(P)
            IF (P .GT. BIG) BIG = P
    5    CONTINUE
         IF (BIG .GT. BIGA) BIGA = BIG
         IF (BIG .EQ. ZERO) GO TO 110
         EQUIL(I) = ONE/BIG
   10 CONTINUE
      DO 105 J=1,N
         JM1 = J-1
         IF (JM1 .LT. 1) GO TO 40
C                                  COMPUTE U(I,J), I=1,...,J-1
         DO 35 I=1,JM1
            SUM = LU(I,J)
            IM1 = I-1
            IF (IDGT .EQ. 0) GO TO 25
C                                  WITH ACCURACY TEST
            AI = ABS(SUM)
            WI = ZERO
            IF (IM1 .LT. 1) GO TO 20
            DO 15 K=1,IM1
               T = LU(I,K)*LU(K,J)
               SUM = SUM-T
               WI = WI+ABS(T)
   15       CONTINUE
            LU(I,J) = SUM
   20       WI = WI+ABS(SUM)
            IF (AI .EQ. ZERO) AI = BIGA
            TEST = WI/AI
            IF (TEST .GT. WREL) WREL = TEST
            GO TO 35
C                                     WITHOUT ACCURACY
   25       IF (IM1 .LT. 1) GO TO 35
            DO 30 K=1,IM1
               SUM = SUM-LU(I,K)*LU(K,J)
   30       CONTINUE
            LU(I,J) = SUM
   35    CONTINUE
   40    P = ZERO
```

```
C                                   COMPUTE U(J,J) AND L(I,J),
I=J+1,...,
         DO 70 I=J,N
            SUM = LU(I,J)
            IF (IDGT .EQ. 0) GO TO 55
C                                   WITH ACCURACY TEST
            AI = ABS(SUM)
            WI = ZERO
            IF (JM1 .LT. 1) GO TO 50
            DO 45 K=1,JM1
               T = LU(I,K)*LU(K,J)
               SUM = SUM-T
               WI = WI+ABS(T)
   45       CONTINUE
            LU(I,J) = SUM
   50       WI = WI+ABS(SUM)
            IF (AI .EQ. ZERO) AI = BIGA
            TEST = WI/AI
            IF (TEST .GT. WREL) WREL = TEST
            GO TO 65
C                                   WITHOUT ACCURACY TEST
   55       IF (JM1 .LT. 1) GO TO 65
            DO 60 K=1,JM1
               SUM = SUM-LU(I,K)*LU(K,J)
   60       CONTINUE
            LU(I,J) = SUM
   65       Q = EQUIL(I)*ABS(SUM)
            IF (P .GE. Q) GO TO 70
            P = Q
            IMAX = I
   70    CONTINUE
C                                   TEST FOR ALGORITHMIC SINGULARITY
         IF (RN+P .EQ. RN) GO TO 110
         IF (J .EQ. IMAX) GO TO 80
C                                   INTERCHANGE ROWS J AND IMAX
         D1 = -D1
         DO 75 K=1,N
            P = LU(IMAX,K)
            LU(IMAX,K) = LU(J,K)
            LU(J,K) = P
   75    CONTINUE
         EQUIL(IMAX) = EQUIL(J)
   80    IPVT(J) = IMAX
         D1 = D1*LU(J,J)
   85    IF (ABS(D1) .LE. ONE) GO TO 90
         D1 = D1*SIXTH
         D2 = D2+FOUR
         GO TO 85
   90    IF (ABS(D1) .GE. SIXTH) GO TO 95
         D1 = D1*SIXTN
```

```
         D2 = D2-FOUR
         GO TO 90
   95    CONTINUE
         JP1 = J+1
         IF (JP1 .GT. N) GO TO 105
C                                    DIVIDE BY PIVOT ELEMENT U(J,J)
         P = LU(J,J)
         DO 100 I=JP1,N
            LU(I,J) = LU(I,J)/P
  100    CONTINUE
  105 CONTINUE
C                                    PERFORM ACCURACY TEST
      IF (IDGT .EQ. 0) GO TO 9005
      P = 3*N+3
      WA = P*WREL
      IF (WA+10.0**(-IDGT) .NE. WA) GO TO 9005
      IER = 34
      GO TO 9000
C                                    ALGORITHMIC SINGULARITY
  110 IER = 129
      D1 = ZERO
      D2 = ZERO
 9000 CONTINUE
C                                    PRINT ERROR
      CALL UERTST(IER,6HLUDATF)
 9005 RETURN
      END
C   IMSL ROUTINE NAME   - LUELMF
C
C-----------------------------------------------------------------------
-
C
C   COMPUTER            - IBM/SINGLE
C
C   LATEST REVISION     - JANUARY 1, 1978
C
C   PURPOSE             - ELIMINATION PART OF SOLUTION OF AX=B
C                           (FULL STORAGE MODE)
C
C   USAGE               - CALL LUELMF (A,B,IPVT,N,IA,X)
C
C   ARGUMENTS    A      - A = LU (THE RESULT COMPUTED IN THE IMSL
C                           ROUTINE LUDATF) WHERE L IS A LOWER
C                           TRIANGULAR MATRIX WITH ONES ON THE MAIN
C                           DIAGONAL. U IS UPPER TRIANGULAR. L AND U
C                           ARE STORED AS A SINGLE MATRIX A AND THE
C                           UNIT DIAGONAL OF L IS NOT STORED. (INPUT)
C                B      - B IS A VECTOR OF LENGTH N ON THE RIGHT HAND
C                           SIDE OF THE EQUATION AX=B. (INPUT)
C                IPVT   - THE PERMUTATION MATRIX RETURNED FROM THE
```

```
C                          IMSL ROUTINE LUDATF, STORED AS AN N LENGTH
C                          VECTOR. (INPUT)
C                N       - ORDER OF A AND NUMBER OF ROWS IN B. (INPUT)
C                IA      - ROW DIMENSION OF A EXACTLY AS SPECIFIED IN
C                          THE DIMENSION STATEMENT IN THE CALLING
C                          PROGRAM. (INPUT)
C                X       - THE RESULT X. (OUTPUT)
C
C   PRECISION/HARDWARE   - SINGLE AND DOUBLE/H32
C                        - SINGLE/H36,H48,H60
C
C   REQD. IMSL ROUTINES - NONE REQUIRED
C
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                          CONVENTIONS IS AVAILABLE IN THE MANUAL
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C
C-----------------------------------------------------------------------
-
C
      SUBROUTINE LUELMF (A,B,IPVT,N,IA,X)
C
      DIMENSION          A(IA,*),B(*),IPVT(*),X(*)
C                                FIRST EXECUTABLE STATEMENT
C                                SOLVE LY = B FOR Y
      DO 5 I=1,N
    5 X(I) = B(I)
      IW = 0
      DO 20 I=1,N
         IP = IPVT(I)
         SUM = X(IP)
         X(IP) = X(I)
         IF (IW .EQ. 0) GO TO 15
         IM1 = I-1
         DO 10 J=IW,IM1
            SUM = SUM-A(I,J)*X(J)
   10    CONTINUE
         GO TO 20
   15    IF (SUM .NE. 0.) IW = I
   20 X(I) = SUM
C                                SOLVE UX = Y FOR X
      DO 30 IB=1,N
         I = N+1-IB
         IP1 = I+1
```

```
         SUM = X(I)
         IF (IP1 .GT. N) GO TO 30
         DO 25 J=IP1,N
            SUM = SUM-A(I,J)*X(J)
   25    CONTINUE
   30 X(I) = SUM/A(I,I)
      RETURN
      END
C
C*DK SPLINE
      SUBROUTINE SPLINE(X,Y,N,A,B,C,D)
      REAL X(*),Y(*),A(*),B(*),C(*),D(*)
C
C  P(X)=A(I)+B(I)*(X-X(I))+C(I)*(X-X(I))**2+D(I)*(X-X(I))**3
C  FOR X(I) <= X < X(I+1)       (D.H. A(I)=Y(I))
C
C  P(X)=A(1)+B(1)*(X-X(1))
C  FOR  X <= X(1)
C
C  P(X)=A(N)+B(N)*(X-X(N))
C  FOR X(N) <= X
C
      NM1=N-1
C   C-ARRAY
      A(1)=2.E0
      C(1)=0.E0
      C(N)=0.E0
      D(1)=0.E0
      B(1)=0.E0
      DX2=X(2)-X(1)
      DY2=(Y(2)-Y(1))/DX2
      DO 1 I=2,NM1
      DX1=DX2
      DY1=DY2
      DX2=X(I+1)-X(I)
      DY2=(Y(I+1)-Y(I))/DX2
      DDX=DX1+DX2
      B(I)=DX2/DDX
      A(I)=1.E0-B(I)
      D(I)=6.E0*(DY2-DY1)/DDX
    1 CONTINUE
      DO 2 I=2,NM1
      J=I-1
      FAC=A(I)/A(J)
      D(I)=D(I)-FAC*D(J)
      A(I)=2.E0-B(J)*FAC
    2 CONTINUE
      K=N
      NMH=N
      DO 3 I=2,NM1
```

```
      K=K-1
      J=NMH-1
      C(J)=(D(K)-B(K)*C(NMH))/A(K)
      NMH=J
    3 CONTINUE
C   A,B,C UND D-ARRAY
      DO 4 J=2,NM1
4     C(J)=C(J)/2.
      DO 5 J=1,NM1
      H=X(J+1)-X(J)
      A(J)=Y(J)
      B(J)=(Y(J+1)-Y(J))/H
      B(J)=B(J)-H/3.*(C(J+1)+2.*C(J))
      D(J)=(C(J+1)-C(J))/(3.*H)
5     CONTINUE
      A(N)=Y(N)
      B(N)=B(NM1)+2.*C(NM1)*(X(N)-X(NM1))+3.*D(NM1)*(X(N)-X(NM1))**2
      RETURN
      END
C
      SUBROUTINE SORT ( EV, LAMBDA, INULL, NOPOS, EPS )
      DOUBLEPRECISION   EV( 3,3 ), LAMBDA( 3 ), EPS,
     >                  HILFL( 3 ), HILFEV( 3,3 ), MERK
C
      INTEGER           INULL
      LOGICAL           NOPOS
      NOPOS = .TRUE.
      J = 0
      DO 10, I=1,3
         IF ( LAMBDA( I ) .GT. EPS ) THEN
            NOPOS = .FALSE.
            HILFL( J+1 ) = LAMBDA( I )
            DO 15, K = 1,3
               HILFEV( K,J+1  ) = EV( K,I )
   15       CONTINUE
            J = J + 1
         ENDIF
   10 CONTINUE
   IF ( J .GE. 2 ) THEN
C
         DO 17, K = 1,J-1
            DO 17, L = K+1,J
C
               IF ( HILFL( K ) .GT. HILFL( L ) ) THEN
                  DO 16, I =1,3
                     MERK         = HILFEV( I,K )
                     HILFEV( I,K )= HILFEV( I,L )
                     HILFEV( I,L )= MERK
   16                CONTINUE
                     MERK       = HILFL( K )


90
```

```
                HILFL( K ) = HILFL( L )
                HILFL( L ) = MERK
             ENDIF
17     CONTINUE
ENDIF
DO 20, I=1,3
IF ( ( ABS( LAMBDA( I ) ) .GT. EPS ) .AND.
  >         (      LAMBDA( I )    .LT. EPS ) ) THEN
   HILFL( J+1 ) = LAMBDA( I )
         DO 25, K = 1,3
            HILFEV( K,J+1 ) = EV( K,I )
25       CONTINUE
         J = J + 1
      ENDIF
20 CONTINUE
DO 30, I = 1,3
      IF (ABS(LAMBDA(I)).LT.EPS) THEN
         HILFL(J+1) = LAMBDA(I)
         DO 35, K = 1,3
            HILFEV( K,J+1 ) = EV(K,I)
35       CONTINUE
         J = J + 1
      ENDIF
30 CONTINUE
DO 40, I=1,3
      LAMBDA( I ) = HILFL( I )
      DO 45, K = 1,3
         EV( K,I ) = HILFEV( K,I )
45    CONTINUE
40 CONTINUE
INULL = 3 - J
   END
C
C
C
      SUBROUTINE PAREBE(EV,LAMBDA,NUE,M,B0,B1,B2,B3,C0,C1,C2,C3,EPS)
      REAL              B0,B1,B2,B3,C0,C1,C2,C3
      DOUBLEPRECISION   LAMBDA( 3 ), EV(3,3),EPS,
     >                  M(3),NUE,NORM,P(3),U(3)
C     DATA              EPS  / 5.D-10 /
*
      U(1) = SQRT(-NUE/LAMBDA(1))
      U(2) = 0.0
      U(3) = 0.0
      B1 = EV(1,1) * U(1)
      B2 = EV(2,1) * U(1)
      B3 = EV(3,1) * U(1)
*
      NORM = B1**2 + B2**2 + B3**2
      NORM = SQRT(NORM)
```

```
*
      B1 = B1 / NORM
      B2 = B2 / NORM
      B3 = B3 / NORM
*     Transformation:
      P(1) = EV(1,1) * U(1) + EV(1,2) + EV(1,3) + M(1)
      P(2) = EV(2,1) * U(1) + EV(2,2) + EV(2,3) + M(2)
      P(3) = EV(3,1) * U(1) + EV(3,2) + EV(3,3) + M(3)
*
      B0 = -(B1 * P(1) + B2 * P(2) + B3 * P(3))
*
      U(1) = -SQRT(-NUE/LAMBDA(1))
      U(2) = 0.0
      U(3) = 0.0
*
      C1 = EV(1,1) * U(1)
      C2 = EV(2,1) * U(1)
      C3 = EV(3,1) * U(1)
*
      NORM = C1**2 + C2**2 + C3**2
      NORM = SQRT(NORM)
      C1 = C1 / NORM
      C2 = C2 / NORM
      C3 = C3 / NORM
*     Transformation:
      P(1) = EV(1,1) * U(1) + EV(1,2) + EV(1,3) + M(1)
      P(2) = EV(2,1) * U(1) + EV(2,2) + EV(2,3) + M(2)
      P(3) = EV(3,1) * U(1) + EV(3,2) + EV(3,3) + M(3)
*
      C0 = -(C1 * P(1) + C2 * P(2) + C3 * P(3))
*
      END
C
      SUBROUTINE DOPEBE(EV,LAMBDA,M,B0,B1,B2,B3,EPS)
*
      DOUBLEPRECISION   LAMBDA( 3 ), EV(3,3),EPS,
     >                  M(3),NORM,P(3)
      REAL              B0,B1,B2,B3
C
C     DATA              EPS  / 5.D-10 /
*     U(1) = 0.0
*     U(2) = 0.0
*     U(3) = 0.0
*
      B1 = M(1)
      B2 = M(2)
      B3 = M(3)
*
      NORM = B1**2 + B2**2 + B3**2
      NORM = SQRT(NORM)
```

```
*
      B1 = B1 / NORM
      B2 = B2 / NORM
      B3 = B3 / NORM
*
*     Transformation:
      P(1) = EV(1,2) + EV(1,3) + M(1)
      P(2) = EV(2,2) + EV(2,3) + M(2)
      P(3) = EV(3,2) + EV(3,3) + M(3)
*
      B0 = -(B1 * P(1) + B2 * P(2) + B3 * P(3))
      END
C
      SUBROUTINE SCHEBE(LAMBDA,EV,M,B0,B1,B2,B3,C0,C1,C2,C3)
*      lambda(1) * u1 ** 2 + lambda(2) * u2**2  = 0                *
*     u1 = sqrt ( -lambda(2)/lambda(1)) * u2                       *
*     u1 = - sqrt ( -lambda(2)/lambda(1)) * u2                     *
*                         e1: bo + b1*x + b2 * y + b3 * z          *
*                         e2: co + b1*x + b2 * y + b3 * z          *
      DOUBLEPRECISION   LAMBDA( 3 ), EV(3,3),
     >                  M(3),NORM,P(3),U(3)
      REAL              B0,B1,B2,B3,C0,C1,C2,C3
      U(1) = 1.0
      U(2) = -SQRT(-LAMBDA(2)/LAMBDA(1))
      U(3) = 0.0
*
      NORM = U(1)**2 + U(2)**2
      NORM = SQRT(NORM)
*
      U(1) = U(1) / NORM
      U(2) = U(2) / NORM
C
      B1 = EV(1,1) * U(1) + EV(1,2) * U(2)
      B2 = EV(2,1) * U(1) + EV(2,2) * U(2)
      B3 = EV(3,1) * U(1) + EV(2,3) * U(2)
*
      NORM = B1**2 + B2**2 + B3**2
      NORM = SQRT(NORM)
*
      B1 = B1 / NORM
      B2 = B2 / NORM
      B3 = B3 / NORM
*
      P(1) = EV(1,1)*SQRT(-LAMBDA(2)/LAMBDA(1)) + EV(1,2)+M(1)
      P(2) = EV(2,1)*SQRT(-LAMBDA(2)/LAMBDA(1)) + EV(2,2)+M(2)
      P(3) = EV(3,1)*SQRT(-LAMBDA(2)/LAMBDA(1)) + EV(3,2)+M(3)
*
      B0 = -(B1 * P(1) + B2 * P(2) + B3 * P(3))

*
```

```
      U(1) = 1.0
      U(2) = SQRT(-LAMBDA(2)/LAMBDA(1))
      U(3) = 0.0

      NORM = U(1)**2 + U(2)**2
      NORM = SQRT(NORM)
*
      U(1) = U(1) / NORM
      U(2) = U(2) / NORM
*
      C1 = EV(1,1) * U(1) + EV(1,2) * U(2)
      C2 = EV(2,1) * U(1) + EV(2,2) * U(2)
      C3 = EV(3,1) * U(1) + EV(3,2) * U(2)
*
      NORM = C1**2 + C2**2 + C3**2
      NORM = SQRT(NORM)
*
      C1 = C1 / NORM
      C2 = C2 / NORM
      C3 = C3 / NORM
*     Transformation:
      P(1) = -EV(1,1)*SQRT(-LAMBDA(2)/LAMBDA(1))+EV(1,2) + M(1)
      P(2) = -EV(2,1)*SQRT(-LAMBDA(2)/LAMBDA(1))+EV(2,2) + M(2)
      P(3) = -EV(3,1)*SQRT(-LAMBDA(2)/LAMBDA(1))+EV(3,2) + M(3)
*
      C0 = -(C1 * P(1) + C2 * P(2) + C3 * P(3))
      END
*
      SUBROUTINE ELLZYL(EV,NUE,M,LAMBDA,X0,Y0,Z0,CX,CY,CZ,R,INDE,EPS)
*     lambda(1) * u1**2 + lambda(2) * u2**2 + nue = 0.              *
*     u1 = sqrt ( (-nue -lambda(2) *u2**2)/ lambda(1) )             *
*
      REAL              X0, Y0, Z0, CX, CY, CZ, R
      DOUBLEPRECISION   LAMBDA(3), EV(3,3), EPS,
     >                  M(3), NUE, NORM, P(3)
C
      INTEGER           INDE
C
C     DATA              EPS  / 5.D-10 /
*
      CX  = EV(1,3)
      CY  = EV(2,3)
      CZ  = EV(3,3)
*
      X0 = M(1)
      Y0 = M(2)
      Z0 = M(3)
*
      IF (ABS(LAMBDA(2)-LAMBDA(1)).LT.EPS) THEN
         INDE = 4
```

```
*        Kreisfoermiger Zylinder
         R = SQRT(- NUE/LAMBDA(1))
      ENDIF
      END
C
C
C
      SUBROUTINE KEGEL(EV,M,LAMBDA,X0,Y0,Z0,CX,CY,CZ,R,EPS)
*     lambda(1) * u1**2 + lambda(2) * u2**2 + lambda(3) * u3**2 =0.  *
*     lambda(1) und lambda(2) sind positiv, lambda(3) ist negativ.   *
*
      REAL              X0, Y0, Z0, CX, CY, CZ, R
      DOUBLEPRECISION   LAMBDA(3), EV(3,3), EPS,
     >                  M(3), NORM
C
C     DATA              EPS  / 5.D-10 /
      NORM = 0.0
      R = 0.0
*
      X0  = M(1)
      Y0  = M(2)
      Z0  = M(3)
*
      CX = EV(1,3) * (-LAMBDA(3))
      CY = EV(2,3) * (-LAMBDA(3))
      CZ = EV(3,3) * (-LAMBDA(3))
      NORM = SQRT (CX ** 2 + CY ** 2 + CZ ** 2)
      CX = CX / NORM
      CY = CY / NORM
      CZ = CZ / NORM
*
      IF (ABS(LAMBDA(2)-LAMBDA(1)).LT.EPS) THEN
      R = ATAN(sqrt(-LAMBDA(3))/sqrt(LAMBDA(1)))
      ENDIF
      END
C
      SUBROUTINE INTER ( NALT, MALT, IALT, XALT, YALT, WALT,
     >                   NNEU, MNEU, INEU, XNEU, YNEU, WNEU )
C
      REAL     XALT( * ), YALT( * ), WALT( IALT,* ),
     >         XNEU( * ), YNEU( * ), WNEU( INEU,* ),
     >         KLFL
      INTEGER  XL, YL
      LOGICAL  XV, YV
      DATA EPS /1.E-20/
C
      DO 10, I = 1, NNEU-1
         XMIN = XNEU( I )
         XMAX = XNEU( I+1 )
         DO 15, J = 1,MNEU-1
```

```
            YMIN = YNEU( J )
            YMAX = YNEU( J+1 )
C           WRITE (6,*) ' XMIN,XMAX ',XMIN,XMAX
C           WRITE (6,*) ' YMIN,YMAX ',YMIN,YMAX

          GESFL=ABS( XMAX - XMIN ) * ABS( YMAX - YMIN )
            KX = 1
   30       IF ( KX + 1 .LE. NNEU ) THEN
               IF ( XALT( KX + 1 ) .LE. XMIN ) THEN
                  KX = KX + 1
                  GOTO 30
               ENDIF
            ENDIF
            KY = 1
   40       IF ( KY + 1 .LE. MNEU ) THEN
               IF ( YALT( KY + 1 ) .LE. YMIN ) THEN
                  KY = KY + 1
                  GOTO 40
               ENDIF
            ENDIF
C           INITIALIZE
               XV    = .FALSE.
               YV    = .FALSE.
               XL    = 0
               YL    = 0
               SUMME = 0.
C
            DO 100, K = KX+1,NALT
               IF ( XALT( K ) .GE. XMAX ) GOTO 105
                  XL = K
                  XV = .TRUE.
                  XG = XMIN
                  IF ( K .GT. 1 ) THEN
                     IF ( XALT( K-1 ) .GT. XMIN ) XG = XALT( K-1 )
                  ENDIF
                  XT = ABS( XALT( K ) - XG )
C
               DO 200, L = KY+1,MALT
                  IF ( YALT( L ) .GE. YMAX ) GOTO 205
                     YL = L
                     YV = .TRUE.
                     WRE = WALT( K-1,L-1 )
                     YG = YMIN
                     IF ( K .GT. 1 ) THEN
                        IF ( YALT( L-1 ) .GT. YMIN ) YG = YALT( L-1 )
                     ENDIF
                     YT    = ABS( YALT( L ) - YG )
                        KLFL  = XT * YT
                        SUMM = SUMM + WRE * KLFL
  200          CONTINUE
```

```
                  WRE   = WALT( KX,YL )
                  KLFL  = XT * YT
                  SUMM = SUMM + WRE * KLFL
               ENDIF
            ENDIF
          IF ( XV .AND. .NOT .YV) THEN
               WRE   = WALT( XL,KY )
               XT    = ABS( XMAX - XALT( XL ) )
               KLFL  = XT * YT
               SUMM = SUMM + WRE * KLFL
          ENDIF
C
            IF ( XV .OR. YV ) THEN
               IF ( GESFL .LT. EPS ) THEN
                  WRITE(*,*) 'FAILURE IN SUBROUTINE INTER !'
                  WRITE(*,*) 'X-COORDINATE :',I
                  WRITE(*,*) 'Y-COORDINATE :',J
               ELSE
                  WNEU( I,J ) = SUMM / GESFL
               ENDIF
            ELSE
               WNEU( I,J ) = WALT( KX,KY )
            ENDIF
C        WRITE (6,*) ' WNEU ',WNEU(I,J)
   15    CONTINUE
   10 CONTINUE
      END
C
      SUBROUTINE FL2O(A00,A1,A2,A3,A4,A5,A6,A7,A8,A9,INDE,X0,Y0,Z0,
     >               CX,CY,CZ,R,B0,B1,B2,B3,C0,C1,C2,C3,EPSIN,NMACH)
C
C     A00, ... ,A9  -
C COEFFICIENTS OF ALGEBRAIC EQN.
C                      A00 + A1*X + A2*Y + A3*Z + A4*X**2 + A5*Y**2
C                      + A6*Z**2 + A7*X*Y + A8*X*Z + A9*Y*Z = 0
C
      DOUBLEPRECISION   A( 3,3 ), LAMBDA( 3 ), EV( 3,3 ), EPS, C, B(3),
     >                  M(3),NUE,NORM,P(3),AMERK(3,3),RES(3),WRK(6)
     >                 ,Q(5,5),DD(3),QEV(5,5)
      REAL              A00,A0,A1,A2,A3,A4,A5,A6,A7,A8,A9,X0,Y0,Z0,
     >                  CX,CY,CZ,R,B0,B1,B2,B3,C0,C1,C2,C3
C
      INTEGER           INDE, INULL, DIM, KBASIS, IW(3)
      LOGICAL           NOPOS
C
C     DATA              EPS  / 5.D-10 /
      EPS=EPSIN
      INDE = 0
      A(1,1) = A4
      A(2,1) = A7/2.D0
```

```
      A(3,1) = A8/2.DO
      A(1,2) = A7/2.DO
      A(2,2) = A5
      A(3,2) = A9/2.DO
      A(1,3) = A8/2.DO
      A(2,3) = A9/2.DO
      A(3,3) = A6
C
      B(1) = A1/2.
      B(2) = A2/2.
      B(3) = A3/2.
      ICOUNT=1
  4   CONTINUE
C
      DIM = 0
C
      DO 2, I=1,3
         DO 2, J=1,3
            IF ( ABS( A(I,J) ) .GT. EPS ) DIM = 1
   2  CONTINUE
      IF ( DIM .EQ. 0 ) THEN
         B0 = 0.DO
         B1 = 0.DO
         B2 = 0.DO
         B3 = 0.DO
C
         IF ( ABS( A1 ) .GT. EPS ) THEN
            B0 = A00 / A1
            B1 = 1.DO
         ELSE IF ( ABS( A2 ) .GT. EPS ) THEN
            B0 = A00 / A2
            B2 = 1.DO
         ELSE
            B0 = A00 / A3
            B3 = 1.DO
         ENDIF
C
         INDE = 1
         GOTO 999

      ELSE
        IF (NMACH.EQ.1) CALL EVCSF( 3,A,3,LAMBDA, EV, 3 )
         DO 4814 I=1,3
4814     IF (ABS(LAMBDA(I)).LT.EPS) LAMBDA(I)=0.
         DO 7, I = 1,3
            NORM = SQRT( EV(1,I)**2 + EV(2,I)**2 + EV(3,I)**2 )
            DO 11, J = 1,3
               IF (NORM.GT.EPS)     EV(J,I) = EV(J,I)/NORM
  11        CONTINUE
  7      CONTINUE


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```

```
C
      ENDIF
C
      CALL SORT( EV, LAMBDA, INULL, NOPOS, EPS )
C
      IF (NOPOS.AND.ICOUNT.EQ.1) THEN
         DO 8, I = 1,3
            DO 9, J = 1,3
                  A(I,J) = -1. * A(I,J)
  9         CONTINUE
            B(I) = - B(I)
  8      CONTINUE
         C = -1. * C
         ICOUNT=2
         GOTO 4
      ELSEIF (NOPOS.AND.ICOUNT.EQ.2) THEN
C
         GOTO 999
      ENDIF
C
      DO 6, I = 1,3
         B(I) = -B(I)
 6    CONTINUE
      IF (NMACH.NE.1) CALL DLSBRR(3,3,A,3,B,EPS,M,RES,KBASIS)
      IF (NMACH.EQ.1) CALL LSBRR(3,3,A,3,B,EPS,M,RES,KBASIS)
C
      DO 17, I = 1,3
        B(I) = -B(I)
17    CONTINUE
C
      DIM = 0
      DO 18, I = 1,3
         IF (ABS(RES(I)).GT.EPS) DIM = DIM + 1
 18   CONTINUE
      IF (DIM.EQ.0) THEN
         NUE = C
         DO 20, I = 1,3
            NUE = NUE + B(I) * M(I)
   20    CONTINUE
         EV(1,1) = EV(2,2)*EV(3,3) - EV(3,2)*EV(2,3)
         EV(2,1) = EV(3,2)*EV(1,3) - EV(3,3)*EV(1,2)
         EV(3,1) = EV(1,2)*EV(2,3) - EV(2,2)*EV(1,3)
C
         NORM = 0.D0
         DO 30, I = 1,3
            NORM = EV(I,1)* EV(I,1) + NORM
 30      CONTINUE
         NORM = SQRT(NORM)
C
         DO 40, I = 1,3


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```

```
            EV(I,1) = EV(I,1) /NORM
40       CONTINUE
         IF (LAMBDA(2).GT. EPS) THEN
            IF (LAMBDA(3).GT. EPS) THEN
               IF (NUE.LT. 0.D0) THEN
                  INDE = 13
               ELSEIF (ABS(NUE).LT.EPS) THEN
                  INDE = 14
               ENDIF
            ELSEIF (LAMBDA(3).LT.-EPS) THEN
               IF (NUE.GT.EPS) THEN
                  INDE = 10
               ELSEIF (NUE.LT.-EPS) THEN
                  INDE = 9
               ELSE
                  INDE = 8
                  CALL KEGEL(EV,M,LAMBDA,X0,Y0,Z0,CX,CY,CZ,R,EPS)
               ENDIF
            ELSE
               IF (NUE.LT.-EPS) THEN
                  INDE = 5
                  CALL ELLZYL(EV,NUE,M,LAMBDA,X0,Y0,Z0,CX,CY,CZ,R,INDE,
     .                        EPS)
               ELSEIF (ABS(NUE).LT.EPS) THEN
               ENDIF
            ENDIF
         ELSEIF (LAMBDA(2).LT.-EPS) THEN
            IF ((ABS(LAMBDA(3)).LT.EPS).AND.(ABS(NUE).LT.EPS)) THEN
               INDE = 3
               CALL SCHEBE(LAMBDA,EV,M,B0,B1,B2,B3,C0,C1,C2,C3)
            ELSEIF (ABS(LAMBDA(3)).LT.EPS) THEN
               INDE = 6
            ENDIF
         ELSE
            IF (ABS(LAMBDA(3)).LT.EPS) THEN
               IF (NUE.LT.0.D0) THEN
C                 ZWEI PARALLELE EBENEN
                  INDE = 2
                  CALL PAREBE(EV,LAMBDA,NUE,M,B0,B1,B2,B3,C0,C1,C2,C3,
     .                        EPS)
               ELSEIF (ABS(NUE).LT.EPS) THEN
                  INDE = 1
                  CALL DOPEBE(EV,LAMBDA,M,B0,B1,B2,B3,EPS)
               ENDIF
            ENDIF
         ENDIF
C      lambda(1)*x1 **2 + lambda(2)*x2 **2 + lambda(3)*x3**2 + nue = 0.
C        Transformation form:
C        X = (ev1,ev2,ev3) * x + m
       ELSEIF ((ABS(LAMBDA(2)).LT.EPS).AND.(ABS(LAMBDA(3)).LT.EPS)) THEN


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```

```
         P(3) = 0.
         DO 80, I = 1,3
            P(3) = P(3) + EV(I,3) * B(I)
   80    CONTINUE
         IF (P(3).GT.0.D0) THEN
            P(3) = -P(3)
            DO 90, I = 1,3
               EV(I,3) = -1.D0 * EV(I,3)
   90       CONTINUE
         ENDIF
C        Lambda(1) * X1 ** 2 + 2 * P(3) * X3 = 0.
         EV(1,1) = EV(2,2)*EV(3,3) - EV(3,2)*EV(2,3)
         EV(2,1) = EV(3,2)*EV(1,3) - EV(3,3)*EV(1,2)
         EV(3,1) = EV(1,2)*EV(2,3) - EV(2,2)*EV(1,3)
C
         NORM = 0.D0
         DO 95, I = 1,3
            NORM = EV(I,1)* EV(I,1) + NORM
   95    CONTINUE
         NORM = SQRT(NORM)
C
         DO 100, I = 1,3
            EV(I,1) = EV(I,1) /NORM
  100    CONTINUE
C        M = (-p1/lambda(1)) * ev1 + 1./ (2.(p3) *
C            (p1**2 /lambda(1) - c) * ev3
C       WITH p1 := ev1  * b
         DO 110,I = 1,3
            M(I) = (-P(1) / LAMBDA(1)) * EV(I,1)
     F             + 1. / (2. * P(3)) * (P(1) ** 2 /LAMBDA(1) -C)
     F             * EV(I,3)
  110    CONTINUE
C
C        Transformation form:
C        X = (EV1,EV2,EV3) * X + M
C
      ELSE
C
         IF (LAMBDA(2).LT.-EPS) THEN
            INDE = 12
         ELSE
            INDE = 11
         ENDIF
         P(3) = 0.
         DO 120, I = 1,3
            P(3) = P(3) + EV(I,3) * B(I)
  120    CONTINUE
         IF (P(3).GT.0.D0) THEN
            P(3) = -P(3)
            DO 130, I = 1,3
```

```
                EV(I,3) = -1.D0 * EV(I,3)
  130        CONTINUE
          ENDIF
C
C         Normal form:
C         lambda(1) * x1 ** 2 + lambda(2) * x2 ** 2 + 2.*p3*x3 = 0.
          EV(1,1) = EV(2,2)*EV(3,3) - EV(3,2)*EV(2,3)
          EV(2,1) = EV(3,2)*EV(1,3) - EV(3,3)*EV(1,2)
          EV(3,1) = EV(1,2)*EV(2,3) - EV(2,2)*EV(1,3)
C
          NORM = 0.D0
          DO 140, I = 1,3
             NORM = EV(I,1)* EV(I,1) + NORM
 140      CONTINUE
          NORM = SQRT(NORM)
C
          DO 150, I = 1,3
             EV(I,1) = EV(I,1) /NORM
 150      CONTINUE
C
C
C     m : = (-p1/lambda(1)) * ev1 + (-p2/lambda(2)) * ev2
C         + 1./2./p3 * (p1**2 / lambda(1) + p2**2/lambda(2)-c)*ev3
C                  t                          t
C     mit p1 := ev1  * b    und p2 := ev2  *b
C

          DO 160, I = 1,2
             P(I) = 0.D0
             DO 170, J = 1,3
                P(I) = P(I) + EV(J,I) * B(J)
  170        CONTINUE
  160     CONTINUE
C
          DO 180, I = 1,3
             M(I) = (-P(1)/LAMBDA(1)) * EV(I,1) +
     F              (-P(2)/LAMBDA(2)) * EV(I,2) +
     F              1.D0/ (2. * P(3)) * ( P(1) ** 2 / LAMBDA(1)
     F                   + P(2)**2/LAMBDA(2) - C) * EV(I,3)
 180      CONTINUE
C
       ENDIF
 999   CONTINUE
C
       END
C
C
       SUBROUTINE MA20A(Q,D,A,R,S,IQ,M,N,TOLER)
       IMPLICIT REAL*8 (A-H,O-Z)
       REAL*8 SUM
```

```
      REAL*8 MIN,MAX
      INTEGER OUT,S(*)
      LOGICAL STAGE,TEST
      REAL*8 Q(IQ,*),A(*),D(*),R(*)
C  ***BIG MUST BE SET EQUAL TO ANY VERY LARGE REAL CONSTANT.
C  ***ITS VALUE HERE IS APPROPRIATE FOR THE IBM 370.
      DATA BIG /1.E75/
C  ***INITIALIZATION
      M2=M+2
      N2=N+2
      M1=M+1
      N1=N+1
      DO 1 J=1,N
      Q(M2,J)=J
    1 A(J)=0.
      DO 3 I=1,M
      Q(I,N2)=N+I
      D(I)=0.
      IF(Q(I,N1).GE.0) GO TO 3
      DO 2 J=1,N2
    2 Q(I,J)=-Q(I,J)
    3 CONTINUE
C  ***COMPUTE MARGINAL COSTS
      DO 5 J=1,N1
      SUM=0.
      DO 4 I=1,M
    4 SUM=SUM+Q(I,J)
    5 Q(M1,J)=SUM
C  ***STAGE I
C  ***DETERMINE VECTOR TO ENTER THE BASIS
      STAGE=.TRUE.
      KOUNT=0
      KR=1
      KL=1
    6 MAX=-1.
      DO 7 J=KR,N
      IF(ABS(Q(M2,J)).GT.N) GO TO 7
      B=ABS(Q(M1,J))
      IF(B.LE.MAX) GO TO 7
      MAX=B
      IN=J
    7 CONTINUE
      IF(Q(M1,IN).GE.0) GO TO 9
      DO 8 I=1,M2
    8 Q(I,IN)=-Q(I,IN)
C  ***DETERMINE VECTOR TO LEAVE THE BASIS
    9 K=0
      DO 10 I=KL,M
      B=Q(I,IN)
      IF(B.LE.TOLER) GO TO 10
```

```
      K=K+1
      R(K)=Q(I,N1)/B
      S(K)=I
      TEST=.TRUE.
   10 CONTINUE
   11 IF(K.GT.0) GO TO 12
      TEST=.FALSE.
      GO TO 14
   12 MIN=BIG
      DO 13 I=1,K
      IF(R(I).GE.MIN) GO TO 13
      J=I
      MIN=R(I)
      OUT=S(I)
   13 CONTINUE
      R(J)=R(K)
      S(J)=S(K)
      K=K-1
C  ***CHECK FOR LINEAR DEPENDENCE IN STAGE I
   14 IF(TEST.OR..NOT.STAGE) GO TO 16
      DO 15 I=1,M2
      B=Q(I,KR)
      Q(I,KR)=Q(I,IN)
   15 Q(I,IN)=B
      KR=KR+1
      GO TO 25
   16 IF(TEST) GO TO 17
      Q(M2,N1)=2.
      GO TO 34
   17 PIVOT=Q(OUT,IN)
      IF(Q(M1,IN)-PIVOT-PIVOT.LE.TOLER) GO TO 19
      DO 18 J=KR,N1
      B=Q(OUT,J)
      Q(M1,J)=Q(M1,J)-B-B
   18 Q(OUT,J)=-B
      Q(OUT,N2)=-Q(OUT,N2)
      GO TO 11
C  ***PIVOT ON Q(OUT,IN)
   19 DO 20 J=KR,N1
      IF(J.EQ.IN) GO TO 20
      Q(OUT,J)=Q(OUT,J)/PIVOT
   20 CONTINUE
      DO 22 I=1,M1
      IF(I.EQ.OUT) GO TO 22
      B=Q(I,IN)
      DO 21 J=KR,N1
      IF(J.EQ.IN) GO TO 21
      Q(I,J)=Q(I,J)-B*Q(OUT,J)
   21 CONTINUE
   22 CONTINUE
```

```
      DO 23 I=1,M1
      IF(I.EQ.OUT) GO TO 23
      Q(I,IN)=-Q(I,IN)/PIVOT
   23 CONTINUE
      Q(OUT,IN)=1./PIVOT
      B=Q(OUT,N2)
      Q(OUT,N2)=Q(M2,IN)
      Q(M2,IN)=B
      KOUNT=KOUNT+1
      IF(.NOT.STAGE) GO TO 26
C  ***INTERCHANGE ROWS IN STAGE I
      KL=KL+1
      DO 24 J=KR,N2
      B=Q(OUT,J)
      Q(OUT,J)=Q(KOUNT,J)
   24 Q(KOUNT,J)=B
   25 IF(KOUNT+KR.NE.N1) GO TO 6
C  ***STAGE II
      STAGE=.FALSE.
C  ***DETERMINE VECTOR TO ENTER THE BASIS
   26 MAX=-BIG
      DO 28 J=KR,N
      B=Q(M1,J)
      IF(B.GE.0) GO TO 27
      IF(B.GT.-2.) GO TO 28
      B=-B-2.
   27 IF(B.LE.MAX) GO TO 28
      MAX=B
      IN=J
   28 CONTINUE
      IF(MAX.LE.TOLER) GO TO 30
      IF(Q(M1,IN).GT.0) GO TO 9
      DO 29 I=1,M2
   29 Q(I,IN)=-Q(I,IN)
      Q(M1,IN)=Q(M1,IN)-2.
      GO TO 9
C  ***PREPARE OUTPUT
   30 L=KL-1
      DO 32 I=1,L
      IF(Q(I,N1).GE.0) GO TO 32
      DO 31 J=KR,N2
   31 Q(I,J)=-Q(I,J)
   32 CONTINUE
      Q(M2,N1)=0.
      IF(KR.NE.1) GO TO 34
      DO 33 J=1,N
      B=ABS(Q(M1,J))
      IF(B.LE.TOLER.OR.2.-B.LE.TOLER) GO TO 34
   33 CONTINUE
      Q(M2,N1)=1.
```

```
   34 DO 37 I=1,M
      K=Q(I,N2)
      B=Q(I,N1)
      IF(K.GT.0) GO TO 35
      K=-K
      B=-B
   35 IF(I.GE.KL) GO TO 36
      A(K)=B
      GO TO 37
   36 K=K-N
      D(K)=B
   37 CONTINUE
      Q(M2,N2)=KOUNT
      Q(M1,N2)=N1-KR
      SUM=0.
      DO 38 I=KL,M
   38 SUM=SUM+Q(I,N1)
      Q(M1,N1)=SUM
C     WRITE (6,*) ' A ',(A(I),I=1,M)
      RETURN
      END
C
C
C##       EA03A          20/03/79
C NAME EA03A(R)                    CHECK
      SUBROUTINE EA03A(A,B,N,ND,E)
      IMPLICIT REAL*8 (A-H,O-Z)
C STANDARD FORTRAN 66 (A VERIFIED PFORT SUBROUTINE)
      DIMENSION A(1),B(1),ARMAX(200),JRMAX(200)
C PURPOSE FINDS ALL THE EIGENVALUES AND EIGENVECTORS OF A REAL
SYMMETRIC
C         BY JACOBI'S METHOD (CLASSICAL METHOD)
C
C ARGUMENTS
C         A(A TWO DIMENSIONAL ARRAY TO THE USER) MUST CONTAIN THE
MATRIX
C          TREATED IN THE FIRST N ROWS AND COLUMNS OF THE ARRAY A.
C              ********* THE ORIGINAL MATRIX WILL BE DESTROYED
C              ********** THE EIGENVALUES WILL BE FOUND IN A(I,I)
I=1,2
C         N THE DIMENSION OF THE MATRIX
C         B THE EIGENVECTORS WILL BE FOUND IN THE COLUMNS OF B
C         ND THE FIRST DIMENSION OF THE ARRAYS A AND B IN THE CALLING
PR
C         MUST BE DIMENSION A(ND,  ),B(ND,  )
C         E ACCURACY CONTROL<<<< THE PROCESS CHOOSES THE OFF DIAGONAL
EL
C         WITH THE LARGEST MODULUS AND PERFORMS AN ORTHOGONAL
TRANSFORMA
```

```
C          REDUCE THE ELEMENT TO ZERO.THE PROCESS IS REPEATED UNTIL THE
L
C          MAGNITUDE AMONG OFF DIAGONAL ELEMENT IS LESS THAN E.
C *******'A IS ASSUMED TO BE SYMMETRIC' ******
C*************************************************************************
*
C
C FINDS THE OFF DIAGONAL ELEMENT WITH THE MAXIMUM MODULUS
C
C*************************************************************************
*
      NDN = ND*N
      DO 1 K=1,NDN
      B(K) = 0.0
    1 CONTINUE
      DO 2 K=1,N
      KK = K*(ND+1)-ND
      ARMAX(K) = 0.0
      B(KK) = 1.0
      DO 3 L=K,N
      IF(L-K)4,3,4
    4 KL = K+ND*(L-1)
      Y = ABS(A(KL))
      IF(ARMAX(K)-Y)5,3,3
    5 ARMAX(K) = Y
      JRMAX(K) = L
    3 CONTINUE
    2 CONTINUE
   11 AMAX = 0.0
      DO 6 K=1,N
      Y = ABS(ARMAX(K))
      IF(AMAX-Y)7,6,6
    7 AMAX = Y
      I = K
    6 CONTINUE
      IF(E-AMAX)8,9,9
    8 NDI = ND*(I-1)
      J = JRMAX(I)
      NDJ = ND*(J-1)
      II = I+NDI
      JJ = J+NDJ
      IJ = I+NDJ
      JI = J+NDI
      AII = A(II)
      AJJ = A(JJ)
      AIJ = A(IJ)
      Y = 2.0*AIJ
      X = AII-AJJ
      T = SIGN(1.0D0,X)*Y/(ABS(X)+SQRT(X**2+Y**2))
      TSQ = T**2
```

```
      C = 1.0/SQRT(1.0+TSQ)
      TY = T*Y
      S = T*C
      CSQ = C**2
      A(II) = CSQ*(AII+TY+AJJ*TSQ)
      A(JJ) = CSQ*(AJJ-TY+AII*TSQ)
      A(IJ) = 0.0
      A(JI) = 0.0
      DO 10 K=1,N
      JTES = (K-I)*(K-J)
      NDK = ND*(K-1)
      KI = K+NDI
      KJ = K+NDJ
      IF(JTES)13,12,13
   13 JK = J+NDK
      IK = I+NDK
      A(KI) = C*A(IK)+S*A(JK)
      A(KJ) =-S*A(IK)+C*A(JK)
      A(JK) = A(KJ)
      A(IK) = A(KI)
   12 X = B(KI)
      B(KI) = C*X+S*B(KJ)
      B(KJ) =-S*X+C*B(KJ)
   10 CONTINUE
C*********************************************************************
*
C
C FINDS THE MAXIMUM MODULUS OFF DIAGONAL ELEMENT BY MODIFIC ATION OF
C PREVIOUS INFORMATION OF OFF DIAGONAL ELEMENTS
C
C*********************************************************************
*
      ARMAX(I) = 0.0
      DO 14 K=1,N
      IF(K-I)15,14,15
   15 IK = I+ND*(K-1)
      Y = ABS(A(IK))
      IF(ARMAX(I)-Y)16,14,14
   16 ARMAX(I) = Y
      JRMAX(I) = K
   14 CONTINUE
      ARMAX(J) = 0.0
      DO 17 K=1,N
      IF(K-J)18,17,18
   18 JK = J+ND*(K-1)
      Y = ABS(A(JK))
      IF(ARMAX(J)-Y)19,17,17
   19 ARMAX(J) = Y
      JRMAX(J) = K
   17 CONTINUE
```

```
      DO 20 K=1,N
      ITES = (K-I)*(K-J)
      KI = K+NDI
      KJ = K+NDJ
      IF(ITES)21,20,21
   21 X = ABS(A(KI))
      Y = ABS(A(KJ))
      JR = J
      IF(X-Y)22,22,23
   23 Y = X
      JR = I
   22 IF(ARMAX(K)-Y)24,20,20
   24 ARMAX(K) = Y
      JRMAX(K) = JR
   20 CONTINUE
      GO TO 11
    9 RETURN
      END
```


Appendix B

Fortran Programme for the collisional radiative model for hydrogen molecules

This Fortran programme computes effective dissociation and dissociative ionization rate coefficients, the rates of production of neutral atoms and ions from the molecules, and the rate of dissociation energy loss. It diaplays all the reaction rate coefficients and results of chapter 3.

```
       IMPLICIT REAL*8(A-H,O-Z)
      PARAMETER (N=1000)
      REAL*4 ZXK(N),ZYK(N),ZXS(10),ZYS(10)
C     COMMON XDATA(N),YDATA(N)
      DIMENSION X(N),Y1(N),Y2(N),Y21(N),Y3(N),Y4(N),Y5(N),Y6(N),
     #               Y7(N),Y8(N),Y9(N),Y91(N),Y10(N),Y11(N),
     #               Y12(N),Y13(N),Y14(N),Y15(N),
     #               Y20(N),Y30(N),Y31(N),Y32(N),Y33(N),
     #               Y34(N),Y35(N),Y36(N),Y37(N),
     #               Y38(N),Y39(N),Y40(N),Y41(N),Y42(N),
     #               Y43(N),Y44(N),Y45(N),Y46(N),Y47(N),Y48(N),Y481(N),
     #               Y49(N),Y50(N),Y51(N),Y52(N),
     #               Y391(N),Y392(N),Y393(N),Y394(N),Y395(N)
      CHARACTER*48 TX(14)
      CALL GRSTRT(35,8)
C     CALL GRSCLC(5.,2.,25.5,20.7)
C     CALL GRSCLV(5.,2.,25.5,20.7)
C     CALL KURVEF(ZXK,ZYK,N,16)
C     WRITE (*,*) 'ENTER I'
C     READ (*,*) I
C     GO TO I
C  RATE COEFFICIENT FOR SINGLET B
      TX(1)='# B SINGLET SIGMA U'
      TX(3)='# C SINGLET PI U'
      TX(5)='# E,F SINGLET SIGMA G'
      TX(7)='# H(1S)+H(2S)'
      TX(8)='#H(1S)+H(3)'
      TX(9)='#H(2S)+H(2P)  RATE COEFFICIENT(CM3/SEC)'
      TX(10)='#H(1S)+H(1S)'
      TX(11)='#IONIZATION(H2+)'
      TX(12)='#DIRECT H(1S)+ H+'
      TX(2)='TEMPERATURE (EV)'
      TX(14)='ELECTRON COLLISION WITH H2'
                A1=-3.081902926338D+01
                B1=1.038866780735D+01
                C1=-4.259768348687D+00
                D1=1.181228673120D+00
                E1=-2.277513907465D-01
                F1=2.900576728856D-02
                G1=-2.287591474628D-03
                H1=1.004346442778D-04
                O1=-1.869930069131D-06
      XMIN=2.DO
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 10 I=1,N
         X(I)=XMIN+(I-1)*DX
         Y1(I)=DEXP(A1+B1*DLOG(X(I))+C1*(DLOG(X(I)))**2+
     #               D1*(DLOG(X(I)))**3+E1*(DLOG(X(I)))**4+
     #               F1*(DLOG(X(I)))**5+G1*(DLOG(X(I)))**6+
```

```
     #               H1*(DLOG(X(I)))**7+O1*(DLOG(X(I)))**8)
      ZXK(I)=X(I)
      ZYK(I)=Y1(I)
C     WRITE(6,*) Y1(I)
10    CONTINUE
C     J=0
C     DO 11 I=1,N,N/9
C       J=J+1
C       ZXS(J)=ZXK(I)
C       ZYS(J)=ZYK(I)
C1    CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
C     CALL KURVEF (ZXS,ZYS,J,1)
      CALL KURVEF (ZXK,ZYK,N,314)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C     GO TO 90
C RATE COEFFICIENT FOR SINGLET C
                A2=-3.348199796300D+01
                B2=1.371702271009D+01
                C2=-5.922607900694D+00
                D2=1.709719148860D+00
                E2=-3.505232830275D-01
                F2=4.834376067841D-02
                G2=-4.131406425550D-03
                H2=1.948388368131D-04
                O2=-3.854278715563D-06
      XMIN=2.D00
      XMAX=1.D03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 20 I=1,N
         x(i)=xmin+(i-1)*dx
         Y2(I)=DEXP(A2+B2*DLOG(X(I))+C2*(DLOG(X(I)))**2+
     #               D2*(DLOG(X(I)))**3+E2*(DLOG(X(I)))**4+
     #               F2*(DLOG(X(I)))**5+G2*(DLOG(X(I)))**6+
     #               H2*(DLOG(X(I)))**7+O2*(DLOG(X(I)))**8)
      ZXK(I)=X(I)
      ZYK(I)=Y2(I)
C     WRITE(6,*) Y2(I)
20    CONTINUE
C     J=0
C     DO 12 I=1,N,N/9
C       J=J+1
C       ZXS(J)=ZXK(I)
C       ZYS(J)=ZYK(I)
C2    CONTINUE
C     CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
```

```
C     CALL KURVEF (ZXS,ZYS,J,2)
      CALL KURVEF (ZXK,ZYK,N,315)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C     GO TO 90
C RATE COEFFICIENT FOR SINGLET E,F
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='E,F SINGLET SIGMA G EXCITATION'
                A21=-3.646589741675D+01
                B21=1.430361969329D+01
                C21=-6.074430521073D+00
                D21=1.677305768580D+00
                E21=-3.128705597349D-01
                F21=3.805424730473D-02
                G21=-2.860085821803D-03
                H21=1.199641410078D-04
                O21=-2.142231851104D-06
      XMIN=3.16D+00
      XMAX=1.D03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 21 I=1,N
         x(i)=xmin+(i-1)*dx
         Y21(I)=DEXP(A21+B21*DLOG(X(I))+C21*(DLOG(X(I)))**2+
     #               D21*(DLOG(X(I)))**3+E21*(DLOG(X(I)))**4+
     #               F21*(DLOG(X(I)))**5+G21*(DLOG(X(I)))**6+
     #               H21*(DLOG(X(I)))**7+O21*(DLOG(X(I)))**8)
      ZXK(I)=X(I)
      ZYK(I)=Y21(I)
C     WRITE(6,*) Y21(I)
21    CONTINUE
C     J=0
C     DO 13 I=1,N,N/9
C       J=J+1
C       ZXS(J)=ZXK(I)
C       ZYS(J)=ZYK(I)
C3    CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,316)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C RATE COEFFICIENT FOR DISSOCIATON INTO H(1S)+H(2S),RXN.2.2.6 JANEV
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION INTO H(1S)+H(2S)'
                A3=-3.454175591367D+01
                B3=1.412655911280D+01
```

```
                C3=-6.004466156761D+00
                D3=1.589476697488D+00
                E3=-2.775796909649D-01
                F3=3.152736888124D-02
                G3=-2.229578042005D-03
                H3=8.890114963166D-05
                O3=-1.523912962346D-06
      XMIN=2.51D+00
      XMAX=1.D03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 30 I=1,N
         x(i)=xmin+(i-1)*dx
         Y3(I)=DEXP(A3+B3*DLOG(X(I))+C3*(DLOG(X(I)))**2+
     #               D3*(DLOG(X(I)))**3+E3*(DLOG(X(I)))**4+
     #               F3*(DLOG(X(I)))**5+G3*(DLOG(X(I)))**6+
     #               H3*(DLOG(X(I)))**7+O3*(DLOG(X(I)))**8)
      ZXK(I)=X(I)
      ZYK(I)=Y3(I)
C     WRITE(6,*) Y3(I)
30    CONTINUE
C     J=0
C     DO 14 I=1,N,N/9
C       J=J+1
C       ZXS(J)=ZXK(I)
C       ZYS(J)=ZYK(I)
C4    CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,6514)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C     CALL GREND
C     GO TO 90
C RATE COEFFICIENT FOR DISSOCIATION INTO H(1S)+H(3),RXN.2.2.8 JANEV
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION INTO H(1S)+H(3)'
                A4=-3.884976142596D+01
                B4=1.520368281111D+01
                C4=-6.078494762845D+00
                D4=1.535455119900D+00
                E4=-2.628667482712D-01
                F4=2.994456451213D-02
                G4=-2.156175515382D-03
                H4=8.826547202670D-05
                O4=-1.558890013181D-06
      XMIN=3.98D+00
      XMAX=1.D03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
```

```
      DO 40 I=1,N
         x(i)=xmin+(i-1)*dx
         Y4(I)=DEXP(A4+B4*DLOG(X(I))+C4*(DLOG(X(I)))**2+
     #               D4*(DLOG(X(I)))**3+E4*(DLOG(X(I)))**4+
     #               F4*(DLOG(X(I)))**5+G4*(DLOG(X(I)))**6+
     #               H4*(DLOG(X(I)))**7+O4*(DLOG(X(I)))**8)
      ZXK(I)=X(I)
      ZYK(I)=Y4(I)
C     WRITE(6,*) Y4(I)
40    CONTINUE
C     J=0
C     DO 15 I=1,N,N/9
C       J=J+1
C       ZXS(J)=ZXK(I)
C       ZYS(J)=ZYK(I)
C5    CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,6515)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C     CALL GREND
C     GO TO 90
C RATE COEFFICIENT FOR DISSOCIATION INTO H(2S)+H(2P),RXN.2.2.7 JANEV
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION INTO H(2S)+H(2P)'
                A5=-4.794288960529D+01
                B5=2.629649351119D+01
                C5=-1.151117702256D+01
                D5=2.991954880790D+00
                E5=-4.949305181578D-01
                F5=5.236320848415D-02
                G5=-3.433774290547D-03
                H5=1.272097387363D-04
                O5=-2.036079507592D-06
      XMIN=5.01D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 50 I=1,N
         x(i)=xmin+(i-1)*dx
         Y5(I)=DEXP(A5+B5*DLOG(X(I))+C5*(DLOG(X(I)))**2+
     #               D5*(DLOG(X(I)))**3+E5*(DLOG(X(I)))**4+
     #               F5*(DLOG(X(I)))**5+G5*(DLOG(X(I)))**6+
     #               H5*(DLOG(X(I)))**7+O5*(DLOG(X(I)))**8)
      ZXK(I)=X(I)
      ZYK(I)=Y5(I)
C     WRITE(6,*) Y5(I)
50    CONTINUE
```

```
C     J=0
C     DO 16 I=1,N,N/9
C       J=J+1
C       ZXS(J)=ZXK(I)
C       ZYS(J)=ZYK(I)
C6    CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,6516)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C     CALL GREND
C     GO TO 90
C RATE COEFFICIENT FOR DISSOCIATION INTO H(1S)+H(1S) THROUGH
C                       TRIPLETS A,B,C
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION INTO H(1S)+H(1S)'
                A6=-2.787217511174D+01
                B6=1.052252660075D+01
                C6=-4.973212347860D+00
                D6=1.451198183114D+00
                E6=-3.062790554644D-01
                F6=4.433379509258D-02
                G6=-4.096344172875D-03
                H6=2.159670289222D-04
                O6=-4.928545325189D-06
      XMIN=1.26D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 60 I=1,N
         x(i)=xmin+(i-1)*dx
         Y6(I)=DEXP(A6+B6*DLOG(X(I))+C6*(DLOG(X(I)))**2+
     #               D6*(DLOG(X(I)))**3+E6*(DLOG(X(I)))**4+
     #               F6*(DLOG(X(I)))**5+G6*(DLOG(X(I)))**6+
     #               H6*(DLOG(X(I)))**7+O6*(DLOG(X(I)))**8)
      ZXK(I)=X(I)
      ZYK(I)=Y6(I)
C     WRITE(6,*) Y6(I)
60    CONTINUE
C     J=0
C     DO 17 I=1,N,N/9
C       J=J+1
C       ZXS(J)=ZXK(I)
C       ZYS(J)=ZYK(I)
C7    CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,616)
```

```
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C     CALL GREND
C     GO TO 90
C IONIZATION RATE COEFFICIENT,RXN.2.2.9 JANEV
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='IONIZATION'
                A7=-3.568640293666D+01
                B7=1.733468989961D+01
                C7=-7.767469363538D+00
                D7=2.211579405415D+00
                E7=-4.169840174384D-01
                F7=5.088289820867D-02
                G7=-3.832737518325D-03
                H7=1.612863120371D-04
                O7=-2.893391904431D-06
      XMIN=2.0D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 70 I=1,N
         x(i)=xmin+(i-1)*dx
         Y7(I)=DEXP(A7+B7*DLOG(X(I))+C7*(DLOG(X(I)))**2+
     #               D7*(DLOG(X(I)))**3+E7*(DLOG(X(I)))**4+
     #               F7*(DLOG(X(I)))**5+G7*(DLOG(X(I)))**6+
     #               H7*(DLOG(X(I)))**7+O7*(DLOG(X(I)))**8)
      ZXK(I)=X(I)
      ZYK(I)=Y7(I)
C     WRITE(6,*) Y7(I)
70    CONTINUE
C     J=0
C     DO 18 I=1,N,N/9
C       J=J+1
C       ZXS(J)=ZXK(I)
C       ZYS(J)=ZYK(I)
C8    CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,4615)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C     CALL GREND
C     GO TO 90
C RATE COEFFICIENT (PART OF IONIZATION ),JANEV RXN.2.2.10
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='IONIZATION LEADING INTO H(1S)+H+'
                A8=-3.834597006782D+01
```

```
                B8=1.426322356722D+01
                C8=-5.826468569506D+00
                D8=1.727940947913D+00
                E8=-3.598120866343D-01
                F8=4.822199350494D-02
                G8=-3.909402993006D-03
                H8=1.738776657690D-04
                O8=-3.252844486351D-06
      XMIN=3.98D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 80 I=1,N
         x(i)=xmin+(i-1)*dx
         Y8(I)=DEXP(A8+B8*DLOG(X(I))+C8*(DLOG(X(I)))**2+
     #               D8*(DLOG(X(I)))**3+E8*(DLOG(X(I)))**4+
     #               F8*(DLOG(X(I)))**5+G8*(DLOG(X(I)))**6+
     #               H8*(DLOG(X(I)))**7+O8*(DLOG(X(I)))**8)
      ZXK(I)=X(I)
      ZYK(I)=Y8(I)
C     WRITE(6,*) Y8(I)
80    CONTINUE
C     J=0
C     DO 19 I=1,N,N/9
C       J=J+1
C       ZXS(J)=ZXK(I)
C       ZYS(J)=ZYK(I)
C9    CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,12616)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C TOTAL IONIZATION RATE COEFFICIENT
      TX(2)='TEMPERATURE (EV)'
      TX(9)='RATE COEFFICIENT (CM3/SEC)'
      TX(14)='TOTAL IONIZATION'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 90 I=1,N
         x(i)=xmin+(i-1)*dx
         Y9(I)=Y7(I)+Y8(I)
      ZXK(I)=X(I)
      ZYK(I)=Y9(I)
C     WRITE(6,*) Y9(I)
90    CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
CC    CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
```

```
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C TOTAL DISSOCIATION COEFFICIENT
      TX(2)='TEMPERATURE (EV)'
      TX(9)='RATE COEFFICIENT (CM3/SEC)'
      TX(14)='TOTAL DISSOCIATION'
      XMIN=1.26D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 91 I=1,N
         x(i)=xmin+(i-1)*dx
         Y91(I)=Y3(I)+Y4(I)+Y5(I)+Y6(I)+
     #          0.295*(Y1(I)+Y21(I))+0.00919*Y3(I)
      ZXK(I)=X(I)
      ZYK(I)=Y91(I)
C     WRITE(6,*) Y91(I)
91    CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C TOTAL INELASTIC COLLISION RATE COEFFICIENT
      TX(2)='TEMPERATURE (EV)'
      TX(9)='RATE COEFFICIENT (CM3/SEC)'
      TX(14)='TOTAL INELASTIC COLLISION'
      XMIN=1.26D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 100 I=1,N
         x(i)=xmin+(i-1)*dx
         Y10(I)=Y1(I)+Y2(I)+Y21(I)+Y3(I)+Y4(I)+Y5(I)+Y6(I)+Y9(I)
      ZXK(I)=X(I)
      ZYK(I)=Y10(I)
C     WRITE(6,*) Y10(I)
100    CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C ENERGY LOSS PER COLLISION
      TX(2)='TEMPERATURE (EV)'
      TX(9)='ENERGY LOSS/COLLISION (EV)'
      TX(14)=' '
      XMIN=1.26D+00
      XMAX=1.D+03


120
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```
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 110 I=1,N
         x(i)=xmin+(i-1)*dx
         Y11(I)=(12.1*Y1(I)+12.4*Y2(I)+12.5*Y21(I)+15.5*Y3(I)+
     #          21.5*Y4(I)+34.6*Y5(I)+10.5*Y6(I)+19.25*Y9(I))/
     #          Y10(I)
      ZXK(I)=X(I)
      ZYK(I)=Y11(I)
C     WRITE(6,*) Y11(I)
110   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D0,1.D3,666.,666.,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C ENERGY LOSS PER IONIZATION
      TX(2)='TEMPERATURE (EV)'
      TX(9)='ENERGY LOSS/IONIZATION(EV)'
      TX(14)=' '
      XMIN=1.26D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 120 I=1,N
         x(i)=xmin+(i-1)*dx
         Y12(I)=(12.1*Y1(I)+12.4*Y2(I)+12.7*Y21(I)+15.5*Y3(I)+
     #          21.5*Y4(I)+34.6*Y5(I)+10.5*Y6(I)+19.25*Y9(I))/
     #          Y9(I)
      ZXK(I)=X(I)
      ZYK(I)=Y12(I)
C     WRITE(6,*) Y12(I)
120   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D0,1.D3,666.,666.,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C ENERGY LOSS PER DISSOCIATION
      TX(2)='TEMPERATURE (EV)'
      TX(9)='ENERGY LOSS/DISSOCIATION(EV)'
      TX(14)=' '
      XMIN=1.26D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 130 I=1,N
         x(i)=xmin+(i-1)*dx
         Y13(I)=(12.1*Y1(I)+12.4*Y2(I)+12.7*Y21(I)+15.5*Y3(I)+
     #          21.5*Y4(I)+34.6*Y5(I)+10.5*Y6(I)+19.25*Y9(I))/
     #          Y91(I)
```

```
      ZXK(I)=X(I)
      ZYK(I)=Y13(I)
C     WRITE(6,*) Y13(I)
130   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D0,1.D3,666.,666.,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C RATE OF PRODUCTION OF GROUND STATE H ATOMS,H(1)
      TX(2)='TEMPERATURE (EV)'
      TX(9)='RATE COEFFICIENT (CM3/SEC)'
      TX(14)='GROUND STATE H ATOMS'
      XMIN=1.26D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 140 I=1,N
         x(i)=xmin+(i-1)*dx
         Y14(I)=2*0.229*(Y1(I)+Y21(I))+2*0.00912*Y2(I)+
     #          Y3(I)+Y4(I)+2*Y6(I)
      ZXK(I)=X(I)
      ZYK(I)=Y14(I)
C     WRITE(6,*) Y14(I)
140   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C RATE OF PRODUCTION OF H(2) ATOMS
      TX(2)='TEMPERATURE (EV)'
      TX(9)='RATE COEFFICIENT (CM3/SEC)'
      TX(14)='H(2) ATOMS'
      XMIN=2.51D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 150 I=1,N
         x(i)=xmin+(i-1)*dx
         Y15(I)=Y3(I)+2*Y5(I)
      ZXK(I)=X(I)
      ZYK(I)=Y15(I)
C     WRITE(6,*) Y15(I)
150   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
```

```
      CALL GRNXTF
C RATE COEFFICIENT FOR DISSOCIATON INTO H+ + H+ ,RXN.2.2.11 JANEV
C DUE TO ELECTRON IMPACT WITH H2+
      TX(1)='#H+ + H+'
      TX(3)='#H(1S) + H+'
      TX(7)='#H(2) + H+'
      TX(8)='#H(1)+H(N>2)'
      TX(5)=' '
      TX(11)=' '
      TX(12)=' '
      TX(10)=' '
      TX(2)='TEMPERATURE (EV)'
      TX(9)='                    RATE COEFFICIENT (CM3/SEC)'
C     TX(2)='TEMPERATURE (EV)'
      TX(14)='ELECTRONIC COLLISION WITH H2+'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION INTO H+ + H+ FROM H2+'
                A20=-3.746192301092D+01
                B20=1.559355031108D+01
                C20=-6.693238367093D+00
                D20=1.981700292134D+00
                E20=-4.044820889297D-01
                F20=5.352391623039D-02
                G20=-4.317451841436D-03
                H20=1.918499873454D-04
                O20=-3.591779705491D-06
      XMIN=3.16D+00
      XMAX=1.D03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 200 I=1,N
         x(i)=xmin+(i-1)*dx
         Y20(I)=DEXP(A20+B20*DLOG(X(I))+C20*(DLOG(X(I)))**2+
     #               D20*(DLOG(X(I)))**3+E20*(DLOG(X(I)))**4+
     #               F20*(DLOG(X(I)))**5+G20*(DLOG(X(I)))**6+
     #               H20*(DLOG(X(I)))**7+O20*(DLOG(X(I)))**8)
       ZXK(I)=X(I)
       ZYK(I)=Y20(I)
C     WRITE(6,*) Y20(I)
200   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,2314)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C RATE COEFFICIENT FOR DISSOCIATON INTO H+ + H(1S), RXN.2.2.12 JANEV
C  FROM H2+
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION INTO H(1S) + H+ FROM H2+'
```

```
                  A30=-1.781416067709D+01
                  B30=2.277799785711D+00
                  C30=-1.266868411626D+00
                  D30=4.296170447419D-01
                  E30=-9.609908013189D-02
                  F30=1.387958040699D-02
                  G30=-1.231349039470D-03
                  H30=6.042383126281D-05
                  O30=-1.247521040900D-06
      XMIN=2.00D-01
      XMAX=1.D03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 300 I=1,N
         x(i)=xmin+(i-1)*dx
         Y30(I)=DEXP(A30+B30*DLOG(X(I))+C30*(DLOG(X(I)))**2+
     #               D30*(DLOG(X(I)))**3+E30*(DLOG(X(I)))**4+
     #               F30*(DLOG(X(I)))**5+G30*(DLOG(X(I)))**6+
     #               H30*(DLOG(X(I)))**7+O30*(DLOG(X(I)))**8)
      ZXK(I)=X(I)
      ZYK(I)=Y30(I)
C     WRITE(6,*) Y30(I)
300   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,2515)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C RATE COEFFICIENT FOR DISSOCIATON INTO H(2) + H+,RXN.2.2.13 JANEV
C  FROM H2+
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION INTO H(2) + H+'
                  A31=-3.408905929046D+01
                  B31=1.573560727511D+01
                  C31=-6.992177456733D+00
                  D31=1.852216261706D+00
                  E31=-3.130312806531D-01
                  F31=3.383704123189D-02
                  G31=-2.265770525273D-03
                  H31=8.565603779673D-05
                  O31=-1.398131377085D-06
      XMIN=2.00D+00
      XMAX=1.D03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 310 I=1,N
         x(i)=xmin+(i-1)*dx
         Y31(I)=DEXP(A31+B31*DLOG(X(I))+C31*(DLOG(X(I)))**2+
     #               D31*(DLOG(X(I)))**3+E31*(DLOG(X(I)))**4+
     #               F31*(DLOG(X(I)))**5+G31*(DLOG(X(I)))**6+
```

```
     #               H31*(DLOG(X(I)))**7+O31*(DLOG(X(I)))**8)
      ZXK(I)=X(I)
      ZYK(I)=Y31(I)
C     WRITE(6,*) Y31(I)
310   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,2716)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C RATE COEFFICIENT FOR DISSOCIATON INTO H(1S)+H(N)(N>1), RXN.2.2.14
JANE
C  FROM H2+
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION INTO H(1S)+H(N>1) FROM H2+'
                A32=-1.670435653561D+01
                B32=-6.035644995682D-01
                C32=-1.942745783445D-08
                D32=-2.005952284492D-07
                E32=2.962996104431D-08
                F32=2.134293274971D-08
                G32=-6.353973401838D-09
                H32=6.152557460831D-10
                O32=-2.025361858319D-11
      XMIN=1.00D-01
      XMAX=1.D03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 320 I=1,N
         x(i)=xmin+(i-1)*dx
         Y32(I)=DEXP(A32+B32*DLOG(X(I))+C32*(DLOG(X(I)))**2+
     #               D32*(DLOG(X(I)))**3+E32*(DLOG(X(I)))**4+
     #               F32*(DLOG(X(I)))**5+G32*(DLOG(X(I)))**6+
     #               H32*(DLOG(X(I)))**7+O32*(DLOG(X(I)))**8)
      ZXK(I)=X(I)
      ZYK(I)=Y32(I)
C     WRITE(6,*) Y32(I)
320   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,2816)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C RADIATIVE ENERGY LOSS
      TX(2)='TEMPERATURE (EV)'
      TX(9)='RADIATIVE ENERGY LOSS/DISSOCIATION(EV)'
      TX(14)=' '
      XMIN=2.00D+00
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```
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 330 I=1,N
         x(i)=xmin+(i-1)*dx
         Y33(I)=(12.1*Y1(I)+12.4*Y2(I)+12.7*Y21(I))/
     #         (Y91(I))
      ZXK(I)=X(I)
      ZYK(I)=Y33(I)
C     WRITE(6,*) Y33(I)
330   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D0,1.D3,666.,666.,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C RATE COEFFICIENT FOR DISSOCIATION OF H2 INTO H+ + H+
      TX(14)='DISSOCIATION OF H2 INTO H+ + H+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 340 I=1,N
         x(i)=xmin+(i-1)*dx
         Y34(I)=Y20(I)*Y7(I)/(Y20(I)+Y30(I)+Y31(I)+Y32(I))
      ZXK(I)=X(I)
      ZYK(I)=Y34(I)
C     WRITE(6,*) Y34(I)
340   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C RATE COEFFICIENT FOR DISSOCIATION OF H2 INTO H(1S)+ H+
      TX(2)='TEMPERATURE (EV)'
      TX(9)='RATE COEFFICIENT (CM3/SEC)'
      TX(14)='DISSOCIATION OF H2 INTO H(1S)+ H+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 350 I=1,N
         x(i)=xmin+(i-1)*dx
         Y35(I)=Y8(I)+Y30(I)*Y7(I)/(Y20(I)+Y30(I)+Y31(I)+Y32(I))
      ZXK(I)=X(I)
      ZYK(I)=Y35(I)
C     WRITE(6,*) Y35(I)
350   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
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```
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C RATE COEFFICIENT FOR DISSOCIATION OF H2 INTO H(2)+ H+
      TX(2)='TEMPERATURE (EV)'
      TX(9)='RATE COEFFICIENT (CM3/SEC)'
      TX(14)='DISSOCIATION OF H2 INTO H(2)+ H+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 360 I=1,N
         x(i)=xmin+(i-1)*dx
         Y36(I)=Y31(I)*Y7(I)/(Y20(I)+Y30(I)+Y31(I)+Y32(I))
      ZXK(I)=X(I)
      ZYK(I)=Y36(I)
C     WRITE(6,*) Y36(I)
360   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C RATE COEFFICIENT FOR DISSOCIATION OF H2 INTO
C H(1)+H(N>1) THROUGH H2+
      TX(2)='TEMPERATURE (EV)'
      TX(9)='RATE COEFFICIENT (CM3/SEC)'
      TX(14)='DISSOCIATION OF H2 INTO H(1)+ H(N>1) THROUGH H2+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 370 I=1,N
         x(i)=xmin+(i-1)*dx
         Y37(I)=Y32(I)*Y7(I)/(Y20(I)+Y30(I)+Y31(I)+Y32(I))
      ZXK(I)=X(I)
      ZYK(I)=Y37(I)
C     WRITE(6,*) Y37(I)
370   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C RATE COEFFICIENT OF PRODUCTION FOR DISSOCIATION OF H2 INTO
C H(1)+H(2) THROUGH H2+
      TX(2)='TEMPERATURE (EV)'
      TX(9)='RATE COEFFICIENT (CM3/SEC)'
      TX(14)='DISSOCIATION OF H2 INTO H(1)+ H(2) THROUGH H2+'
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```
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 380 I=1,N
         x(i)=xmin+(i-1)*dx
         Y38(I)=0.10*Y37(I)
      ZXK(I)=X(I)
      ZYK(I)=Y38(I)
C     WRITE(6,*) Y38(I)
380   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C RATE COEFFICIENT OF PRODUCTION FOR DISSOCIATION OF H2 INTO
C H(1)+H(3) THROUGH H2+
      TX(2)='TEMPERATURE (EV)'
      TX(9)='RATE COEFFICIENT (CM3/SEC)'
      TX(14)='DISSOCIATION OF H2 INTO H(1)+ H(3) THROUGH H2+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 390 I=1,N
         x(i)=xmin+(i-1)*dx
         Y39(I)=0.45*Y37(I)
      ZXK(I)=X(I)
      ZYK(I)=Y39(I)
C     WRITE(6,*) Y39(I)
390   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C RATE COEFFICIENT OF PRODUCTION FOR DISSOCIATION OF H2 INTO
C H(1)+H(4) THROUGH H2+
      TX(2)='TEMPERATURE (EV)'
      TX(9)='RATE COEFFICIENT (CM3/SEC)'
      TX(14)='DISSOCIATION OF H2 INTO H(1)+ H(4) THROUGH H2+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 400 I=1,N
         x(i)=xmin+(i-1)*dx
         Y40(I)=0.22*Y37(I)
      ZXK(I)=X(I)
      ZYK(I)=Y40(I)
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C RATE COEFFICIENT OF PRODUCTION FOR DISSOCIATION OF H2 INTO
C H(1)+H(N>6) THROUGH H2+
      TX(2)='TEMPERATURE (EV)'
      TX(9)='RATE COEFFICIENT (CM3/SEC)'
      TX(14)='DISSOCIATION OF H2 INTO H(1)+ H(N>6) THROUGH H2+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 430 I=1,N
         x(i)=xmin+(i-1)*dx
         Y43(I)=0.04*Y37(I)
      ZXK(I)=X(I)
      ZYK(I)=Y43(I)
C     WRITE(6,*) Y43(I)
430   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,16)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C TOTAL RATE OF PRODUCTION OF GROUND STATE H ATOMS,H(1)
      TX(1)='#H(1)'
      TX(3)='#H(2)'
      TX(7)='#H(3)'
      TX(8)='#H(4)'
      TX(10)='#H(5)'
      TX(11)='#H(6)'
      TX(12)='#H(N>6)'
      TX(2)='TEMPERATURE (EV)'
      TX(9)='  RATE COEFFICIENT (CM3/SEC)'
      TX(14)='PRODUCTION OF NEUTRAL ATOMS'
      TX(5)=' '
      XMIN=1.26D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 440 I=1,N
         x(i)=xmin+(i-1)*dx
         Y44(I)=Y14(I)+Y35(I)+Y37(I)
      ZXK(I)=X(I)
      ZYK(I)=Y44(I)
C     WRITE(6,*) Y44(I)
440   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,314)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C TOTAL RATE OF PRODUCTION OF H(2) ATOMS
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C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='TOTAL H(2) ATOMS'
      XMIN=2.51D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 450 I=1,N
         x(i)=xmin+(i-1)*dx
         Y45(I)=Y15(I)+Y36(I)+Y38(I)
      ZXK(I)=X(I)
      ZYK(I)=Y45(I)
C     WRITE(6,*) Y45(I)
450   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,315)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C TOTAL RATE OF PRODUCTION OF H(3)
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION OF H2 INTO H(1)+ H(3) THROUGH H2+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 3910 I=1,N
         x(i)=xmin+(i-1)*dx
         Y391(I)=Y4(I)+Y39(I)
      ZXK(I)=X(I)
      ZYK(I)=Y391(I)
C     WRITE(6,*) Y391(I)
3910   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,316)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C TOTAL RATE OF PRODUCTION OF H(4)
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION OF H2 INTO H(1)+ H(4) THROUGH H2+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 3920 I=1,N
         x(i)=xmin+(i-1)*dx
         Y392(I)=0.22*Y37(I)
      ZXK(I)=X(I)
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```
      ZYK(I)=Y392(I)
C     WRITE(6,*) Y392(I)
3920  CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,4514)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C TOTAL RATE OF PRODUCTION OF H(5)
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION OF H2 INTO H(1)+ H(5) THROUGH H2+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 3930 I=1,N
         x(i)=xmin+(i-1)*dx
         Y393(I)=0.12*Y37(I)
      ZXK(I)=X(I)
      ZYK(I)=Y393(I)
C     WRITE(6,*) Y393(I)
3930  CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,4515)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C TOTAL RATE OF PRODUCTION OF H(6)
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION OF H2 INTO H(1)+ H(6) THROUGH H2+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 3940 I=1,N
         x(i)=xmin+(i-1)*dx
         Y394(I)=0.069*Y37(I)
      ZXK(I)=X(I)
      ZYK(I)=Y394(I)
C     WRITE(6,*) Y394(I)
3940  CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,4516)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C TOTAL RATE OF PRODUCTION OF H(N>6)
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C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION OF H2 INTO H(1)+ H(N>6) THROUGH H2+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 3950 I=1,N
         x(i)=xmin+(i-1)*dx
         Y395(I)=0.04*Y37(I)
      ZXK(I)=X(I)
      ZYK(I)=Y395(I)
C     WRITE(6,*) Y395(I)
3950  CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,6616)
      CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
      CALL GRLGND(TX)
      CALL GRNXTF
C EFFECTIVE DISSOCIATION RATE COEFFICIENT OF DISSOCIATION OF H2 INTO
C H + H
      TX(1)='#H + H'
      TX(3)='#H + H+'
      TX(7)='#H+ + H+'
      TX(8)='#SUM'
      TX(5)=' '
      TX(10)=' '
      TX(11)=' '
      TX(12)=' '
      TX(13)=' '
      TX(2)='TEMPERATURE (EV)'
      TX(9)='EFFECTIVE DISSOCIATION RATE COEFFICIENT(CM3/SEC)'
      TX(14)=' '
      TX(2)='TEMPERATURE (EV)'
C     TX(9)='EFFECTIVE DISSOCIATION RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATION OF H2 INTO H + H'
      XMIN=1.26D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 460 I=1,N
         x(i)=xmin+(i-1)*dx
         Y46(I)=0.229*(Y1(I)+Y21(I))+0.00912*Y2(I)+Y3(I)+Y4(I)+
     #          Y5(I)+Y6(I)
      ZXK(I)=X(I)
      ZYK(I)=Y46(I)
C     WRITE(6,*) Y46(I)
460   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,2314)
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C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C EFFECTIVE DISSOCIATION RATE COEFFICIENT OF DISSOCIATION OF H2 INTO
C H + H+
C     TX(14)='DISSOCIATIVE IONIZATION OF H2 INTO H + H+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 470 I=1,N
         x(i)=xmin+(i-1)*dx
         Y47(I)=Y35(I)+Y36(I)
      ZXK(I)=X(I)
      ZYK(I)=Y47(I)
C     WRITE(6,*) Y47(I)
470   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,2515)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C EFFECTIVE DISSOCIATION RATE COEFFICIENT OF DISSOCIATION OF H2 INTO
C H+ + H+
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='EFFECTIVE RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='DISSOCIATIVE IONIZATION OF H2 INTO  H+ + H+'
      XMIN=2.00D+00
      XMAX=1.D+03
      DX=(XMAX-XMIN)/DFLOAT(N-1)
      DO 480 I=1,N
         x(i)=xmin+(i-1)*dx
         Y48(I)=Y34(I)
      ZXK(I)=X(I)
      ZYK(I)=Y48(I)
C     WRITE(6,*) Y48(I)
480   CONTINUE
      CALL GRSCLC (1.,2.,39.5,28.7)
C     CALL GRSCLV (5.,2.,25.5,20.7)
      CALL KURVEF (ZXK,ZYK,N,2716)
C     CALL GRBLD (30.,20.,-101,-101,1.D-1,1.D3,1.D-11,1.D-6,-666)
C     CALL GRLGND(TX)
C     CALL GRNXTF
C EFFECTIVE DISSOCIATION RATE COEFFICIENT OF DISSOCIATION OF H2 INTO
C TWO PARTICLES
C     TX(2)='TEMPERATURE (EV)'
C     TX(9)='EFFECTIVE RATE COEFFICIENT (CM3/SEC)'
C     TX(14)='TOTAL DISSOCIATION OF H2 INTO TWO PARTICLES'
      XMIN=1.26D+00
      XMAX=1.D+03
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