A
STEADY-STATE CALCULATION OF
COLUMN DENSITIES OF INTERSTELLAR SPECIES
TOWARD ζ OPHIUCHI, ο PERSEI AND LYNDS 134

BY

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ABSTRACT

Calculations of column densities of some 100 interstellar species based on a steady-state analysis are carried out for interstellar clouds toward ζOph, οPer, and Lynds 134, using appropriate cloud models and physical conditions.

The observed column densities of CH, OH, and CO are well reproduced by calculations. However, the calculated column densities of CH$^+$ and C$_2$ show somewhat large discrepancies from the observed values. No explanation was found for these discrepancies. Column densities of species including ^{13}C are also calculated for L134.

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I. INTRODUCTION

It is already over 35 years since the first detection of the ultra-violet lines of interstellar CN, CH^+, and CH in the 1930's and now we can count over 40 molecular species in the list of interstellar molecules detected (APPENDIX A). The size of molecules ranges from diatomic molecules such as CH, CN to nine-atomic ones such as C_2H_5OH, ethylalcohol. These molecules have been observed from optical to the radio wavelength region: however, the majority has been discovered by means of radio telescopes in the centimeter and millimeter bands.

Molecular species sufficiently abundant for easy detection form more or less dense regions. Those regions are rich in dust grains which significantly reduce the transparency of the clouds to background star light. Therefore, frequently, the stellar radiation cannot be a source of interstellar absorption lines. On the other hand, radio waves can penetrate even through the dense clouds, so that they can be detected from the radio emission.

When we depict our Milky Way in our minds, the spiral arms, the disk, and the halo are the large scale structures. If the material organized into this structure, which is mainly neutral hydrogen atoms, were distributed uniformly, the mean density would be ~ 3 atoms/cm^3 (Rank, et al. 1971). On the small scale, however, interstellar material is distributed irregularly. Dust grains and gas components are concentrated into small areas to form relatively cool, dense regions called 'clouds'.

The interstellar clouds have irregular shapes and occupy approximately 5% of the volume of our galaxy and are strongly concentrated to the galactic plane. The sizes of the clouds are 0.1 to 50 light years and the gas densities are 10 to 10^7 cm^{-3} (Rank, et al. 1971). Most clouds have kinetic temperatures of 10 to 200°K, except in HII regions, and contain $\sim 1\%$ mass of dust grains of approximately 0.1 microns in size (Rank, et al. 1971; Hollenbach, et al. 1971).

Relatively low density clouds of $10 \leq n \leq 10^3$ cm^{-3} (Snow 1976) are called diffuse interstellar clouds, and are relatively transparent to the background stellar radiation, while dark interstellar clouds with densities of 10^4-10^7 cm^{-3} and $A_V \gtrsim 5$ mag are more opaque to the stellar radiation, but transparent to high energy cosmic ray protons. This difference of transparency is closely related to the chemistry in interstellar clouds.

Since the discovery of interstellar molecules, several general processes have been considered to interpret the observed molecular lines and to understand the chemistry in the clouds. Probably molecules are continuously produced in and removed from the clouds by various mechanisms. The relatively low density clouds are transparent to the background ultra-violet radiation field. Therefore, ionization and dissociation by ultra-violet radiation are important mechanisms for the destruction of molecules in the clouds. As the density of clouds increases, the clouds become opaque to the ultra-violet radiation, and hence photoionization and photodissociation become less important to the chemistry of the clouds. For these dense clouds, on the other hand, cosmic ray protons play an important role by ionizing H_2 and He. The cosmic ray ionization rate itself is small compared with photoionization in diffuse clouds, but this process creates reactive species, and hence is important to the chemistry of dense clouds.

Another process which may occur in interstellar clouds is the freezing out of molecules on the surface of dust grains. Although this process is slower than the photoionization of unshielded molecules (Herbst, et al. 1976), it may have non-negligible effects on the abundance of molecules since it can occur even in shielded dense clouds.

Chemical reactions such as ion-neutral reactions, recombination reactions with electrons, and neutral-neutral reactions are, of course, the major mechanisms for removing certain species from the clouds. Since molecules suffer destruction processes, one or several efficient formation mechanisms are essential to maintain the observed abundance of molecules.

In the first place, the gas phase chemical reactions mentioned above are probably the most important processes for the formation of molecules in the clouds. Since the densities of clouds are low compared with stellar atmospheres, many-body collisions are very unlikely and hence, two atomic or molecular collisions are the principal reaction schemes in the clouds. Secondaly, formation of molecular species on the surface of dust grains may take place efficiently. Interstellar grains have irregular shape (Abell 1974) and supply chemically active surfaces which act as catalysts to atomic or molecular species impinging on them. Molecules may be formed on these active sites and may be released into interstellar space. Molecules may also be formed in the atmospheres of stars which are much denser than interstellar clouds and can be blown off the stellar surface. It is, however, questionable whether the molecules formed in stellar atmospheres can survive the radiation of the star which formed the molecules.

Interstellar molecules are good indicators of the physical conditions at the place where the molecules are found: observed molecular line strengths directly give us information on the constitution, location, and radial velocities of the clouds. Careful analysis of these molecular lines, combined with quantities measured in the laboratory, provides indirect information on the physical conditions and dynamics of the clouds. Since the gaseous components of clouds are probably not in thermodynamic equilibrium, the interpretation of line intensities is not simple since many factors must be considered, such as cloud temperature, the radiation field, cosmic rays, ultra-violet radiation, the 2.7°K black body radiation, electron density,etc.

Several general models have been used to interpret the molecular observations. As a first approximation, time-independent (steady-state) analysis have had considerable success in the interpretation of the abundances of molecules. Of molecular parameters, column densities are the only directly measurable quantities, and hence, to test models of clouds, it is best to consider the agreement between observed and calculated column densities of molecular species.

From this consideration, column density calculations based on the steady-state analysis were carried out using appropriate cloud models and physical conditions toward the interstellar clouds ζ Oph, ο Per, and Lynds 134, and some results are presented here. The method of calculation is found in Chapter III, and the results are presented in Chapters IV (for ζ Oph cloud), V (for ο Per cloud), and VI (for Lynds 134).

II. CHEMISTRY IN INTERSTELLAR CLOUDS

Since the most abundant element in interstellar clouds is hydrogen, the form of hydrogen is important in describing the properties of the clouds.

In the calculation, only gas phase reactions have been considered, neglecting processes of acretion and release of molecules on the surface of dust grains except for hydrogen molecules. The reasons for this are described by Herbst and Klemperer (1973), i.e.

1. The constituent(s) and the properties of the surfaces of dust grains are not well-studied.
2. The molecular ions N_2H^+ and HCO^+ have been detected, and hence even if surface catalysed reactions are considered, gas phase reactions must be involved in describing the chemistry of the interstellar medium.
3. The rate constants for gas phase reactions can sometimes be obtained through laboratory measurement or theoretical consideration. Gas phase processes including several important reactions are also described below.

(1) Hydrogen in interstellar clouds

Interstellar hydrogen mainly takes three forms, i.e. H^+, H, and H_2. Hydrogen ions, H^+, are found mainly near the hot stars as the constituents of HII regions. In cooler clouds, H and H_2 are the most abundant hydrogen species. Hollenbach, et al. (1971) demonstrated the formation of hydrogen molecules, H_2, on the surface of dust grains under the conditions usually found in interstellar clouds.

$$H + H + \text{grain surface} \dashrightarrow H_2(\text{gas}) \qquad (418)^*$$

is the most efficient process to interpret the observed abundance of H_2. Two properties of hydrogen make this process the most preferable for making hydrogen molecules; one is the mobility of hydrogen atom on the surface of grain even at low temperature; and the other is the low binding energy of H_2 to grain surfaces which permit the release of H_2 from the surfaces of the grains. The rate, R, of the reaction 418 is expressed by the formula

$$R = 10^{-17}\, n\, n_H \ \text{cm}^{-3}\text{sec}^{-1}$$

where n and n_H are the number densities of the total hydrogen atom and the hydrogen atom in the atomic form (Hollenbach, et al.

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[*] The reaction numbers are those in APPENDIX B.

1971).

It is well established that hydrogen molecules are the major constituent of dense clouds. In less dense ($n \lesssim 10^3$) clouds where ultra-violet radiation can penetrate, photodissociation of H_2 molecules is important:

$$H_2 \xrightarrow{h\nu} H + H$$

The rate for this process is given by

$$\text{Rate (D)} = 2 \times 10^{-17}\, n\, \frac{1-f}{f}$$

where $f = \dfrac{x}{x + \sqrt{x} + 1}$

n is the total density: $n = n(H) + 2n(H_2)$ cm^{-3}

and $x = 10^{-4}\, n^2\, \tau_c \exp(5\tau_c)$ (Hollenbach, et al. 1971).

In the above expressin τ_c is the optical depth measured at the cloud centre. Optical depth and visual absorption are related by

$$A_v = 1.086\, \tau_v \quad \text{and hence}$$

$$\tau_c = \frac{A_v}{1.086}\,\frac{1}{2} \quad \text{(cloud centre)}$$

Visual absorption for each cloud is taken from observed data.

In dense clouds where ultra-violet radiation cannot penetrate because of a large shielding effect, the major destruction process of the H_2 molecule is the ionization caused by high energy cosmic rays which have the energy $\gtrsim$100 Mev. The ionization rate is well established and found to be $\sim 10^{-17}$ sec^{-1} (Hollenbach, et al. 1971; Mitchell, et al. 1977). In the dense clouds exposed to these cosmic rays, hydrogen atoms suffer from ionizations:

$$H + p \text{ -----> } H^{+} + e^{-} + p \qquad (596)$$

Hydrogen molecules are destroyed in three ways:

$$H_2 + p \text{ -----> } H_2^{+} + e^{-} + p \qquad (601)$$

$$H_2 + p \text{ -----> } H^{+} + H + e^{-} + p \qquad (602)$$

$$H_2 + p \text{ -----> } H + H + p \qquad (603)$$

The rates for these processes are given by Hollenbach, et al. (1971), Glassgold and Langer (1974), and Watson (1974).

Gas phase processes

As described above, only two-body gas phase reactions are assumed for formation of molecules other than H_2 in interstellar clouds. The low temperatures of clouds set another restriction to the chemistry of the clouds: Reactions must be exothermic (Herbst and Klemperer 1973). The rate constants for bimolecular reactions are often expressed as

$$K = Ae^{-Ea/kT} \ \mathrm{cm}^3/\mathrm{sec}$$

where A is a constant,

Ea is called activation energy and is the minimum energy barrier to the reaction,

and k is the Boltzmann constant.

In the case of neutral-neutral reactions, the activation energy is often much greater than kT and hence $K \dashrightarrow 0$, i.e. neutral-neutral reactions are often of less importance. Only atom-reactive species reactions are the exceptions.

Under the low density and low temperature conditions of clouds, exothermic ion-molecules reactions are the major processes in forming various species, as they hardly need activation energy.

<u>TABLE 1</u> in APPENDIX B lists the ion-neutral reactions used in the calculations.

3) Photodestruction (photoionization and photodissociation) processes

In diffuse cloud, the background radiation field is quite important in the ionization and dissociation of many species. In TABLE 3 of APPENDIX B, photodestruction processes used in the calculation are listed. All these are taken from Mitchell et al. (1977b). Rates for photodestruction processes are calculated by Black and Dalgarno (1977).

The rate, R, of each photoionization or photodissociation is expressed as

$$R = \int_{\nu_t}^{\nu_L} \phi(\nu)\sigma(\nu)\,d\nu$$

where $\phi(\nu)$ is the intensity of the radiation field at frequency ν, $\sigma(\nu)$ is the cross section of that process in cm^2.

Integration is made from the threshold frequency, ν_t, to the Lyman limit of atomic hydrogen, ν_L. Intensity, $\phi(\nu)$, of the radiation penetrating through a cloud with no internal radiation source has the form using boundary intensity, $\phi_o(\nu)$,

$$\phi(\nu) = \phi_o(\nu)\,e^{-K\tau(\nu)}$$

where τ is the optical depth,
and κ is linear absorption coefficient.

In this expression, τ is related to the corresponding absorption in magnitude by

$$A_\nu = 1.086 \tau_\nu$$

Using these expressions, Black and Dalgarno evaluated the rate of the photodestruction processes and obtained approximate expression of the rate as

$$R = A \exp(-B \times A_v) \ \mathrm{sec}^{-1}$$

where A and B are constants,
A_v is the visual absorption which is taken from observed data.

In TABLE 3 in APPENDIX B, values of A and B are listed for various reactions. These values are estimated for a background radiation energy normalized to 4×10^{-17} erg cm^{-3} $\mathrm{Å}^{-1}$ at 1000 Å.

III. THE METHOD OF CALCULATION

In the calculation, the following quantities may be needed to specify the cloud properties. These quantities are usually taken from observed data for each cloud.

(1) Total Density, n

Hydrogen atoms and molecules are the most abundant species in any cloud and others are minor constituents compared with hydrogen. Thus the total density of clouds is defined by the number density of hydrogen nuclei, namely,

$$n = n(H) + 2n(H_2)$$

where $n(x)$ describes the number density of species x in cm^{-3}.

(2) Element Abundances

In the calculation, nine elements are included except for the calculation of ^{13}C abundances in Lynds 134. Those are H, He, C, O, N, S, Mg, Fe, and Si.

Morton (1975) found depletion in the abundance of many elements compared with solar element abundances in the direction of ζ Oph. Snow (1976) has reported the depletion of element abundances toward o Per. The relative abundances of elements used in these calculations are listed in <u>TABLE 1</u>.

TABLE 1

ELEMENT ABUNDANCES (H = 1.00)

	Solar	ζ Oph	o Per
He	0.14	0.14	0.14
C	3.72(-4)	7.41(-5)	3.35(-5)
N	1.15(-4)	2.14(-5)	3.57(-6)
O	6.76(-4)	1.76(-4)	1.51(-5)
Mg	3.47(-5)	1.02(-6)	2.51(-6)
Si	3.55(-5)	8.32(-7)	3.72(-7)
S	1.62(-5)	8.32(-6)	1.22(-6)
Fe	2.51(-5)	2.69(-7)	1.35(-7)

According to the column density and the element depletion data presented by Morton and Snow, however, the element abundances observed have large uncertainties.

Since the element abundances toward L134 have not been observed, the same depleted abundances used for the calculation of ζ Oph are assumed in the L134 calculation.

(3) Optical Depth

Many photodestruction processes are involved in these calculations. By the rate equation described previously,

$$R = A \exp(-B \times A_V),$$

the rate of photodestruction processes depends on the optical depth, i.e. the distance into the cloud. The optical depth at a particular point in the cloud is calculated from τ_c using the working model of each cloud which is described later.

When the visual extinction or the total optical depth is not available from the observations, the total optical depth is calculated by the relation (Hollenbach et al. 1971):

$$\tau_c = \left(\frac{M}{500}\right)^{1/3} \left(\frac{n}{260}\right)^{2/3}$$

where M is the cloud mass in $M_\odot$, and n is the total density of the cloud.

(4) Ultra-violet Radiation Field Strength

Probably the ultra-violet radiation field in interstellar clouds is not simple, especially for clouds near hot stars (e.g. ζ Oph and o Per). In the calculation, however, all effects of the radiation field caused by the stars are neglected even in the case of o Per in which the star is imbedded in the cloud. The radiation field considered is the mean isotropic intercloud radiation field. The unattenuated radiation field strength is expressed (Black and Dalgarno 1977) as

$$\phi_o(\nu) = 2.0 \times 10^{-17} \lambda^3 I \text{ photons cm}^{-2} \text{ sec}^{-1} \text{ Hz}^{-1}$$

for $\lambda = 912 - 3300$ Å, I is the radiation energy density normalized to 4×10^{-17} erg cm^{-3} Å^{-1} at 1000 Å. All A and B values appearing in TABLE 3 in APPENDIX B are calculated for this value, i.e. $I = 1$.

From the method of derivation of A and B, photodestruction rates, R, are directly proportional to I (Black and Dalgarno 1976). Where a stronger radiation field is appropriate, the rate, R, is simply multiplied by a factor which differs from unity (for example, 2.5 for the ζ Oph cloud).

(5) Cloud Temperature

In some reactions the reaction rate coefficients are temperature dependent, and hence cloud temperature is needed. Temperature estimates are taken from the observed data for each cloud. In the calculation, the temperature ranges from 10°K to 110°K.

(6) Cloud Size

To compute the column densities of species, cloud size must be involved. The size is taken from the observed data, if available, or computed from the cloud mass and the total hydrogen density, n, assuming spherical shape.

The chemical reactions used and their rates are listed in TABLE 1 to TABLE 5 in APPENDIX B. These include ion-neutral reactions, neutral-neutral reactions, photodestruction processes, ion-electron recombinations and cosmic ray induced destructions. In these reactions 100 molecular and atomic species are concerned. They are listed in TABLE 2. Additional species including the isotope ^{13}C are used in a calculation for the globule L134.

Steady-state column densities are calculated as follows: Each species must appear at least once as a reactant and at least once as a product in the series of chemical reactions. Then a set of simultaneous equations can be set up. The method is illustrated in the example below.

Example:

Let the chemical reactions and their rate constants K_i(cm^3/sec) be given as follows:

TABLE 2

SPECIES USED FOR CALCULATIONS

H
H^+
H_2^+
H_3^+
H_2

He
He^+

C
C^+
C_2
C_2^+
CH
CH^+
CH_2^+
CH_2
CH_3^+
C_2H^+
C_2H
$C_2H_2^+$
C_3
C_3^+
C_3H^+
CH_3
CH_4^+
CH_4
CH_5^+

^{13}C
$^{13}C^+$
^{13}CH
$^{13}CH^+$
$^{13}CH_2$
$^{13}CH_2^+$
$^{13}CH_3^+$
^{13}CO
$H^{13}CO^+$
$^{13}CO^+$
$H^{13}CO$
$H_2{}^{13}CO^+$

O
O^+
O_2
OH
O_2^+
OH^+
CO
H_2O
H_2O^+
H_3O^+
HCO^+
CO^+
HCO
CO_2
CO_2^+
H_2CO
O_2H^+
H_2CO^+
HCO_2^+
H_3CO^+
CH_2OH^+

N
N^+
NH
NH^+
NH_2
NH_2^+
NH_3
NH_3^+
NH_4^+
NO
NO^+
N_2
N_2^+
CN
CN^+
N_2H^+
HCN
HCN^+
H_2CN^+
C_2N^+
CH_4N^+

S
S^+
SH^+
H_2S^+
SH
SO^+
SN^+
SO
SN
H_2S
HCS^+
H_3S^+
CS^+
CS
OCS
SO_2
S_2^+
CH_3S^+
H_2CS
H_3CS^+
H_2CS^+

Si
Si^+
H_2Si^+
SiO^+
SiO
$HSiO^+$

Mg
Mg^+

Fe
Fe^+

e^-

$$H \xrightarrow[k_1]{p} H^+ + e^-$$

$$H_2 \xrightarrow[k_2]{p} H^+ + H + e^-$$

$$H_2 \xrightarrow[k_3]{p} H_2^+ + e^-$$

$$H^+ + O \xrightarrow[k_4]{} O^+ + H$$

$$H_2^+ + O \xrightarrow[K_5]{} OH^+ + H$$

$$H_2^+ + H \xrightarrow[k_6]{} H^+ + H_2$$

Then the simultaneous equations are as follows:

For H: $K_1\, n(H) + K_6\, n(H_2^+)\, n(H)$

$$= K_2\, n(H_2) + K_4\, n(H^+) n(O) + K_5\, n(H_2^+)\, n(O)$$

For H^+: $K_4\, n(H^+)\, n(O)$

$$= K_1\, n(H) + K_2\, n(H_2) + K_6\, n(H_2^+)\, n(H)$$

For H_2^+: $K_5\, n(H_2^+)\, n(O) + K_6\, n(H_2^+)\, n(H) = K_3\, n(H_2)$

and so on.

These equations set up for each species are solved by Newton's method of iteration, and the abundance for each species is obtained as the converged value after several iterations. The computing program created by Drs. Kuntz, Mitchell, and Ginsburg was used. The detailed method of solution is described in Kuntz, Mitchell, and Ginsburg (1976). To obtain column densities, a spherical, shell-divided, onion-like configuration was assumed as a cloud model. The parameters described above specify this simplified cloud. The division into 10 homogeneous shells corresponds to the variation of optical depth at the various depths from the outside of the cloud to the centre. The optical depth is proportional to the distance (or depth).

If the actual cloud has revealed the existence of a denser part, for example a dense core around the centre, then, the cloud model was assigned to have multiple-density components as shown in <u>FIGURE 1</u>. The computing program calculates the abundances of the species for each shell which has corresponding optical depth and density n, multiplies by shell-thickness and sums up from one "edge" of the cloud to another "edge".

Thus, the working equation for species i is simply

$$N_i = \sum n_{ij} \cdot \Delta R_j$$

where N_i is the column density of species i,

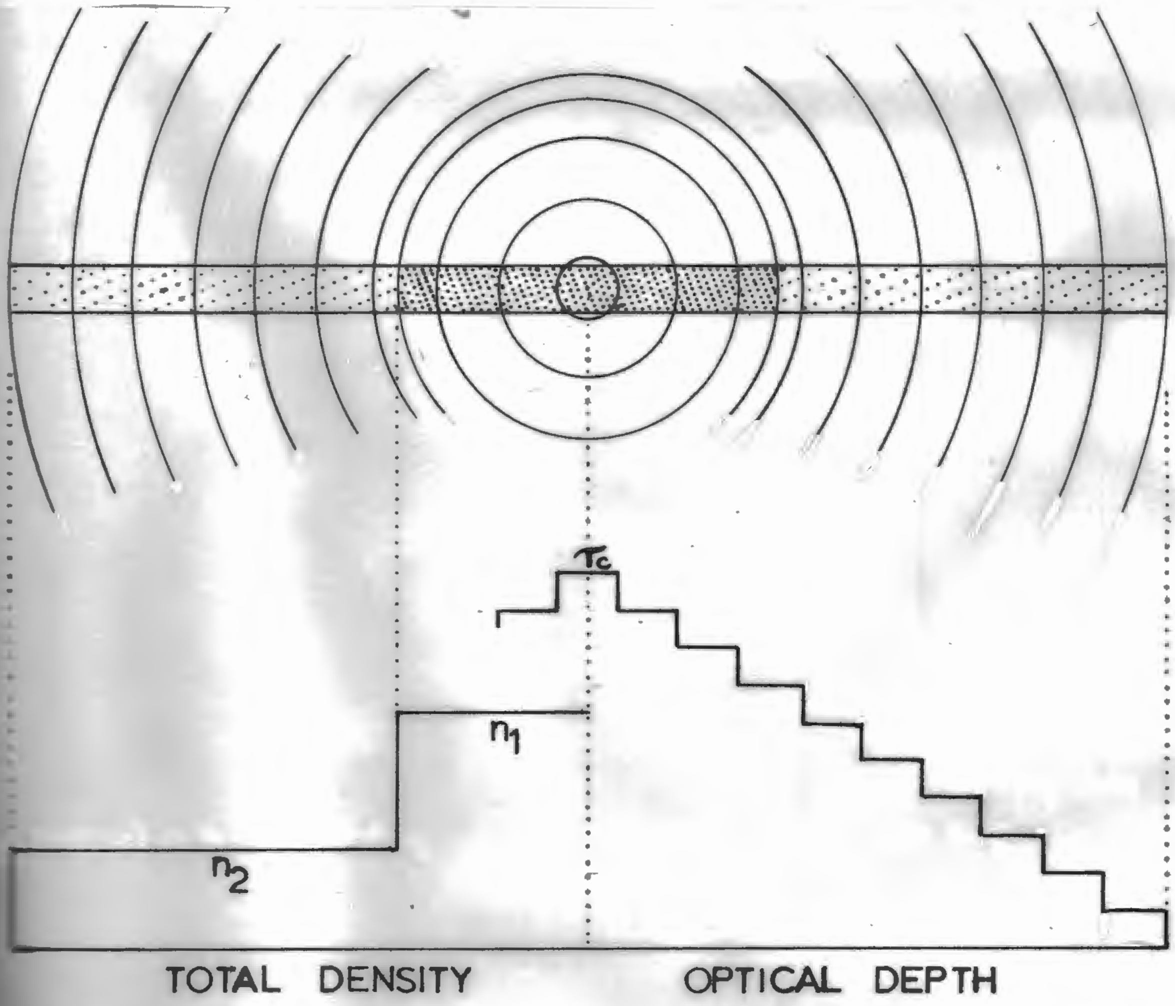
n_{ij} is the calculated abundance of species i in the shell j,

and ΔR_j is the thickness of the shell j.

FIGURE 1

CLOUD MODEL FOR CALCULATION SHOWING

AN EXAMPLE OF DENSITY AND OPTICAL DEPTH VARIATION



IV. ζ OPHIUCHI CLOUD

The ζ Ophiuchi and o Persei clouds are, perhaps, the best-studied clouds over the infrared, ultraviolet, and radio regions. Extensive observations by the high-resolution ultraviolet spectrometer on the Copernicus satellite have been carried out for these stars. ζ Ophiuchi (HD149757) itself is a bright 09.5V star with many absorption lines in the ultraviolet region. There is some evidence of continuous mass loss from this star (Black and Dalgarno 1977). Other physical parameters about ζ Ophiuchi (Morton 1975) are:

$m_v = 2.56$

$B - V = +0.02$

$(B - V)_o = -0.30$ for 09.5V

Hence, $E_{B - V} = 0.32$ mag

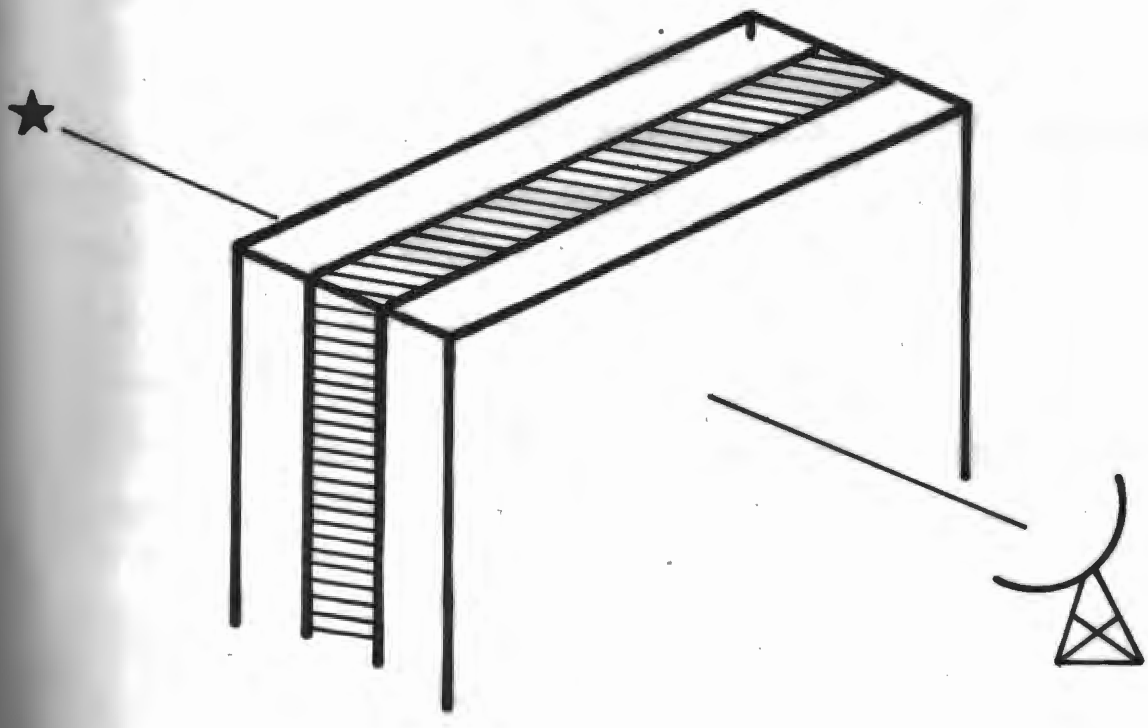
and $A_v = 3.0 \times E_{B-V} = 0.96$

This extinction is due to the interstellar medium between ζ Oph and the sun. The distance to the star is calculated as

200 pc for $M_v = -4.9$ (Morton 1975).

There exists a model of ξ Ophiuchi cloud in which the cloud is a thin disc with the thickness of 0.05 pc (Morton 1975). From the observations, there are at least 6 velocity components in the clouds. However, from the distribution of the excited states of CI and H_2, a two-component model with different total density for each component has been proposed (Black and Dalgarno 1976). This model consists of two regions (FIGURE 2): one is a

FIGURE 2
A CLOUD MODEL OF ξ OPHIUCHI
WITH TWO-DENSITY-COMPONENT



core-like region which occupy 1/10 of the total size with higher density and lower kinetic temperature, while another is a halo-like region with lower density and higher temperature. The core size is 2.06 x 10^{17} cm along the line of sight, with a temperature of 22°K, and a density of 2500 cm^{-3}. The total halo size is 1.71 x 10^{18}cm, its temperature is 110°K and its density is 500cm^{-3}. Black and Dalgarno also suggest that the radiation field intensity for this cloud is characterised by

$$I = 2.5 \quad \text{instead of} \quad I = 1.0$$

Using this model, they achieved fairly good agreement between theoretical and observed values for column densities of some species. In the present calculation, their model as well as a one-density-component model is used.

For a one-density-component model, it is possible to obtain a good guess of the conditions for calculation by plotting several calculated abundances, n(x), divided by the H_2 abundance, $n(H_2)$ (i.e. $n(x)/n(H_2)$) against total density and by comparing the result with the observed values of $n(x)/n(H_2)$. The plottings are shown on FIGURE 3 to FIGURE 6. On the right hand side, the observed values of $n(x)/n(H_2)$ are shown for various species.

FIGURE 3

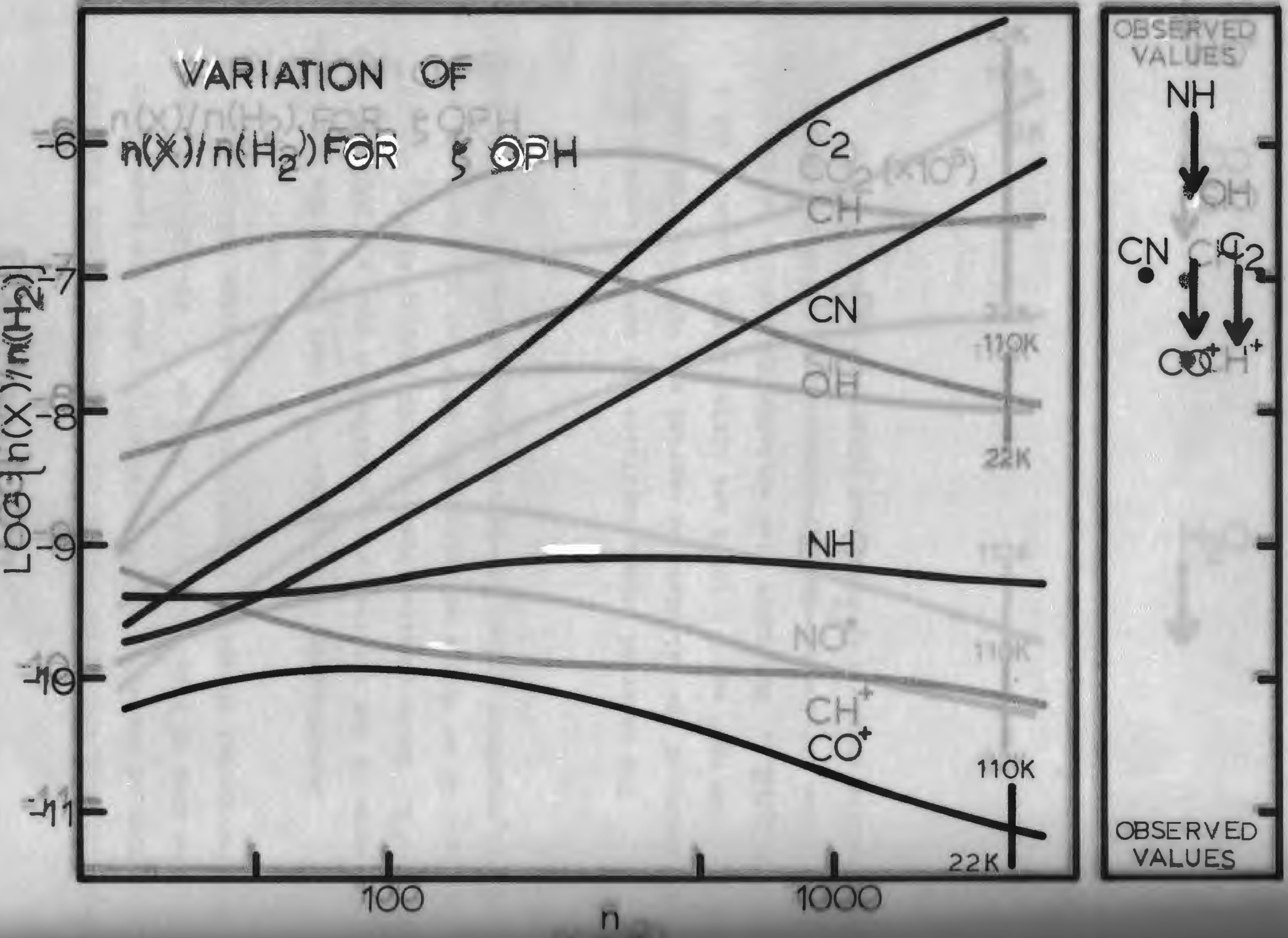

VARIATION OF
n(X)/n(H2) FOR ζ OPH
LOG{n(X)/n(H2)}
-6
-7
-8
-9
-10
-11
100
1000
n
C2
CN
NH
CO+
110K
22K
110K
22K
OBSERVED VALUES
NH
CN
C2
CO+
CH+
OBSERVED VALUES

FIGURE 4

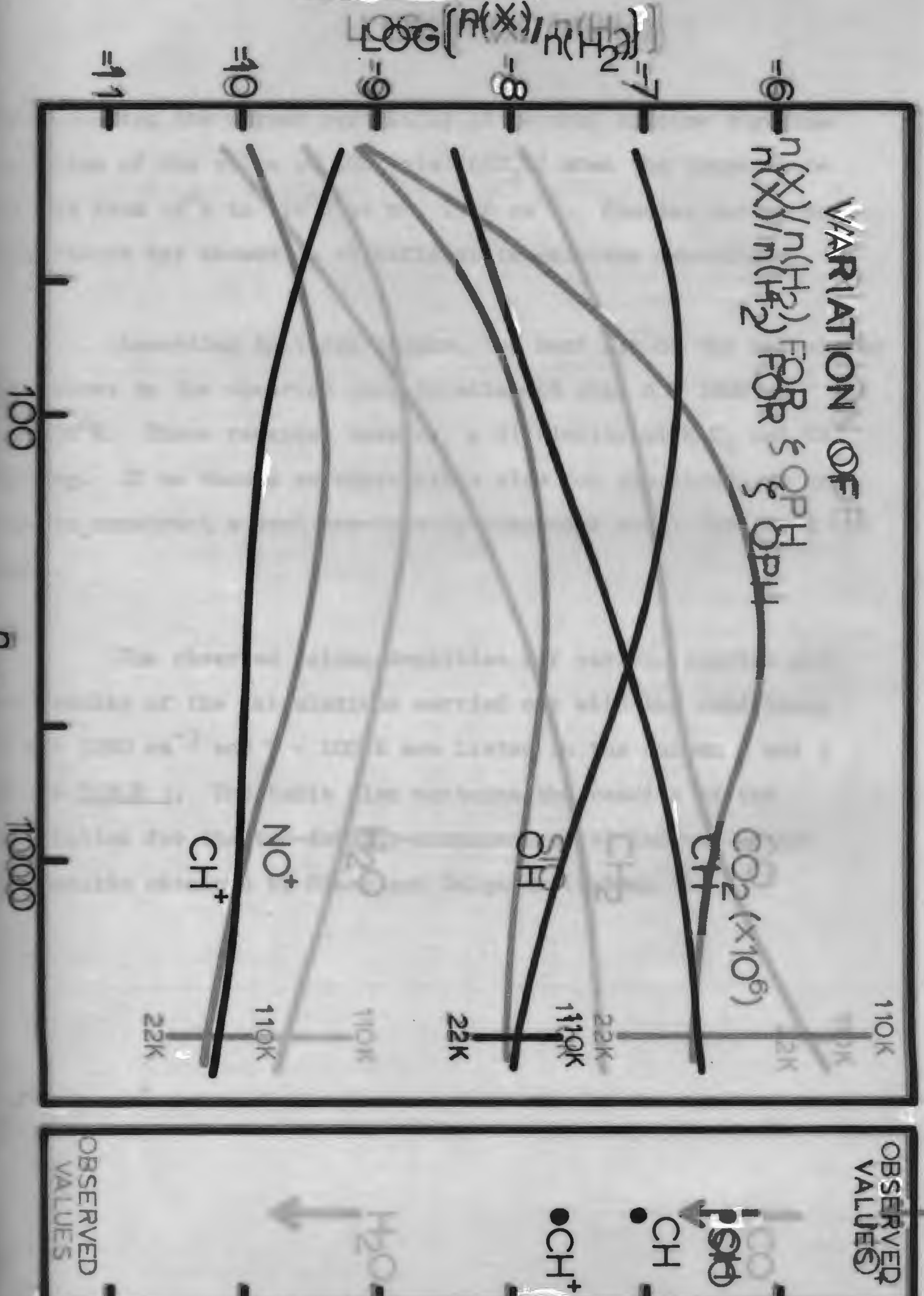

VARIATION OF
n(X)/n(H2) FOR ζ OPH
LOG[n(X)/n(H2)]
-6
-7
-8
-9
-10
-11
100
1000
n̄
(cm-3)
CO2 (×10^6)
CH
OH
NO+
CH+
110K
22K
110K
22K
OBSERVED VALUES
CH
CH+

FIGURE 5

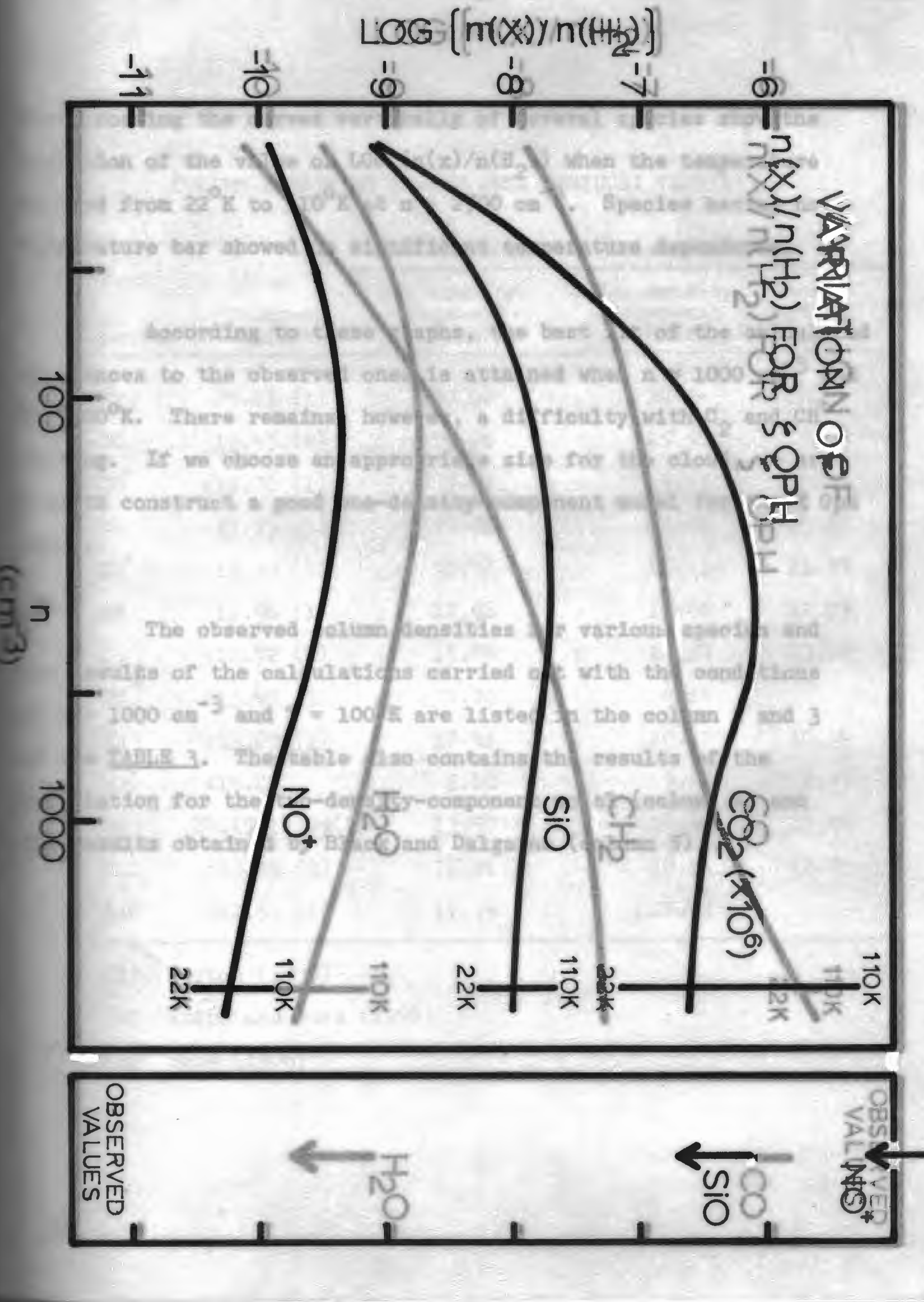
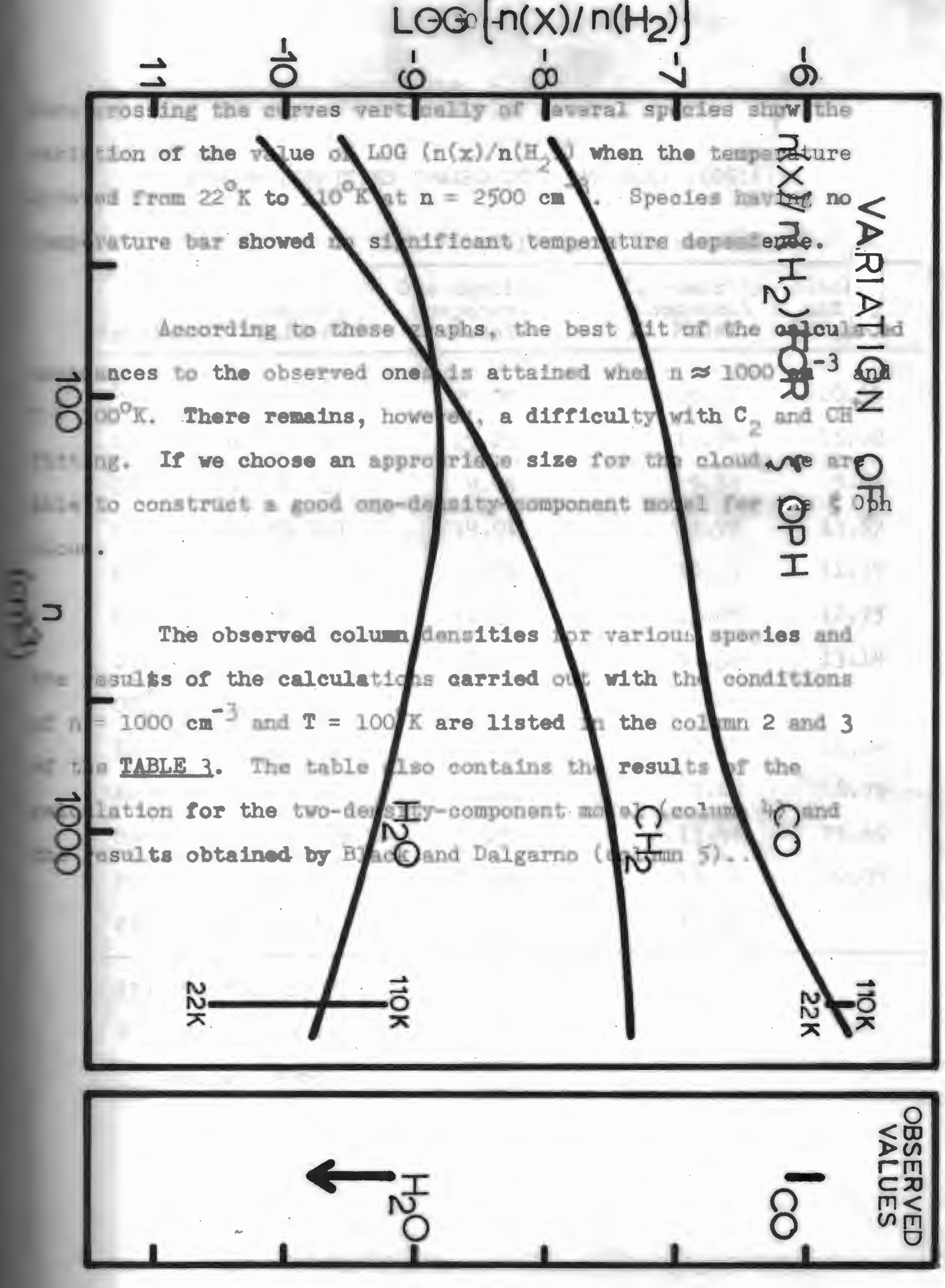

VARIATION OF
n(X)/n(H$_2$) FOR ζ OPH
LOG [n(X)/n(H$_2$)]
-6
-7
-8
-9
-10
-11
n
(cm^{-3})
100
1000
CO$_2$ (×10^6)
CO
CH$_2$
SiO
H$_2$O
NO$^+$
110K
22K
OBSERVED VALUES

FIGURE 6



...rossing the curves vertically of several species show the variation of the value of LOG $(n(x)/n(H_2))$ when the temperature ...ed from 22°K to 110°K at $n = 2500\ cm^{-3}$. Species having no temperature bar showed no significant temperature dependence.

According to these graphs, the best fit of the calculated ...ances to the observed ones is attained when $n \approx 1000\ cm^{-3}$ and ...00°K. There remains, however, a difficulty with C_2 and CH fitting. If we choose an appropriate size for the cloud, we are able to construct a good one-density-component model for the ζ Oph cloud.

The observed column densities for various species and the results of the calculations carried out with the conditions of $n = 1000\ cm^{-3}$ and T = 100°K are listed in the column 2 and 3 of the TABLE 3. The table also contains the results of the calculation for the two-density-component model (column 4) and the results obtained by Black and Dalgarno (column 5).

Bars crossing the curves vertically of several species show the variation of the value of LOG $(n(x)/n(H_2))$ when the temperature altered from 22°K to 110°K at $n = 2500$ cm^{-3}. Species having no temperature bar showed no significant temperature dependence.

According to these graphs, the best fit of the calculated abundances to the observed ones is attained when $n \approx 1000$ cm^{-3} and $T \geq 100$°K. There remains, however, a difficulty with C_2 and CH^+ fitting. If we choose an appropriate size for the cloud, we are able to construct a good one-density-component model for the ξ Oph cloud.

The observed column densities for various species and the results of the calculations carried out with the conditions of $n = 1000$ cm^{-3} and $T = 100$°K are listed in the column 2 and 3 of the TABLE 3. The table also contains the results of the calculation for the two-density-component model (column 4) and the results obtained by Black and Dalgarno (column 5)..

TABLE 3

COLUMN DENSITIES TOWARD ZETA OPHIUCHI (LOG(X))

		Calculated Values		
Species	Observed Values	One-density Component Model	Two-density-Component Model	Black and Dalgarno
H_2	20.62 (1)	20.90	20.74	20.38
CO	15.45 (2)	15.28	15.54	15.02
CO^+	<12.76 (1)	9.46	9.33	9.83
CH	13.53 (1)	14.01	13.90	13.57
CH^+	12.97 (1)	10.98	10.75	11.39
CN	12.94 (1)	12.58	13.08	12.75
C_2	<12.72 (1)	13.84	14.30	13.14
CO_2	<13.47 (3)	7.02	6.66	
NH	<13.87 (1)	10.61	10.47	10.14
NO^+	<14.03	9.20	9.08	8.79
OH	14.19-14.29(3)	13.57	13.46	13.69
H_2O	<12.49 (3)	12.91	12.71	12.03
SiO	<12.51 (1)	11.14	10.83	

(1) Morton (1975)

(2) Knapp and Jura (1976)

(3) Snow (1976)

These are discussed later. The chemical reactions which significantly contribute to the formation and destruction of certain species at this density (1000 cm^{-3}) for ζ Oph cloud are listed in TABLE 4. The plus sign denotes the contribution to formation and the minus sign denotes destruction. The numbers outside the brackets are the chemical reaction numbers listed in APPENDIX B and the numbers appearing in the brackets are rates in units of molecules/cm^3/sec relative to the largest formation or destruction rates.

TABLE 4

CONTRIBUTIONS OF INDIVIDUAL CHEMICAL REACTIONS TO FORMATION AND DESTRUCTION OF SPECIES FOR ζ OPH

$n = 1000$ cm^{-3}
$0.047 \leq \tau \leq 0.47$

$\tau = 0.047$	$\tau = 0.28$	$\tau = 0.47$
201 (-1.00) 474 (+0.82)	201 (-1.00) 474 (+0.82)	201 (-1.00) 474 (+0.73) 67 (+0.28)
474 (-1.00) 544 (+0.90) 487 (+0.61) 475 (-0.52) 485 (+0.36) 66 (-0.23)	487 (+1.00) 474 (-0.86) 544 (+0.65) 475 (-0.61) 485 (+0.41) 66 (-0.40)	487 (+1.00) 474 (-0.57) 475 (-0.51) 66 (-0.45) 544 (+0.42) 485 (+0.31) 67 (-0.22)
502 (+1.00) 499 (-0.82) 476 (-0.42)	502 (+1.00) 499 (-0.72) 476 (-0.39)	502 (+1.00) 499 (-0.67) 476 (-0.39)

As can be seen in column 2 and 3 of TABLE 3, agreement with the observed column densities is excellent for H_2, CO, and CN, and fairly good for CH . However, the calculated column density of CH^+ is somewhat low and C_2 column density is somewhat high compared with the observation. This discrepancy between the observed and calculated values of CH^+ is difficult to understand (Mitchell, et al. 1977a;1977b). Although quite a number of factors are involved in the calculation of column densities, the possibilities of obtaining better agreement should be sought for.

At this density OH^+ is mainly removed by the reactions

$$CH^+ + H_2 \text{ -----> } CH_2^+ + H \qquad (201)$$
$$CH^+ + e^- \text{ -----> } C + H \qquad (535)$$

both for large and small τ, and formed mainly by the reactions (cf. TABLE 4).

$$CH + h\nu \text{ -----> } CH^+ + e^- \qquad (474)$$
$$C^+ + CH \text{ -----> } CH^+ + C \qquad (67)$$

CH^+ is directly formed by photoionization of CH through reaction 474 above. Thus CH, in turn, is mainly formed by the various photodestruction processes at this density, namely,

$$\mathrm{CH_2} + h\nu \dashrightarrow \mathrm{CH} + \mathrm{H} \tag{485}$$

$$\mathrm{C_2H} + h\nu \dashrightarrow \mathrm{CH} + \mathrm{C} \tag{487}$$

$$\mathrm{CH_3} + h\nu \dashrightarrow \mathrm{CH} + \mathrm{H_2} \tag{505}$$

It is, therefore, expected that if the radiation field strength is increased CH abundance and, in turn, $\mathrm{CH^+}$ abundance might be increased. At this point, it should be noted that CH formed by the above reactions suffers from photodestruction process to yield C and H instead of $\mathrm{CH^+}$, i.e.

$$\mathrm{CH} + h\nu \dashrightarrow \mathrm{C} + \mathrm{H} \tag{475}$$

However, at this density ($n=1000\mathrm{cm}^{-3}$), the reaction 474 dominates for all values of τ (cf. <u>TABLE 4</u>).

Next, the possibility exists of increasing the $\mathrm{CH^+}$ abundance through the reaction 67:

$$\mathrm{C^+} + \mathrm{CH} \dashrightarrow \mathrm{CH^+} + \mathrm{C} \tag{67}$$

Since we have seen the reactions which increase the abundance of CH, the problem is to increase the abundance of $\mathrm{C^+}$. The major formation process of C^+ at this density is the photoionization of carbon, i.e.

$$C + h\nu \longrightarrow C^+ + e^- \qquad (469)$$

This reaction is also the major destruction process of carbon atoms. Hence, if the radiation field strength is increased, C^+ abundance increases rapidly and after all CH^+ abundance may be raised.

In spite of this expectation, however, attempts to raise significantly the abundance of CH^+ by increasing the radiation field strength have failed (Mitchell, et al. 1977a). They could not get sufficient CH^+ to explain the observations. Black and Dalgarno (1977), who also could not get sufficient CH^+, suggest that the observed CH^+ abundance occurs in an HII region instead of in the ζ Oph cloud, the HII region consisting of the matter ejected from the star and surrounding the star.

The calculated abundance of C_2 is high compared with the observed value. At this density C_2 is removed from the cloud by the reactions

$$C_2 + h\nu \longrightarrow C_2^+ + e^- \qquad (499)$$

$$C_2 + h\nu \dashrightarrow C + C \qquad (476)$$

and is formed mainly by the reactions

$$C_3 + h\nu \dashrightarrow C_2 + C \qquad (502)$$

$$C_3^+ + e^- \dashrightarrow C_2 + C \qquad (562)$$

Of these reactions, 499, 476 and 502 are photodestruction processes. 499 and 502 have the same rate. Hence, an increase in the radiation field may lower the abundance of C_2: However, this has not yet been tested.

The two-component cloud model proposed by Black and Dalgarno (1977) is used here for calculation of column densities. The details of the model is described in the previous section.

TABLE 3 includes the results of the calculation of the two-component model and those of Black and Dalgarno for comparison, too. Excellent agreement with the observed column densities is attained for H_2, CO, CH, and CN, but the agreement with observation for CH^+ and C_2 is again not satisfactory. The same tendency can be seen in the results of Black and Dalgarno.

V. ο PERSEI CLOUD

This cloud has also been extensively investigated, especially in the ultra-violet region, by the Copernicus satellite (eg. Snow 1975, 1976). ο Persei is a B1 III star imbedded in the Perseus complex region as a member of the Perseus II association. For ο Per,

$$E_{B-V} = 0.32 \text{ mag}$$

and

$$\frac{A_V}{E_{B-V}} = 2.72 \quad \text{Hence, } A_V = 0.87 \text{ (Snow, 1976)}$$

This amount of extinction is produced by the cloud intervening between ο Persei and the sun. However, there is some evidence that the star is located at the near edge of the molecular cloud. The radiation from the imbedded star might effect the chemistry of the cloud, although it is neglected in the calculations. There is another uncertainty for this cloud. As mentioned in the earlier section, observed values of element abundances, especially of C, O, and N, have large uncertainties compared with those reported for the ζ Ophiuchi cloud.

Snow (1976) suggests possible density variation in the cloud and the existence of all molecules in a very dense portion. It is therefore, worthwhile to compute a two-component model for this cloud. The total density ($n = n(H) + 2n(H_2)$) for this cloud is not well-established.

Since the star o Per is imbedded in the cloud, the column density calculation is somewhat different from that for ζ Oph cloud.

As mentioned in the previous chapter, only the intercloud radiation field is considered and the stellar radiation field is neglected, even from the star imbedded in the cloud. The cloud optical depth is highest at the point of the star and decreasing toward the "edge" of the cloud in the calculation (FIGURE 7).

Since the uncertainty of the observed total density, n, is somewhat large, the best fit condition is looked for as for ζ Oph cloud, by plotting

$$\log n(x)/n(H_2) \quad \text{vs.} \quad n$$

where $n(x)$ is the calculated abundance of species x for various n with $\tau = 0.4$

n is the total density ($= n(H) + 2n(H_2)$).

FIGURE 8 and 9 show these plots. In this case, the effects of temperature variation are not checked since the kinetic temperature of the cloud is well estimated (Snow, 1976) and is $T = 20^{\circ}K$. On the right side, observed values of $\log n(x)/n(H_2)$ are marked.

According to the graph, n = 1000-1200 is likely for some species except CH^+ and C_2 again for this cloud. The total density derived from the observed column density of H_2 is higher (Snow, 1976), i.e.

$$1120 \leqq n(H) \leqq 7450 \text{ cm}^{-3}$$

$$n(H) = 1200 \text{ cm}^{-3}$$ is chosen for the calculation.

There is another uncertainty of the observation toward this cloud: Element abundances, especially those of C and O, have large uncertainties. Calculations are carried out both for C/O = 50 and C/O = 0.08 which approximately correspond to the extremes of the uncertainty (Snow, 1976).

In this calculation, the cloud size (from A to B in FIGURE 7) is estimated from the observed column density of H nuclei and the assumed total density, namely

$$\dot{N}(H) = N(H) + 2N(H_2) = 1.41 - 1.72 \times 10^{21} \text{ cm}^{-2}$$

$$n(H) = n(H) + 2n(H_2) = 1200 \text{ cm}^{-3}$$

Then size = 1.18×10^{18} cm.

FIGURE 7

A CLOUD MODEL FOR o PER

The optical depth is highest at the position of the star.

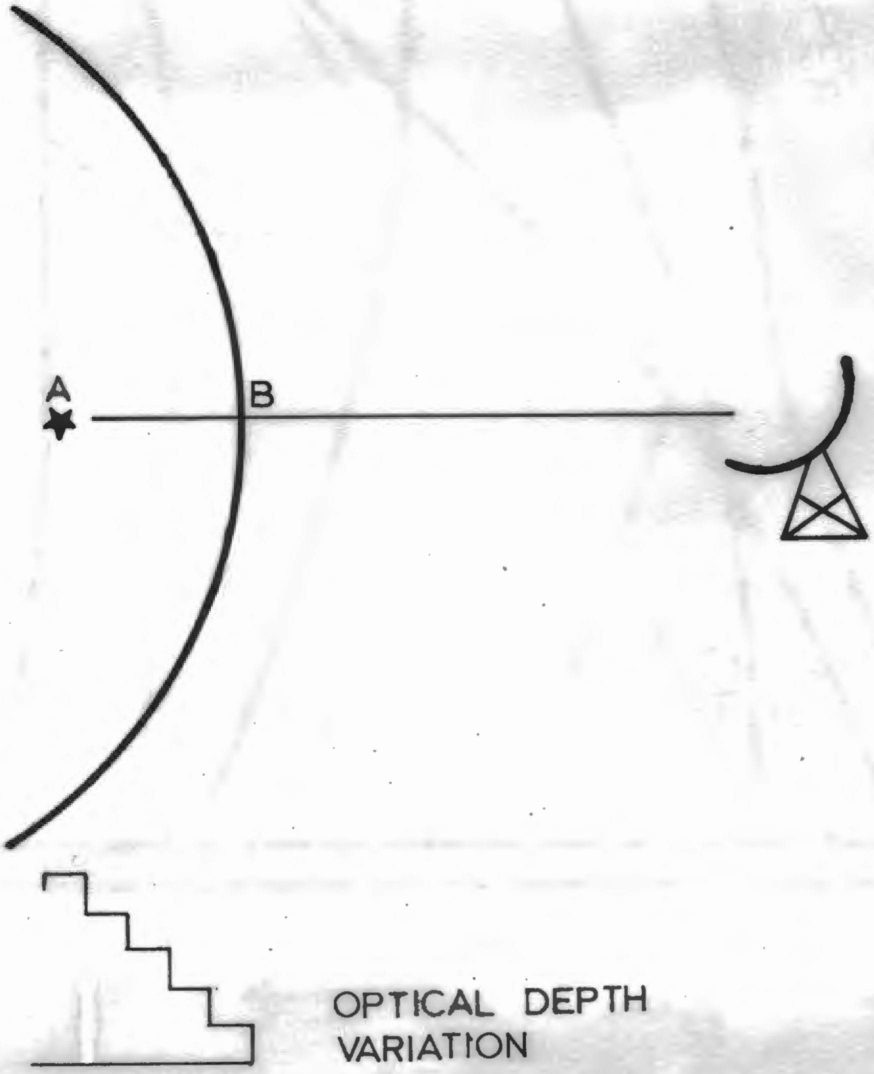


FIGURE 8

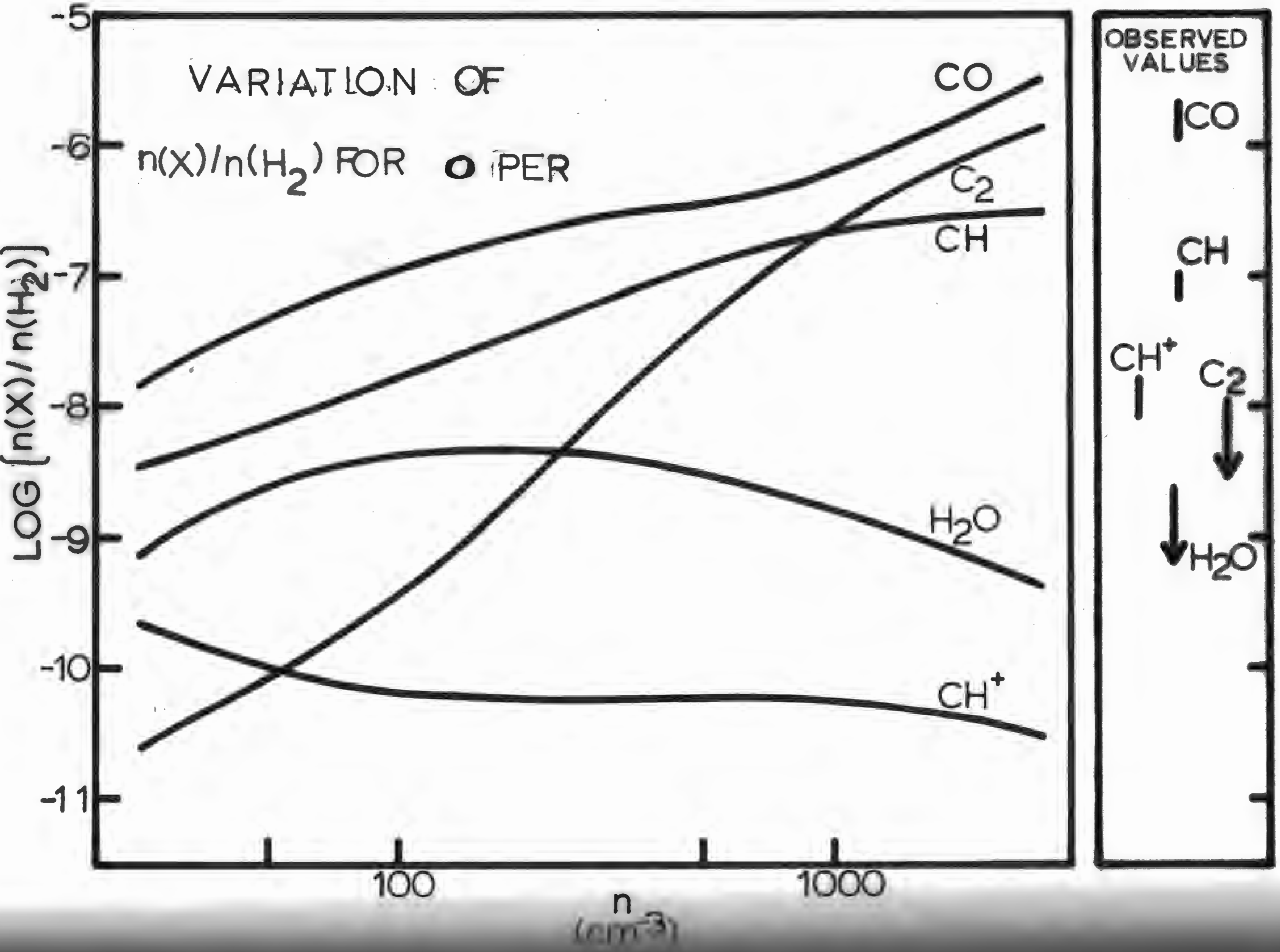

VARIATION OF
$n(X)/n(H_2)$ FOR o PER
LOG $[n(X)/n(H_2)]$
-5
-6
-7
-8
-9
-10
-11
100
1000
n
(cm^{-3})
CO
C_2
CH
H_2O
CH^+
OBSERVED VALUES
CO
CH
CH^+
C_2
H_2O

FIGURE 9

VARIATION OF $n(X)/n(H_2)$ FOR ο PER

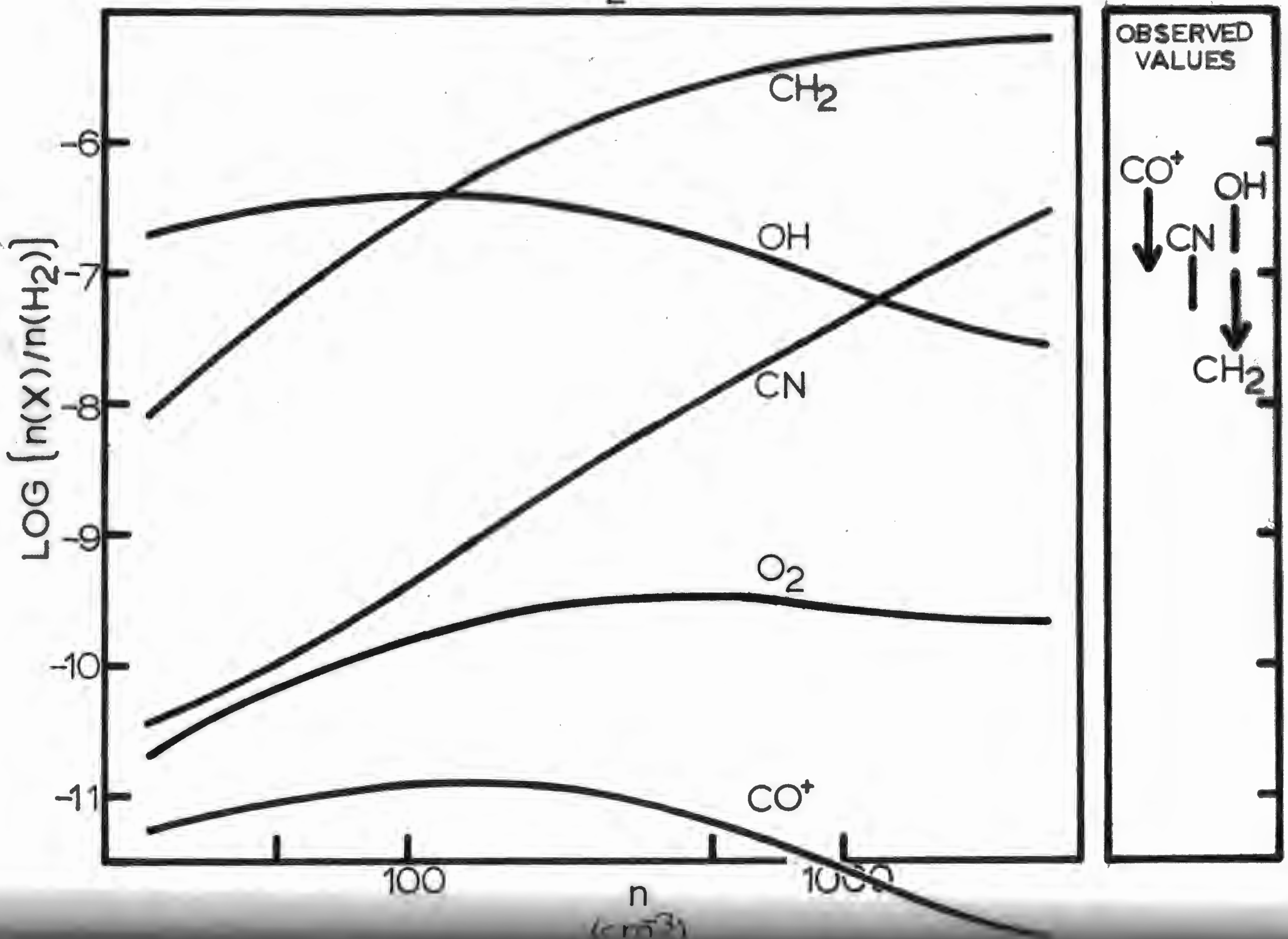


TABLE 5

COLUMN DENSITIES TOWARD ο PER

Species	Observed Values	C/O = 50	C/O = 0.08
H_2	20.58-20.64	20.76	20.80
CH	13.44-13.62	13.88	12.70
CH^+	12.55-12.81	10.98	9.06
CO	14.68-14.95	15.72	13.31
CO^+	$\leqq 13.23$	7.24	6.38
CN	12.34-12.70	13.95	11.83
C_2	$\leqq 12.64$	15.91	10.62
CH_2	$\leqq 12.60$	14.15	13.58
NO^+	$\leqq 14.43$	4.59	8.14
OH	12.79-13.09	10.50	12.39
H_2O	$\leqq 11.99$	8.54	11.23
SiO	$\leqq 12.60$	7.23	10.43
N_2	$\leqq 13.32$	8.53	9.72
O_2	$\leqq 13.54$	7.28	9.96
SH	$\leqq 12.16$	4.40	5.41
H	21.15-21.24	20.30	

The results as well as the observed values are listed in TABLE 5. It is interesting to see that in TABLE 5, CH and CO column densities decrease by a factor of ~100 and the OH column density increases by a factor of ~75 when the C/O ratio is changed from 50 to 0.08. For CH, CO, and CN, the observed values lie between the values calculated for C/O = 50 and 0.08. For example, in the case of CO, the observed value $14.68 \leq \log N \leq 14.95$ is between the $\log N = 15.72$ for C/O = 50 and the $\log N = 13.31$ for C/O = 0.08. Agreement with observations is, therefore, satisfactory in this case. Other species such as CH and CN also show satisfactory agreement with observed column densities. Again for this cloud, the calculated CH^+ abundance is far below the observed value and the calculated C_2 abundance is too high.

In our chemical scheme, the majority of CN is removed at this density (1200 cm^{-3}) by the photodissociation process (cf. TABLE 6).

TABLE 6

CONTRIBUTIONS OF INDIVIDUAL CHEMICAL REACTIONS
TO FORMATION AND DESTRUCTION OF SPECIES FOR o PER

$n = 1200\ cm^{-3}$
$0.087 \leq \tau \leq 0.87$

$\tau = 0.087$	$\tau = 0.52$	$\tau = 0.87$
482(-1.00) 421(+0.96)	482(-1.00) 421(+0.99)	421(+1.00) 482(-0.99)

$$CN + h\nu \text{ -----> } C + N \qquad (482)$$

and the majority is formed by

$$C_2 + N \text{ -----> } CN + C \qquad (421)$$

Increasing the radiation field strength might not be the appropriate solution to lower the CN abundance for C/O = 50 because, as seen in previous section, C_2 might be increased by increasing the radiation field, and the CN abundance might be steady or at least moderately changed through 421 with increased C_2 and through 482 with the increased destruction rate.

The rate coefficient of 421 is uncertain (Solomon and Klemperer 1972). If the rate is decreased, the CN abundance may be lowered.

It is worth looking for a more efficient process for destroying CN. The following is proposed by Dalgarno and Black (1977):

$$CN + O \text{ -----> } CO + N \qquad (439)$$

Putting this reaction into the chemical reaction scheme, Mitchell (1977) can decrease the CN abundance by a large factor.

The OH column density obtained from the calculation is somewhat low (TABLE 5). The OH abundance is sensitive to the primary cosmic ray ionization rate ζ_0 , through (Mitchell, et al. 1977b; Black and Dalgarno 1977).

$H + P \longrightarrow H^+ + e^- + p$ (596)

$H^+ + O \longrightarrow O^+ + H$ (1)

$O^+ + H_2 \longrightarrow OH^+ + H$ (109)

$OH^+ + H_2 \longrightarrow H_2O^+ + H$ (206)

$H_2O^+ + H_2 \longrightarrow H_3O^+ + H$ (298)

$H_3O^+ + e \longrightarrow OH + 2H$ (554)

Mitchell, et al. found that at high densities, the abundances of OH, CH, HCO^+, and N_2H^+ decreased with decreasing ζ_0. However, to increase the cosmic ray ionization rate might not be a solution for increasing the OH column density because there is no good reason to believe that ζ_0 is higher than 10^{-17} s^{-1}.

VI. LYNDS 134

Lynds (1962) has studied and listed a large number of interstellar clouds: This object is one of them. L134 is a small, isolated dark globule with an opaque core. The lower limit of the absorption at the cloud centre is fairly large, $A_v \gtrsim 8$ mag (Heiles 1968). This number, based on star counts, is rather poorly determined.

A lower limit of the cloud mass is estimated by the virial theorem to be 18 $M_\odot$ (Brooks, et al. 1976). However, another recent estimate of the lower mass limit (Dickman 1977) is

$$M \geqq 66\ M_\odot$$

In the calculation, 75 $M_\odot$ is used. The total density, n, is not well known and $n = 10^4\ \mathrm{cm}^{-3}$ is assumed in the calculation as the standard value. Because of the very uncertain central extinction, the optical depth at the cloud centre, τ_c, is estimated from the assumed mass and the assumed total density using

$$\tau_c = \left(\frac{M}{500}\right)^{1/3} \left(\frac{n}{260}\right)^{2/3}$$

where M is the cloud mass in $M_\odot$.

Since a systematic velocity pattern has been observed, it has been suggested that the cloud is rotating in a solid body fashion. The distance estimate to the cloud (200 pc) is uncertain, and the proposed real size of the cloud (0.9 x 0.6 pc.) is also poorly known. The kinetic temperature determined from CO observations is $\sim 7^{\circ}$K (Brooks, et al. 1976). While many molecular species have been detected in molecular clouds associated with HII region, fewer species have been found in dark clouds. The molecular species detected in L134 are OH, CH, H_2CO, CO, HCO^+ and HCN (Snyder and Hollis 1976). In this cloud, three isotopic forms of CO have been detected (Mahoney, et al. 1976). Dickman, et al. (1976) studied the fractionation of CO and found that there is considerable enrichment of $^{13}C^{16}O$ in the outer part of the cloud.

Using the isotope exchange reaction (Watson, et al. 1976)

$$^{13}C^{+} + {}^{12}CO \text{ -----> } {}^{13}CO + {}^{12}C^{+} \qquad (107)$$

the abundances of various carbon isotope species across the cloud are calculated as well as column densities for ^{13}CO.

Two cloud models are used: one is a one-density-component model with total density n = 10^4 cm^{-3}, and the other is a two-density-component model with an inner part of n = 10^5 cm^{-3} having half the mass and an outer part of n = 10^4 cm^{-3} having another half of the mass.

TABLE 7

COLUMN DENSITIES TOWARD LYNDS 134

Species	Observed Values	Calculated values One-Density-Component Model	Two-Density-Component Model
H	21.8(1)	19.05	19.29
H_2	21.04-21.83(1)	21.51	22.73
CH	14(2)	14.28	14.60
OH	15.11(3)	13.93	14.84
H_2CO	13(4)	11.87	13.90
CO	17.9(5)	17.63	18.89
HCN	11.87-12.41(5)	14.25	15.23

(1) Sancisi (1971)
(2) Rydbeck, et al. (1976)
(3) Turner (1973)
(4) Dieter (1973)
(5) Milman, et al. (1975)
(6) Snyder and Hollis (1976)

TABLE 7 lists the observed column densities and the calculated ones for the one- and the two-density-component models. As seen in the table, the two-density-component model reproduced fairly well the observed column densities. For example, Rydbeck, et al. (1976) reports the column density of CH toward L134 as 10^{14} cm^{-2} from radio observation. The same order of column density is obtained from the two-density-component model. The one-density-component model also shows good agreement for the CH column density. However, the calculated column density of HCN is too high compared with the observed one.

TABLE 8

CONTRIBUTIONS OF INDIVIDUAL CHEMICAL REACTIONS
TO FORMATION AND DESTRUCTION OF SPECIES FOR L134

$n = 10^4$ cm^{-3}
$0.4 \leq \tau \leq 4.0$

$\tau = 0.4$		$\tau = 2.4$		$\tau = 4.0$	
443 (+1.00)	77 (-0.91)	443 (+1.00)	77 (-0.91)	77 (-1.00) 569 (+0.27)	443 (+0.87)
469 (+1.00)	524 (-0.33)	32 (+1.00)	64 (-0.70)	32 (+1.00)	73 (-0.33)
597 (+1.00)	32 (-0.94)			597 (+1.00)	32 (-0.92)

The major destruction process of HCN (cf. TABLE 8) at this density ($n = 10^4$ cm^{-3}) is

$$C^+ + HCN \text{ -----> } C_2N^+ + H \qquad (77)$$

C^+ is, in turn, mainly formed by the reaction

$$He^+ + CO \text{ -----> } C^+ + O + He \qquad (32)$$

In dense clouds such as L134, He^+ is supplied by cosmic ray induced ionization

$$He + P \text{ -----> } He^+ + e + P \qquad (597)$$

For L134, abundances of species including ^{13}C are calculated using the same one-density-component model. Dickman, et al (1977) point out that the ratio $^{12}C/^{13}C$ for L134 is approximately 10^4 and that the abundance of $^{13}C^{16}O$ is considerably enriched in the outer regions of L134 where an exchange reaction

$$^{13}C^+ + {}^{12}CO \text{ -----> } {}^{12}C^+ + {}^{13}CO \qquad (107)$$

proceeds effectively to give the observed column density.

The calculation is carried out to demonstrate this suggestion using the exchange reaction with a suggested reaction rate of $k = 2.0 \times 10^{-10}$ cm^3 sec^{-1} as well as the reactions which contribute considerably to formation and destruction of carbon species.

TABLE 9

CALCULATED ABUNDANCES OF SPECIES INCLUDING ^{13}C FOR VARIOUS OPTICAL DEPTH

					τ					
Species	0.4	0.8	1.2	1.6	2.0	2.4	2.8	3.2	3.6	4.0
$^{13}C^+$	0.21(-3)	0.45(-4)	0.13(-4)	0.57(-5)	0.37(-5)	0.32(-5)	0.30(-5)	0.26(-5)	0.20(-5)	0.14(-5)
^{13}CH	0.69(-5)	0.17(-5)	0.54(-6)	0.23(-6)	0.15(-6)	0.13(-6)	0.12(-6)	0.11(-6)	0.80(-7)	0.58(-7)
$^{13}CH^+$	0.46(-13)	0.39(-14)	0.70(-15)	0.31(-15)	0.29(-15)	0.40(-15)	0.67(-15)	0.12(-14)	0.17(-14)	0.23(-14)
$^{13}CH_2^+$	0.29(-9)	0.63(-10)	0.19(-10)	0.80(-11)	0.52(-11)	0.45(-11)	0.42(-11)	0.37(-11)	0.28(-11)	0.20(-11)
$^{13}CH_2$	0.43(-4)	0.11(-4)	0.34(-5)	0.15(-5)	0.95(-6)	0.81(-6)	0.75(-6)	0.66(-6)	0.50(-6)	0.30(-6)
$^{13}CH_3^+$	0.14(-7)	0.53(-8)	0.20(-8)	0.10(-8)	0.84(-9)	0.97(-9)	0.13(-8)	0.18(-8)	0.25(-8)	0.27(-8)
^{13}CO	0.14(-1)	0.14(-1)	0.14(-1)	0.14(-1)	0.14(-1)	0.14(-1)	0.14(-1)	0.14(-1)	0.15(-1)	0.15(-1)
$H^{13}CO^+$	0.33(-8)	0.29(-8)	0.32(-8)	0.40(-8)	0.58(-8)	0.99(-8)	0.20(-7)	0.47(-7)	0.13(-6)	0.27(-6)
$^{13}CO^+$	0.68(-12)	0.45(-12)	0.25(-12)	0.17(-12)	0.18(-12)	0.27(-12)	0.50(-12)	0.12(-11)	0.33(-11)	0.63(-11)
$H^{13}CO$	0.11(-5)	0.41(-6)	0.20(-6)	0.13(-6)	0.13(-6)	0.18(-6)	0.30(-6)	0.52(-6)	0.11(-5)	0.26(-5)
^{13}C	0.45(-3)	0.34(-3)	0.26(-3)	0.21(-3)	0.17(-3)	0.14(-3)	0.13(-3)	0.95(-4)	0.48(-4)	0.30(-4)

Eleven ^{13}C species listed in TABLE 2 are used. The carbon isotope ratio is chosen as $^{12}C/^{13}C = 50$, which is approximately the middle of the observed range for this cloud. As a first approximation from which the iteration proceeds, it is assumed that all ^{13}C species are fractionated in ^{13}C and ^{12}C by the same ratio as $^{12}C/^{13}C$ i.e. 50. Because of computer capacity, all sulfur species were dropped in the calculation.

TABLE 10

CALCULATED COLUMN DENSITIES
OF SPECIES INCLUDING ^{13}C

Species	Log N
$^{13}C^+$	13.6
^{13}CH	12.1
$^{13}CH^+$	3.9
$^{13}CH_2^+$	7.7
$^{13}CH_2$	12.9
$^{13}CH_3^+$	9.6
^{13}CO	16.3
$H^{13}CO^+$	10.7
$^{13}CO^+$	6.1
$H^{13}CO$	11.8
^{13}C	16.6

The calculated abundances in cm^{-3} for different τ (i.e. for different depths of the cloud) and the column densities are listed in TABLE 9 and TABLE 10. As seen in the TABLE 9, the tendency of enrichment of $^{13}C^{16}O$ in the outer region is not reproduced. ^{13}CO abundances at various depths of the cloud are fairly steady, and rather more abundant in the inner region.

The major formation process of ^{13}CO in the outer (small τ) region of the cloud is

$$^{12}CO + ^{13}C^{+} \longrightarrow ^{12}C^{+} + ^{13}CO \qquad (504)$$

and the major destruction process is the photodestruction of ^{13}CO, i.e.

$$^{13}CO + h\nu \longrightarrow ^{13}C + O \qquad (505)$$

Since the radiation field is strong in the outer region, the photodestruction process (505) dominates the destruction process. Therefore, even if ^{13}CO is formed efficiently through the reaction (504), it suffers from the photodestruction.

As a result, it is expected from the reaction (505) that ^{13}C might accumulate in the outer region of the cloud.

This tendency is clearly seen in TABLE 9, where the ^{13}C abundance for small τ is more than 10 times larger than that for large τ. However, this is not consistent with the observation in which the enrichment of ^{13}CO in the outer region has been found. To interpret this observation, assumptions in the calculation, such as isotope ratio, fractionation, or reaction coefficient of isotope process might be altered.

SUMMARY

Under the assumption of a steady-state, column densities of some 100 interstellar species are calculated using the conditions found in three interstellar clouds, the cloud toward ζ Oph, o Per and Lynds 134. For the calculation, spherical cloud models are employed which are divided into 10 homogeneous shells corresponding to the optical depth variation. For the clouds in which density variation has been observed, a two-component cloud model is used.

For the ζ Oph cloud, calculations are made for two cloud models. One is a one-density-component model which has a total density of $n = 1000 \text{ cm}^{-3}$ and temperature 100°K, and the other is a two-density-component model which has two regions of different densities and temperatures, namely $n = 500 \text{ cm}^{-3}$, $T = 110^{\circ}$K for outer region and $n = 2500 \text{ cm}^{-3}$, $T = 110^{\circ}$K for inner region. The optical depth at the cloud centre is estimated from $A_v = 0.96$ for this cloud and has the value of $\tau_c = 0.4$. The calculation showed good agreement with the observed values for the species of H_2, CO, CH, and OH. However, CH^+ and C_2 showed considerable discrepancy between observed and calculated values. Uncertainties in the radiation field strength are unlikely to resolve these discrepancies.

For the calculation of the o Per cloud, n = 1200 cm^{-3} and T = 20°K are assumed from the observed data. Observation toward this cloud has shown an uncertainty in [C] / [O] ratio which ranges from 76 to 0.06 (Snow, 1976). Two separate calculations with [C]/ [O] = 50 and 0.08 are used here. Since the star o Per is inbedded in the cloud, the optical depth in the calculation is highest at the position of the star.

Fairly good agreements are attained between the observed and the calculated column densities of various species; C_2 and CH^+ again are discrepant.

In the case of dark globule L134, there are several uncertainties. A lower limit of the mass of the cloud is proposed (Dickman, 1977) and 75 $M_\odot$ is used as the cloud mass to estimate optical depth at the centre of the cloud. The total density is not well-known and n = $10^4 cm^{-3}$ is assumed. Calculations were carried out for one and two-density-component models. The calculated column densities of various species showed good agreement with observed values. One exception was the high column density of HCN compared with the observed value. This discrepancy cannot be understood from the chemistry used here.

For L134, abundances of species including ^{13}C are also calculated. Carbon isotope ratio is chosen as $^{12}C/^{13}C = 50$. The isotope exchange reaction

$$^{13}C^{+} + {}^{12}CO \dashrightarrow {}^{13}CO + {}^{12}C^{+}$$

which has been suggested as the mechanism leading to the observed enhancement of ^{13}CO was included.

The calculated abundance of ^{13}CO did not reproduce the observed fact that ^{13}CO is enriched in the outer part of L134, casting doubt on this mechanism.

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APPENDIX A

INTERSTELLAR MOLECULES DETECTED

CH	Methyline	CH^+	methyline ion
CN	cyanogen	CO	carbon monoxide
H_2	hydrogen	OH	hydroxyl
CS	carbon monosulphide	SiO	silicon monoxide
SO	sulphur monoxide	NS	nitrogen sulphide
SiS	silicon sulphide		
HDO	heavy water	H_2S	hydrogen sulphide
HCN	hydrogen cyanide	HNC	
OCS	carbonyl sulphide	SO_2	sulphur dioxide
N_2H^+	protonated nitrogen	HCO^+	protonated carbon monoxide
C_2H	ethynyl	HCO	formyl
NH_3	ammonia	H_2CO	formaldehyde
H_2CS	thioformaldehyde	HNCO	isocyanic acid
HCOOH	formic acid	HC_3N	cyanoacetylene
NH_2CN	cyanamide	CH_2NH	methanimine
CH_3OH	methanol	CH_3CN	acetonitrile
NH_2HCO	formamide		
CH_3C_2H	methyl acetylene	CH_3HCO	acetaldehyde
CH_3NH_2	methylamine	HC_5N	cyanodiacetylene
CH_2CHCN	acrylonitrile	$(CH_2)_2O$	ethylene oxide
CH_3C_3N	methyl cyanoacetylene	$HCOOCH_3$	methyl formate
$(CH_3)_2O$	dimethyl ether	CH_3CH_2OH	ethanol
		HC_7N	cyanotriacetylene

APPENDIX B

CHEMICAL REACTIONS USED IN THE CALCULATIONS

All reactions are taken from Mitchell, et al. (1977b). Reactions marked with asterisk (*) are those used only for calculations of ^{13}C species in L134.

TABLE 1 ION-NEUTRAL REACTIONS
2 NEUTRAL-NEUTRAL REACTIONS
3 PHOTODESTRUCTION PROCESSES
4 ION-ELECTRON RECOMBINATION REACTIONS
5 COSMIC RAY DESTRUCTION PROCESSES

TABLE 1. ION-NEUTRAL REACTIONS

	Reaction	Rate ($cm^3 s^{-1}$)
1.	$H^+ + O \rightarrow O^+ + H$	$1.0 \times 10^{-9}\ e^{-232/T}$
2.	$H^+ + O_2 \rightarrow O_2^+ + H$	1.2 (-9)
3.	$H^+ + C_2 \rightarrow C_2^+ + H$	1.0 (-9)
4.	$H^+ + OH \rightarrow OH^+ + H$	1.0 (-9)
5.	$H^+ + NO \rightarrow NO^+ + H$	1.9 (-9)
6.	$H^+ + NH \rightarrow NH^+ + H$	1.0 (-9)
7.	$H^+ + CH \rightarrow CH^+ + H$	1.0 (-9)
8.	$H^+ + CH_2 \rightarrow CH_2^+ + H$	1.0 (-9)
9.	$H^+ + H_2O \rightarrow H_2O^+ + H$	8.2 (-9)
10.	$H^+ + CO_2 \rightarrow HCO^+ + O$	3.0 (-9)
11.	$H^+ + C_2H \rightarrow C_2H^+ + H$	1.0 (-9)
12.	$H^+ + HCO \rightarrow HCO^+ + H$	1.0 (-9)
13.	$H^+ + NH_3 \rightarrow NH_3^+ + H$	5.2 (-9)
14.	$H^+ + H_2CO \rightarrow H_2CO^+ + H$	1.0 (-9)
15.	$H^+ + CH_4 \rightarrow CH_4^+ + H$	1.5 (-9)
16.	$H^+ + CH_4 \rightarrow CH_3^+ + H_2$	2.3 (-9)
17.	$H^+ + H_2S \rightarrow H_2S^+ + H$	7.6 (-9)
18.	$H^+ + OCS \rightarrow SH^+ + CO$	1.0 (-9)
19.	$H^+ + SH \rightarrow SH^+ + H$	1.0 (-9)
20.	$H^+ + C_3 \rightarrow C_3^+ + H$	1.0 (-9)
21.	$H^+ + CH_3 \rightarrow CH_3^+ + H$	1.0 (-9)
22.	$He^+ + H \rightarrow H^+ + He$	$1.9 \times 10^{-15} (1 + 5/T)$
23.	$He^+ + H_2 \rightarrow H^+ + H + He$	1.0 (-13)
24.	$He^+ + C_2 \rightarrow C^+ + C + He$	1.0 (-9)

25.	$He^+ + C_2 \rightarrow C_2^+ + He$	5.0 (-10)
26.	$He^+ + N_2 \rightarrow N^+ + N + He$	7.5 (-10)
27.	$He^+ + N_2 \rightarrow N_2^+ + He$	4.4 (-10)
28.	$He^+ + O_2 \rightarrow O^+ + O + He$	1.0 (-9)
29.	$He^+ + CH \rightarrow CH^+ + He$	5.0 (-10)
30.	$He^+ + CH \rightarrow H^+ + C + He$	3.0 (-10)
31.	$He^+ + OH \rightarrow H^+ + O + He$	3.0 (-10)
32.	$He^+ + CO \rightarrow C^+ + O + He$	1.6 (-9)
33.	$He^+ + CN \rightarrow C^+ + N + He$	2.0 (-9)
34.	$He^+ + NO \rightarrow N^+ + O + He$	1.4 (-9)
35.	$He^+ + NO \rightarrow O^+ + N + He$	2.2 (-10)
36.	$He^+ + CH_2 \rightarrow CH_2^+ + He$	5.0 (-10)
37.	$He^+ + C_2H \rightarrow C_2H^+ + He$	5.0 (-10)
38.	$He^+ + H_2O \rightarrow H_2O^+ + He$	7.5 (-11)
39.	$He^+ + H_2O \rightarrow OH^+ + H + He$	3.6 (-10)
40.	$He^+ + CO_2 \rightarrow CO^+ + O + He$	8.2 (-10)
41.	$He^+ + CO_2 \rightarrow O^+ + CO + He$	1.4 (-10)
42.	$He^+ + CO_2 \rightarrow C^+ + O_2 + He$	4.0 (-11)
43.	$He^+ + NH_3 \rightarrow NH_3^+ + He$	2.6 (-10)
44.	$He^+ + NH_3 \rightarrow NH_2^+ + H + He$	1.8 (-9)
45.	$He^+ + NH_3 \rightarrow NH^+ + H_2 + He$	1.8 (-10)
46.	$He^+ + HCN \rightarrow CN^+ + H + He$	1.6 (-9)
47.	$He^+ + HCN \rightarrow CH^+ + N + He$	5.9 (-10)
48.	$He^+ + HCN \rightarrow C^+ + N + H + He$	6.8 (-10)
49.	$He^+ + HCN \rightarrow N^+ + C + H + He$	1.9 (-10)
50.	$He^+ + H_2CO \rightarrow CH_2^+ + O + He$	1.0 (-9)
51.	$He^+ + CH_4 \rightarrow CH_2^+ + H_2 + He$	9.3 (-10)
52.	$He^+ + CH_4 \rightarrow CH^+ + H_2 + H + He$	2.4 (-10)

53.	He^+ + H_2S --> S^+ + H_2 + He	3.6 (-9)
54.	He^+ + H_2S --> SH^+ + H + He	4.8 (-10)
55.	He^+ + H_2S --> H_2S^+ + He	3.1 (-10)
56.	He^+ + C_3 --> C_3^+ + He	1.0 (-9)
57.	He^+ + CS --> CS^+ + He	1.0 (-9)
58.	He^+ + NH_2 --> NH_2^+ + He	1.0 (-9)
59.	He^+ + SiO --> SiO^+ + He	1.0 (-9)
60.	He^+ + CH_3 --> CH_3^+ + He	1.0 (-9)
61.	He^+ + HCO --> HCO^+ + He	1.0 (-9)
*62.	He^+ + ^{13}CO --> $^{13}C^+$ + O + He	1.6 (-9)
63.	C^+ + H --> CH^+ + $h\nu$	1.0 (-17)
64.	C^+ + H_2 --> CH_2^+ + $h\nu$	1.0 (-15)
65.	C^+ + O_2 --> CO^+ + O	1.1 (-9)
66.	C^+ + CH --> C_2^+ + H	2.0 (-9)
67.	C^+ + CH --> CH^+ + C	1.0 (-9)
68.	C^+ + OH --> H^+ + CO	8.0 (-10)
69.	C^+ + OH --> CO^+ + H	8.0 (-10)
70.	C^+ + NO --> NO^+ + C	9.0 (-10)
71.	C^+ + NH --> H^+ + CN	2.0 (-9)
72.	C^+ + CH_2 --> C_2H^+ + H	2.0 (-9)
73.	C^+ + H_2O --> HCO^+ + H	2.0 (-9)
74.	C^+ + CO_2 --> CO^+ + CO	1.9 (-9)
75.	C^+ + C_2H --> C_3^+ + H	1.0 (-9)
76.	C^+ + HCO --> CH^+ + CO	1.0 (-9)
77.	C^+ + HCN --> C_2N^+ + H	1.9 (-9)
78.	C^+ + NH_2 --> H^+ + HCN	2.0 (-9)
79.	C^+ + NH_3 --> H_2CN^+ + H	1.1 (-9)
80.	C^+ + NH_3 --> NH_3^+ + C	1.1 (-9)
81.	C^+ + NH_3 --> HCN^+ + H_2	4.6 (-11)

82.	$C^+ + H_2CO$ --> $CH_2^+ + CO$	1.0 (-9)
83.	$C^+ + H_2CO$ --> $H_2CO^+ + C$	1.0 (-9)
84.	$C^+ + CH_3$ --> $C_2H_2^+ + H$	1.0 (-9)
85.	$C^+ + H_2CS$ --> $H_2CS^+ + C$	1.0 (-9)
86.	$C^+ + H_2S$ --> $HCS^+ + H$	1.8 (-9)
87.	$C^+ + SO$ --> $S^+ + CO$	1.0 (-9)
88.	$C^+ + SO$ --> $CO^+ + S$	1.0 (-9)
89.	$C^+ + SN$ --> $S^+ + CN$	1.0 (-9)
90.	$C^+ + SO_2$ --> $SO^+ + CO$	1.0 (-9)
91.	$C^+ + OCS$ --> $CS^+ + CO$	1.0 (-9)
92.	$C^+ + SH$ --> $CS^+ + H$	1.0 (-9)
93.	$C^+ + SiO$ --> $Si^+ + CO$	1.0 (-9)
94.	$C^+ + O_2$ --> $O^+ + CO$	4.4 (-10)
95.	$C^+ + CH_4$ --> $C_2H_2^+ + H_2$	1.4 (-9)
96.	$C^+ + H_2S$ --> $H_2S^+ + C$	5.6 (-10)
97.	$C^+ + H_2CO$ --> $HCO^+ + CH$	9.2 (-10)
98.	$C^+ + CH_3$ --> $CH_3^+ + C$	1.0 (-9)
* 99.	$^{13}C^+ + H_2$ --> $^{13}CH_2^+$	1.0 (-15)
* 100.	$^{13}C^+ + O_2$ --> $^{13}CO^+ + O$	1.1 (-9)
* 101.	$^{13}C^+ + H_2O$ --> $H^{13}CO^+ + H$	2.0 (-9)
* 102.	$^{13}C^+ + H^{13}CO$ --> $^{13}CH^+ + {}^{13}CO$	1.0 (-9)
* 103.	$^{13}C^+ + NH_3$ --> $NH_3^+ + {}^{13}C$	1.1 (-9)
* 104.	$^{13}C^+ + NO$ --> $NO^+ + {}^{13}C$	9.0 (-10)
* 105.	$^{13}C^+ + SO$ --> $^{13}CO^+ + S$	1.0 (-9)
* 106.	$^{13}C^+ + O_2$ --> $O^+ + {}^{13}CO$	4.4 (-10)
* 107.	$^{13}C^+ + CO$ --> $C^+ + {}^{13}CO$	2.0 (-10)

108.	O^+ + H --> H^+ + O	1.0 (-9)
109.	O^+ + H_2 --> OH^+ + H	1.6 (-9)
110.	O^+ + C_2 --> C^+ + CO	1.0 (-9)
111.	O^+ + N_2 --> NO^+ + N	1.0 (-13)
112.	O^+ + CN --> NO^+ + C	1.0 (-9)
113.	O^+ + H_2O --> H_2O^+ + O	2.3 (-9)
114.	O^+ + NH_3 --> NH_3^+ + O	1.0 (-9)
115.	N^+ + H_2 --> NH^+ + H	4.8 (-10)
116.	N^+ + C_2 --> C^+ + CN	1.0 (-9)
117.	N^+ + O_2 --> NO^+ + O	5.0 (-10)
118.	N^+ + CO --> CO^+ + N	5.0 (-10)
119.	N^+ + CN --> C^+ + N_2	1.0 (-9)
120.	S^+ + O_2 --> SO^+ + O	2.0 (-11)
121.	S^+ + H_2S --> H_2S^+ + S	2.1 (-10)
122.	S^+ + H_2S --> S_2^+ + H_2	2.5 (-10)
123.	S^+ + Fe --> Fe^+ + S	3.0 (-9)
124.	S^+ + CH_4 --> SCH_3^+ + H	1.4 (-10)
125.	S^+ + NH_3 --> MH_3^+ + S	1.3 (-9)
126.	S^+ + CH_3 --> CH_3^+ + S	1.0 (-9)
127.	S^+ + NO --> NO^+ + S	1.0 (-9)
128.	S^+ + HCO --> HCO^+ + S	1.0 (-9)
129.	Si^+ + O_2 --> SiO^+ + O	1.0 (-9)
130.	Si^+ + H_2 --> SiH_2 + $h\nu$	1.0 (-16)
131.	Si^+ + OH --> SiO^+ + H	1.0 (-9)
132.	Si^+ + Mg --> Mg^+ + Si	2.0 (-9)
133.	H_2^+ + H --> H^+ + H_2	5.8 (-10)
134.	H_2^+ + C --> CH^+ + H	1.0 (-9)

135.	H_2^+ + N --> NH^+ + H	1.0 (-9)
136.	H_2^+ + O --> OH^+ + H	1.0 (-9)
137.	H_2^+ + H_2 --> H_3^+ + H	2.1 (-9)
138.	H_2^+ + N_2 --> N_2H^+ + H	2.0 (-9)
139.	H_2^+ + O_2 --> O_2H^+ + H	1.9 (-9)
140.	H_2^+ + O_2 --> O_2^+ + H_2	7.8 (-10)
141.	H_2^+ + CO --> HCO^+ + H	2.2 (-9)
142.	H_2^+ + CO --> CO^+ + H_2	6.4 (-10)
143.	H_2^+ + H_2O --> H_3O^+ + H	3.4 (-9)
144.	H_2^+ + H_2O --> H_2O^+ + H_2	3.9 (-9)
145.	H_2^+ + NH_3 --> NH_3^+ + H_2	5.7 (-9)
146.	H_2^+ + H_2S --> H_2S^+ + H_2	2.7 (-9)
147.	H_2^+ + H_2S --> SH^+ + H + H_2	8.6 (-10)
148.	H_2^+ + H_2S --> S^+ + H_2 + H_2	7.7 (-10)
149.	H_3^+ + C --> CH^+ + H_2	2.0 (-9)
150.	H_3^+ + C --> CH_2^+ + H	1.0 (-9)
151.	H_3^+ + S --> SH^+ + H_2	2.0 (-9)
152.	H_3^+ + S --> H_2S^+ + H	2.0 (-9)
153.	H_3^+ + Mg --> Mg^+ + H_2 + H	1.0 (-9)
154.	H_3^+ + Si --> Si^+ + H_2 + H	1.0 (-9)
155.	H_3^+ + Fe --> Fe^+ + H_2 + H	1.0 (-9)
156.	H_3^+ + N --> NH_2^+ + H	1.0 (-9)
157.	H_3^+ + O --> H_2O^+ + H	4.0 (-10)
158.	H_3^+ + N_2 --> N_2H^+ + H_2	1.7 (-9)
159.	H_3^+ + CO --> HCO^+ + H_2	1.7 (-9)
160.	H_3^+ + OH --> H_2O^+ + H_2	2.0 (-9)
161.	H_3^+ + CN --> HCN^+ + H_2	2.0 (-9)

162.	$H_3^+ + H_2O \longrightarrow H_3O^+ + H_2$	5.9 (-9)
163.	$H_3^+ + CO_2 \longrightarrow HCO_2^+ + H_2$	1.9 (-9)
164.	$H_3^+ + HCO \longrightarrow H_2CO^+ + H_2$	1.0 (-9)
165.	$H_3^+ + HCN \longrightarrow H_2CN^+ + H_2$	8.0 (-9)
166.	$H_3^+ + NH_3 \longrightarrow NH_4^+ + H_2$	2.7 (-9)
167.	$H_3^+ + NH_3 \longrightarrow NH_3^+ + H_2 + H$	2.0 (-9)
168.	$H_3^+ + H_2CO \longrightarrow H_3CO^+ + H_2$	2.0 (-9)
169.	$H_3^+ + C_2 \longrightarrow C_2H^+ + H_2$	1.0 (-9)
170.	$H_3^+ + CH_3 \longrightarrow CH_4^+ + H_2$	1.0 (-9)
171.	$H_3^+ + CH_4 \longrightarrow CH_5^+ + H_2$	2.4 (-9)
172.	$H_3^+ + H_2S \longrightarrow H_3S^+ + H_2$	3.7 (-9)
173.	$H_3^+ + SH \longrightarrow H_2S^+ + H_2$	1.0 (-9)
174.	$H_3^+ + NH \longrightarrow NH_2^+ + H_2$	1.0 (-9)
175.	$H_3^+ + CS \longrightarrow HCS^+ + H_2$	1.0 (-9)
176.	$H_3^+ + C_2H \longrightarrow C_2H_2^+ + H_2$	1.0 (-9)
177.	$H_3^+ + CH \longrightarrow CH_2^+ + H_2$	1.0 (-9)
178.	$H_3^+ + NH_2 \longrightarrow NH_3^+ + H_2$	1.0 (-9)
179.	$H_3^+ + CH_2 \longrightarrow CH_3^+ + H_2$	1.0 (-9)
*180.	$H_3^+ + H^{13}CO \longrightarrow H_2{}^{13}CO^+ + H_2$	1.0 (-9)
*181.	$H_3^+ + {}^{13}C \longrightarrow {}^{13}CH_2^+ + H$	1.0 (-9)
*182.	$H_3^+ + {}^{13}CO \longrightarrow H^{13}CO^+ + H_2$	1.7 (-9)
183.	$C_2^+ + C \longrightarrow C^+ + C_2$	1.0 (-9)
184.	$C_2^+ + N \longrightarrow C^+ + CN$	1.0 (-9)
185.	$C_2^+ + O \longrightarrow C^+ + CO$	1.0 (-9)
186.	$C_2^+ + H_2 \longrightarrow C_2H^+ + H$	1.0 (-9)

187.	O_2^+ + C --> C^+ + O_2	1.0 (-9)
188.	O_2^+ + N --> NO^+ + O	1.8 (-10)
189.	O_2^+ + NH_3 --> NH_3^+ + O_2	2.6 (-9)
190.	O_2^+ + Mg --> Mg^+ + O_2	1.0 (-9)
191.	O_2^+ + Si --> Si^+ + O_2	1.0 (-9)
192.	O_2^+ + S --> S^+ + O_2	1.0 (-9)
193.	O_2^+ + Fe --> Fe^+ + O_2	1.0 (-9)
194.	N_2^+ + H --> H^+ + N_2	1.0 (-9)
195.	N_2^+ + O --> NO^+ + N	2.5 (-10)
196.	N_2^+ + H_2 --> N_2H^+ + H	1.7 (-9)
197.	CH^+ + H --> C^+ + H_2	$7.5 \times 10^{-15} \times T^{1.25}$
198.	CH^+ + C --> C_2^+ + H	1.0 (-9)
199.	CH^+ + N --> H^+ + CN	1.0 (-9)
200.	CH^+ + O --> CO^+ + H	1.0 (-9)
201.	CH^+ + H_2 --> CH_2^+ + H	1.0 (-9)
202.	CH^+ + H_2S --> HCS^+ + H_2	6.6 (-10)
*203.	$^{13}CH^+$ + H_2 --> $^{13}CH_2^+$ + H	1.0 (-9)
204.	OH^+ + C --> H^+ + CO	1.0 (-9)
205.	OH^+ + O --> O_2^+ + H	1.0 (-9)
206.	OH^+ + H_2 --> H_2O^+ + H	1.0 (-9)
207.	OH^+ + H_2O --> H_2O^+ + OH	1.6 (-9)
208.	OH^+ + H_2O --> H_3O^+ + O	1.3 (-9)
209.	OH^+ + H_2S --> H_3S^+ + O	9.1 (-10)
210.	OH^+ + CO_2 --> HCO_2^+ + O	1.0 (-9)
211.	OH^+ + CH_3 --> CH_4^+ + O	1.0 (-9)

212.	$OH^+ + CH_4 \rightarrow CH_5^+ + O$	1.0 (-9)
213.	$OH^+ + NH \rightarrow NH_2^+ + O$	1.0 (-9)
214.	$OH^+ + CO \rightarrow HCO^+ + O$	1.0 (-9)
215.	$OH^+ + OH \rightarrow H_2O^+ + O$	1.0 (-9)
216.	$OH^+ + C \rightarrow CH^+ + O$	1.0 (-9)
217.	$OH^+ + CS \rightarrow HCS^+ + O$	1.0 (-9)
218.	$OH^+ + HCO \rightarrow H_2CO^+ + O$	1.0 (-9)
219.	$OH^+ + S \rightarrow SH^+ + O$	1.0 (-9)
220.	$OH^+ + C_2H \rightarrow C_2H_2^+ + O$	1.0 (-9)
221.	$OH^+ + SH \rightarrow H_2S^+ + O$	1.0 (-9)
222.	$OH^+ + C_2 \rightarrow C_2H^+ + O$	1.0 (-9)
223.	$OH^+ + H_2CO \rightarrow H_3CO^+ + O$	1.0 (-9)
224.	$OH^+ + HCN \rightarrow H_2CN^+ + O$	1.0 (-9)
225.	$OH^+ + CH \rightarrow CH_2^+ + O$	1.0 (-9)
226.	$OH^+ + NH_2 \rightarrow NH_3^+ + O$	1.0 (-9)
227.	$OH^+ + CH_2 \rightarrow CH_3^+ + O$	1.0 (-9)
228.	$OH^+ + NH_3 \rightarrow NH_4^+ + O$	1.0 (-9)
229.	$CO^+ + H \rightarrow H^+ + CO$	1.0 (-9)
230.	$CO^+ + N \rightarrow NO^+ + C$	1.0 (-11)
231.	$CO^+ + H_2 \rightarrow HCO^+ + H$	1.4 (-9)
232.	$CO^+ + OH \rightarrow CO_2^+ + H$	1.0 (-9)
233.	$CO^+ + NO \rightarrow NO^+ + CO$	6.0 (-10)
234.	$CO^+ + H_2O \rightarrow H_2O^+ + CO$	1.0 (-9)
235.	$CO^+ + NH_3 \rightarrow NH_3^+ + CO$	2.1 (-9)
*236.	$^{13}CO^+ + H_2 \rightarrow H^{13}CO^+ + H$	1.4 (-9)

237.	$NH^+ + C \dashrightarrow H^+ + CN$	1.0 (-9)
238.	$NH^+ + N \dashrightarrow H^+ + N_2$	1.0 (-9)
239.	$NH^+ + O \dashrightarrow NO^+ + H$	1.0 (-9)
240.	$NH^+ + H_2 \dashrightarrow NH_2^+ + H$	9.5 (-10)
241.	$CN^+ + H \dashrightarrow H^+ + CN$	1.0 (-9)
242.	$CN^+ + N \dashrightarrow C^+ + N_2$	2.0 (-10)
243.	$CN^+ + O \dashrightarrow NO^+ + C$	2.0 (-10)
244.	$CN^+ + H_2 \dashrightarrow HCN^+ + H$	1.2 (-9)
245.	$SH^+ + O \dashrightarrow SO^+ + H$	1.0 (-9)
246.	$SH^+ + O \dashrightarrow S^+ + OH$	1.0 (-9)
247.	$SH^+ + N \dashrightarrow S^+ + NH$	1.0 (-9)
248.	$SH^+ + Mg \dashrightarrow Mg^+ + SH$	1.0 (-10)
249.	$SH^+ + S \dashrightarrow S^+ + SH$	1.0 (-10)
250.	$SH^+ + Si \dashrightarrow Si^+ + SH$	1.0 (-10)
251.	$SH^+ + C_2H \dashrightarrow C_2H_2^+ + S$	1.0 (-9)
252.	$SH^+ + H_2O \dashrightarrow H_3O^+ + S$	1.0 (-9)
253.	$SH^+ + SH \dashrightarrow H_2S^+ + S$	1.0 (-9)
254.	$SH^+ + C_2 \dashrightarrow C_2H^+ + S$	1.0 (-9)
255.	$SH^+ + H_2CO \dashrightarrow H_3CO^+ + S$	1.0 (-9)
256.	$SH^+ + HCN \dashrightarrow H_2CN^+ + S$	1.0 (-9)
257.	$SH^+ + H_2S \dashrightarrow H_3S^+ + S$	1.0 (-9)
258.	$SH^+ + CH \dashrightarrow CH_2^+ + S$	1.0 (-9)
259.	$SH^+ + NH_2 \dashrightarrow NH_3^+ + S$	1.0 (-9)
260.	$SH^+ + CH_2 \dashrightarrow CH_3^+ + S$	1.0 (-9)
261.	$SH^+ + NH_3 \dashrightarrow NH_4^+ + S$	1.0 (-9)

262.	$SO^+ + N \rightarrow SN^+ + O$	5.0 (-11)
263.	$SO^+ + Mg \rightarrow Mg^+ + SO$	1.0 (-10)
264.	$CS^+ + H_2 \rightarrow HCS^+ + H$	1.0 (-9)
265.	$CS^+ + H \rightarrow H^+ + CS$	1.0 (-9)
266.	$SN^+ + O \rightarrow NO^+ + S$	1.0 (-10)
267.	$SiO^+ + H_2 \rightarrow HSiO^+ + H$	1.0 (-9)
268.	$SiO^+ + Mg \rightarrow Mg^+ + SiO$	1.0 (-9)
269.	$SiO^+ + Fe \rightarrow Fe^+ + SiO$	1.0 (-9)
270.	$CH_2^+ + C \rightarrow C_2H^+ + H$	1.0 (-9)
271.	$CH_2^+ + N \rightarrow HCN^+ + H$	1.0 (-9)
272.	$CH_2^+ + O \rightarrow HCO^+ + H$	1.0 (-9)
273.	$CH_2^+ + H_2 \rightarrow CH_3^+ + H$	7.1 (-10)
274.	$CH_2^+ + H_2O \rightarrow CH_2OH^+ + H$	5.2 (-10)
275.	$CH_2^+ + NH_3 \rightarrow NH_4^+ + CH$	3.1 (-10)
276.	$CH_2^+ + NH_3 \rightarrow CH_2NH_2^+ + H$	1.2 (-9)
277.	$CH_2^+ + H_2S \rightarrow HCS^+ + H_2 + H$	2.0 (-10)
278.	$CH_2^+ + H_2S \rightarrow CH_2SH^+ + H$	3.9 (-10)
*279.	$^{13}CH_2^+ + H_2 \rightarrow {}^{13}CH_3^+ + H$	7.1 (-10)
280.	$CH_3^+ + C \rightarrow C_2H^+ + H_2$	1.0 (-9)
281.	$CH_3^+ + N \rightarrow H_2CN^+ + H$	6.7 (-11)
282.	$CH_3^+ + O \rightarrow HCO^+ + H_2$	4.4 (-10)
283.	$CH_3^+ + NH_3 \rightarrow NH_4^+ + CH_2$	1.7 (-10)
284.	$CH_3^+ + NH_3 \rightarrow CH_2NH_2^+ + H_2$	6.6 (-10)
285.	$CH_3^+ + H_2 \rightarrow CH_5^+ + h$	1.0 (-16)
286.	$CH_3^+ + S \rightarrow H_2CS^+ + H$	1.0 (-9)

287.	$CH_3^+ + H_2S \longrightarrow CH_2SH^+ + H_2$	5.0 (-10)
288.	$CH_3^+ + Mg \longrightarrow Mg^+ + CH_3$	2.0 (-9)
289.	$CH_3^+ + Fe \longrightarrow Fe^+ + CH_3$	2.0 (-9)
290.	$CH_3^+ + Si \longrightarrow Si^+ + CH_3$	2.0 (-9)
291.	$CH_3^+ + O_2 \longrightarrow HCO^+ + H_2O$	4.3 (-11)
292.	$CH_3^+ + NO \longrightarrow NO^+ + CH_3$	9.4 (-10)
293.	$CH_3^+ + H_2CO \longrightarrow HCO^+ + CH_4$	1.0 (-9)
*294.	$^{13}CH_3^+ + O \longrightarrow H^{13}CO^+ + H_2$	4.4 (-10)
295.	$CH_4^+ + H_2 \longrightarrow CH_5^+ + H$	4.1 (-11)
296.	$CH_4^+ + O \longrightarrow CH_3^+ + OH$	1.0 (-9)
297.	$H_2O^+ + C \longrightarrow HCO^+ + H$	1.0 (-9)
298.	$H_2O^+ + H_2 \longrightarrow H_3O^+ + H$	6.1 (-10)
299.	$H_2O^+ + H_2O \longrightarrow H_3O^+ + OH$	2.0 (-9)
300.	$H_2O^+ + H_2S \longrightarrow H_3S^+ + OH$	7.0 (-10)
301.	$H_2O^+ + H_2S \longrightarrow H_2S^+ + H_2O$	8.9 (-10)
302.	$H_2O^+ + H_2S \longrightarrow H_3O^+ + SH$	5.9 (-10)
303.	$H_2O^+ + CS \longrightarrow HCS^+ + OH$	1.0 (-9)
304.	$H_2O^+ + HCO \longrightarrow H_2CO^+ + OH$	1.0 (-9)
305.	$H_2O^+ + S \longrightarrow SH^+ + OH$	1.0 (-9)
306.	$H_2O^+ + C_2H \longrightarrow C_2H_2^+ + OH$	1.0 (-9)
307.	$H_2O^+ + SH \longrightarrow H_2S^+ + OH$	1.0 (-9)
308.	$H_2O^+ + C_2 \longrightarrow C_2H^+ + OH$	1.0 (-9)
309.	$H_2O^+ + H_2CO \longrightarrow H_3CO^+ + OH$	1.0 (-9)
310.	$H_2O^+ + HCN \longrightarrow H_2CN^+ + OH$	1.0 (-9)
311.	$H_2O^+ + CH \longrightarrow CH_2^+ + OH$	1.0 (-9)

312.	$H_2O^+ + NH_2 \rightarrow NH_3^+ + OH$	1.0 (-9)
313.	$H_2O^+ + CH_2 \rightarrow CH_3^+ + OH$	1.0 (-9)
314.	$H_2O^+ + NH_3 \rightarrow NH_3^+ + H_2O$	2.2 (-9)
315.	$H_2O^+ + NH_3 \rightarrow NH_4^+ + OH$	9.4 (-10)
316.	$H_3O^+ + C \rightarrow HCO^+ + H_2$	2.0 (-9)
317.	$H_3O^+ + NH_3 \rightarrow NH_4^+ + H_2O$	2.3 (-9)
318.	$H_3O^+ + SH \rightarrow H_2S^+ + H_2O$	1.0 (-9)
319.	$H_3O^+ + C_2 \rightarrow C_2H^+ + H_2O$	1.0 (-9)
320.	$H_3O^+ + H_2CO \rightarrow H_3CO^+ + H_2O$	1.0 (-9)
321.	$H_3O^+ + HCN \rightarrow H_2CN^+ + H_2O$	1.0 (-9)
322.	$H_3O^+ + H_2S \rightarrow H_3S^+ + H_2O$	1.0 (-9)
323.	$H_3O^+ + CH \rightarrow CH_2^+ + H_2O$	1.0 (-9)
324.	$H_3O^+ + NH_2 \rightarrow NH_3^+ + H_2O$	1.0 (-9)
325.	$H_3O^+ + CH_2 \rightarrow CH_3^+ + H_2O$	1.0 (-9)
326.	$HCO^+ + C \rightarrow CH^+ + CO$	1.0 (-9)
327.	$HCO^+ + H_2 \rightarrow H_3CO^+ + h$	2.0 (-17)
328.	$HCO^+ + OH \rightarrow HCO_2^+ + H$	1.0 (-9)
329.	$HCO^+ + CH \rightarrow CH_2^+ + CO$	1.0 (-9)
330.	$HCO^+ + CH_2 \rightarrow CH_3^+ + CO$	1.0 (-9)
331.	$HCO^+ + NH \rightarrow NH_2^+ + CO$	1.0 (-9)
332.	$HCO^+ + NH_2 \rightarrow NH_3^+ + CO$	1.0 (-9)
333.	$HCO^+ + NH_3 \rightarrow NH_4^+ + CO$	2.6 (-9)
334.	$HCO^+ + H_2CO \rightarrow H_3CO^+ + CO$	1.0 (-9)
335.	$HCO^+ + H_2O \rightarrow H_3O^+ + CO$	2.7 (-9)
336.	$HCO^+ + HCN \rightarrow H_2CN^+ + CO$	3.5 (-9)

337.	$HCO^+ + H_2S \dashrightarrow H_3S^+ + CO$	1.6 (-9)
338.	$HCO^+ + H_2CS \dashrightarrow H_3CS^+ + CO$	1.0 (-9)
339.	$HCO^+ + Mg \dashrightarrow Mg^+ + HCO$	1.0 (-9)
340.	$HCO^+ + Si \dashrightarrow Si^+ + HCO$	1.0 (-9)
341.	$HCO^+ + Fe \dashrightarrow Fe^+ + HCO$	1.0 (-9)
342.	$HCO^+ + CS \dashrightarrow HCS^+ + CO$	1.0 (-9)
343.	$HCO^+ + HCO \dashrightarrow H_2CO^+ + CO$	1.0 (-9)
344.	$HCO^+ + S \dashrightarrow SH^+ + CO$	1.0 (-9)
345.	$HCO^+ + C_2H \dashrightarrow C_2H_2^+ + CO$	1.0 (-9)
346.	$HCO^+ + SH \dashrightarrow H_2S^+ + CO$	1.0 (-9)
347.	$HCO^+ + C_2 \dashrightarrow C_2H^+ + CO$	1.0 (-9)
*348.	$H^{13}CO^+ + {}^{13}C \dashrightarrow {}^{13}CH^+ + {}^{13}CO$	1.0 (-9)
*349.	$H^{13}CO^+ + Mg \dashrightarrow Mg^+ + H^{13}CO$	1.0 (-9)
*350.	$H^{13}CO^+ + Fe \dashrightarrow Fe^+ + H^{13}CO$	1.0 (-9)
*351.	$H^{13}CO^+ + H^{13}CO \dashrightarrow H_2{}^{13}CO^+ + {}^{13}CO$	1.9 (-9)
352.	$C_3^+ + H_2 \dashrightarrow C_3H^+ + H$	1.0 (-9)
353.	$CO_2^+ + H_2 \dashrightarrow HCO_2^+ + H$	1.0 (-9)
354.	$NH_2^+ + H_2 \dashrightarrow NH_3^+ + H$	1.2 (-10)
355.	$NH_2^+ + NH_3 \dashrightarrow NH_3^+ + NH_2$	1.4 (-9)
356.	$NH_2^+ + NH_3 \dashrightarrow NH_4^+ + NH$	9.7 (-10)
357.	$NH_3^+ + CH \dashrightarrow NH_4^+ + C$	1.0 (-9)
358.	$NH_3^+ + NH \dashrightarrow NH_4^+ + N$	1.0 (-9)
359.	$NH_3^+ + OH \dashrightarrow NH_4^+ + O$	1.0 (-9)
360.	$NH_3^+ + HCO \dashrightarrow NH_4^+ + CO$	1.0 (-9)
361.	$NH_3^+ + H_2O \dashrightarrow NH_4^+ + OH$	4.3 (-10)

362.	NH_3^+ + HCN --> NH_4^+ + CN	1.0 (-11)
363.	NH_3^+ + H_2CO --> NH_4^+ + HCO	2.3 (-9)
364.	NH_3^+ + NH_3 --> NH_4^+ + NH_2	2.3 (-9)
365.	NH_3^+ + CH_4 --> NH_4^+ + CH_3	3.9 (-10)
366.	NH_3^+ + H_2 --> NH_4^+ + H	3.0 (-13)
367.	NH_3^+ + CH_2 --> CH_3^+ + NH_2	1.0 (-9)
368.	HCN^+ + H_2 --> H_2CN^+ + H	9.6 (-10)
369.	HCN^+ + NH_3 --> NH_3^+ + HCN	1.0 (-9)
370.	N_2H^+ + CO --> HCO^+ + N_2	1.0 (-9)
371.	N_2H^+ + CO_2 --> HCO_2^+ + N_2	1.0 (-9)
372.	N_2H^+ + CH_3 --> CH_4^+ + N_2	1.0 (-9)
373.	N_2H^+ + CH_4 --> CH_5^+ + N_2	1.0 (-9)
374.	N_2H^+ + NH --> NH_2^+ + N_2	1.0 (-9)
375.	N_2H^+ + OH --> HCO^+ + N_2	1.0 (-9)
376.	N_2H^+ + C --> CH^+ + N_2	1.0 (-9)
377.	N_2H^+ + CS --> HCS^+ + N_2	1.0 (-9)
378.	N_2H^+ + HCO --> H_2CO^+ + N_2	1.0 (-9)
379.	N_2H^+ + S --> SH^+ + N_2	1.0 (-9)
380.	N_2H^+ + C_2H --> $C_2H_2^+$ + N_2	1.0 (-9)
381.	N_2H^+ + H_2O --> H_3O^+ + N_2	1.0 (-9)
382.	N_2H^+ + SH --> H_2S^+ + N_2	1.0 (-9)
383.	N_2H^+ + C_2 --> C_2H^+ + N_2	1.0 (-9)
384.	N_2H^+ + H_2CO --> H_3CO^+ + N_2	1.0 (-9)
385.	N_2H^+ + HCN --> H_2CN^+ + N_2	1.0 (-9)

386.	$N_2H^+ + H_2S \text{ --> } H_3S^+ + N_2$	1.0 (-9)
387.	$N_2H^+ + CH \text{ --> } CH_2^+ + N_2$	1.0 (-9)
388.	$N_2H^+ + NH_2 \text{ --> } NH_3^+ + N_2$	1.0 (-9)
389.	$N_2H^+ + CH_2 \text{ --> } CH_3^+ + N_2$	1.0 (-9)
390.	$N_2H^+ + NH_3 \text{ --> } NH_4^+ + N_2$	1.0 (-9)
391.	$C_2H_2^+ + H_2 \text{ --> } C_2H_2^+ + H$	1.0 (-9)
392.	$C_2H_2^+ + N \text{ --> } C_2N^+ + H_2$	1.0 (-9)
393.	$C_2H_2^+ + H_2O \text{ --> } H_3O^+ + C_2H$	2.2 (-10)
394.	$C_2H_2^+ + SH \text{ --> } H_2S^+ + C_2H$	1.0 (-9)
395.	$C_2H_2^+ + C_2 \text{ --> } C_2H^+ + C_2H$	1.0 (-9)
396.	$C_2H_2^+ + H_2CO \text{ --> } H_3CO^+ + C_2H$	1.0 (-9)
397.	$C_2H_2^+ + HCN \text{ --> } H_2CN^+ + C_2H$	1.0 (-9)
398.	$C_2H_2^+ + H_2S \text{ --> } H_3S^+ + C_2H$	1.0 (-9)
399.	$C_2H_2^+ + CH \text{ --> } CH_2^+ + C_2H$	1.0 (-9)
400.	$C_2H_2^+ + NH_2 \text{ --> } NH_3^+ + C_2H$	1.0 (-9)
401.	$C_2H_2^+ + CH_2 \text{ --> } CH_3^+ + C_2H$	1.0 (-9)
402.	$C_2H_2^+ + NH_3 \text{ --> } NH_4^+ + C_2H$	1.0 (-9)
403.	$H_2CN^+ + NH_3 \text{ --> } NH_4^+ + HCN$	2.2 (-9)
404.	$H_2S^+ + H_2O \text{ --> } H_3O^+ + SH$	7.0 (-10)
405.	$H_2S^+ + O \text{ --> } SH^+ + OH$	1.0 (-9)
406.	$H_2S^+ + Mg \text{ --> } Mg^+ + H_2S$	1.0 (-10)
407.	$H_2S^+ + S \text{ --> } S^+ + H_2S$	1.0 (-10)
408.	$H_2S^+ + Si \text{ --> } Si^+ + H_2S$	1.0 (-10)
409.	$HCS^+ + H_2 \text{ --> } H_3CS^+ + h\nu$	2.0 (-17)
410.	$HCS^+ + H_2O \text{ --> } H_3O^+ + CS$	3.0 (-9)
411.	$NH_3^+ + H_2S \text{ --> } NH_4^+ + SH$	6.5 (-10)

412.	$NH_3^+ + H_2S \rightarrow H_3S^+ + NH_2$	1.1 (-10)
413.	$H_2CO^+ + S \rightarrow S^+ + H_2CO$	2.0 (-9)
414.	$H_2CO^+ + Mg \rightarrow Mg^+ + H_2CO$	2.0 (-9)
415.	$H_2CO^+ + Fe \rightarrow Fe^+ + H_2CO$	2.0 (-9)
416.	$H_2CO^+ + Si \rightarrow Si^+ + H_2CO$	2.0 (-9)
417.	$H_3^+ + O \rightarrow OH^+ + H_2$	4.0 (-10)

TABLE 2. NEUTRAL-NEUTRAL REACTIONS

	Reaction	Rate (cm^3s^{-1})
418.	$H + H \dashrightarrow H_2$ (grains)	1.0 (-17)
419.	$C + H \dashrightarrow CH + h\nu$	1.0 (-17)
420.	$O + H \dashrightarrow OH + h\nu$	4.0 (-19)
421.	$C_2 + N \dashrightarrow CN + C$	4.0 (-11)
422.	$C_2 + O \dashrightarrow CO + C$	4.0 (-11)
423.	$CH + H \dashrightarrow C + H_2$	1.0 (-14)
424.	$CH + C \dashrightarrow C_2 + H$	4.0 (-11)
425.	$CH + N \dashrightarrow CN + H$	4.0 (-11)
426.	$CH + O \dashrightarrow CO + H$	4.0 (-11)
427.	$CH + O \dashrightarrow HCO^+ + e$	1.0 (-11)
428.	$NH + C \dashrightarrow CN + H$	4.0 (-11)
429.	$NH + N \dashrightarrow N_2 + H$	4.0 (-11)
430.	$NH + O \dashrightarrow NO + H$	4.0 (-11)
431.	$OH + C \dashrightarrow CO + H$	4.0 (-11)
432.	$OH + N \dashrightarrow NO + H$	7.0 (-11)
433.	$OH + O \dashrightarrow O_2 + H$	5.0 (-11)
*434.	$OH + {}^{13}C \dashrightarrow {}^{13}CO + H$	4.0 (-11)
435.	$NO + C \dashrightarrow CO + N$	4.0 (-11)
436.	$NO + N \dashrightarrow N_2 + O$	2.2 (-11)
*437.	$NO + {}^{13}C \dashrightarrow {}^{13}CO + N$	4.0 (-11)
438.	$CN + N \dashrightarrow N_2 + C$	1.0 (-14)
439.	$CN + O \dashrightarrow CO + N$	1.0 (-12)
440.	$CO + OH \dashrightarrow CO_2 + H$	$5.0 \times 10^{-13} e^{-300/T}$

441.	CH_2 + O --> CH + OH	8.0 (-12)
442.	CH_2 + O --> HCO + H	1.0 (-11)
443.	CH_2 + N --> HCN + H	4.0 (-11)
*444.	$^{13}CH_2$ + O --> ^{13}CH + OH	8.0 (-12)
*445.	$^{13}CH_2$ + O --> $H^{13}CO$ + H	1.0 (-11)
446.	C_2H + O --> CO + CH	4.0 (-11)
447.	NH_2 + O --> NH + OH	4.0 (-11)
448.	HCO + C --> CH + CO	1.0 (-11)
*449.	$H^{13}CO$ + ^{13}C --> ^{13}CH + ^{13}CO	1.0 (-11)
450.	CH_3 + O --> H_2CO + H	3.0 (-11)
451.	H_2CO + O --> HCO + OH	1.8 (-13)
452.	SH + O --> SO + H	2.0 (-10)
453.	SH + N --> SN + H	2.0 (-10)
454.	SO + N --> NO + S	8.0 (-13)
455.	SO + N --> SN + O	1.0 (-12)
456.	CH + S --> CS + H	1.0 (-11)
*457.	^{13}CH + O --> $H^{13}CO^+$ + e	1.0 (-11)
*458.	^{13}CH + O --> ^{13}CO + H	4.0 (-11)
459.	CH_3 + S --> H_2CS + H	1.0 (-11)
460.	CS + OH --> OCS + H	1.0 (-13)
461.	CO + SH --> OCS + H	1.0 (-13)
462.	SO + OH --> SO_2 + H	5.0 (-11)
463.	CS + O --> CO + S	1.0 (-11)
464.	SN + N --> N_2 + S	1.0 (-11)
465.	SN + O --> NO + S	1.0 (-11)

466.	$NH + S \rightarrow SN + H$	1.0 (-11)
467.	$SN + C \rightarrow CS + N$	1.0 (-11)
468.	$SO + O \rightarrow SO_2 + h\nu$	7.0 (-16)

TABLE 3

PHOTODESTRUCTION PROCESSES: RATES HAVE THE FORM $a \exp(-bA_V) s^{-1}$

Reaction	a	b
469. $C + h\nu \dashrightarrow C^{+} + e$	1.31 (-10)	2.415
470. $S + h\nu \dashrightarrow S^{+} + e$	7.2 (-10)	2.39
471. $Mg + h\nu \dashrightarrow Mg^{+} + e$	4.45 (-11)	1.435
472. $Fe + h\nu \dashrightarrow Fe^{+} + e$	1.17 (-10)	1.536
473. $Si + h\nu \dashrightarrow Si^{+} + e$	1.20 (-9)	1.622
474. $CH + h\nu \dashrightarrow CH^{+} + e$	2.89 (-10)	2.75
475. $CH + h\nu \dashrightarrow C + H$	1.4 (-10)	1.54
476. $C_2 + h\nu \dashrightarrow C + C$	5.0 (-11)	1.72
477. $O_2 + h\nu \dashrightarrow O_2^{+} + e$	6.2 (-12)	3.10
478. $O_2 + h\nu \dashrightarrow O + O$	3.3 (-10)	1.4
479. $OH + h\nu \dashrightarrow OH^{+} + e$	1.6 (-12)	3.09
480. $OH + h\nu \dashrightarrow O + H$	7.2 (-12)	1.81
481. $CO + h\nu \dashrightarrow C + O$	5.0 (-12)	3.0
482. $CN + h\nu \dashrightarrow C + N$	5.0 (-11)	1.72
483. $H_2O + h\nu \dashrightarrow H_2O^{+} + e$	2.1 (-11)	3.09
484. $H_2O + h\nu \dashrightarrow OH + H$	3.2 (-10)	1.68
485. $CH_2 + h\nu \dashrightarrow CH + H$	5.0 (-11)	1.72
486. $CH_2 + h\nu \dashrightarrow CH_2^{+} + e$	1.0 (-9)	2.28
487. $C_2H + h\nu \dashrightarrow CH + C$	1.4 (-10)	1.72
488. $HCO + h\nu \dashrightarrow CO + H$	8.8 (-10)	1.61
489. $HCN + h\nu \dashrightarrow CN + H$	1.0 (-10)	1.80
490. $NH_3 + h\nu \dashrightarrow NH_2 + H$	5.0 (-10)	2.0

491.	$NH_3 + h\nu \dashrightarrow NH + H_2$	5.0 (-11)	2.0
492.	$H_2CO + h\nu \dashrightarrow CO + H_2$	4.4 (-10)	1.61
493.	$H_2CO + h\nu \dashrightarrow CO + 2H$	4.4 (-10)	1.61
494.	$H_2CO + h\nu \dashrightarrow H_2CO^+ + e$	1.4 (-11)	3.09
495.	$NH + h\nu \dashrightarrow N + H$	1.4 (-10)	1.54
496.	$NH + h\nu \dashrightarrow NH^+ + e$	1.0 (-11)	2.0
497.	$NO + h\nu \dashrightarrow N + O$	1.0 (-11)	2.0
498.	$NO + h\nu \dashrightarrow NO^+ + e$	2.0 (-10)	2.0
499.	$C_2 + h\nu \dashrightarrow C_2^+ + e$	1.0 (-10)	2.0
500.	$N_2 + h\nu \dashrightarrow N + N$	5.0 (-11)	2.0
501.	$CO_2 + h\nu \dashrightarrow CO + O$	1.0 (-10)	2.0
502.	$C_3 + h\nu \dashrightarrow C_2 + C$	1.0 (-10)	2.0
503.	$NH_2 + h\nu \dashrightarrow NH + H$	1.0 (-10)	2.0
504.	$C_2H + h\nu \dashrightarrow C_2H^+ + e$	1.5 (-11)	2.0
505.	$CH_3 + h\nu \dashrightarrow CH + H_2$	3.0 (-11)	1.72
506.	$CH_3 + h\nu \dashrightarrow CH_2 + H$	3.0 (-11)	1.72
507.	$CH_3 + h\nu \dashrightarrow CH_3^+ + e$	1.0 (-10)	2.069
508.	$CH_4 + h\nu \dashrightarrow CH + H_2 + H$	1.59 (-10)	2.17
509.	$CH_4 + h\nu \dashrightarrow CH_2 + H_2$	4.78 (-10)	2.17
510.	$CH_4 + h\nu \dashrightarrow CH_3 + H$	1.59 (-10)	2.17
511.	$SH + h\nu \dashrightarrow S + H$	1.5 (-10)	3.092
512.	$SO + h\nu \dashrightarrow S + O$	3.3 (-10)	1.4
513.	$SN + h\nu \dashrightarrow SN^+ + e$	1.0 (-11)	2.0
514.	$H_2S + h\nu \dashrightarrow SH + H$	3.2 (-10)	1.677
515.	$CS + h\nu \dashrightarrow C + S$	1.0 (-11)	2.0
516.	$OCS + h\nu \dashrightarrow CO + S$	1.0 (-11)	2.0

517.	$SO_2 + h\nu \rightarrow SO + O$	1.0 (-11)	2.0
518.	$H_2CS + h\nu \rightarrow H_2CS^+ + e$	8.0 (-11)	2.8
519.	$H_2CS + h\nu \rightarrow HCS^+ + H + e$	1.4 (-11)	3.09
520.	$H_2CS + h\nu \rightarrow CS + H_2$	8.0 (-10)	1.6
521.	$SiO + h\nu \rightarrow Si + O$	1.0 (-10)	2.0
522.	$H_2 + h\nu \rightarrow H + H$		

TABLE 4 ION-ELECTRON RECOMBINATION REACTIONS

	Reaction	Rate (cm^3s^{-1})
523.	$H^+ + e \dashrightarrow H + h$	$1.9 \times 10^{-10}T^{-0.7}$
524.	$C^+ + e \dashrightarrow C + h$	$7.6 \times 10^{-12}(100/T)^{0.7}$
*525.	$^{13}C^+ + e \dashrightarrow {}^{13}C + h\nu$	$7.6 \times 10^{-12}(100/T)^{0.7}$
526.	$N^+ + e \dashrightarrow N + h$	$1.3 \times 10^{-10}T^{-0.62}$
527.	$O^+ + e \dashrightarrow O + h$	$1.2 \times 10^{-10}T^{-0.626}$
528.	$He^+ + e \dashrightarrow He + h$	$2.1 \times 10^{-10}T^{-0.67}$
529.	$S^+ + e \dashrightarrow S + h$	$1.4 \times 10^{-10}T^{-0.63}$
530.	$Si^+ + e \dashrightarrow Si + h$	$1.5 \times 10^{-10}T^{-0.641}$
531.	$Fe^+ + e \dashrightarrow Fe + h$	$1.5 \times 10^{-10}T^{-0.65}$
532.	$Mg^+ + e \dashrightarrow Mg + h$	$3.7 \times 10^{-10}T^{-0.855}$
533.	$H_3^+ + e \dashrightarrow H_2 + H$	1.5 (-7)
534.	$H_3^+ + e \dashrightarrow 3H$	1.5 (-7)
535.	$CH^+ + e \dashrightarrow C + H$	1.0 (-7)
536.	$C_2^+ + e \dashrightarrow C + C$	2.0 (-7)
537.	$OH^+ + e \dashrightarrow O + H$	1.0 (-7)
538.	$CO^+ + e \dashrightarrow C + O$	1.0 (-7)
539.	$O_2^+ + e \dashrightarrow O + O$	2.1 (-7)
540.	$NH^+ + e \dashrightarrow N + H$	1.0 (-7)
541.	$NO^+ + e \dashrightarrow N + O$	4.1 (-7)
542.	$N_2^+ + e \dashrightarrow N + N$	3.0 (-7)
543.	$CN^+ + e \dashrightarrow C + N$	3.0 (-7)
544.	$CH_2^+ + e \dashrightarrow CH + H$	3.0 (-7)
545.	$CH_2^+ + e \dashrightarrow C + H_2$	3.0 (-7)

546.	CH_3^+ + e --> CH_2 + H	3.0 (-7)
*547.	$^{13}CH_3^+$ + e --> $^{13}CH_2$ + H	3.0 (-7)
548.	C_2H^+ + e --> C_2 + H	1.0 (-7)
549.	$C_2H_2^+$ + e --> C_2H + H	3.0 (-7)
550.	H_2O^+ + e --> OH + H	3.0 (-7)
551.	HCO^+ + e --> CO + H	3.0 (-7)
*552.	$H^{13}CO^+$ + e --> ^{13}CO + H	3.0 (-7)
553.	H_3O^+ + e --> H_2O + H	1.0 (-6)
554.	H_3O^+ + e --> OH + 2H	1.0 (-6)
555.	H_3CO^+ + e --> H_2CO + H	1.0 (-6)
556.	H_3CO^+ + e --> CO + H_2 + H	1.0 (-6)
557.	H_2CO^+ + e --> CO + 2H	6.0 (-7)
*558.	$H_3{}^{13}CO^+$ + e --> ^{13}CO + 2H	6.0 (-7)
559.	HCO_2^+ + e --> CO_2 + H	1.0 (-6)
560.	HCO_2^+ + e --> CO + O + H	1.0 (-6)
561.	C_3H^+ + e --> C_3 + H	3.0 (-7)
562.	C_3^+ + e --> C_2 + C	3.0 (-7)
563.	CO_2^+ + e --> CO + O	3.0 (-7)
564.	O_2H^+ + e --> O_2 + H	3.0 (-7)
565.	CH_2OH^+ + e --> CH_2 + OH	3.0 (-7)
566.	N_2H^+ + e --> N_2 + H	6.0 (-7)
567.	NH_3^+ + e --> NH + 2H	6.0 (-7)
568.	H_2CN^+ + e --> CH + 2H	1.0 (-6)
569.	H_2CN^+ + e --> HCN + H	1.0 (-6)
570.	NH_4^+ + e --> NH_3 + H	1.8 (-6)
571.	NH_4^+ + e --> NH_2 + 2H	2.0 (-7)

572.	$CH_2NH_2^+ + e \longrightarrow HCN + H_2 + H$	3.0 (-7)
573.	$NH_2^+ + e \longrightarrow NH + H$	3.0 (-7)
574.	$HCN^+ + e \longrightarrow CN + H$	3.0 (-7)
575.	$C_2N^+ + e \longrightarrow C_2 + N$	3.0 (-7)
576.	$CH_3^+ + e \longrightarrow CH_3 + h$	3.0 (-10)
577.	$CH_4^+ + e \longrightarrow CH_3 + H$	6.0 (-7)
578.	$CH_5^+ + e \longrightarrow CH_4 + H$	6.0 (-7)
579.	$H_2S^+ + e \longrightarrow SH + H$	1.0 (-6)
580.	$H_2S^+ + e \longrightarrow H_2S + h$	1.0 (-10)
581.	$SH^+ + e \longrightarrow S + H$	1.0 (-7)
582.	$H_3S^+ + e \longrightarrow H_2S + H$	1.0 (-6)
583.	$H_3S^+ + e \longrightarrow SH + H_2$	1.0 (-6)
584.	$HCS^+ + e \longrightarrow CS + H$	1.0 (-6)
585.	$SO^+ + e \longrightarrow S + O$	1.0 (-7)
586.	$SN^+ + e \longrightarrow S + N$	1.0 (-7)
587.	$S_2^+ + e \longrightarrow S + S$	1.0 (-7)
588.	$CH_2SH^+ + e \longrightarrow CH_2 + SH$	1.0 (-6)
589.	$H_2CS^+ + e \longrightarrow CS + H_2$	1.0 (-6)
590.	$H_3CS^+ + e \longrightarrow H_2CS + H$	1.0 (-6)
591.	$H_3CS^+ + e \longrightarrow CS + H_2 + H$	1.0 (-6)
592.	$CS^+ + e \longrightarrow C + S$	1.0 (-7)
593.	$HSiO^+ + e \longrightarrow SiO + H$	1.0 (-6)
594.	$SiH_2^+ + e \longrightarrow Si + H_2$	3.0 (-7)
595.	$SiO^+ + e \longrightarrow Si + O$	3.0 (-7)

TABLE 5 COSMIC RAY DESTRUCTION PROCESSES

	Reaction	Rate (s^{-1})
596.	$H + P \dashrightarrow H^+ + e + P$	1.5 (-17)
597.	$He + P \dashrightarrow He^+ + e + P$	1.5 (-17)
598.	$C + P \dashrightarrow C^+ + e + P$	1.8 (-17)
599.	$N + P \dashrightarrow N^+ + e + P$	2.1 (-17)
600.	$O + P \dashrightarrow O^+ + e + P$	2.8 (-17)
601.	$H_2 + P \dashrightarrow H_2^+ + e + P$	2.3 (-17)
602.	$H_2 + P \dashrightarrow H^+ + H + e + P$	4.6 (-19)
603.	$H_2 + P \dashrightarrow H + H + P$	1.15 (-17)
604.	$C_3 + P \dashrightarrow C_3^+ + e + P$	3.0 (-17)

```
      PROGRAM HALFAX(DAT,OUTPUT,OTL105,TAPE11=DAT,TAPE12=OUTPUT,
     +TAPE13=OTL105)
C     THIS PROGRAM COMPUTES THE STEADY STATE ABUNDANCES CONC(I) FOR A
C     SCHEME OF NEQ CHEMICAL REACTIONS ASSUMING EACH SPECIES IS IN
C     A STEADY STATE,  THE RATES OF APPEARANCE AND DISAPPEARANCE OF THE
C     SPECIES ARE COMPUTED FROM A RATE CONSTANT AND THE NUMBER OF SPECIES
C     ON THE  LEFT HAND SIDE OF THE CHEMICAL EQUATIONS.
C
C
C                RESTRICTIONS AND CONVENTIONS
C     NUMBER OF CHEMICAL REACTIONS LE 150
C     NUMBER OF SPECIES LE 100
C     NUMBER OF ELEMENTS INCLUDING ELECTRONS LE 6
C     RESTRAINT EQUATION FOR ELEMENT H MUST BE READ IN LAST
C     CHEMICAL EQUATION FOR FORMATION OF H2 ON A GRAIN
C     SURFACE MUST COME FIRST, SINCE ITS RATE IS COMPUTED DIFFERENTLY
C     FROM ALL OTHER RATES.
C
C
C                DATA NEEDED
C     CARD     LIST      FORMAT
C     KR,KW,KWS(FROM DEVICE 1)  3I3
C     DATA FOR SUBROUTINE REED
C     NDEN      3I4
C     DEN,KTP    F10.3,I4
C     CARD 4 AND 5 ARE REPEATED AS NEEDED
C     SPE,CON    1XA4,E12.5
C     CARD 5 IS REPEATED NSS TIMES AND IS ONLY USED IF KTP IS NE 0
C
C            GLOSSARY OF TERMS
C     KR      INPUT DEVICE NUMBER
C     KW      OUTPUT DEVICE NUMBER
C     NDEN    NUMBER OF DENSITIES AT WHICH CALCULATION IS TO BE DONE
C     DEN     DENSITY AT WHICH CALCULATION IS TO BE DONE
C     KTP     =0 IF PREVIOUS VALUES OF SPECIES CONCENTRATIONS ARE TO
C             BE USED AS A FIRST APPROXIMATION TO THE SOLUTION
C     SPE     SPECIES NAME
C     CON     SPECIES CONCENTRATION
C
C             SUBROUTINES NEEDED
C     ROUTINE         PURPOSE
C     REED    REED IN THE DATA FOR THE SCHEME
C     CRAT    COMPUTES RATE COEFFICIENTS AT THE GIVEN DENSITY
C             IN CASE THEY ARE DENSITY DEPENDANT
C     BOUND   COMPUTES THE CONCENTRATIONS OF THE ELEMENTAL SPECIES FROM
C             THE RESTRAINT EQUATIONS
C     SOLVE   SOLVES THE STEADY STATE EQUATIONS BY ITERATION
C     NORMA   COMPUTES THE CONTRIBUTIONS FROM EACH CHEMICAL EQUATION
C             TO THE DESTRUCTION OR FORMATION OF EACH SPECIES AT THE
C             STEADY STATE CONCENTRATION
C
C
      DIMENSION CONCLG(100),RCONC(100),RCNCLG(100),CONCT(100,10),
     +WTTAU(10),CLMND(100,3),TLCON(100,3),FLLG(120),
     +CMDLG(100,3),CONCI(100),FLCON(100),FLCMD(100)
      COMMON/CNTRL/NERTS,NURTS,NSS,NRES,NEQ,NITER,PTOL,NSPEC,NSING
      COMMON/DEVICE/KR,KW,KWS
      COMMON/TTAU/KTAU,NTAU,XTAU(10),TAUC,NDEN,KTAUST
      COMMON/MAIN/CONC(100),CRS(10),CRST(10),RATE(600),SPEC(100)
      COMMON/MAIT/ASW(100,600),ICODE(600)
      COMMON/SIZE/IR(600),IP(600),NEACT(600,3),NPROD(600,4),NRS(10,125)
     1,IER(10),NPIER(10),NUM(600)
      KR=11
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```
      KW=12
      KWS=13
      WRITE(KW,1050)
 1050 FORMAT(////20X"PROGRAM HALIFAX - STEADY STATE"1X"ANALYSIS - VERSI
     1ON HAL02 - OCT 8/75")
      CALL REED(NCLD)
      DO 150 I=1,NEQ
  150 ICODE(I)=NUM(I)
C     READ IN INITIAL GUESS FOR THE STEADY STATE SPECIES
      DO 440 NUMCD=1,NCLD
      DO 160 I=1,NSPEC
  160 CONC(I)=0.
      PDEN=1.
      READ(KR,1060) NDEN,KTAUST,KTAUED
 1060 FORMAT(3I7)
      DO 260 KDEN=1,NDEN
      DELR=1.11E17
      TAUC=6.05
      KTAU=10
      NTAU=KTAUST
      NSING=0
  330 IF(NTAU.NE.KTAUST) GO TO 340
      READ(KR,1070) DEN,KTP
 1070 FORMAT(F8.1,I6)
      WRITE(KW,1080) DEN,DELR,TAUC,KTAU,KTAUST,KTAUED
      WRITE(KWS,1080) DEN,DELR,TAUC,KTAU,KTAUST,KTAUED
 1080 FORMAT(1H0,"TOT H DEN="E15.5,4X,"DELTA R=",E10.4,4X,
     +"CNTR TAU=",F5.2,4X,"KTAU=",I2,4X,"TAU IS FROM ",I2," TO",I2,/)
      DO 170 I=1,NRES
  170 CRS(I)=CRST(I)*DEN
  340 CALL CRAT(DEN,RATE,NEQ,NUM)
      IF(NTAU.NE.KTAUST)  GO TO 200
      WRITE(KW,1090)
 1090 FORMAT(30X"RATES AT THIS DENSITY ARE")
      WRITE(KW,1100)(NUM(JI),RATE(JI),JI=1,NEQ)
 1100 FORMAT(6(I4,1XE12.5))
      IF(KTP.EQ.0) GO TO 200
      DO 190 I=1,NSS
      READ(KR,1110)SPE,CON
      DO 180 IS=1,NSPEC
      IF(SPE.NE.SPEC(IS))GO TO 180
 1110 FORMAT(1XA4,E12.5)
      CONC(IS)=CON
      GO TO 190
  180 CONTINUE
  190 CONTINUE
      GO TO 220
  200 DO 210 I=1,NSS
  210 CONC(I)=CONC(I)*DEN/PDEN
  220 CALL BOUND
      PDEN=DEN
      WRITE(KW,1120)(SPEC(I),CONC(I),I=1,NSPEC)
 1120 FORMAT(1H ,2X,"INITIAL CONCENTRATION"/6(3X,A4,1XE12.5))
      WRITE(KW,1190)
 1190 FORMAT(1H ,2X,"INITIAL CONCENTRATIONS")
      DO 270 I100=1,20
      I110=I100+80
      WRITE(KW,1180) ((SPEC(I),CONC(I)),I=I100,I110,20)
 1180 FORMAT(5(3X,A4,1X,E12.5))
  270 CONTINUE
      LTS=0
      DO 230 I=1,NSPEC
      IF(CONC(I).GE.0.) GO TO 230
      LTS=1
      NERTS=1
  230 CONTINUE
      IF(LTS.NE.0) WRITE(KW,1130)
 1130 FORMAT(" NEGATIVE CONCS OCCUR")
```

```
      IF(NERTS.EQ.0) GO TO 240
      WRITE(KW,1140)
 1140 FORMAT(" BAD DATA")
      CALL EXIT
  240 IF (NURTS.EQ.1)WRITE(KW,1150)
 1150 FORMAT(" SUSPECT RESULTS POSSIBLE")
      LRITE=1
      CALL SOLVE(DEN,LRITE,LCONV)
      DO 350 I=1,NSPEC
  350 CONCT(I,NTAU)=CONC(I)
      WRITE(KW,1160)(SPEC(IWR),CONC(IWR),IWR=1,NSPEC)
 1160 FORMAT(1H ,2X"FINAL CONCENTRATIONS"/(6(3X,A4,1XE12.5)))
      WRITE(KW,1220)
      WRITE(KWS,1220)
 1220 FORMAT(1H ,2X,"FINAL CONCENTRATIONS")
      DO 280 I120=1,20
      I130=I120+80
      WRITE(KW,1270) ((SPEC(I),CONC(I)),I=I120,I130,20)
      WRITE(KWS,1270)   ((SPEC(I),CONC(I)),I=I120,I130,20)
 1270 FORMAT(5(3X,A4,1X,E12.5))
  280 CONTINUE
      DO 290 I140=1,NSPEC
      RCONC(I140)=CONC(I140)/CONC(4)
  290 CONTINUE
      WRITE(KW,1230)
 1230 FORMAT(1H ,2X,"RELATIVE CONCENTRATIONS TJ H2")
      DO 300 I150=1,20
      I160=I150+80
      WRITE(KW,1240) ((SPEC(I),RCONC(I)),I=I150,I160,20)
 1240 FORMAT(5(3X,A4,1X,E12.5))
  300 CONTINUE
      DO 250 IWR=1,NSPEC
      CLOG=CONC(IWR)/DEN
  250 CONCLG(IWR)=ALOG10(CLOG)
      WRITE(KW,1170)(SPEC(IWR),CONCLG(IWR),IWR=1,NSPEC)
      WRITE(KWS,1170)(SPEC(IWR),CONCLG(IWR),IWR=1,NSPEC)
 1170 FORMAT(1H ,2X"LOG OF THE REDUCED CONCENTRATIONS"/(6(3X,A4,1XF10.5,
     12X)))
      DO 310 I170=1,NSPEC
      RCNCLG(I170)=CONCLG(I170)-CONCLG(4)
  310 CONTINUE
      WRITE(KW,1250)
 1250 FORMAT(1H ,2X,"LOG OF THE RELATIVE CONCENTRATIONS TO H2")
      DO 320 I180=1,20
      I190=I180+80
      WRITE(KW,1260) ((SPEC(I),RCNCLG(I)),I=I180,I190,20)
 1260 FORMAT(5(3X,A4,1X,F12.5))
  320 CONTINUE
      CALL NORMA(NSPEC,NEQ)
      IF(KTAU.EQ.1) GO TO 260
      NTAU=NTAU-1
      IF(NTAU.GE.KTAUED) GO TO 330
      IF(KTP.EQ.0) GO TO 400
      READ(KR,1280) (WTTAU(I),I=1,10)
 1280 FORMAT(1X,10(F6.4,1X))
  400 DO 360 I=1,NSPEC
  360 TLCON(I,NUMCD)=0.
      DO 370 I=1,NSPEC
      KTAU9=KTAU-1
      DO 380 J=1,KTAU9
  380 TLCON(I,NUMCD)=TLCON(I,NUMCD)+CONCT(I,J)*WTTAU(J)
      TLCON(I,NUMCD)=2*TLCON(I,NUMCD)+CONCT(I,KTAU)*WTTAU(KTAU)
      CLMND(I,NUMCD)=TLCON(I,NUMCD)*DELR
      CMDLG(I,NUMCD)=ALOG10(CLMND(I,NUMCD))
  370 CONTINUE
      DATA BLNK/"              "/
      DO 530 I=1,NSPEC
      DO 540 J=1,10
```

```
  540 IF(WTTAU(J).EQ.0.0000) CONCT(I,J)=BLNK
  530 CONTINUE
      WRITE(KW,1290)  (WTTAU(I),I=1,10)
 1290 FORMAT(/,3X,"COLUMN DENSITIES"/4X,"(",10F9.3,")")
      WRITE(KW,1300)
 1300 FORMAT(50X,"TAU",45X,"TTL CONC",2X,"CLMN DEN",2X,"LOG N")
      WRITE(KW,1310) (XTAU(I),I=1,KTAU)
 1310 FORMAT(7X,10(F6.4,3X))
      DO 390 I=1,NSPEC
      WRITE(KW,1320) SPEC(I),(CONCT(I,J),J=1,KTAU),TLCON(I,NUMCD),
     +CLMND(I,NUMCD),CMDLG(I,NUMCD),SPEC(I)
 1320 FORMAT(1X,A4,10E9.3,E11.4,E10.4,F7.2,2X,A4)
      WRITE(KWS,1350)  SPEC(I),TLCON(I,NUMCD)
 1350 FORMAT(1X,A4,E12.5)
  390 CONTINUE
  260 CONTINUE
  440 CONTINUE
      IF(NCLD.EQ.1)  GO TO 520
      DO 450 I=1,NSPEC
      DO 460 NUMCD=1,NCLD
  460 FLCON(I)=FLCON(I)+TLCON(I,NUMCD)
  450 CONTINUE
      DO 470 I=1,NSPEC
      FLCMD(I)=FLCON(I)*DELR
  470 FLLG(I)=ALOG10(FLCMD(I))
      WRITE(KW,1330)
 1330 FORMAT(//,1X,3("      TTL CONC COLM DEN LOG N",10X))
      DO 480 I=1,40
      J=I+80
      IF(I.GE.21)J=I+40
      WRITE(KW,1340)  ((SPEC(K),FLCON(K),FLCMD(K),FLLG(K)),K=I,J,40)
 1340 FORMAT(1X,3(A4,2E9.3,F6.2,10X))
  480 CONTINUE
      WRITE(KWS,1360)  ((SPEC(I),FLCON(I)),I=1,NSPEC)
 1360 FORMAT(1X,A4,E12.5)
  520 STOP
      END
      SUBROUTINE NORMA(NSPEC,NRATE)
      COMMON/MAIT/ASW(100,600),ICODE(600)
C     FINDS THE LARGEST ELEMENT IN ASW AND NORMALISES ALL ELEMENTS TO
C     THIS AND THEN ARRANGES THE ELEMENTS OF EACH ROW IN DECREASING
C     ORDER, PRINTING THE RESULTS
      COMMON/MAIN/CONC(100),CRS(10),CRST(10),RATE(600),SPEC(100)
      COMMON/DEVICE/KR,KW,KWS
      DIMENSION NCODE(100),BIG(100),IPCOD(600)
C     NSPEC IS THE TOTAL NUMBER OF SPECIES
C     NRATE IS THE NUMBER OF RATES WHOSE VARIATION IS BEING CONSIDERED
C     ICODE(NRATE) LABELS THE VARIOUS RATES, NCODE THE VARIOUS SPECIES
      WRITE(KW,1050)
 1050 FORMAT(1H0)
      DO 160 I=1,NSPEC
      NCODE(I)=I
      BIG(I)=0.
      DO 150 J=1,NRATE
      TEST=ABS(ASW(I,J))
      IF(TEST.GT.BIG(I)) BIG(I)=TEST
  150 CONTINUE
  160 CONTINUE
C     NORMALISE EACH ROW TO BIG(I)
      DO 170 I=1,NSPEC
      ABIG=BIG(I)
      DO 170 J=1,NRATE
  170 ASW(I,J)=ASW(I,J)/ABIG
C     ARRANGE ROWS IN ORDER OF BIG(I)
      NM=NSPEC-1
      DO  190 I=1,NM
      IP=I+1
      DO 190 J=IP,NSPEC
```

```
      IF(BIG(I).GE.BIG(J)) GO TO 190
      TEMP=BIG(I)
      BIG(I)=BIG(J)
      BIG(J)=TEMP
      DO 180 K=1,NRATE
      TEMP=ASW(I,K)
      ASW(I,K)=ASW(J,K)
  180 ASW(J,K)=TEMP
      TEMP=NCODE(I)
      NCODE(I)=NCODE(J)
      NCODE(J)=TEMP
  190 CONTINUE
      WRITE(KW,1080)
 1080 FORMAT(1HO 1X"SPECIES"1X"UNIT FOR ROW" 10X"CONTRIBUTIONS"
     1"TO FORMATION AND DESTRUCTION OF SPECIES FROM EACH EQN."
     11X":FORMAT(EQUATION #ASW)")
C     ARRANGE ELEMENTS IN DECREASING ORDER FOR EACH ROW
      NM=NRATE-1
      DO 240 K=1,NSPEC
      DO 200 I=1,NRATE
  200 IPCOD(I)=ICODE(I)
      DO 210 I=1,NM
      IP=I+1
      DO 210 J=IP,NRATE
      IF(ABS(ASW(K,I)).GE.ABS(ASW(K,J))) GO TO 210
      TEMP=ASW(K,I)
      ASW(K,I)=ASW(K,J)
      ASW(K,J)=TEMP
      TEMP=IPCOD(I)
      IPCOD(I)=IPCOD(J)
      IPCOD(J)=TEMP
  210 CONTINUE
C
C     FIND IMAX, THE NUMBER OF NON-ZERO ELEMENTS IN ROW K OF ASW
      IMAX=0
      DO 220 I=1,NRATE
      IF(ABS(ASW(K,I)).LT.1.E-05) GO TO 220
      IMAX=IMAX+1
  220 CONTINUE
C
C     CHECK THAT THE MATRIX CORRESPONDS TO A STEADY STATE SOLUTION
      TOTAL=0.
      DO 224 I=1,NRATE
  224 TOTAL=TOTAL+ASW(K,I)
      IF(ABS(TOTAL).LE.1.E-05) GO TO 230
      WRITE(KW,1090)TOTAL
 1090 FORMAT(8X"***NOT A STEADY STATE TO WITHIN"1XE15.5,1X"RELATIVE RATE
     1 UNITS")
  230 NSQ=7
      IF(IMAX.LT.7)NSQ=IMAX
      N=NCODE(K)
      WRITE(KW,1100)SPEC(N),BIG(K),(IPCOD(I),ASW(K,I),I=1,NSQ)
 1100 FORMAT(3XA4,E13.5,7(1X"("I3,1XF8.5,")"))
      IF(IMAX.LE.7) GO TO 240
      WRITE(KW,1120)(IPCOD(I),ASW(K,I),I=8,IMAX)
 1120 FORMAT((20X7(1X"("I3,1XF8.5,")")))
  240 CONTINUE
      RETURN
      END
      SUBROUTINE BOUND
C             THIS ROUTINE CALCULATES THE RESTRAINT SPECIES
C             CONCENTRATIONS FROM THE STEADY-STATE SPECIES CONCENTRATIONS
C             AND THE ATOMIC ABUNDANCES CRS(I). THE RESTRAINT
C             SPECIES ARE ASSUMED TO BE THE ELEMENTS THEMSELVES
C             OR THE ELECTRON.
C
C                        GLOSSARY OF TERMS
C NSS         NUMBER OF STEADY-STATE SPECIES.
```

```
C NRES        NUMBER OF RESTRAINT SPECIES.
C CONC(I)     CONCENTRATION OF THE ITH SPECIES.
C CRS(I)      ABUNDANCE OF THE ITH ELEMENT.
C IER         NUMBER OF SPECIES ENTERING THE RESTRAINT EQUATION
C NPIER       NUMBER OF THE IER WHICH ENTER THE RESTRAINT
C             EQUATION WITH A POSITIVE COEFFICIENT.
C NRS(I,J)    CODE NUMBER LABELLING THE JTH SPECIES ENTERING
C             THE ITH RESTRAINT EQUATION.
      COMMON/MAIN/CONC(100),CRS(10),CRST(10),RATE(600),SPEC(100)
      COMMON/CNTRL/NERTS,NURTS,NSS,NRES,NEQ,NITER,PTOL,NSPEC,NSING
      COMMON/SIZE/IR(600),IP(600),NEACT(600,3),NPROD(600,4),NRS(10,125)
     1,IER(10),NPIER(10),NUM(600)
       NEND=NSS+NRES
      NST=NSS+1
C
C             SET THE RESTRAINT SPECIES CONCENTRATIONS TO
C             THEIR ATOMIC ABUNDANCES.
      DO 170 IS=NST,NEND
      I=IS-NSS
      CONC(IS)=CRS(I)
C
C             IN THE CASE OF ELECTRONS, INCREMENT THE CONCENTRATION
C              OF THE RESTRAINT SPECIES BY THAT OF ALL POSITIVE SPECIES.
      JKS=IER(I)
      DO 160 J=1,JKS
      IF(J.GT.NPIER(I)) GO TO 150
      JC=NRS(I,J)
      CONC(IS)=CONC(IS)+CONC(JC)
      GO TO 160
C
C             DECREMENT THE CONCENTRATION BY THE CONCENTRATION
C             OF ALL SPECIES CONTAINING THE ATOM IN QUESTION,
C             OR IN THE CASE OF ELECTRONS, BY ALL NEGATIVE IONS.
 150  JC=NRS(I,J)
      CONC(IS)=CONC(IS)-CONC(JC)
 160  CONTINUE
      IF(CONC(IS).LT.0.)CONC(IS)=1.E-31
 170  CONTINUE
      RETURN
      END
      SUBROUTINE SOLVE(DEN,LRITE,LCONV)
C
C             THIS ROUTINE CALCULATES THE STEADY-STATE ABUNDANCES OF
C             ALL SPECIES AT A GIVEN DENSITY DEN, GIVEN AN INITIAL
C             APPROXIMATION TO THE CONCENTRATIONS CONC(I)
C
C                  THE PROCEDURE USED IS AN ITERATIVE NEWTON'S METHOD
C             IN THE SPACE OF THE STEADY-STATE SPECIES, THE RESTRAINT
C             CONCENTRATIONS BEING OBTAINED AFTER EVERY ITERATION BY
C             CALLING THE SUBROUTINE BOUND.  THE NEQ RATE EQUATIONS ARE
C             SCANNED ONCE PER ITERATION, AND THE RATE OF CHANGE OF
C             EACH SPECIES, FI(I), AS WELL AS THE DERIVATIVES OF THESE
C             W.R.T. THE CONCENTRATIONS, FIJ(I,J), ARE BUILT UP FROM
C             A KNOWLEDGE OF THE REAGENTS AND PRODUCTS OCCURRING
C             IN EACH REACTION.  A SYSTEM OF SIMULTANEOUS LINEAR ALGEBRAIC
C             EQUATIONS IS SET UP FOR THE CORRECTIONS TO THE STEADY-
C             STATE SPECIES CONCENTRATIONS WHICH WOULD MAKE THE RATES OF
C             CHANGE OF ALL SPECIES VANISH IN FIRST ORDER.  THIS
C             SYSTEM OF EQUATIONS IS SOVED BY THE ROUTINE GAJODF.  IF
C             NEGATIVE STEADY-STATE CONCENTRATIONS RESULT, THEY ARE PUT
C             EQUAL TO 1.E-31 BEFORE COMPUATION OF THE RESTRAINT SPECIES.
C
C              ***SUBROUTINES NEEDED**
C                BOUND
C                GAJODF
C
C                     ***GLOSSARY OF TERMS***
C KW          OUTPUT DEVICE FOR MESSAGES.
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C DEN           DENSITY AT WHICH CALCULATION IS TO BE DONE.
C LRITE         =0 IF NO INFORMATION IS TO COME OUT AT EACH
C               ITERATION, ELSE THE CONCENTRATIONS AT EVERY ITERATION
C               ARE PRINTED.
C LCONV         =0 IF SOLUTION IS OK
C               =1 IF THERE WAS NO CONVERGENCE
C               V2 IF THERE WAS A SINGULAR MATRIX
C
C ASW(I,J)      MATRIX CONTAINING THE CONTRIBUTION TO THE
C               FORMATION RATE OF SPECIES I FROM RATE EQUATION J.
C CONC(I)       CONCENTRATION OF SPECIES I
C CRS(I)        TOTAL CONCENTRATION OF ELEMENT I
C CRST(I)       RELATIVE TOTAL CONCENTRATION OF ELEMENT I IN
C               TERMS OF THE DENSITY.
C FI(I)         A.    BEFORE SOLUTION OF THE LINEAR EQUATIONS, FI
C                     CONTAINS THE RHS OF THE EQUATIONS: I.E. THE
C                     OVERALL RATE OF DESTRUCTION OF THE STEADY-STATE
C                     SPECIES I.
C               B.    AFTER THE SOLUTION OF THE LINEAR EQUATIONS, FI
C                     CONTAINS THE CORRECTIONS TO THE STEADY-STATE
C                     CONCENTRATIONS.
C FIJ(I,J)      THE DERIVATIVE OF FI(I) W.R.T. THE STEADY-
C               STATE CONCENTRATIONS CONC(J).  IN THE PROGRAM, FIJ IS
C               SINGLY DIMENSIONED BY KSUB=I+(J-1)*NSS
C ICON          FLAG TO INDICATE NO CONVERGENCE.
C IER(I)        NUMBER OF SPECIEE ENTERING THE RESTRAINT EQUATION
C               FOR ELEMENT I
C IP(I)         NUMBER OF PRODUCTS ENTERING THE ITH RATE  EQUATION
C IR(I)         NUMBER OF REAGENTS ENTERING THE ITH RATE
C               EQUATION.
C ITER          CURRENT ITERATION INDEX
C NEACT(I,J)    CODE NUMBER LABELLING THE J REAGENT
C               SPECIES ENTERING REACTION I.
C NEQ           NUMBER OF RATE EQUATIONS IN THE REACTION SCHEME.
C NPIER(I)      NUMBER OF SPECIES ENTERING THE ITH RESTRAINT
C               EQUATION WITH A POSITIVE COEFFICIENT.
C NPROD(I,J)    CODE NUMBER LABELLING THE J PRODUCT
C               SPECIES ENTERING REACTION I
C NRS(I,J)      INTERNAL CODE NUMBER LABELLING THE JTH SPECIES
C               ENTERING THE RESTRAINT EQUATION I.
C NSING         NUMBER OF TIMES A SINGULAR MATRIX IS ENCOUNTERED.
C               IF NSING.GT.30 STOP.
C NRES          NUMBER OF RESTRAINT EQUATIONS
C NSS           NUMBER OF STEADY-STATE EQUATIONS.
C NCON          NUMBER OF NO CONVERGENCE CASES. IF NCON .GT. 50 STOP.
C NUM(U
C NUM(I)        CODE NUMBER OF THE ITH RATE EQUATION.
C PTOL          PARAMETER TO TEST FOR CONVERGENCE OF THE STEADY-
C               STATE CONCENTRATIONS. IF ABS(FI(I)/CONC(I)).LT.PTOL FOR
C               ALL I, THEN ITERATION IS DISCONTINUED.
C RATE(KEQ)     RATE COEFFICIENT FOR THE RATE EQUATION KEQ.
C NSPEC         NUMBER OF SPECIES OCCURRING IN THE WHOLE SCHEME.
      COMMON/CNTRL/NERTS,NURTS,NSS,NRES,NEQ,NITER,PTOL,NSPEC,NSING
      COMMON/MAIN/CONC(100),CRS(10),CRST(10),RATE(600),SPEC(100)
      COMMON/SIZE/IR(600),IP(600),NEACT(600,3),NPROD(600,4),NRS(10,125)
     1,IER(10),NPIER(10),NUM(600)
      COMMON/MAIT/ASW(100,600),ICODE(600)
      COMMON/DEVICE/KR,KW,KWS
      DIMENSION FI(100),FIJ(10000),IT(10)
      DATA NOCON/0/
      LCONV=0
C
C               CHECK FOR ARRAY OVERFLOW
△     IF(NSS.LE.100.AND.NRES.LE.10) GO TO 140
      WRITE(KW,1040)NSS,NRES
 1040 FORMAT(20X"***ARRAY OVERFLOW.NSS="1XI5,3X"NRES="1XI5)
      STOP
C               BEGIN NEWTON METHOD ITERATIONS.
```

```
  140 DO 320 ITER=1,NITER
C
C                 INITIALISE ARRAYS.
      DO 150 I=1,NSPEC
      DO 150 J=1,NEQ
  150 ASW(I,J)=0.
      ICON=0
      DO 160 I=1,NSS
  160 FI(I)=0.
      NSSS=NSS*NSS
      DO 170 J=1,NSSS
  170 FIJ(J)=0.
C
C                 COMPUTE THE MATRIX FIJ BY SCANNING OVER ALL
C                 RATE EQUATIONS
      DO 260 KEQ=1,NEQ
      IRKEQ=IR(KEQ)
      DO 230 L=1,IRKEQ
C
C                 COMPUTE THE RATE CONTRIBUTION FROM THE CURRENT
C                 REACTION AND STORE THE REAGENT SPECIES LABELS IN IT.
      CUMD=RATE(KEQ)
      DO 180 LZ=1,IRKEQ
      JC=NEACT(KEQ,LZ)
      IT(LZ)=JC
      IF(LZ.EQ.L) GO TO 180
      CUMD=CUMD*CONC(JC)
  180 CONTINUE
C
C                 SPECIAL TREATMENT FOR REACTION 1
      IF(KEQ.EQ.1) CUMD=RATE(KEQ)*CRS(NRES)
C
C                 STORE THE PRODUCT SPECIES LABELS IN IT
      IPKEQ=IP(KEQ)
      DO 190 LZ=1,IPKEQ
      JC=IR(KEQ)+LZ
  190 IT(JC)=NPROD(KEQ,LZ)
C
C                 COMPUTE THE CONTRIBUTION TO FIJ FROM THE STEADY
C                 -STATE SPECIES OCCURRING AMONG THE REAGENTS OF
C                 EQUATION KEQ.
      NIT=IR(KEQ)+IP(KEQ)
      JSUB=NEACT(KEQ,L)
      DO 220 IS=1,NIT
      ISUB=IT(IS)
      IF(ISUB.EQ.0.OR.JSUB.EQ.0) GO TO 220
      P=1.
      IF(IS.GT.IR(KEQ))P=-P
      IF(ISUB.GT.NSS) GO TO 220
      IF(JSUB.GT.NSS) GO TO 200
      KSUB=ISUB+(JSUB-1)*NSS
      FIJ(KSUB)=FIJ(KSUB)+P*CUMD
      GO TO 220
C
C                 COMPUTE THE CONTRIBUTION TO FIJ FROM THE RESTRAINT
C                 SPECIES OCCURRING AMONG THE REAGENTS OF
C                 EQUATION KEQ.
  200 NSPC=JSUB-NSS
      IERNS=IER(NSPC)
      DO 210 NP=1,IERNS
      PZ=P
      IF(NP.GT.NPIER(NSPC)) PZ=-P
      JS=NRS(NSPC,NP)
      KSUB=ISUB+(JS-1)*NSS
  210 FIJ(KSUB)=FIJ(KSUB)+PZ*CUMD
  220 CONTINUE
  230 CONTINUE
C
```

```
C             CALCULATE THE CONTRIBUTION OF EQUATION KEQ TO THE RATE
C             OF CHANGE OF EACH STEADY-STATE SPECIES.
      CUM=RATE(KEQ)
      DO 240 L=1,IRKEQ
      JC=NEACT(KEQ,L)
  240 CUM=CUM*CONC(JC)
      IF(KEQ.EQ.1) CUM=RATE(KEQ)*CONC(NSPEC)*CRS(NRES)
      DO 250 IS=1,NIT
      P=1.
      ISUB=IT(IS)
      IF(ISUB.LE.0) GO TO 250
      IF(IS.GT.IR(KEQ)) P=-P
      CUMP=CUM*P
      ASW(ISUB,KEQ)=ASW(ISUB,KEQ)-CUMP
      IF(ISUB.GT.NSS) GO TO 250
      FI(ISUB)=FI(ISUB)+CUMP
  250 CONTINUE
  260 CONTINUE
C
C             SOLVE THE SYSTEM OF SIMULTANEOUS EQUATIONS TO GET
C             THE FIRST ODER CORRECTIONS TO THE CONCENTRATIONS.
      IRANG=NSS
      CALL SIMQ(FIJ,FI,NSS,KS)
      IF (KS.GT.0)GO TO 270
      GO TO 290
C
C             ERROR FLAG IS RETURNED FROM GAJODF
  270 WRITE(KW,1050)
 1050 FORMAT(20X"SINGULAR MATRIX")
      LCONV=2
      NSING=NSING+1
      IF(NSING.GT.30)STOP
      WRITE(KW,1060)
 1060 FORMAT(30X"RATES AT THIS POINT ARE")
      WRITE(KW,1070)(NUM(JR),RATE(JR),JR=1,NEQ)
 1070 FORMAT(6(I4,1XE15.7))
      WRITE(KW,1080)(SPEC(JR),CONC(JR),JR=1,NSPEC)
 1080 FORMAT(20X"CONCENTRATION"/(4X(8X,A4,1XE12.5)))
      DO 280 JR=1,NSS
      IF(CONC(JR).GT.1.E-30) GO TO 280
      CONC(JR)=DEN*1.E-08
  280 CONTINUE
      CALL BOUND
      RETURN
C
C             CORRECT THE STEADY-STATE SPECIES CONCENTRATIONS AND TEST
C             FOR CONVERGENCE
  290 DO 300 I=1,NSS
      CONC(I)=CONC(I)-FI(I)
      IF(CONC(I).EQ.0.) GO TO 300
      TEST=ABS(FI(I)/CONC(I))
      IF (TEST.GT.PTOL) ICON=1
      IF(CONC(I).LT.0.) CONC(I)=1.E-31
  300 CONTINUE
C
C             COMPUTE THE RESTRAINT SPECIES CONCENTRATIONS.
      CALL BOUND
      IF(LRITE.EQ.0) GO TO 310
      WRITE(KW,1090)ITER
 1090 FORMAT(2X"CONCENTRATIONS AFTER"1XI6,1X"ITERATIONS")
      WRITE(KW,1100)(SPEC(JR),CONC(JR),JR=1,NSPEC)
 1100 FORMAT(6(3X,A4,1XE12.5))
  310 IF(ICON.EQ.0) GO TO 330
  320 CONTINUE
      WRITE(KW,1110) NITER
 1110 FORMAT(//," ","NO CONVERGENCE AFTER ",I4," ITERATIONS")
      LCONV=1
      STOP
```

```
  330 RETURN
      END
      SUBROUTINE REED(NCLD)
C
C                   THIS ROUTINE READS IN THE DATA FOR THE STEADY-STATE
C                   PROGRAM. INPUT DEVICE IS KR, OUTPUT IS KW. THE DATA
C                   IS CHECKED FOR INCONSISTENCIES; IF THESE ARE FATAL,
C                   NERTS IS SET EQUAL TO 1 AND THE PROGRAM EVENTUALLY
C                      STOPS; IF NOT, NURTS IS SET EQUAL TO 1 AND ERROR
C                   MESSAGES ARE GIVEN BEFORE THE PROGRAM IS RUN.
C
C                             ***** INPUT DATA *****
C CARD NUMBER           LIST                                 FORMAT
C  1                TITLE(I),I=1,15                          15A4
C  2                NRES,NSS                                 3I4
C  3                SPEC(I),I=1,NSS                          14(1XA4)
C  4                LER,IER,NPIER,CRS,NSPR(I),I=1,11         1XA4,2I3,D12.4,
C                                                            11(1XA4)
C                   NSPR(I),I=12,IER                         16(1XA4)
C  ** CARD 4 IS REPEATED NRES TIMES.
C  5                NEQ                                      3I4
C  6                NUM,IX,JX,RAT,(REACT(I),I=1,IX),         1XI4,2I2,D12.5,
C                   (PROD(I),I=1,JX)                         6(1XA4)
C  ** CARD 6 IS REPEATED NEQ TIMES.
C
C                             ***** GLOSSARY OF TERMS *****
C TITLE             A 60-LETTER CODE IDENTIFYING THE JOB.
C NRES              NUMBER OF RESTRAINT SPECIES ( AND EQUATIONS )
C NSS               NUMBER OF STEADY-STATE SPECIES
C SPEC(I)           CODE NAME FOR SPECIES I
C LER               CODE NAME FOR THE CURRENT RESTRAINT SPECIES.
C IER               NUMBER OF TERMS ENTERING THE RHS OF THE ITH
C                   RESTRAINT EQUATION.
C NPIER             NUMBER OF POSITIVE TERMS ENTERING THE RHS
C                   OF THE ITH RESTRAINT EQUATION.
C CRS               ABUNDANCE (RELATIVE TO H) OF THE ITH RESTRAINT
C                   SPECIES.
C NSPR(I)           CODE NAMES OF THE SPECIES FORMING THE TERMS
C                   ON THE RHS OF THE CURRENT RESTRAINT EQUATION.
C NEQ               NUMBER OF CHEMICAL REACTIONS (RATE EQUATIONS)
C                   IN THE CURRENT SCHEME.
C NUM               CODE NUMBER OF THE CURRENT REACTION
C IX                NUMBER OF SPECIES ON THE LHS (REGENTS)
C                   OF THE CURRENT RATE EQUATION.
C JS                NUMBER OF SPECIES ON THE RHS (PRODUCTS) OF THE
C                   CURRENT RATE EQUATION.
C NEACT(I)          CODE NAME OF THE ITH REAGENT SPECIES.
C NPROD (I)         CODE NAME OF THE ITH PRODUCT SPECIES.
C                            ********************************
      DIMENSION NRFL(100),NPFL(100),REACT(3),PROD(4),NSPR(100)
      COMMON/CNTRL/NERTS,NURTS,NSS,NRES,NEQ,NITER,PTOL,NSPEC,NSING
      COMMON/MAIN/CONC(100),CRS(10),CRST(10),RATE(600),SPEC(100)
      COMMON/SIZE/IR(600),IP(600),NEACT(600,3),NPROD(600,4),NRS(10,125)
     1 ,IER(10),NPIER(10),NUM(600)
      COMMON/DEVICE/KR,KW,KWS
      DIMENSION NTITLE(15)
      REAL LER,NSPR
      DATA TSTNB/"   H"/
C
C                   INITIALISE ARRAYS.
      DO 150 I=1,600
      DO 150 J=1,3
  150 NEACT(I,J)=0
      DO 151 I=1,600
      DO 151 J=1,4
  151 NPROD(I,J)=0
      DO 160 I=1,100
      NRFL(I)=0
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  160 NPFL(I)=0
      NURTS=0
      NERTS=0
C
C             READ THE TITLE AND THE SPECIES INFORMATION.
      READ(KR,1050)(NTITLE(I),I=1,15)
      WRITE(KW,1060)(NTITLE(I),I=1,15)
 1050 FORMAT(15A4)
 1060 FORMAT(25X15A4)
C     IF NURTS BECOMES 1 SOMETHING IS FISHY WITH DATA BUT CALC IS DONE
C     IF NERTS BECOMES 1 SOMETHING IS WRONG WITH DATA AND PROGRAM STOPS
      READ(KR,1070)NRES,NSS
      WRITE(KW,1070)NRES,NSS
      NSPEC=NRES+NSS
      NSTRT=NSS+1
 1070 FORMAT(2I4)
      IF(NSPEC.LE.100) GO TO 180
C     NSPEC MAY BE LIMITED BY THE DIMENSION OF FI IN SOLVE
      WRITE(KW,1080) NSPEC
 1080 FORMAT(" ","ARRAY OVERFLOW NSPEC= ",I6)
  170 CALL EXIT
  180 READ(KR,1090) (SPEC(I),I=1,NSS)
 1090 FORMAT(14(1XA4))
C
C             READ IN INFORMATION FOR THE RESTRAINT EQUATIONS.
      DO 240 KER=1,NRES
      READ(KR,1110) LER,IER(KER),NPIER(KER),CRS(KER),(NSPR(LC),LC=1,11)
      CRST(KER)=CRS(KER)
      IF(KER.NE.NRES) GO TO 190
C
C             CHECK THAT THE LAST RESTRAINT EQUATION IS FOR HYDROGEN
      IF(LER.EQ.TSTNB) GO TO 190
      NERTS=1
      WRITE(KW,1100) LER,TSTNB
 1100 FORMAT(" ","SPECIES ",A4," IN LAST RESTRAINT EQ SHOULD BE ",A4)
  190 CONTINUE
 1110 FORMAT(1XA4,2I3,E12.5,11(1XA4))
      IERKE=IER(KER)
      IF(IERKE.LE.11) GO TO 200
      READ(KR,1120) (NSPR(LC),LC=12,IERKE)
 1120 FORMAT(16(1XA4))
  200 NSP=NSS+KER
C
C             WRITE OUT THE RESTRAINT EQUATION INFORMATION.
      SPEC(NSP)=LER
      WRITE(KW,1130) NSP,SPEC(NSP)
 1130 FORMAT(20X"SPEC(",I4,")=",A4)
C
C             ASSIGN THE INTERNAL LABELS NRS TO THE SPECIES
C             OCCURRING IN THE RESTRAINT EQUATIONS.
      DO 230 I=1,IERKE
      DO 220 J=1,NSS
      IF(NSPR(I).NE.SPEC(J)) GO TO 210
      NRS(KER,I)=J
      GO TO 230
C
C             CHECK THAT THE SPECIES IS A STEADY-STATE SPECIES.
  210 IF(J.LT.NSS) GO TO 220
      NERTS=1
      WRITE(KW,1140) NSPR(I),KER
 1140 FORMAT(" ","NON-STEADY-ST. VAR. ",A4," APPEARS ON RIGHT"
     11X"SIDE OF ",I3," RESTRAINT EQ.")
  220 CONTINUE
  230 CONTINUE
      WRITE(KW,1150) LER,CRS(KER),(NSPR(LC),LC=1,IERKE)
 1150 FORMAT(2XA4,"="E12.5/(19X20(1XA4)))
      WRITE(KW,1160)  (NRS(KER,I),I=1,IERKE)
 1160 FORMAT(19X20I5)
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  240 CONTINUE
      WRITE(KW,1170) NSPEC
 1170 FORMAT(   I6," SPECIES USED..")
      WRITE(KW,1090) (SPEC(I),I=1,NSPEC)
C
C             READ IN INFORMATION FOR EACH RATE EQUATION.
      READ(KR,1070) NEQ
 1180 FORMAT(I6,"EQUATIONS USED..")
      WRITE(KW,1180) NEQ
      DO 600 KEQ=1,NEQ
      READ(KR,1190)NUM(KEQ),IX,JX,RAT,(REACT(I),I=1,IX),(PROD(I),I=1,JX)
 1190 FORMAT(1XI4,2I2,E12.5,7(1XA4))
      IR(KEQ)=IX
      IP(KEQ)=JX
      RATE(KEQ)=RAT
C
C             ASSIGN INTERNAL LABELS NEACT TO THE SPECIES
C             MAKING UP THE REAGENTS.
  660 DO 270 I=1,IX
      DO 260 IS=1,NSPEC
      IF(REACT(I).NE.SPEC(IS)) GO TO 250
      NEACT(KEQ,I)=IS
      NRFL(IS)=NRFL(IS)+1
      GO TO 270
  250 IF(IS.LT.NSPEC) GO TO 260
      NERTS=1
C
C             ONE OF THE REAGENT SPECIES CANNOT BE IDENTIFIED
C             WITH ANY OF THOSE IN THE ARRAY SPEC(I)
      WRITE(KW,1220) REACT(I),KEQ
 1220 FORMAT(" ","UNKNOWN SPECIES ",A4," AMONG REACTANTS EQ ",I4)
  260 CONTINUE
  270 CONTINUE
C
C             ASSIGN INTERNAL LABELS NPROD TO THE SPECIES
C             MAKING UP THE PRODUCTS.
      DO 300 I=1,JX
      DO 290 IS=1,NSPEC
      IF(PROD(I).NE.SPEC(IS)) GO TO 280
      NPROD(KEQ,I)=IS
      NPFL(IS)=NPFL(IS)+1
      GO TO 300
  280 IF(IS.LT.NSPEC) GO TO 290
      NURTS=1
C
C             ONE OF THE PRODUCT SPECIES CANNOT BE IDENTIFIED
C             WITH ANY OF THOSE IN THE ARRAY SPEC.
      WRITE(KW,1230)PROD(I),KEQ
 1230 FORMAT(" ","UNKNOWN SPECIES ",A4," AMONG PRODUCTS IN EQ ",I4)
  290 CONTINUE
  300 CONTINUE
C
C     SEGMENT TO CHECK THAT A SPECIES DOES NOT APPEAR ON
C     BOTH SIDES OF AN EQUATION.
C
C
C     FIRST SUM OVER ALL SPECIES.
      DO 550 IS=1,NSPEC
C
C     DOES THE SPECIES OCCUR AMONG THE REAGENTS?
C     IF SO SET LRTEST=1
      LPTEST=0
      LRTEST=0
      DO 510 I=1,IX
      IF(REACT(I).NE.SPEC(IS))GO TO 510
      LRTEST=1
      GO TO 520
  510 CONTINUE
C
```

```
C     IF SPECIES OCCURS AMONG PRODUCTS SET LPTEST=1
  520 DO 530 I=1,JX
      IF(PROD(I).NE.SPEC(IS)) GO TO 530
      LPTEST=1
      GO TO 540
  530 CONTINUE
C
C     TEST FOR SPECIES AMONG REAGENTS AND PRODUCTS.
  540 IF(LRTEST.EQ.0.OR.LPTEST.EQ.0) GO TO 550
      NERTS=1
      WRITE(KW,1310)SPEC(IS),KEQ
 1310 FORMAT(10X"SPECIES"1XA4,1X"APPEARS ON BOTH SIDES"
     11X"OF EQN"1XI5)
  550 CONTINUE
  600 CONTINUE
C
C             CHECK THAT ALL SPECIES OCCUR AT LEAST ONCE AS
C    C        A REAGENT AND ONCE AS A PRODUCT IN THE RATE SCHEME.
      DO 620 I=1,NSPEC
      IF(NRFL(I).GT.0) GO TO 610
      WRITE(KW,1320) SPEC(I)
 1320 FORMAT(10X"SPECIES "A4,1X"NEVER APPEARS AS A REACTANT")
      NERTS=1
  610 IF (NPFL(I).GT.0) GO TO 620
      WRITE(KW,1330) SPEC(I)
 1330 FORMAT(10X"SPECIES "A4,1X"NEVER APPEARS AS A PRODUCT")
      NERTS=1
  620 CONTINUE
C     SEGMENT TO CHECK THAT NO REACTION APPEARS TWICE
C     AND THAT THE LABELS FOR ALL REACTIONS ARE DISTINCT
      NQM=NEQ-1
      DO 650 I=1,NQM
      JL=I+1
      DO 650 J=JL,NEQ
      NSUM=0
      IRTST=0
      DO 630 K=1,3
      IF(NEACT(I,K).NE.NEACT(J,K)) GO TO 632
  630 CONTINUE
      IRTEST=1
  632 DO 634 K=1,3
      IF(NPROD(I,K).NE.NPROD(J,K))GO TO 640
  634 CONTINUE
      IF(IRTST.EQ.0)GO TO 640
      WRITE(KW,1332)NUM(I),NUM(J)
 1332 FORMAT(20X"***REACTIONS"1XI4,1X"AND"1XI4,1X"ARE"1X"IDENTICAL")
      NURTS=1
  640 IF(NUM(I).NE.NUM(J))GO TO 650
      WRITE(KW,1334)NUM(J)
 1334 FORMAT(20X"***THE LABEL"1XI4,1X"APPEARS MORE"1X
     1"THAN ONCE IN THE LIST OF REACTIONS")
      NERTS=1
  650 CONTINUE
      READ(KR,1340) PTOL,NITER,NCLD
 1340 FORMAT(F7.5,2I7)
      WRITE(KW,1350)NCLD, PTOL,NITER
      WRITE(KWS,1350)  NCLD,PTOL,NITER
 1350 FORMAT(/,2X,"NUMBER OF CLOUD=",I2,4X," ER TOL="F10.6,
     +4X," MAX ITER="I4)
      RETURN
      END
      SUBROUTINE SERIAL(NCODE,NMAX,KIN,KOUT,KW)
      DIMENSION NCODE(600)
C
C     A SERIAL ARRAY 1 TO NMAX HAS ITS ELEMENTS CODED
C      BY THE ARRAY NCODE(I) FOR I=1,NMAX. FOR A GIVEN
C       CODE NUMBER KIN, THIS ROUTINE FINDS THE
C      CORRESPONDING SERIAL INDEX KOUT. THAT IS, GIVEN KIN,
```

```
C         FIND KOUT SUCH THAT NCODE(KOUT)=KIN
C         KW IS THE OUTPUT DEVICE FOR THE ERROR MESSAGE.
C
C         CODE NUMBER KIN, THIS ROUTINE FINDS THE
C         CODES IN THE ARRAY NCODE(I). IF AN EQUALITY IS
C         FOUND FOR A PARTICULAR I, THEN KOUT IS SET=I.
C         IF NO EQUALITY IS FOUND FOR ALL I, A MESSAGE IS GIVEN.
C
          DO 150 I=1,NMAX
          IF(NCODE(I).NE.KIN)GO TO 150
          KOUT=I
          GO TO 170
   150    CONTINUE
          WRITE(KW,2050)KIN
  2050    FORMAT(20X"***THE CODE"1XI4,1X"DOES NOT"
        11X"CORRESPOND TO ANY OF THE FOLLOWING")
          WRITE(KW,2060)(NCODE(I),I=1,NMAX)
  2060    FORMAT((5X20(1XI4)))
   170    RETURN
          END
          SUBROUTINE SIMQ(A,B,N,KS)
          DIMENSION A(1),B(1)
          TOL=0.0
          KS=0
          JJ=-N
          DO 65 J=1,N
          JY=J+1
          JJ=JJ+N+1
          BIGA=0.0
          IT=JJ-J
          DO 30 I=J,N
          IJ=IT+I
          IF(ABS(BIGA)-ABS(A(IJ))) 20,30,30
    20    BIGA=A(IJ)
          IMAX=I
    30    CONTINUE
          IF(ABS(BIGA)-TOL)  35,35,40
    35    KS=1
          RETURN
    40    I1=J+N*(J-2)
          IT=IMAX-J
          DO 50 K=J,N
          I1=I1+N
          I2=I1+IT
          SAVE=A(I1)
          A(I1)=A(I2)
          A(I2)=SAVE
    50    A(I1)=A(I1)/BIGA
          SAVE=B(IMAX)
          B(IMAX)=B(J)
          B(J)=SAVE/BIGA
          IF(J-N) 55,70,55
    55    IQS=N*(J-1)
          DO 65 IX=JY,N
          IXJ=IQS+IX
          IT=J-IX
          DO 60 JX=JY,N
          IXJX=N*(JX-1)+IX
          JJX=IXJX+IT
    60    A(IXJX)=A(IXJX)-(A(IXJ)*A(JJX))
    65    B(IX)=B(IX)-(B(J)*A(IXJ))
    70    NY=N-1
          IT=N*N
          DO 80 J=1,NY
          IA=IT-J
          IB=N-J
          IC=N
          DO 80 K=1,J
```

```
      B(IB)=B(IB)-(A(IA)*B(IC))
      IA=IA-N
   80 IC=IC-1
      RETURN
      END
      SUBROUTINE CRAT(DEN,RATE,NEQ,NUM)
      DIMENSION RATE(600),NUM(600),A(700),B(700)
      COMMON/DEVICE/KR,KW,KWS
      COMMON/TTAU/KTAU,NTAU,XTAU(10),TAUC,NDEN,KTAUST
      IF(NTAU.NE.KTAUST) GO TO 14
      READ(KR,100)CLDM,T,RAD
  100 FORMAT(E8.1,F7.0,F8.1)
   14 IF(NDEN.EQ.1)  GO TO 15
      XTAU(NTAU)=((CLDM/500.)**.33333333)*((DEN/260.)**.66666666)
      GO TO 16
   15 XTAU(NTAU)=(TAUC*NTAU)/KTAU
   16 AV=1.086*XTAU(NTAU)
      WRITE(KW,101)CLDM,XTAU(NTAU),T,RAD
  101 FORMAT(/,5X"CLDM="E10.3,5X"TAU="E10.3,4X,"T=",F4.0,4X,
     +"RAD=",F3.1,/)
      WRITE(KWS,102)  CLDM,XTAU(NTAU),T,RAD
  102 FORMAT(5X,"CLDM=",E10.3,5X,"TAU=",E10.3,4X,"T=",F4.0,4X,
     +"RAD=",F3.1)
      CALL  SERIAL(NUM,NEQ,2,KOUT,KW)
      RATE(KOUT)=0.1E-08*EXP(-232./T)
      CALL  SERIAL(NUM,NEQ,8,KOUT,KW)
      RATE(KOUT)=0.19E-14*(1.+(5./T))
      CALL  SERIAL(NUM,NEQ,9,KOUT,KW)
      RATE(KOUT)=0.16E-12*EXP(-160./T)
      CALL  SERIAL(NUM,NEQ,48,KOUT,KW)
      RATE(KOUT)=0.75E-14*(T**1.25)
      CALL  SERIAL(NUM,NEQ,200,KOUT,KW)
      RATE(KOUT)=0.19E-09/(T**0.7)
      CALL  SERIAL(NUM,NEQ,201,KOUT,KW)
      RATE(KOUT)=0.21E-09/(T**0.67)
      CALL  SERIAL(NUM,NEQ,202,KOUT,KW)
      RATE(KOUT)=0.76E-11*((100./T)**0.7)
      CALL  SERIAL(NUM,NEQ,203,KOUT,KW)
      RATE(KOUT)=0.12E-09/(T**0.626)
      CALL  SERIAL(NUM,NEQ,231,KOUT,KW)
      RATE(KOUT)=0.13E-09/(T**0.62)
      CALL  SERIAL(NUM,NEQ,280,KOUT,KW)
      RATE(KOUT)=0.14E-09/(T**0.63)
      CALL  SERIAL(NUM,NEQ,357,KOUT,KW)
      RATE(KOUT)=0.1E-17*DEN
      CALL  SERIAL(NUM,NEQ,412,KOUT,KW)
      RATE(KOUT)=0.5E-12*(EXP(-300./T))
      CALL  SERIAL(NUM,NEQ,602,KOUT,KW)
      RATE(KOUT)=1.5E-10/(T**0.641)
      CALL  SERIAL(NUM,NEQ,603,KOUT,KW)
      RATE(KOUT)=1.5E-10/(T**0.65)
      CALL  SERIAL(NUM,NEQ,604,KOUT,KW)
      RATE(KOUT)=3.7E-10/(T**0.855)
      IF(XTAU(NTAU)-50.)11,11,12
   11 A(262)=3.0E-11
      B(262)=1.72
      A(263)=3.0E-11
      B(263)=1.72
      A(264)=1.0E-10
      B(264)=2.069
      A(265)=1.59E-10
      B(265)=2.17
      A(266)=4.78E-10
      B(266)=2.17
      A(267)=1.59E-10
      B(267)=2.17
      A(270)=7.2E-10
      B(270)=2.39
```

```
A(271)=1.5E-10
B(271)=3.092
A(272)=3.3E-10
B(272)=1.4
A(273)=1.0E-11
B(273)=2.0
A(274)=3.2E-10
B(274)=1.677
A(275)=1.0E-11
B(275)=2.0
A(276)=1.0E-11
B(276)=2.0
A(277)=1.0E-11
B(277)=2.0
A(278)=8.0E-11
B(278)=2.8
A(279)=1.4E-11
B(279)=3.09
A(294)=8.0E-10
B(294)=1.6
A(307)=1.31E-10
B(307)=2.416
A(309)=2.89E-10
B(309)=2.75
A(310)=1.4E-10
B(310)=1.544
A(312)=5.0E-11
B(312)=1.72
A(315)=6.2E-12
B(315)=3.1
A(316)=3.3E-10
B(316)=1.4
A(317)=1.5E-10
B(317)=3.092
A(318)=1.6E-12
B(318)=3.092
A(320)=5.0E-12
B(320)=3.0
A(321)=3.2E-10
B(321)=1.677
A(322)=2.1E-11
B(322)=3.094
A(327)=5.0E-11
B(327)=1.72
A(328)=1.0E-09
B(328)=2.284
A(332)=1.4E-10
B(332)=1.72
A(333)=4.39E-10
B(333)=1.613
A(334)=4.39E-10
B(334)=1.613
A(335)=8.0E-11
B(335)=2.812
A(337)=8.8E-10
B(337)=1.613
A(338)=1.0E-10
B(338)=2.0
A(339)=1.0E-10
B(339)=2.0
A(341)=5.0E-11
B(341)=1.72
A(342)=1.0E-10
B(342)=1.8
A(343)=5.0E-10
B(343)=2.0
A(344)=5.0E-11
B(344)=2.0
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```
      A(345)=1.4E-10
      B(345)=1.54
      A(346)=1.0E-10
      B(346)=2.0
      A(347)=1.0E-11
      B(347)=2.0
      A(348)=5.0E-11
      B(348)=2.0
      A(368)=1.0E-11
      B(368)=2.0
      A(369)=1.0E-10
      B(369)=2.0
      A(370)=2.0E-10
      B(370)=2.0
      A(371)=1.5E-11
      B(371)=2.0
      A(610)=4.45E-11
      B(610)=1.435
      A(611)=1.17E-10
      B(611)=1.536
      A(612)=1.20E-09
      B(612)=1.622
      A(613)=1.0E-10
      B(613)=2.0
      DO 13 I=262,613
   13 A(I)=RAD*A(I)
      DO 1 I=262,267
      CALL SERIAL(NUM,NEQ,I,KOUT,KW)
    1 RATE(KOUT)=A(I)*EXP(-B(I)*AV)
      DO 2 I=270,279
      CALL SERIAL(NUM,NEQ,I,KOUT,KW)
    2 RATE(KOUT)=A(I)*EXP(-AV*B(I))
      DO 3 I=315,318
      CALL SERIAL(NUM,NEQ,I,KOUT,KW)
    3 RATE(KOUT)=A(I)*EXP(-AV*B(I))
      DO 4 I=320,322
      CALL SERIAL(NUM,NEQ,I,KOUT,KW)
    4 RATE(KOUT)=A(I)*EXP(-AV*B(I))
      DO 5 I=332,335
      CALL SERIAL(NUM,NEQ,I,KOUT,KW)
    5 RATE(KOUT)=A(I)*EXP(-AV*B(I))
      DO 6 I=610,613
      CALL SERIAL(NUM,NEQ,I,KOUT,KW)
    6 RATE(KOUT)=A(I)*EXP(-AV*B(I))
      DO 7 I=337,339
      CALL SERIAL(NUM,NEQ,I,KOUT,KW)
    7 RATE(KOUT)=A(I)*EXP(-AV*B(I))
      DO 8 I=341,348
      CALL SERIAL(NUM,NEQ,I,KOUT,KW)
    8 RATE(KOUT)=A(I)*EXP(-AV*B(I))
      DO 9 I=368,371
      CALL SERIAL(NUM,NEQ,I,KOUT,KW)
    9 RATE(KOUT)=A(I)*EXP(-AV*B(I))
      CALL SERIAL(NUM,NEQ,294,KOUT,KW)
      RATE(KOUT)=A(294)*EXP(-AV*B(294))
      X=0.1E-03*(DEN**2)*XTAU(NTAU)*EXP(5.*XTAU(NTAU))
      F=X/(1.+SQRT(X)+X)
      CALL SERIAL(NUM,NEQ,307,KOUT,KW)
      RATE(KOUT)=A(307)*EXP(-AV*B(307))
      CALL SERIAL(NUM,NEQ,308,KOUT,KW)
      RATE(KOUT)=0.2E-16*DEN*RAD*((1.-F)/F)
      CALL SERIAL(NUM,NEQ,309,KOUT,KW)
      RATE(KOUT)=A(309)*EXP(-AV*B(309))
      CALL SERIAL(NUM,NEQ,310,KOUT,KW)
      RATE(KOUT)=A(310)*EXP(-AV*B(310))
      CALL SERIAL(NUM,NEQ,312,KOUT,KW)
      RATE(KOUT)=A(312)*EXP(-AV*B(312))
      CALL SERIAL(NUM,NEQ,327,KOUT,KW)
```

```
      RATE(KOUT)=A(327)*EXP(-AV*B(327))
      CALL SERIAL(NUM,NEQ,328,KOUT,KW)
      RATE(KOUT)=A(328)*EXP(-AV*B(328))
      CALL SERIAL(NUM,NEQ,337,KOUT,KW)
      RATE(KOUT)=A(337)*EXP(-AV*B(337))
      CALL SERIAL(NUM,NEQ,339,KOUT,KW)
      RATE(KOUT)=A(339)*EXP(-AV*B(339))
   12 CONTINUE
      RETURN
      END
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16.26.42.BMIT,T15.
16.26.43.ACCOUNT,SMAS002,.
16.26.43.GET,HF1.
16.26.45.COPYSBF(HF1)
16.26.47. END OF INFORMATION ENCOUNTERED.
16.26.47.EXIT.
16.26.48.UEAD,         0.001KUNS.
16.26.48.UEPF,         0.037KUNS.
16.26.48.UEMS,         0.655KUNS.
16.26.48.UECP,         0.605SECS.
16.26.48.AESR,         4.000UNTS.
16.26.48.AEJC,         0.290 DOLLARS.
16.29.06.UCLP, 54,         1.216 KLNS.
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