

TIME DEPENDENT CHEMICAL STUDY OF CONTRACTING INTERSTELLAR CLOUDS. I. ABUNDANCES OF NITROGEN- AND CARBON-BEARING MOLECULES

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Abstract. We have constructed a reaction system containing the chemical families of H, C, O, N, S, Si, Cl, metals (Me) and grains. A total of 104 species have been included and a network of 557 reactions has been studied. The chemical kinetic equations were integrated as a function of time by using gear program. The chemical reaction system was followed at low, intermediate and high cloud densities i.e. from $10\text{--}10^7$ particles cm^{-3} . The calculated fractional abundances of N_2 , CN, HCN, and CH which are in good agreement with the results of observations and with those of previous theoretical studies.

1. Introduction

It is now generally recognized that chemistry plays a critical role in regulating the dynamics of core and star formation. This is primarily achieved by creating the coolants that regulate the energy balance and ionized matter which affects the magnetic field. The chemical composition of a cloud responds to the physical changes so that composition measurements can be used to probe various events. In the formation of low mass stars, the dynamical history of material must be incorporated into the description of the evolving chemistry (Hartquist *et al.*, 1993).

Many authors dealt with gas phase reactions by considering one species or one family of molecules (e.g., Prasad and Huntress, 1978; Kirby and Dalgarno, 1978). Alternatively, various other authors, e.g. Langer and Gredel (1989), considered a large number of species involved in many reactions. While most of the models were built on the steady state approximation (e.g., Herbst and Klemperer, 1973, Mitchell *et al.*, 1978), some scientists have included time dependence in their models. An early model was given by Gerola and Glassgold (1978). Prasad and Huntress (1980a, b) published the first detailed pseudo time-dependent model, in which chemical abundances evolved under fixed physical conditions. They investigated some of the transient phenomena that occur before the steady state conditions are reached. Several time-dependent models were presented by Langer and Co-workers e.g. (Graedel *et al.*, 1982; Langer *et al.*, 1984; Langer and Graedel, 1989). The above authors probed such topics as the dependence of the chemistry on element abundances, gas density and nature of isotopic fractionation. Other authors, e.g. Millar and Nejad (1985), Millar *et al.* (1987), Leung *et al.* (1984), Herbst and

Leung (1986a, b), Millar and Freeman (1984b) and Suzuki (1983) addressed the question of how and in what quantities moderately complex molecules could be synthesized. A much more extensive time dependent model was given by Tarafdar *et al.* (1985). Amin *et al.* (1991) presented models in the shock region involving simulations of hydrodynamic collapse. They included a large chemical network and realistic changes of physical conditions with time in a gas phase. Calculations on the excitation and abundance of H_3O^+ were presented by Phillips *et al.* (1992) with some approximations. Caselli *et al.* (1993) studied a massive spherical cloud containing a luminous protostar able to heat the circumstellar environment. They presented a dynamical chemical model of massive star formation regions, in which gas and dust grains are included. Pineau des Forets *et al.* (1993), calculated the structure of magnetohydrodynamic shocks in a dense cloud, with particular attention to sulphur bearing species.

The objective of this paper is two-fold:

1. To investigate whether diffuse and dark clouds are different evolutionary phases of the same interstellar cloud which is gravitationally contracting from an initial diffuse to a final dense state on the verge of star formation.

2. To follow the gas phase production and annihilation of a large number of charged and uncharged atomic, and molecular species during a magnetohydrodynamic contraction of an interstellar cloud. This paper is the first of a three part series concerning the chemistry in a contracting magnetized cloud. The dynamical model is given in Section 2. The reactions of the molecules and their rate coefficients are discussed in Section 3. The numerical method and the assumptions are introduced in Section 4. The results are given in Section 5. Finally the conclusions are summarized in Section 6.

2. The Dynamical Model

The equations governing the contraction of an interstellar cloud of density ρ , velocity v , gas pressure P , magnetic field B , and gravitational potential ψ are:

$$\frac{\partial}{\partial t}\rho + \bar{\nabla} \cdot (\rho\bar{v}) = 0, \quad (1)$$

$$\frac{\partial}{\partial t}(\rho\bar{v}) + \bar{\nabla} \cdot \rho\bar{v}\bar{v} = -\bar{\nabla}p - \rho\bar{\nabla}\psi + \frac{\bar{J}}{c} \times \bar{B} + \bar{F}, \quad (2)$$

$$\nabla^2\psi = 4\pi\rho G, \quad (3)$$

$$\frac{\partial}{\partial t}\rho\phi + \bar{\nabla} \cdot \rho\phi\bar{v}_i = 0. \quad (4)$$

Where G is the gravitational constant. \bar{F} is the fractional force and v_i is the ion velocity. These four equations of contraction were solved using the finite difference

method given by Black and Bodenheimer (1975) and later refined and adopted by El Nawawy *et al.* (1988) to study the contraction of magnetized cloud. Cylindrical polar coordinates were used in solving equations (1)–(4). The coordinates were constructed to move approximately with the matter, but with the inner zone under a constraint of a constant mass. We aim to follow numerically the details of ambipolar diffusion. Therefore the details of the contraction processes and hence the problem of ambipolar diffusion are left to a following article.

3. Molecules, Reactions and Rate Equations

The various molecular, atomic, and ionic species included in our calculations are listed in Table I. Altogether they are 104 species from the families of H, C, O, N, S, Si, Cl, metals and grains. The number of possible mutual interactions between the 104 species is extremely large. We have considered only reactions involving two body interactions and only those for which values of rate coefficients are available. Photo-dissociation and cosmic ray ionization were considered for all species. For every species, there were at least two reactions leading to its formation and two leading to its destruction except the least significant ones, e.g., HC_2O_2^+ . For each one of the more significant species, e.g. CO, H_2O , HCO, and SO, many more reactions were considered for its formation and annihilation. This resulted in a large network involving 557 reactions including the 104 species as compiled by Amin (1994). For each of 104 species we performed a mass balance using the relevant first order rate equations. These resulted in 94 simultaneous first order differential equations involving the concentration of the 104 species. These were combined with 10 equations representing the conservation of mass for each family of the elements shown in Table II except He and Grains. The variables in these equations are non-separable. The solution of this system for each species yields the time dependence of its number density within the cloud.

For modeling interstellar cloud chemistry, it is necessary to know the reaction rate coefficients for a very large number of ion-molecular reactions at temperatures below 100 K. Only a small number of these reactions has been studied in the laboratory, so it was necessary to calculate the reaction rate coefficients for many of these reactions. The Langevin value was frequently used where no laboratory data exist (Langer and Graedel, 1989). Various investigators assumed that the Langevin model was correct for ion-molecule reactions and that the rate coefficients measured at room temperature prevailed at temperatures as low as 10 K. While this view is frequently adopted, it is now recognized that ion-molecule reactions, in which the neutral reactant has a permanent dipole moment behave, differently. Recently, extensive theoretical calculations of the rate coefficients have been made. Some of these reactions were studied at temperature down to 10 K in the laboratory and were found to possess a peculiar temperature dependence (Herbst, 1987).

TABLE I
The chemical species involved in developing the model

Main element of group	Groups of various species
e	e
H	H, H ⁺ , H ⁻ , H ₂ , H ₂ ⁺ , H ₃ ⁺
C	C, C ⁺ , C ⁻ , C ₂ , C ₂ ⁺ CH, CH ⁺ , CH ⁻ , CH ₂ , CH ₂ ⁺ , CH ₃ , CH ₃ ⁺ , CH ₄ , CH ₄ , C ₂ H, C ₂ H ⁺ , C ₂ H ₂ ⁺ , C ₂ H ₃ ⁺
O	O, O ⁺ , O ⁻ , O ₂ , O ₂ ⁺ OH, OH ⁺ , H ₂ O, H ₂ O ⁺ , H ₃ O ⁺ , CO, CO ⁺ , CO ₂ , CO ₂ ⁺ , C ₂ O, HCO, HCO ⁺ , H ₂ CO, H ₂ CO ⁺ , H ₃ CO ⁺ , HCO ₂ ⁺ , HC ₂ O ⁺ , HC ₂ O ₂ ⁺
N	N, N ⁺ , N ₂ , N ₂ ⁺ , NH, NH ⁺ , NH ₂ , NH ₂ ⁺ , NH ₃ , NH ₃ ⁺ , NH ₄ , NH ₄ ⁺ , CN, CN ⁺ , CN ⁻ , C ₂ N ⁺ , HCN, HCN ⁺ , H ₂ CN ⁺ , NO, NO ⁺ , NO ₂
S	S, S ⁺ , S ⁻ , HS, HS ⁺ , H ₂ S, H ₂ S ⁺ , H ₃ S ⁺ , CS, CS ⁺ , HCS ⁺ , H ₂ CS, H ₂ CS ⁺ , SO, SO ⁺ , OCS, SN, SN ⁺ , ONS
Cl	Cl, Cl ⁺ , HCl, HCl ⁺ , H ₂ Cl ⁺
He	He, He ⁺
Si	Si, Si ⁺
Me	Mg, Mg ⁺ , Fe, Fe ⁺ , Na, Na ⁺

For strongly polar molecules, the permanent dipole moment increases the attractive forces for the incoming ions. Hence it should lead to a cross section larger than the Langevin value (Langer and Graedel, 1989). Many observed interstellar molecules have rather large values of dipole moment (D), (Millar *et al.*, 1991).

Values of the rate coefficients of the reactions included in this chemical system were taken from the following sources: the UMIST ratefile given by Millar *et al.* (1991) and Anicich (1993), Pineau des Forets *et al.* (1993), Amin (1990), Hollenbach and Mckee (1989), Pineau des Forets *et al.* (1987), Graff and Dalgarno (1987), Flower *et al.* (1986), Pineau des Forets *et al.* (1986a, b), Trafadar *et al.* (1985), Leung *et al.* (1984), Herbst (1983), Mitchell and Deveau (1983), Graedel *et al.* (1982), Henning (1981) and Prasad and Huntress (1980a).

4. Numerical Method and Chemical Assumptions

The chemical kinetic equations were integrated as a function of time. The abundances of each species at time step $t = t_0 + \Delta t$ was taken from that at the previous

TABLE II
Solar element abundance

Element	Abundance	Element	Abundance
H	1	Mg	3.50 (-05)
C	3.72 (-4)	Na	1.74 (-06)
O	6.80 (-4)	Fe	2.50 (-05)
N	1.15 (-4)	Cl	4.40 (-07)
S	1.60 (-5)	He	1.40 (-01)
Si	3.50 (-5)	Grain	2.64 (-12)

time step. The corresponding density at the same time was taken from the contraction equations. Our procedure falls short of simultaneous integration of the chemical rate equations and the magnetohydrodynamic equations. To achieve this objective a computer with high capacity is required in addition to much longer computer time. The fractional abundance of a species is denoted by X , where

$$X = n(x)/n, \quad \text{and} \quad n = n(\text{H}) + 2n(\text{H}_2). \quad (5)$$

In order to obtain the solution, several physical assumptions were made. These are:

1. The evolution is assumed to proceed isothermally at $T = 10$ k.
2. The hydrodynamical parameters (e.g., density, velocity, ...) remain unchanged during a run, so the calculations simply follow the time contraction of a volume element of constant mass.
3. The interstellar radiation field is taken from the contraction model, and the value adopted for the cosmic ray primary ionization rate is $4 \times 10^{-17} \text{ s}^{-1}$ as recommended by (Hollenbach and Mckee, 1989)
4. The initial values of the fractional abundance of the elements are assumed to be those of H, He, C, O, N, S, Si, Cl, Me, and grain. These are listed in Table II.
5. The rate coefficients for all the polar molecules in our reaction network were estimated using the formula of Langer and Graedel (1989), i.e.,

$$K = 50K(l)T^{-0.5}$$
 where $K(l)$ is the Langvien value.
6. The radiative association rates for C^+ and CH_3^+ with H_2 probably should be increased (Herbst, 1985).
7. The initial abundances of all molecules and ionic species equal zero. This is necessary so that we obtain a model of general applicability and in order to compare its predictions with different observations.
8. There is no effect of magnetic field on the chemical reactions network.

9. The time of chemical evolution in our model is that for contraction. Note that the time of contraction at the end of a run code is equal to $1.7\tau_{\text{ff}}$. Where τ_{ff} is the free fall time of contraction which is equal to 1.4×10^7 year.
10. The density of the central zone is used in the model of chemical evolution. The mass involved in the chemical model is not important. Since we do not calculate the column density of the species, the mass of the central zone is always fixed.
11. The element depletion is taken equal to zero because we take only this reaction

$$\text{H} + \text{H} + \text{grain} \longrightarrow \text{H}_2 + \text{grain},$$
 i.e., the condensation on dust grain was not considered here.

5. Results

In the following results we discuss only the abundance of the various neutral species within the different chemical families. The ionic species will be dealt with in a latter paper. In the shielded regions, the neutral-neutral reactions will be dominant over the ion-neutral reactions; the former leading to decay of the abundance of neutrals. Nevertheless, since there are no destruction process left except further chemical reactions, even unstable species may live long enough to accumulate or to be a necessary step in a ladder leading to complex molecules. If shielded cloudlets have enough time to evolve, high densities of molecules can be achieved. Since the time scale for the molecular formation is larger than the time scale for dynamical stability, the general results for the shielded regions have existed before the shielding occurred. i.e., gas phase reactions cannot account for a high amount of molecules within the relatively short lifetime of small dense clouds. Furthermore no steady state is reached.

Our results are compared with the observations of Irvine *et al.* (1987), Hydbek and Hjalmarson (1985) and Duley and Williams (1984), and with the results of the theoretical studies of Langer and Gredel (1989), Herbst and Leung (1989), Nejad *et al.* (1990), Williams and Hartquist (1991), Caselli *et al.* (1993), and Hasegawa and Herbst (1993), it should be noted that:

1. The initial values of abundance of H, N, C, O, S, Si, Cl, metals and grains taken in our model not exactly equal to those taken by the others.
2. The time of chemical evolution in our model is that for contraction. This assumption has not been considered by the authors.
3. The optical depth τ (or visual extinction A_v) is taken from the model of contraction. i.e., $A_v = 1.068\tau$.
4. There is continuous development in the values of the rate coefficients and we have used the most available recent values.
5. Since there are numerous differences between this model and many previous ones, it is not possible to trace down all the differences between this and the previous models.

5.1. NITROGEN CHEMISTRY

The nitrogen chemistry depends upon the initial distribution of nitrogen between N, N₂ and NH₃. The interstellar cloud synthesis of many of the nitrogen bearing molecules such as NH₃, N₂H⁺ and HCN is a more difficult problem than those of oxygen and carbon. This is because the initiation reactions by which atomic nitrogen is introduced into the ion-molecule chemistry are poorly understood (Langer and Graedel, 1989). In interstellar clouds, nitrogen is primarily neutral because its ionization potential, about 14 eV, is beyond the Lyman limit. However N⁺ can be produced directly by cosmic rays, i.e.



Following that, nitrogen bearing molecules are presented, via He⁺ dissociative ionization of molecules (N₂, CN, . . . etc.).

Herbst *et al.* (1987) performed a theoretical study on the reaction H₃⁺+N. They concluded that it has a significant activation barrier. Thus the reaction will be rather slow under interstellar cloud conditions. The measurements of Adams and Smith (1985) confirmed that



does not occur. Therefore, the rate coefficient of this reaction was taken equal to zero.

The chemical network for the various species in the nitrogen family are shown graphically in Figures 1 and 2 in diffuse and dense regions, respectively. The abundance profiles of the various species are shown in Figure 3. The comparison with the observations are given in Table III.

In this group we find extremely important molecules from the results of observational and theoretical studies, i.e., the diatomic molecules N₂, CN and NO. They are formed in common by neutral-neutral reactions. They are fairly stable species and hence they accumulate with time. In diffuse region, negative ion-neutral reactions cause the production of NO. The contribution of N₂ to the formation of nitrohydrides is small the relevant reactions are given by Amin (1994). Comparing our results with those of observations and with the values obtained by other authors, one can see that:

1. The concentration of N₂ at densities of 10⁴–10⁵ cm⁻³ is in agreement with the observation in TMC-1 cloud.
2. The maximum concentration of CN at densities of 10³ cm⁻³ is in agreement with the observation of TMC-1 cloud, and Orion plateau. In diffuse region the abundance of CN is less than that observed in ζ Oph cloud.
3. Our calculated value for N₂ is nearly equal to the value calculated by Hasegawa and Herbst (1993).

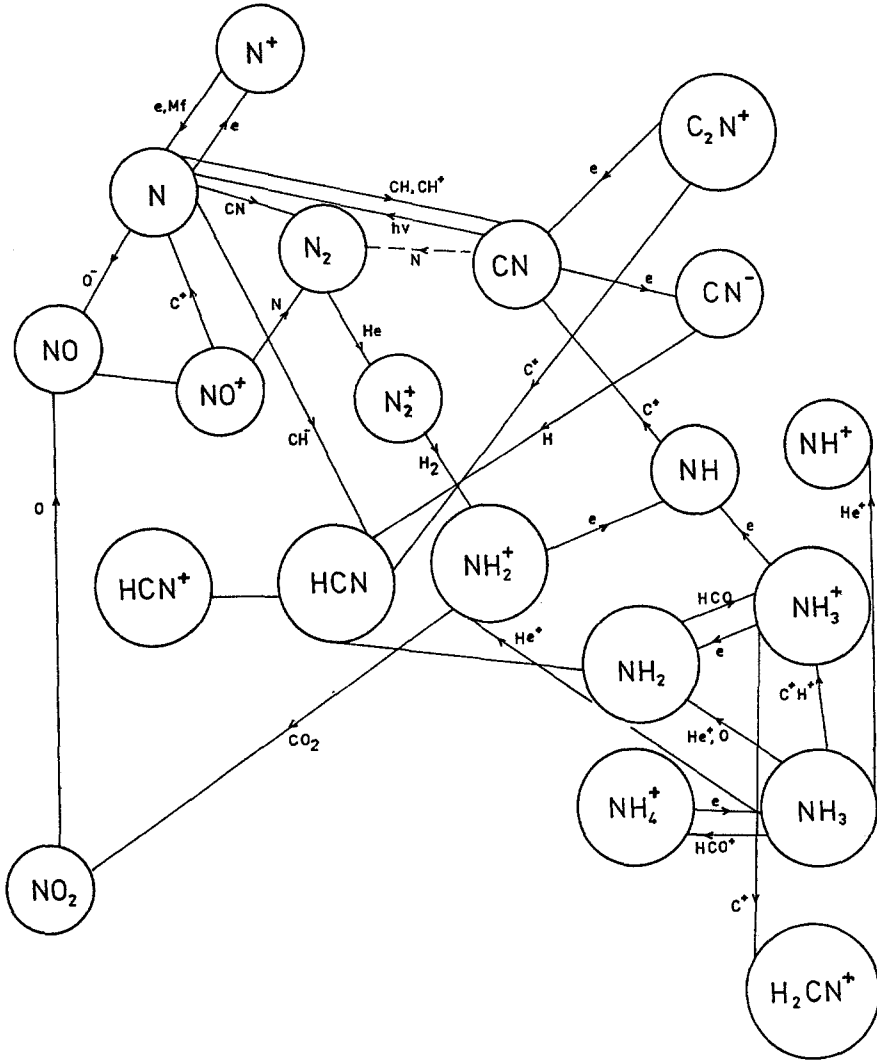


Fig. 1. The chemical network for nitrogen family in the diffuse region.

4. The maximum fractional abundance of CN is several-fold smaller than the values reported by Langer and Graedel (1989), Nejad *et al.* (1990), and Hasegawa and Herbst (1993).
5. The fractional abundance of NO occurs at densities of 10^4 to 10^5 cm^{-3} which is in agreement with the results calculated by Nejad *et al.* (1990). Furthermore, the concentration of NO is about one order of magnitude greater than that of Herbst and Leung (1989).

The neutral species of nitrogen hydrides are formed by dissociative recombination of the ions containing more hydrogen. These ions are formed by molecular

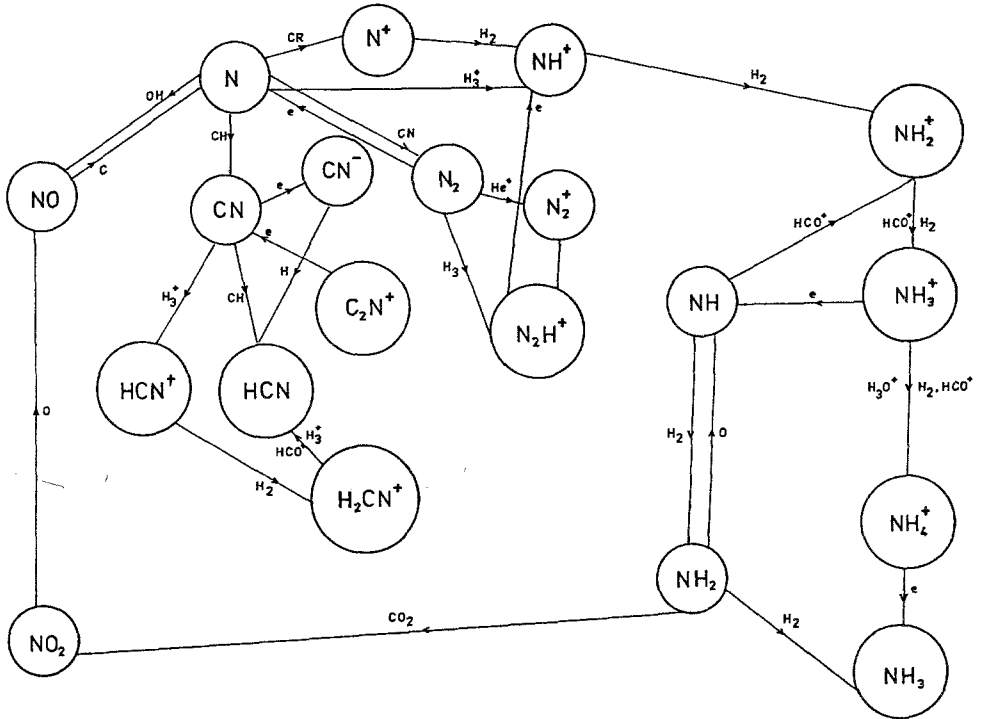


Fig. 2. The chemical network for nitrogen family in the dense region.

TABLE III

The maximum fractional abundance for Nitrogen bearing molecules

Species	Our calculated value	Observed value	
		TMC-1 ^A	Orion
N ₂	4.20 (-08)	5.00 (-08)	
CN	1.40 (-08)	2.00 (-08)	6.00 (-08) ^O 3.00 (-07) ^F
NH ₃	5.20 (-09)	2.00 (-08)	2.00 (-06) ^O 3.00 (-07) ^F
HCN	9.00 (-07)	2.00 (-08)	2.00 (-08) ^F 7.00 (-07) ^O

$a(-b)$ signifies $a \times 10^{-b}$.

A: For TMC-1 cloud observed by Irvine *et al.*, 1987.

O: For Orion plateau cloud observed by Hydebeck and Hjalmarson, 1985.

F: For Orion ridge cloud by Hydebeck and Hjalmarson, 1985.

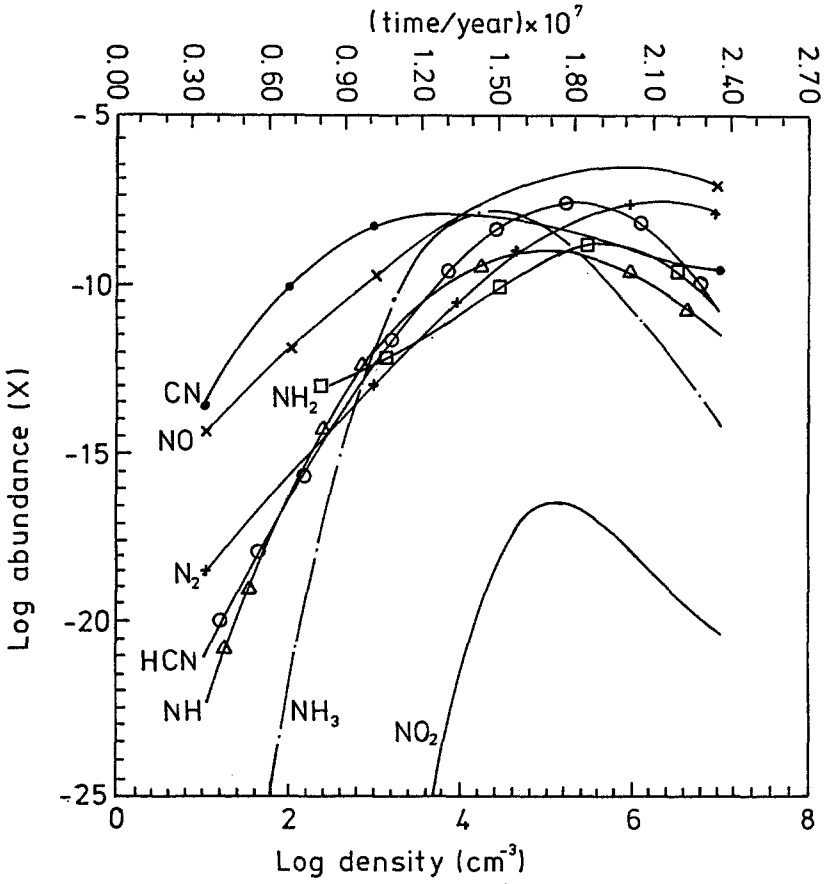


Fig. 3. The abundance profiles of the nitrogen family with respect to density and time in a contracting cloud.

hydrogen attachment reactions. Because the molecular hydrogen attachment reactions leading to NH_4^+ are often endothermic the chain ceases at the NH_3 . Therefore NH_3 is the most abundant neutral molecule in the family of nitrogen hydrides up to a density of 10^6 particles/ cm^{-3} . At higher densities NH_3 is depleted frequently with the depletion of both NH_4^+ and electrons.

The neutral molecules of nitrogen hydrides are mainly removed by reactions with C^+ , O in the outer and with S in the inner parts of the cloud, respectively, rather than by photo-dissociation. This latter gives birth to CN, NO, and SN molecules.

The fractional abundance of NH, NH_2 , and NH_3 confirm that the maximum fractional abundance of NH_3 at a density of 10^5 cm^{-3} is one order of magnitude smaller than the observations of TMC-1 cloud, two orders of magnitude smaller than that of Orion ridge and three orders of magnitude smaller than that of Orion plateau, respectively. We also note the following:

1. Our maximum value for NH occurs at densities of 10^3 to 10^5 cm^{-3} is in agreement with that of Herbst and Leung (1989), and Hasegawa and Herbst (1993).
2. The maximum concentration of NH_2 at a density of 10^5 cm^{-3} is in agreement with the values reported by Langer and Graedel (1989).
3. The fractional abundance of NH_3 is in agreement with that of Langer and Graedel (1989), and Hasegawa and Herbst (1993).

The important reactions producing HCN are,



HCN is dissociated by the reactions of HCO^+ and He^+ . The abundance of HCN increases to 9×10^{-7} at a density of 10^5 cm^{-3} , and decreases to 1.6×10^{-11} at the end of the run code. The maximum fractional abundance of HCN is in agreement with the observation of Orion plateau. It is one order of magnitude greater than that observed for both TMC-1 cloud, and Orion ridge. Furthermore this value is in agreement with the values reported by Herbst and Leung (1989), and Caselli *et al.* (1993).

5.2. CARBON CHEMISTRY

Because the ionization energy of atomic carbon is below the cut-off limit in the galactic radiation caused by the ionized hydrogen, carbon atoms exist mainly as C^+ in diffuse clouds (Crutcher and Watson, 1985). Their ionization provides free electrons in diffuse clouds (Crutcher and Watson, 1985).

The exchange reaction



requires an activation energy of 0.4 eV for reactants in their ground state. Therefore, it is completely negligible at the standard temperature of diffuse cloud, i.e., 100 k.

The radiative association reaction



is very important in ion-molecular chemistry (Dalgarno, 1976). The above reaction produces neither CH nor CH^+ directly. Subsequent reactions and photo-processes serve to recycle the carbon back into CH and CH^+ . For the reaction



TABLE IV
The maximum fractional abundance for carbon bearing molecules

Species	Our calculated value	Observed value	
		TMC-1 ^A	Orion
C ₂	4.90 (-10)	5.00 (-08)	
CH	3.20 (-08)	2.10 (-08)	
C ₂ H	6.80 (-07)	8.00 (-08)	3.00 (-08) ^F
H ₂ CO	1.20 (-08)	2.00 (-08)	8.00 (-08) ^F

$a(-b)$ signifies $a \times 10^{-b}$.

The symbols are the same as those of Table I.

we have used the theoretical reaction rate coefficient estimated by Herbst (1985) for this reaction.

Figures 4 and 5 summarize the chemical network for the carbon compounds in the diffuse and dense regions, respectively. The corresponding abundance profiles are shown in Figure 6. The comparison with the observations are given in Table IV.

In the interstellar space, carbon is present in three forms: neutral, ionized, and chemically bound in CO which is the most abundant molecule after H₂. The chemistry of carbon oxides is strongly coupled to the chemistry of HCO, and H₂CO (Henning, 1981).

In the unshielded region, the whole chemistry is practically reduced to an interaction between C and C⁺ in which the ion plays the major role.

C₂ has a moderate influence. While this molecule suffers from photo-dissociation in the unshielded region, it is rapidly converted into CO by its affinity to oxygen in the inner part of the cloud. The maximum abundance of C₂ at a density of 10³ cm⁻³ is smaller than the observed value in TMC-1 cloud. Also in diffuse region the abundance of C₂ is less than that observed in ζ Oph cloud. Comparison with theoretical values calculated by other authors reveals the following:

1. Our value of C₂ is about one order of magnitude smaller than that of Langer and Graedel (1989) (calculated at a density 10⁴ cm⁻³, and C/O = 0.7).
2. Although the rate of cosmic ray ionization in our models equals 4×10^{-17} s⁻¹, the maximum fractional abundance of C₂ is about one order of magnitude greater than that of Nejad *et al.* (1990), who used a value of 10⁻¹⁶ s⁻¹. This indicates that cosmic ray ionization does not have a strong influence on the abundance of C₂ in our model.

The first observed interstellar molecules were CH and CH⁺. Many difficulties arose in clarifying their chemistry. They are still the subject of great consideration

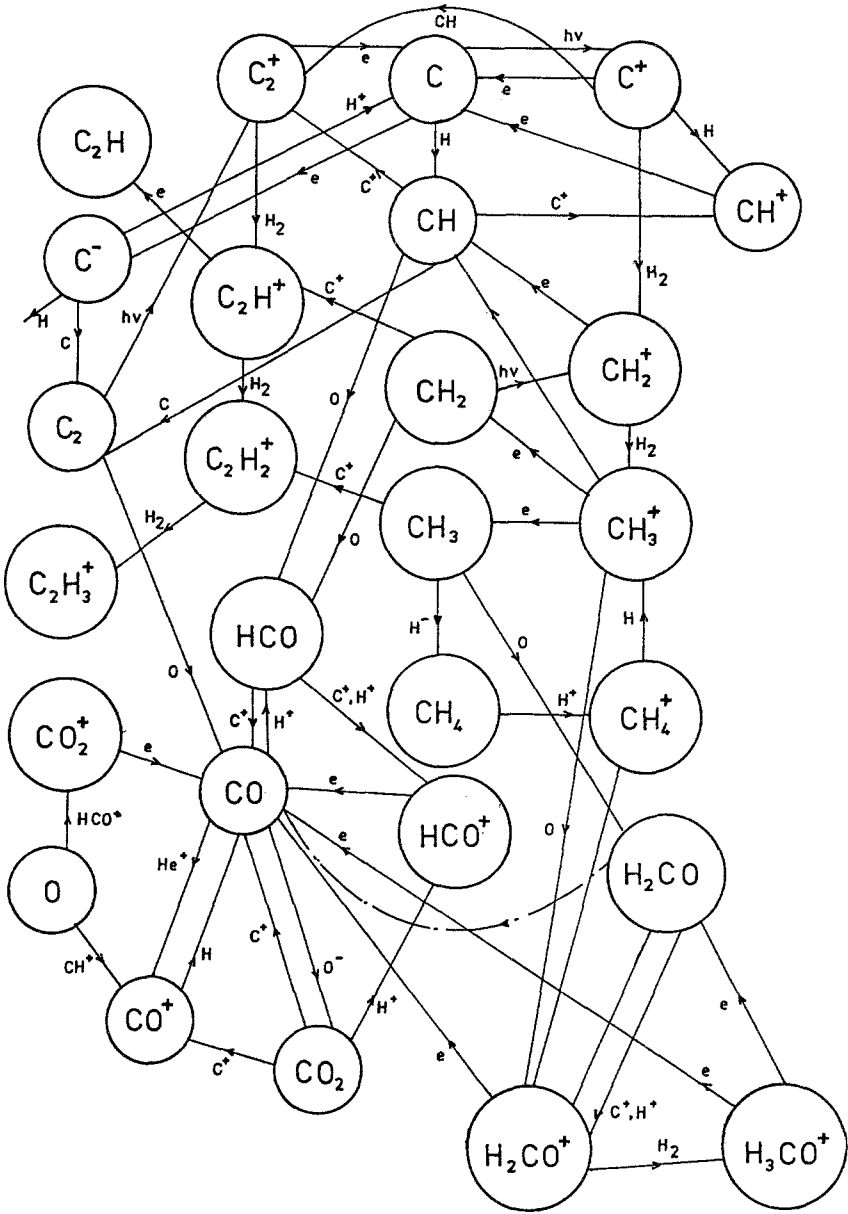


Fig. 4. The chemical network for carbon family in the diffuse region.

in the literature. Many authors have dealt with this family in observations and experiments (Henning, 1981).

Comparisons of the concentration of carbon hydrides at a density of 10^5 cm^{-3} with other observational and theoretical studies shows that:

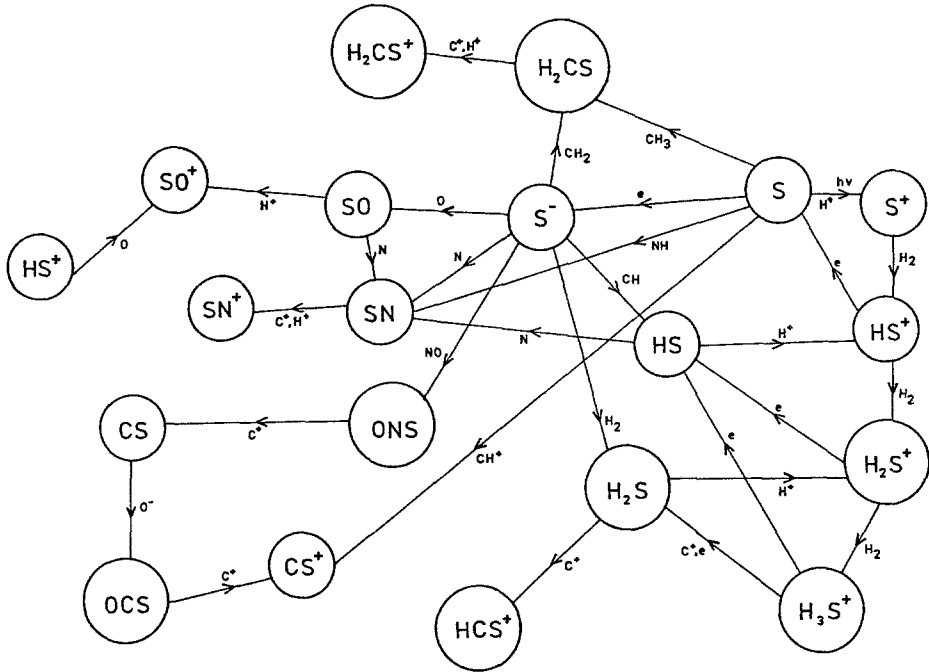


Fig. 5. The chemical network for carbon family in the dense region.

1. The maximum fractional abundance of CH is in agreement with the observed value in the TMC-1 cloud.
2. The maximum fractional abundance of C_2H is one order of magnitude greater than that observed in the TMC-1 cloud, and the Orion ridge.
3. Our calculated value for CH agrees with that of Langer and Graedel (1989), and Herbst and Leung (1989). It is one or two orders of magnitude greater than that of Nejad *et al.* (1990) and Pineau des Forets *et al.* (1992), respectively.
4. The calculated value of maximum concentration for CH_2 is about one order of magnitude smaller than that of Langer and Graedel (1989), Nejad *et al.* (1990) and Pineau des Fortes *et al.* (1992).
5. The maximum concentration of CH_4 is in agreement with that of Pineau des Forets *et al.* (1992).
6. The maximum concentration of C_2H is one order of magnitude greater than that of Herbst and Leung (1989), two orders of magnitude greater than that of Langer and Graedel (1989), and three orders of magnitude greater than that of Nejad *et al.* (1990), respectively.

The concentration of CH_3 is very small because its formation rate is less than its destruction rate.

The CH species is not involved in the synthesis of the heavier carbon hydrides but makes the main contribution to the starting point of the C_2H_n molecules as

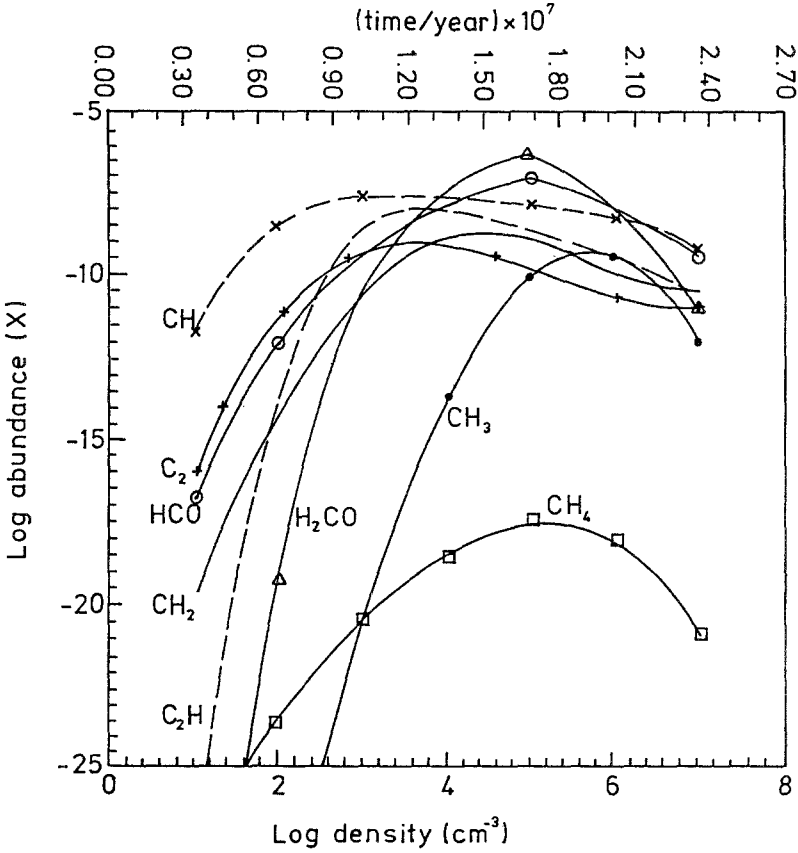


Fig. 6. The abundance profiles of carbon family with respect to density and time in a contracting cloud.

long as a sufficient concentration of C^+ is available Langer and Gredel (1989). Going deeper into the cloud the situation changes with decreasing the abundance of the electrons. The dissociative reactions are no longer effective, and the CH_2 which is primarily concerned has to be synthesized via the long reaction chain.

The least abundant molecule, C_2H in particular, reaches the same concentration as that of the CH . Both belong to the most important species at the edge of the cloud. In the inner region, too, its concentration is comparable to that of CH_2 with which it is coupled via ion-neutral reactions. These results differ from that of Henning (1981), who found that the concentration of C_2H in the inner region is comparable to that of CH_3 .

Since formaldehyde is not only easily observable but also abundant, a detailed knowledge about the formaldehyde chemistry is of great importance. For a long time severe difficulties arose in explaining the amount of H_2CO observed. This

is because no molecular hydrogen attachment reaction is possible between HCO^+ and H_2CO^+ , and also because the radiative association reaction, i.e.,



is very slow (Fehsenfeld *et al.*, 1974; and Herbst, 1976).

In looking at the carbon family as shown in Figures 4 and 5, one sees that the H_nCO family consists of only two weakly bound subfamilies. The members are synthesized from CH_n molecules in reactions with oxygen rather than within the subfamilies themselves. These reactions produce adequate amounts of H_2CO and HCO to explain the observation. Our results indicate that:

1. HCO reaches its maximum concentration of 1.3×10^{-7} at a density of 10^5 cm^{-3} , and decreases to 4.6×10^{-10} at the end of the run of the model.
2. H_2CO reaches its maximum concentration of 1.2×10^{-8} in the shielded part of the cloud. It has a lower concentration in the diffuse part.
3. The concentration of HCO at a density of 10^5 cm^{-3} is two orders of magnitude greater than that of Langer and Graedel (1989) and Herbst and Leung (1989).
4. Our value of H_2CO agrees well with the observations of TMC-1 cloud, and Orion ridge. The maximum concentration of H_2CO is in agreement with the values of Hasegawa and Herbst (1993).

6. Conclusion

We presented a contraction model for an isothermal cloud with the density progressively increasing up to $n = 10^9$ particles/ cm^3 . In the initial model the abundances of all molecules are assumed equal zero, $n = 10$ particles/ cm^3 . We have run the contraction assuming that the cloud model is isothermal with $T = 10 \text{ K}$, which is nearly the case for density lower than $n \simeq 10^9$ particles/ cm^3 (Larson, 1969). As the density increases, the program is developed to study the chemical structure at densities from 10 to 10^7 particles/ cm^3 . It has been found that in diffuse region CN and CH are the most abundant. The time of chemical evolution in our model was assumed equal to the time of contraction. In the diffuse region the time of contraction (10^5 year) is still smaller than the time required to reach steady state. Therefore the calculated abundance of C_2 and CN are less than that observed in the ζ Oph cloud. As the density increases to intermediate values the abundances of the molecules CN, NO, N_2 , HCN, NH, and NH_3 , shown in Figure 3 and of the molecules CH, C_2 , HCO, CH_2 , C_2H and H_2CO shown in Figure 6 increases relative to their values in the diffuse region. However CN and CH molecules are still the most dominant. As the contraction proceeds to the dense region the abundance of all molecules increase to their maximum values. As shown in Figures (3 and 6) NO, HCO, and H_2CO are the most dominant molecules. Our chemical model produces fractional abundances of N_2 , CN, HCN, and CH which are in good agreement with

the results of observations. The calculated abundances of N₂, CN, HCN and CH are in agreement with the results of previous theoretical studies. It is interesting to follow simultaneously the contraction of interstellar cloud and study the time dependent chemical evolution. This represents a second generation model which will be considered in further work.

In the following papers we discuss our results on oxygen- and sulphur-bearing molecule abundances and the charge distribution in interstellar clouds.

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