TIME DEPENDENT CHEMICAL STUDY OF CONTRACTING INTERSTELLAR CLOUDS. III. THE CHARGE DISTRIBUTION IN INTERSTELLAR CLOUDS

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Abstract. We have constructed a chemical reaction model in a contracting interstellar cloud including 104 species which are involved in a network of 557 reactions. The chemical kinetic equations were integrated as a function of time by using gear package. The evolution of the system was followed in the density range 10–10^7 particles cm^{-3}.

The calculated fractional abundances of the charged species are in good agreement with those given by other investigators. The charge density has been followed in diffuse, intermediate and dense regions. The most dominant ionic species are metallic ions, HCO^+ and H_3^+ in the shielded regions and atomic ions H^+, C^+, Si^+, He^+, S^+ and metal ions in the diffuse and intermediate regions. The abundances of negatively charged ions were found to be negligible. The results of the calculations on the different metallic ions are interpreted.

1. Introduction

Ionized particles play an important role in interstellar chemistry and the dynamics of the interstellar gas, because the ions mediate the coupling of the neutral gas to the magnetic field.

The fractional ionization is relatively low in molecular or dark clouds. The degree of ionization in molecular clouds is intricately related to various processes, e.g., ionization of H_2 and He by cosmic ray (Solomon and Werner, 1971), formation and dissociative recombination of molecular ions (Herbst and Klempere, 1973) charge transfer between molecular ions and metallic atoms (Oppenheimer and Dalgarno, 1974b), radiative recombination of metallic ions, recombination of ions on grains, and of electrons to grains (Umebayashi and Nakano. 1980). Photoionization, adsorption of ions and capture of electrons on grain surface, recombination of ions and electrons due to grain-grain collisions, desorption of charged particles off grain surface, recombination due to association reaction and negative ions (El Nawawy *et al*,. 1992).

Many observational efforts have been made to derive the density of charged particles in interstellar clouds (e.g., Van Dishoeck *et al*,. 1992; Petrie *et al*,. 1991; Balm and Jura 1992; Vladilo *et al*,. 1993; Phillips *et al*,. 1992; Turner 1993 and Heck *et al*,. 1993). On the other hand, the physical parameters affecting the charge state, in diffuse and dense interstellar clouds, have been followed by many authors

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(Oppenheimer and Dalgarno, 1974a,b; Elmegreen 1979; Umebayashi and Nakano 1980; Umebayashi 1983; Langer 1985 and El nawawy *et al*,. 1992). More intensive studies of grain surface reactions (for charged particles) have been done by Watson and Salpeter (1972), Umebayashi and Nakano (1980), d'Hendecourt *et al.* (1985), Brown and Charnely (1990) and Hasegawa and Herbst (1993).

Reactions of charged particles with grains have been neglected in this work. They have been treated in detail by Hasegawa and Herbst (1993).

The metal abundance is a potentially important contributor to the electron abundance in clouds (Graedel *et al.* 1982). In the previous model calculations the metal abundance was an important factor in determining the chemistry through its influence on the abundance of polyatomic ions, especially H_3^+. From observation of molecules and molecular ions it is possible to place some limits on the electron abundance in clouds (Langer, 1985 and Dalgarno and Lepp, 1984) and given a model of the contribution of the metals to the electron abundance, a limit on the metal abundance is defined. Note, however, that if polycyclic aromatic hydrocarbons (PAHS) are abundant (χ(PAHS) $> 10^{-8}$) they will play a more important role in the electron balance than will the metals (Lepp and Dalgarno, 1988). In the current work we neglect the effect of PAHS.

The objective of this work is to develop a time dependent model which describes the ion chemistry of the less complex carbon, nitrogen, oxygen and sulphur bearing molecules during contraction of a magnetized gas cloud. The model also take proper account of the effects of metallic elements and neutral grains. The details of the physical and chemical scheme, the numerical method of solution, the rate coefficients and the abundances of nitrogen- and carbon-bearing species were presented earlier in part (I), Amin *et al.* (1995a). The abundances of oxygen-, chlorine- and sulphur-bearing molecules are given in part (II), Amin *et al.* (1995b). The reaction scheme was compiled by Amin (1994). In this paper we specifically aim to obtain a detailed distribution of the charged particles in a contracting interstellar cloud and follow its evolution from the low neutral densities of $n = 10^{-3}$ cm up to the protostellar densities of $n = 10^7$ cm^{-3}.

2. Results

Figures 1–5, represent the fractional abundances of the important atomic ions and molecular ions, respectively. From these figures, we can represent the fractional abundance of electrons by the equation

$$X(e) = an^{-0.5},$$

where $a = 5 \times 10^{-3}$ in the diffuse part and 2×10^{-4} in a highly dense cloud. Figure 6 shows a comparison between the predictions of the above relation of electron density based on time dependent calculations and those based on steady

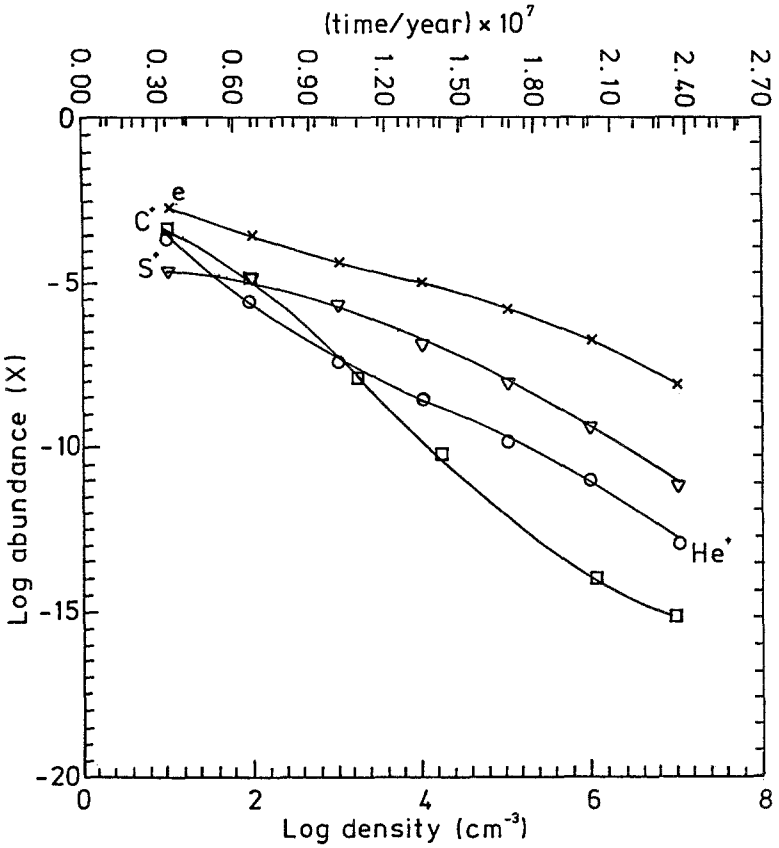

Fig. 1. The abundance profiles of e, C^+, He^+, and S^+ with respect to density and time in a contracting cloud.

state calculations by Nakano (1984) (curve a), and El Nawawy *et al.* (1992) (curve b). From this figure we note the following:

1. The values of electron density are greater than that of El Nawawy up to $n(H_2) < 10^6$ cm^{-3}, above which the values of El Nawawy are greater than the present values.
2. Our calculated values for electron density are greater than those of Nakano (1984). At the end of the calculations i.e. ($n(H_2)$ equals to 10^7 cm^{-3}, the value of Nakano is smaller than the present value by about one-half order of magnitude.

In the diffuse region, the H^+ concentratlon is strongly coupled to the electron directly, i.e., Photo-ionization and recombination, but involves charge transfer with oxygen and metals

$$H + h\nu \longrightarrow H^+ + e \qquad \text{(reaction No. 84)}$$

$$H + CR \longrightarrow H^+ + e \qquad \text{(reaction No. 82)}$$

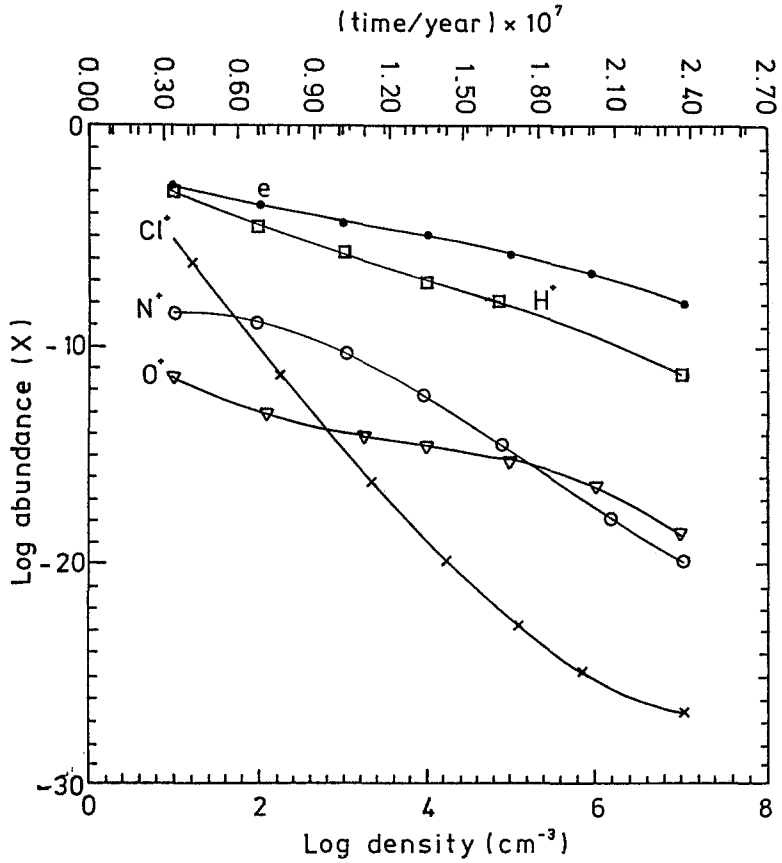

Fig. 2. The abundance profiles of e, H^+, Cl^+, N^+ and O^+ with respect to density and time in a contracting cloud.

$$H^+ + Me \longrightarrow Me^+ + H \qquad \text{(reactions No. 142–144)}$$

$$H^+ + O \longrightarrow O^+ + H. \qquad \text{(reactions No. 123)}$$

In the dense region, the metal reactions are the main cause of removal of H^+. On the other hand, the generation of H^+ results from cosmic ray ionization of H_2.

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. As recombination is very rapid, only a major part of the C^+ is allowed to initiate other reaction channels. As the radiation field begins to attenuate, the situation changes. For H_2, the fractional abundance increases. The charge of C^+ is transferred to other species, so that C^+ will become either neutralized or chemically bound (i.e the fractional abundance of C^+ decreases).

Due to the high abundances of S, Si, He, and Me, and the effect of photoionization and cosmic ray ionization, the fractional abundances of S^+, Si^+, He^+, and Me^+ range from 10^{-4} to 10^{-6} in the diffuse region.

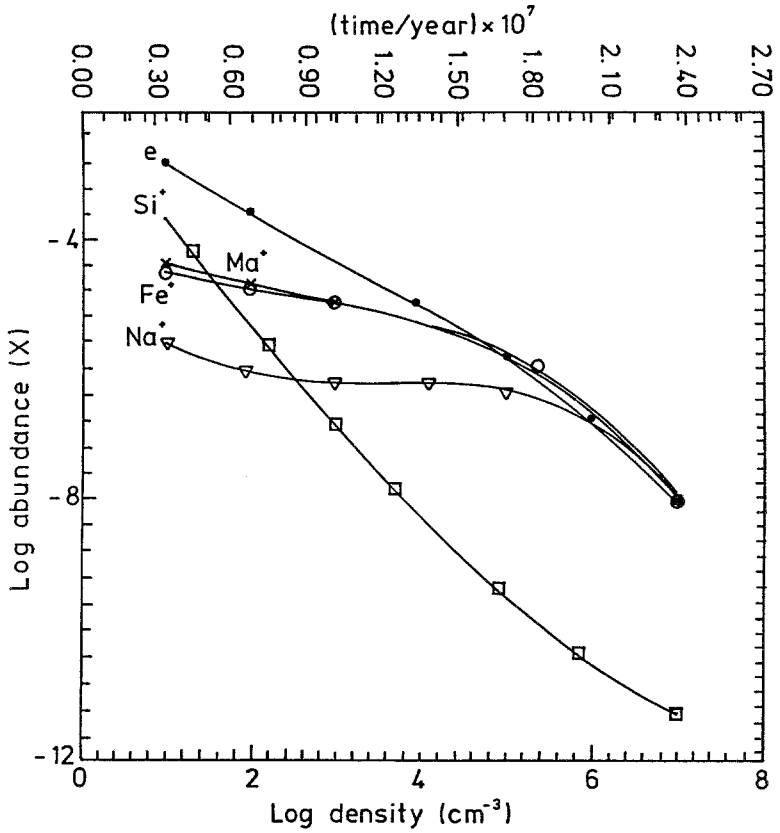

Fig. 3. The abundance profiles of e, Si^+, Ma^+, Na^+ and Fe^+ with respect to density and time in a contracting cloud

The importance of metals to the ion balance in molecular cloud was pointed out by Oppenhimer and Dalgarno (1974a). Metal atoms are ionized principally by the charge exchange processes of the form :

$$H_3^+ + Me \longrightarrow Me^+ + H_2 + H, \qquad \text{(reactions No. 234–236)}$$

and are neutralized by relatively slow processes of radiative recombination i.e.,

$$e + Me^+ \longrightarrow Me + h\nu. \qquad \text{(reactions No. 79–81)}$$

Figure (7) describes the relative abundances of metalic ions. Note that Mg^+ and Fe^+ have higher abundances during evolution that Na^+ ion. They have the same values at a density of 10^7 cm^{-3}. This could be explained by the following reactions

$$Fe^+ + Na \longrightarrow Na^+ + Fe, \qquad \text{(reaction No. 556)}$$

$$Mg^+ + Na \longrightarrow Na^+ + Mg. \qquad \text{(reaction No. 557)}$$

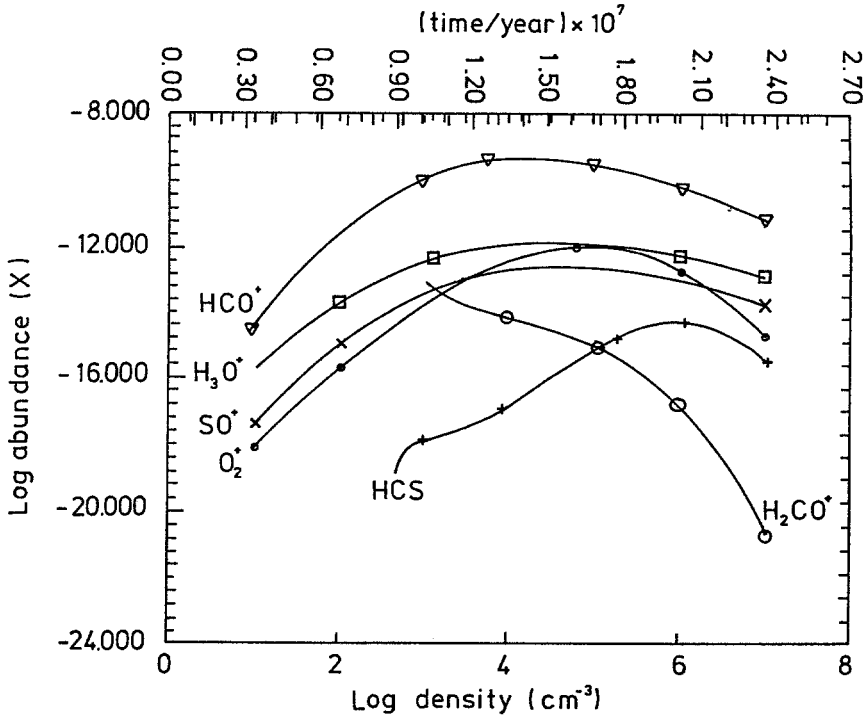

Fig. 4. The abundance profiles of HCO^+, H_3O^+, SO^+, HCS^+, H_2CO^+ and O^+_2 with respect to density and time in a contracting cloud

These reactions show that the abundance of Na^+ increases with the abundances of both Fe^+ and Mg^+. This result agrees well with that given by Oppenhimer and Dalgarno (1974a). Pineau des Forets *et al.* (1992) gave a similar value for the abundance of Fe^+. If we consider the effect of negative charged grains on ion reactions, the abundance of Me^+ will decrease via the reaction

$$g^- + Me^+ \longrightarrow g + Me.$$

On the other hand Si^+ has large values in the diffuse regions and sharply decays at the dense regions. Comparison between our result and that of Prasad and Huntress (1980b), reveals the following:

1. In the diffuse region the abundances of Mg^+ and Fe^+ are one or two orders of magnitude greater than those of Prasad and Huntress, respectively. Our calculated value for Na^+ is one order of magnitude greater than those of Prasad and Huntress. This is due to the difference of the initial values of the species Mg, Fe and Na in our and in their model. In addition, the values of A_v in our model differ from that in their model.
2. In the dense region, i.e., at a density of 10^5 cm^{-3}, the maximum abundance of Mg^+ is one order of magnitude greater than that of Prasad and Huntress. But

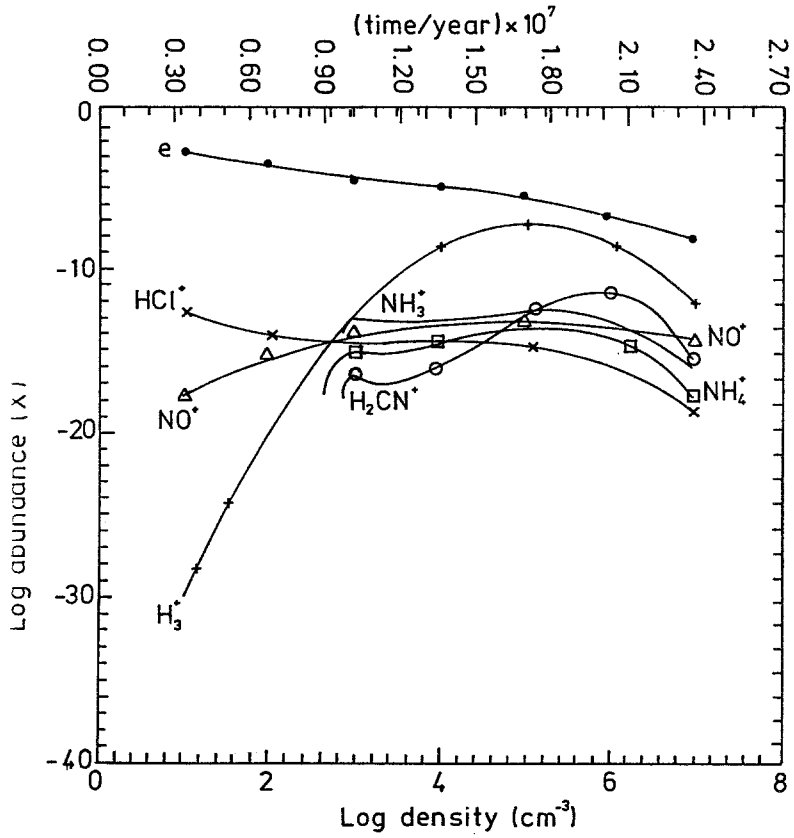

Fig. 5. The abundance profiles of e, NH^+_3, HCl^+, NH^+_4, H_2CN^+, $H^+_3$and NO^+ with respect to density and time in a contracting cloud

the maximum fractional abundance of Na^+ agrees well with that of Prasad and Huntress. The value for Fe^+ is about two orders of magnitude greater than that given by Prasad and Huntress.

It is not surprising that molecular ions have only a slight influence on the charge balance, as long as the cosmic ray ionization rate is larger than 5×10^{-19} s^{-1}. This is contrary to the opinion of early authors, Solomon and Klemperer (1972) and Herbst and Klemperer (1973). In the shielded region, ionization is maintained by cosmic rays. The efficiency of cosmic ray ionization, however, is much lower than that of direct ionization. Moreover most of the positive charge is accumulated by the Me^+ ions and so prevented from inducing new ion-neutral reaction chains (at least in the reaction scheme considered here). The important molecular ions in our model are: H_3^+, O_2^+, H_3O^+, HCO^+, SO^+, HCS^+, NH_3^+, HN_4^+, NO^+, H_2CN^+, H_2Cl^+, and HCO_2^+.

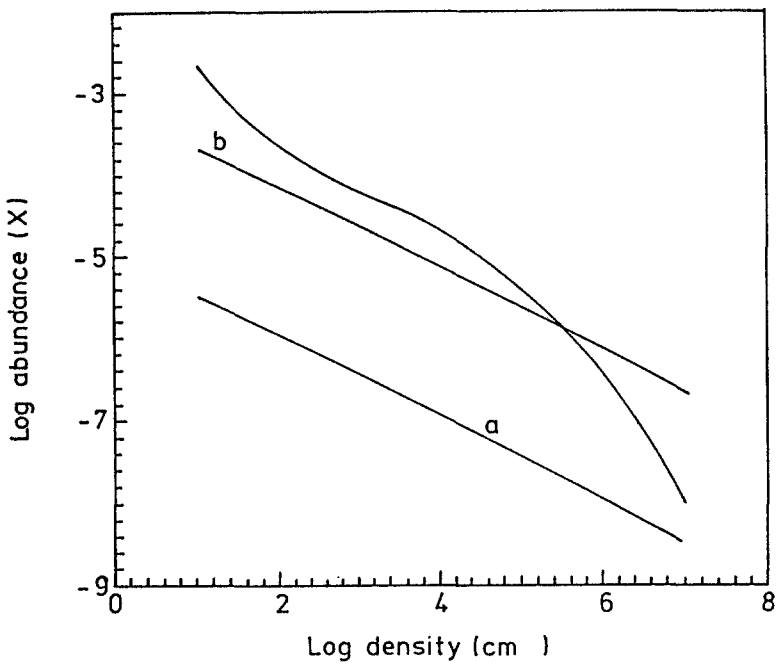

Fig. 6. The comparison between our result and both of that of El Nawawy *et al.* (curve b) and Nakano (curve a) for the abundance profile of electron in a contracting cloud.

Due to the chemical properties of H_3^+, it is the most important ion of the hydrogen family since it allows molecular hydrogen attachment through ion-neutral reaction, i.e.,

$$H_2^+ + H_2 \longrightarrow H_3^+ + H. \qquad \text{(reaction No. 157)}$$

Its sensitivity towards photo-destruction and the necessity of H_2 for its synthesis confine this molecule to the denser regions inside the contracting cloud. In the heavily shielded regions, in particular, it is of great importance in the synthesis of hydrides. A large number of H_3^+ reactions was included in this model, which leads to a maximum concentration of H_3^+ of 1.7×10^{-7} at a density of 10^3 cm^{-3}. It decreases to 7.5×10^{-12} at the end of the calculations.The destructive mechanisms of H_3^+ involved in our model decreases the fractional abundance of H_3^+ to the above mentioned value. This is shown in Figure 8, which represents the abundance of the important atomic and molecular ions in our model during the contraction . Comparing our result for H_3^+ with that given by other authors, one can see that:

1. Our calculated value of H_3^+ agrees well with that of Langer and Graedel. (1989).
2. The maximum fractional abundance of H_3^+ is about two orders of magnitude greater than that of Herbst and Leung (1989).

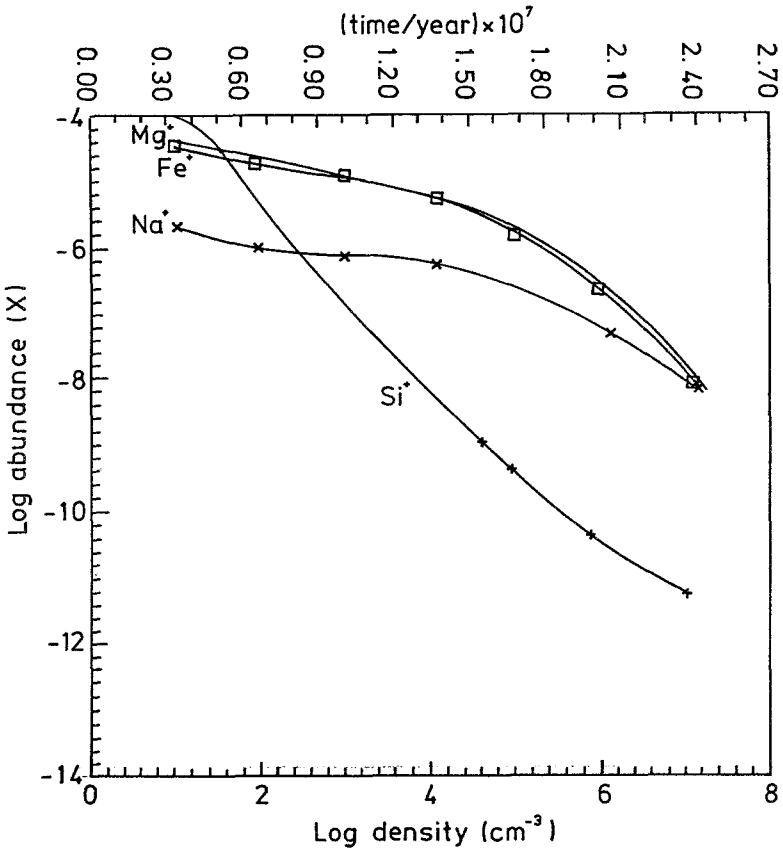

Fig. 7. The abundance profiles of Mg^+, Fe^+, Na^+ and Si^+ with respect to density and time in a contracting cloud.

3. At density of 10^5 cm^{-3} our fractional abundance for H_3^+ agrees well with that of Millar *et al.* (1991).

HCO^+ is one of the most important molecular ions in the shielded region. It is essential for the production of more complex molecules. The maximum abundance of HCO^+ is 1.4×10^{-9} at a density of 10^5 cm^{-3}. In dense regions, this value is in agreement with that observed in Orion Ridge cloud, (Caselli *et al.*, 1993). A similar value was also predicted by Millar *et al.* (1991) and Pineau de Forets *et al.* (1992). The abundance of HCO^+ at low density is less than that observed in diffuse clouds or that calculated by Prasad and Huntress (1980b). This result is due to several reasons:

1. The initial abundances of the elements in our model are different from those used in the model of Prasad and Huntress.
2. The contraction time in our model was less than the required steady state time.

At a density of 10^7 cm^{-3} our calculated fractional abundance of HCO^+ decreases due to the destruction by hydrogen molecules.

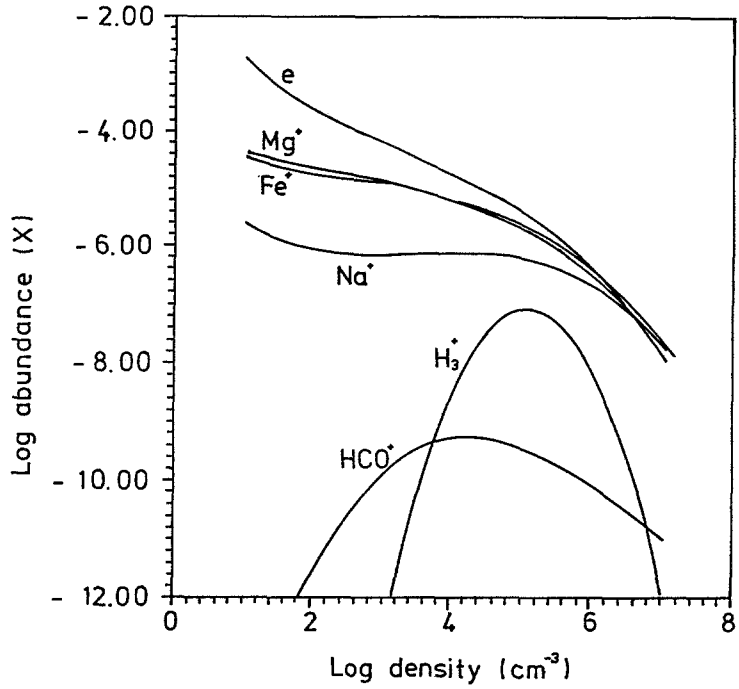

Fig. 8. The abundance profiles of e, $H^+{}_3$, Mg^+, Na^+, Fe^+ and HCO^+ with respect to density and time in a contracting cloud.

In the shielded regions H_3O^+ is one of the most abundant ions. It is the product of a molecular hydrogen attachment reaction whose beginning is set by H_3^+, e.g.,

$$H_2^+ + H_2 \longrightarrow H_3^+ + H, \qquad \text{(reaction No. 57)}$$

and

$$H_3^+ + H_2O \longrightarrow H_2 + H_3O^+. \qquad \text{(reaction No. 217)}$$

In the diffuse region, the abundance of H_3O^+ is 1.7×10^{-14}. This value agrees well with that of Prasad and Huntress (1980b). At a density of 10^5 cm^{-3} the maximum fractional abundance of H_3O^+ agrees well with that of Prasad and Huntress (1980b), while it is two orders of magnitude smaller than that given by Langer and Graedel (1989).

Negative ion – atomic collisions have been the subject of detailed and accurate experimental measurements. They have provided the opportunity of developing new theoretical methods to deal with bound state continuum interactions. In an $A^- - B$ collision, electron detachment is the most important process (Gauyacq, 1980):

$$A^- + B \longrightarrow A + B + e.$$

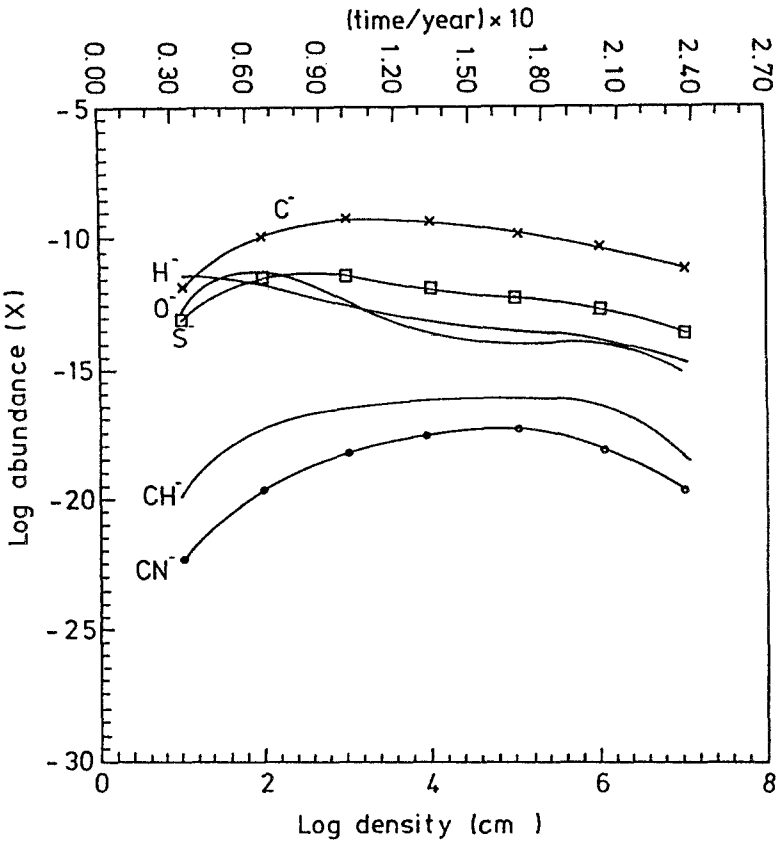

Fig. 9. The abundance profiles of negative species, with respect to density and time in a contracting cloud.

Figures 9 and 10 show that the abundance of H^- depends on the concentration of hydrogen atoms. The abundance of H^- in the diffuse region is smaller than the values reported by Henning (1981), and Black and Dalgarno (1977). Conversely, our results are larger than their values in the shielded region. At a density of 10^4 cm^{-3}, the fractional abundance of H^- equals 1.1×10^{-13}, which agrees well with that of Millar *et al.* (1991).

Our model predicts similar behaviour for results of the concentration of O^- as that of Henning (1981). In the diffuse region our concentration of O^- is less than that of Rudkjoebing (1976) by 4 orders of magnitude. This may be attributed to the fact that we did not account for the reaction

$$OH + e \longrightarrow O^- + H.$$

At a density of 10^4 cm^{-3} the abundance of O^- is three orders of magnitude greater than that of Millar *et al.* (1991). This is attributed to the greater value of electron fractional abundance in our model as compared to that of Millar *et al.*. The fractional

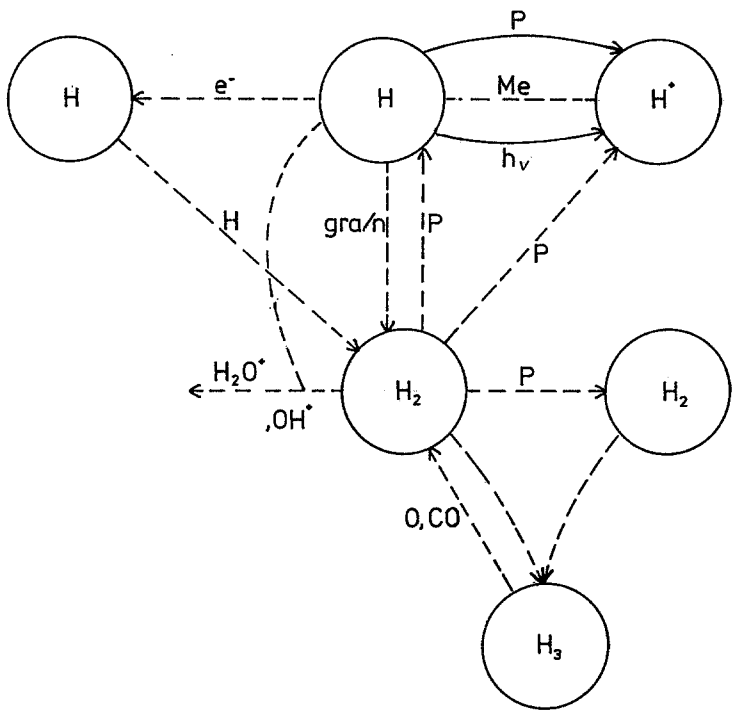

Fig. 10. The chemical network for hydrogen family in both diffuse and dense regions.

abundances of C^- and S^- are 5 orders of magnitude greater than that of Millar *et al.* (1991). This is because our electron fractional abundance is greater than that of Millar *et al.*.The fractional abundance of CN^- is three orders of magnitude smaller than that of Millar *et al.* This is because our fractional abundance of CN is one order of magnitude smaller than that of Millar *et al.*, e.g.,

$$CN + e \longrightarrow CN + h\nu$$

In future we plan to study the negative ions in detail.

3. Conclusion

The fractional abundances of the charged species have been followed in this paper. The results of the fractional abundances of the dominant ionic species are in good agreement with the published works. The conclusions are summarized as follows:

1. The electron fractional abundance $x(e)$ changes from 10^{-3} to 10^{-4} in the diffuse region. In the intermediate region we have $x(e) \simeq 10^{-5}$ and in the dense region $x(e)$ decreases from 10^{-6} to less than 10^{-8}.

2. The most dominant ionic species in the shielded region are metallic ions, HCO^+ and H_3^+. In the diffuse and intermediate regions the atomic ions H^+, C^+, Si^+, He^+, S^+ and metal ions are more dominant than molecular species.
3. Negative ions are negligible.
4. The fractional abundance of electrons $x(e)$ is given by
   $$x(e) = an^{-0.5}$$
   where a ranges between 6×10^{-3} and 2×110^{-4}.
5. Detailed calculations of metallic ions were followed. Our value of Fe^+ is similar to that given by Pineau des Fortes *et al.* (1992). The values of the other metal ion species are also in agreement with the previous theoretical calculations.
6. In the shielded regions, H_3O^+ is one of the most abundant ions.
7. Our calculated value of HCO^+ is in agreement with the observation in both TMC-1 and Orion clouds.
8. In the diffuse region the electron fractional concentration shows values between 10^{-3}, and 10^{-4}. In the intermediate region we have $X(e) = 10^{-5}$ and in the shielded region the electron densities were in the range of 10^{-6} to 10^{-8}.
9. The charge balance is determined by H^+ and C^+ in the diffuse region, by Me^+ (Mg^+, Fe^+, Na^+) in the shielded region, and by H^+, C^+, Si^+, He^+, S^+, and Me^+ in the intermediate region. He^+ has no influence on the ionization balance at high densities.

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