

TIME DEPENDENT CHEMICAL STUDY OF CONTRACTING INTERSTELLAR CLOUDS. II. ABUNDANCES OF OXYGEN- AND SULPHUR-BEARING MOLECULES

M. Y. AMIN¹, M. S. EL NAWAWY², B. G. ATEYA³ and A. AIAD⁴

¹*Astronomy Department, Faculty of Science, Cairo University;* ²*Physics Department, Faculty of Science, U.A.E. Univ., Al-Ain United Arab Emirates;* ³*Chemistry Department, Faculty of Science, Cairo University;* ⁴*Astronomy Department, Faculty of Science, King Saud University*

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Abstract. Abstract. We have constructed a chemical reaction system in a contracting interstellar cloud. In paper (I) we have presented the details of the physical and chemical scheme and the method of solution. The results of our chemical model produce fractional abundances of H₂CO, CO, OH, H₂O, SO and OCS which are in good agreement with the results of observations. On the other hand, the results of chlorine-bearing species are not in agreement with those of the observations. The calculated abundances of H₂CO, CO, OH, H₂O, SO, OCS and Cl⁺ are in agreement with the results of previous theoretical studies.

1. Introduction

The time dependent chemical structure of interstellar clouds during contraction in attracting considerable attention. In part (I) of this series (Amin *et al.*, 1995a), we presented a model which gave abundances on nitrogen- and carbon-bearing molecules during contraction. In this paper, we present the model predictions regarding the abundance of oxygen-, chlorine-, and sulphur-bearing molecules. The reaction scheme was given by Amin (1994) while the formulation of the model, the basic assumption and the solution technique were detailed in part (I), Amin *et al.* (1995a). The abundances of the species at time step $t = t_0 + \Delta t$ was taken from the previous time step while the density was updated from the contraction model. The chemical kinetic equations were integrated as a function of time using gear program. The fractional abundance of a species is denoted by X , where

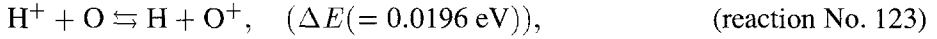
$$X = n(x)/n \text{ and } n = n(\text{H}) + 2n(\text{H}_2).$$

In Section 2 the results are given and the conclusions are summarized in Section 3.

2. Results

2.1. OXYGEN CHEMISTRY

Oxygen has an ionization energy that is almost equal to that of hydrogen. The charge transfer reaction



has a rate coefficient of $7 \times 10^{-10} \exp(-232/T)$ in the exothermic direction, Millar *et al.* (1991). The laboratory measurements by Federer *et al.* (1984) and Watson (1973) and the calculations of Chambaud *et al.* (1980) indicated a rapid charge transfer in the forward reaction with a rate coefficient of about $5 \times 10^{-10} \text{ cm}^{-3} \text{ s}^{-1}$ for exothermic reaction (reverse direction). Both these values were used in the present calculations.

The species O^+ reacts with H_2 ultimately to produce OH and H_2O , as shown below,



In this case further reactions with H_2 are possible and occur rapidly (Watson, 1973, and Black and Dalgarno, 1973),



followed by



More complex molecules containing oxygen (e.g., CO_2 , HCO , CO_2^+ , HCO_2^+ , OCS , H_3O^+) are then formed by the reactions with OH and H_2O . Neutral-neutral reactions with the OH radical are more important in the shielded regions than the neutral-ion or ion-ion reactions since carbon, sulphur, ... etc. exist predominantly as neutral species. For example, the reaction



leads to the formation of HCO^+ which is the first molecular ion detected in the dense shielded clouds. Early support for the ion molecular scheme in dense clouds arose from its success in predicting the HCO^+ abundance. It is a molecular species

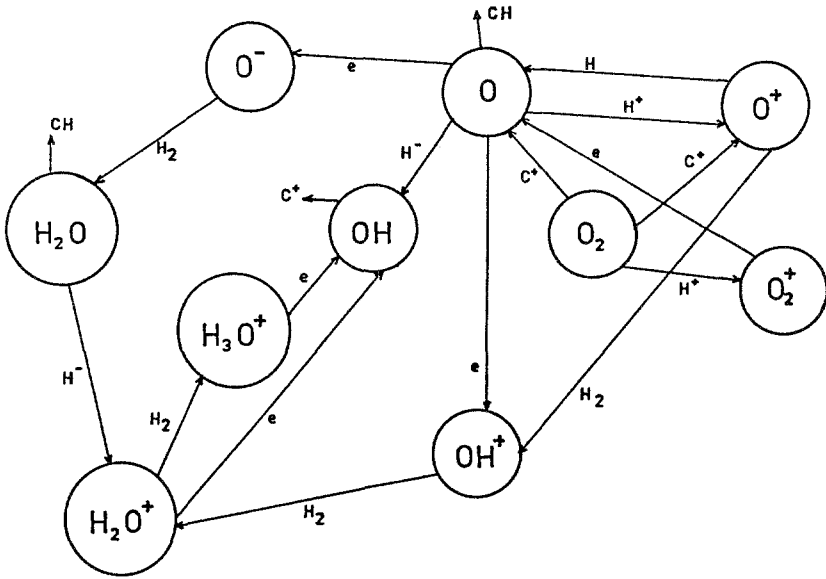


Fig. 1. The chemical network for oxygen family in the diffuse region.

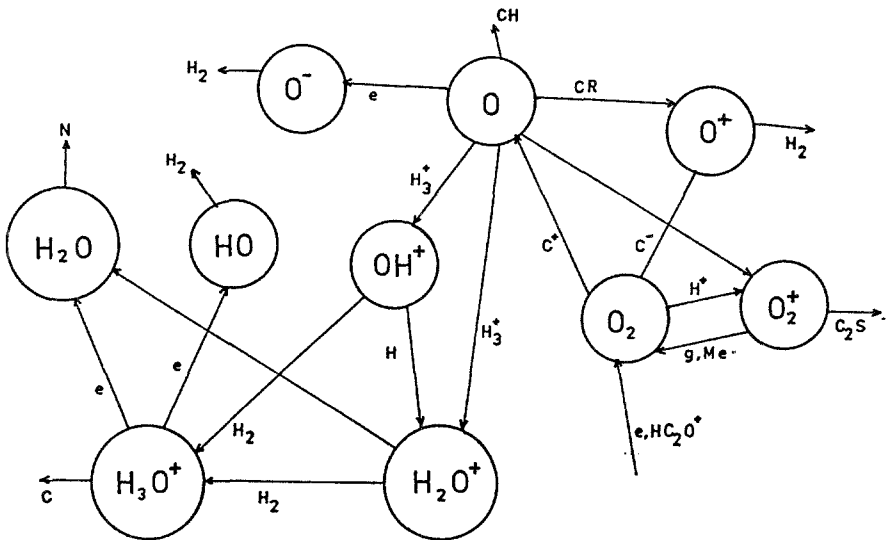


Fig. 2. The chemical network for oxygen family in the dense region.

whose production was hard to establish by any chemical scheme other than the ion-molecule chemistry .

Figures 1, 2 and 3 represent the chemical network of the oxygen family in diffuse and dense regions, respectively, while Figure 3 shows the abundance profiles for

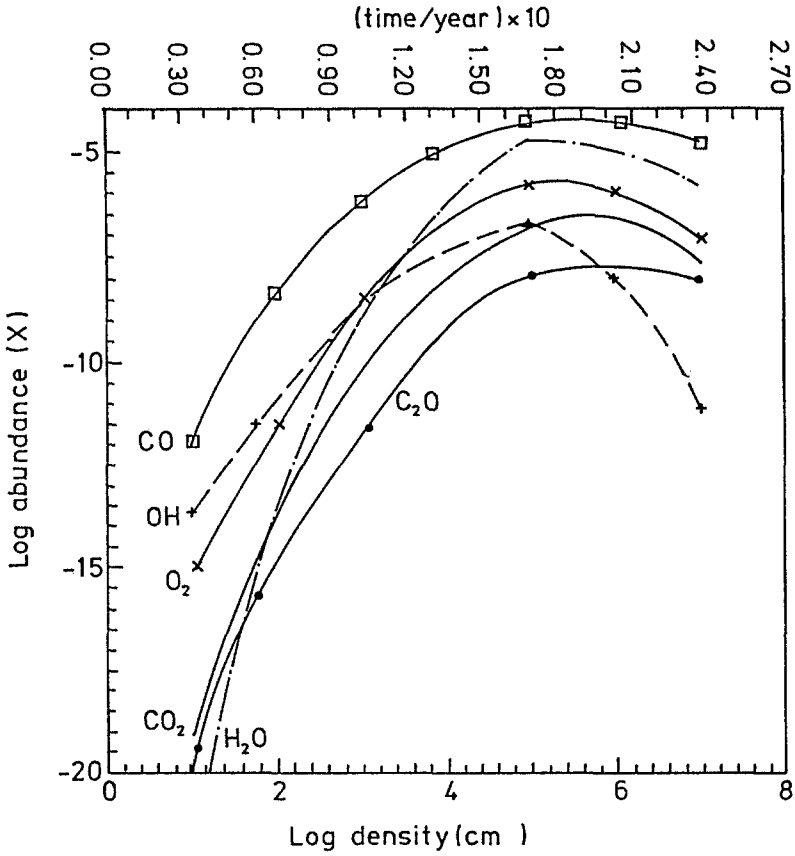


Fig. 3. The abundance profiles of oxygen family with respect to density and time in a contracting cloud.

TABLE I

The maximum fractional abundance for oxygen bearing molecules

Species	Our calculated value	Observed value	
		TMC-1 ^A	Orion
CO	5.70 (-05)	8.00 (-5)	8.00 (-5) ^{F,O}
OH	1.80 (-07)	3.00 (-7)	
H ₂ O	2.10 (-07)		2.00 (-07) ^B

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

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

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

F: For Orion ridge cloud by Hydbeck and Hjalmarson 1985.

B: Black *et al.* (1987).

the various neutral species of the oxygen family. Comparisons with the results of observations are given in Table I.

In our model O_2 is formed by the reactions



and by some other charge transfer reactions. It is destroyed by photo-dissociation and ion-molecular reactions.

The abundance of O_2 increases to a value of 1.6×10^{-6} at a density of 10^5 cm^{-3} , and decreases to a value of 1×10^{-7} at the end of the calculations. The above greater value agrees well with that reported by Herbst and Leung (1989) and Langer and Graedel (1989).

Carbon Monoxide, CO, is produced in the diffuse region mainly by destruction of HCO^+ , i.e.



Here it is nearly coupled to CO^+ via charge exchange, i.e.



With decreasing ion concentration in the shielded regions, the neutral-neutral attachment reactions became more important for CO.

The carbon Monoxide shows a high abundance in the dense region. It is one of the most important molecules in this region. This is because CO is the most strongly bound diatomic molecule, hence it is not easily destroyed. In view of the high stability of CO, the only significant destructive reaction for it is the dissociative charge transfer by He^+ , i.e.



It is also a fractionalization product of many heavier H—C—O molecules. As only few molecules and rates of this kind were included in this model, it is probable that an extension of the chemistry in this direction would bring even higher concentration of CO_2 . Comparison of our calculated maximum abundances of both CO and CO_2 with observations show that our value for CO is in agreement with that observed in TMC-1 cloud, Orion ridge and Orion plateau. But the abundance of CO in the diffuse region is smaller than that observed in ζ Oph cloud. Comparison with theoretical values calculated by other authors reveals the following:

1. Our value of CO is in agreement with that of Nejad *et al.* (1990), Pineau des Forets *et al.* (1992), Hasegawa and Herbst (1993) and Caselli *et al.* (1993).

2. The maximum fractional abundance of CO₂ is one or two orders of magnitude greater than that of Caselli *et al.* (1993) and Hasegawa and Herbst (1993).

The OH chemistry is widely different in the diffuse and the shielded regions. In diffuse part of the cloud, the abundance of OH is less than that observed in the ζ Oph cloud. The abundance of OH increases quickly to a maximum value of 1.8×10^{-7} at a density of 10^5 cm^{-3} and decreases to 7.5×10^{-12} at the end of the calculation. The H₂O concentration remains below that of the OH until the OH decreases and is converted into H₂O.

Our calculated values of OH and H₂O are in agreement with those observed in the TMC-1 cloud, and the compact region of the Orion cloud, respectively. The maximum fractional abundance of OH is in agreement with that calculated by Herbst and Leung (1989), Nejad *et al.* (1990), and Hasegawa and Herbst (1993). However, this value is about one order of magnitude greater than that given by Pineau des Forets *et al.* (1992). The maximum fractional abundance calculated for H₂O is in agreement with the values given by Pineau des Forets *et al.* (1992) and Hasegawa and Herbst (1993).

2.2. CHLORINE CHEMISTRY

In present model, the chlorine family is only weakly coupled to the other molecules. Figures 4 and 5 show, respectively, the chemical network and abundance profiles for the chlorine species. Our results show similar trends to those of Henning (1981), Dalgarno *et al.* (1974) and Jura (1974a,b). From Figure 5 we note the following:

1. The concentration of Cl⁺ in the diffuse region starts at a maximum value, which agrees well with that of Henning (1981). The maximum calculated fractional abundance for Cl⁺ is smaller than the observation in ζ Oph cloud. This possibly arose from the dependence of Cl⁺ formation on the visual extinction A_v . In a dense region, the concentration of Cl⁺ decreases quickly due to



2. The maximum fractional abundance of HCl⁺ is one order of magnitude smaller than that of Henning (1981) in both diffuse and dense regions. This is because the formation and destruction rates of HCl⁺ depends on A_v , H⁺, CL⁺, and on e , $h\nu$, and H₂, respectively, these variables were used with values different from those of Henning (1981).
3. The maximum concentration of HCl occurs at a density of 10^5 – 10^6 cm^{-3} . This maximum is one order of magnitude smaller than that reported by Henning (1981). In the diffuse region, the concentration of HCl decreases because of the following reactions:



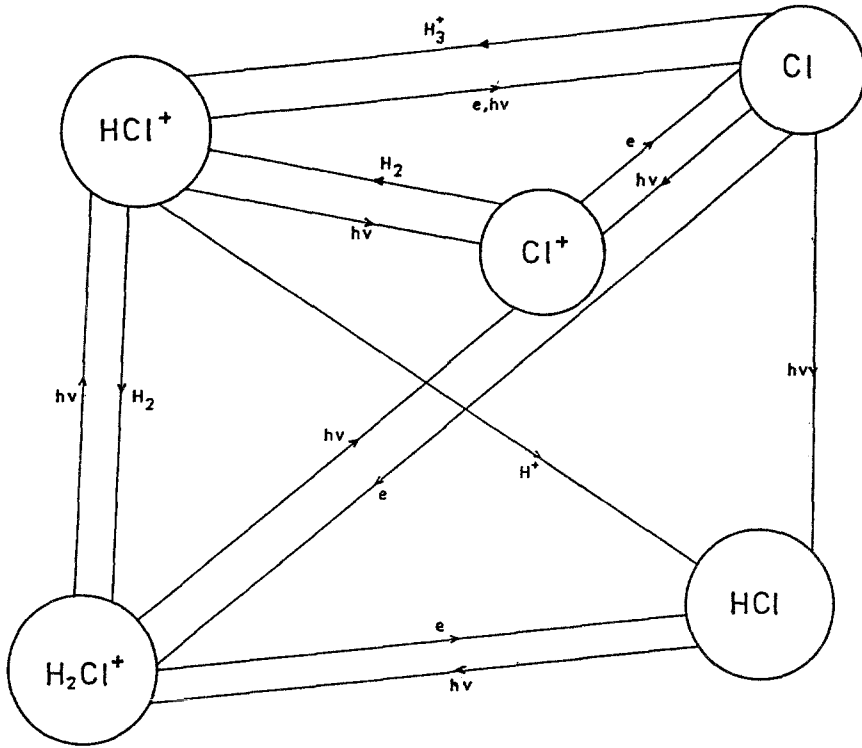


Fig. 4. The chemical network for chlorine family in both dense and diffuse regions.

4. The abundance profile of H₂Cl⁺ is similar to that of HCl, due to the reactions:



In the future we plan to study the chlorine chemistry in diffuse and dense clouds with new calculations of rate constants.

2.3. SULPHUR CHEMISTRY

The sulphur chemistry differs from that of carbon and oxygen. Even though the reaction



is exothermic (Amin *et al.*, 1991), the subsequent reaction of HS⁺ with H₂ is not. Oppenheimer and Dalgarno (1974a) suggested the use of the exothermic reaction



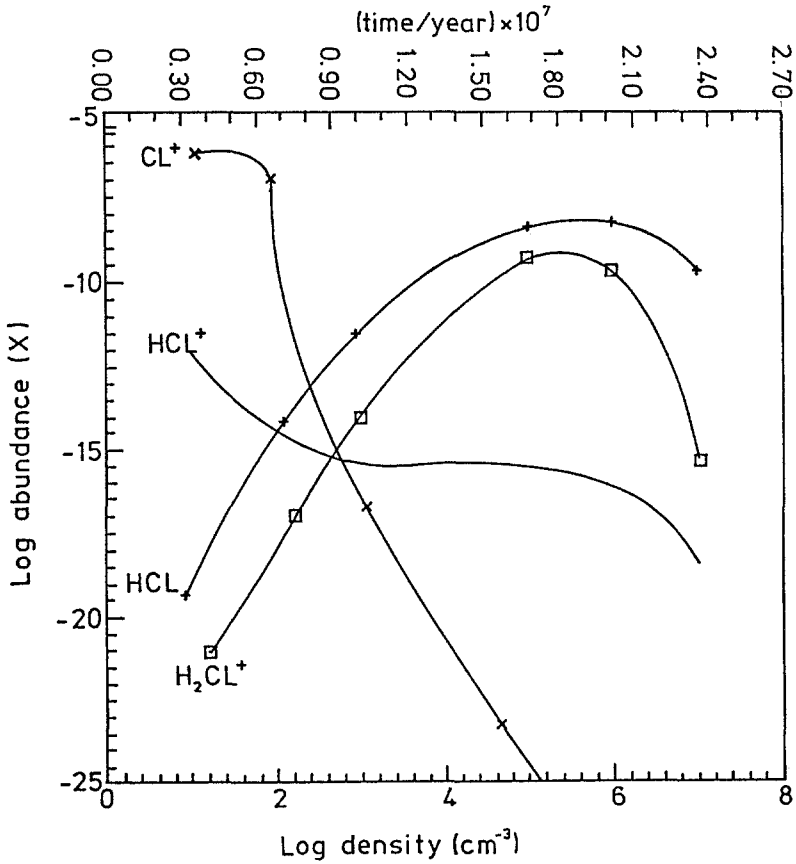


Fig. 5. The abundance profiles of chlorine family with respect to density and time in a contracting cloud.

The dominant form of sulphur in diffuse interstellar clouds is S^+ . Atomic sulphur, like atomic carbon, has an ionization potential which is less than that of hydrogen. Furthermore, the reaction:



is more endothermic than the analogous reactions (Millar *et al.*, 1986)



The possibility of detecting HS^+ in the interstellar medium and in other astrophysical objects has been considered by Horani *et al.* (1985). These authors gave the relevant spectroscopic data which, together with a prediction of the expected column density of the molecular ion, enables equivalent widths to be estimated. A good summary of sulphur chemistry in clouds can be found in Pineau des Forets *et al.* (1986b).

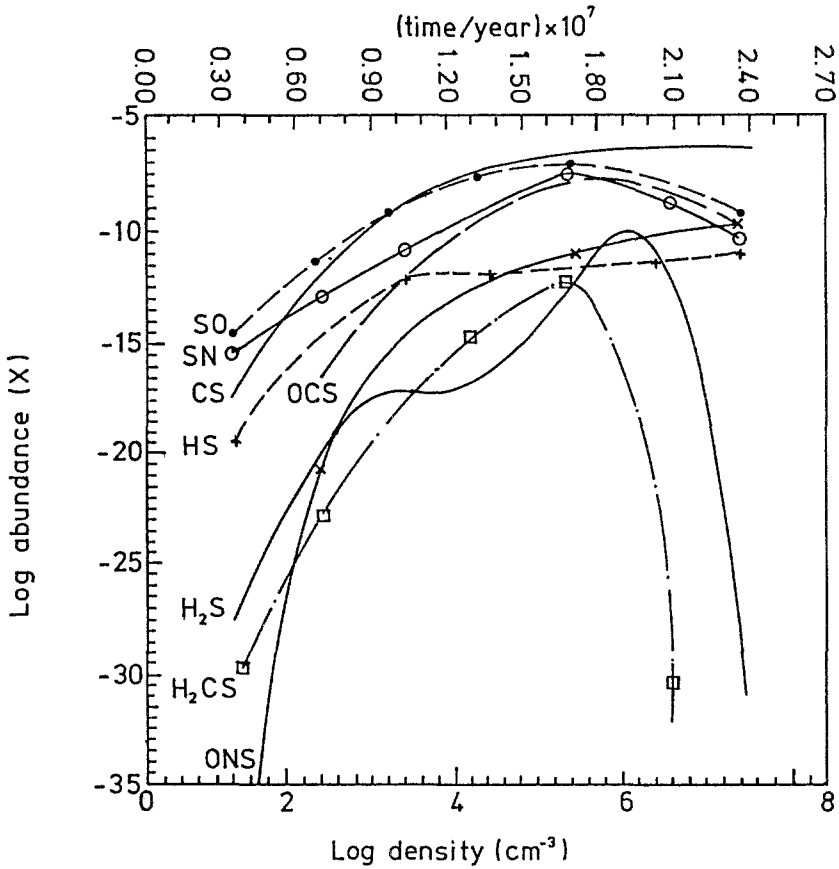


Fig. 6. The abundance profiles of sulphur family with respect to density and time in a contracting cloud.

Figures 6, 7 and 8 represent the maximum fractional abundances and chemical network for sulphur chemistry. The comparison with the observations are given in Table II.

The chemical reactions that produce diatomic sulphur molecules in our model include primarily reactions of sulphur with carbon, oxygen, and nitrogen-bearing molecules, Amin (1994).

As shown in Figure 6 in the diffuse region, SO has a maximum value, and in the shielded region CS has the maximum value of the diatomic molecules in this family. SN is formed in the diffuse region with the aid of S^- while in the shielded regions it is formed via neutral-neutral reactions. The abundance of OCS is greater than that of SN. This result differs from that of Henning (1981). The ONS species has a small value in this family.

Comparison of the maximum fractional abundances of this family with the observations reveals that:

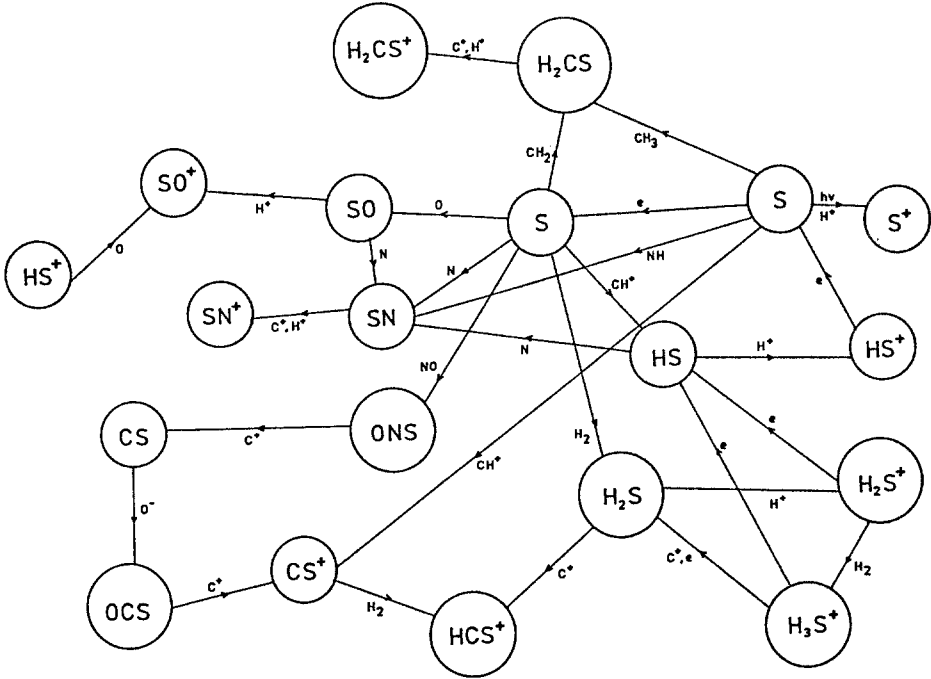


Fig. 7. The chemical network for sulphur family in the diffuse region.

TABLE II

The maximum fractional abundance for sulphur bearing molecules

Species	Our calculated value	Observed value	
		TMC-1 ^A	Orion
CS	8.80 (-07)	1.00 (-08)	5.00 (-09) ^F
			5.00 (-08) ^O
			2.00 (-06) ^O
SO	9.90 (-08)	5.00 (-09)	5.00 (-09) ^F
			2.00 (-08) ^C
			2.00 (-08) ^O
OCS	1.70 (-08)	2.00 (-09)	9.00 (-09) ^F
			1.00 (-08) ^O
			1.00 (-07) ^O
H ₂ S	1.40 (-10)	3.00 (-09) ^F	3.00 (-09) ^F
			3.00 (-09) ^F
H ₂ CS	7.70 (-13)		3.00 (-09) ^F

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

Other symbols are the same as those of Table I.

C: Caselli *et al.*, 1993.

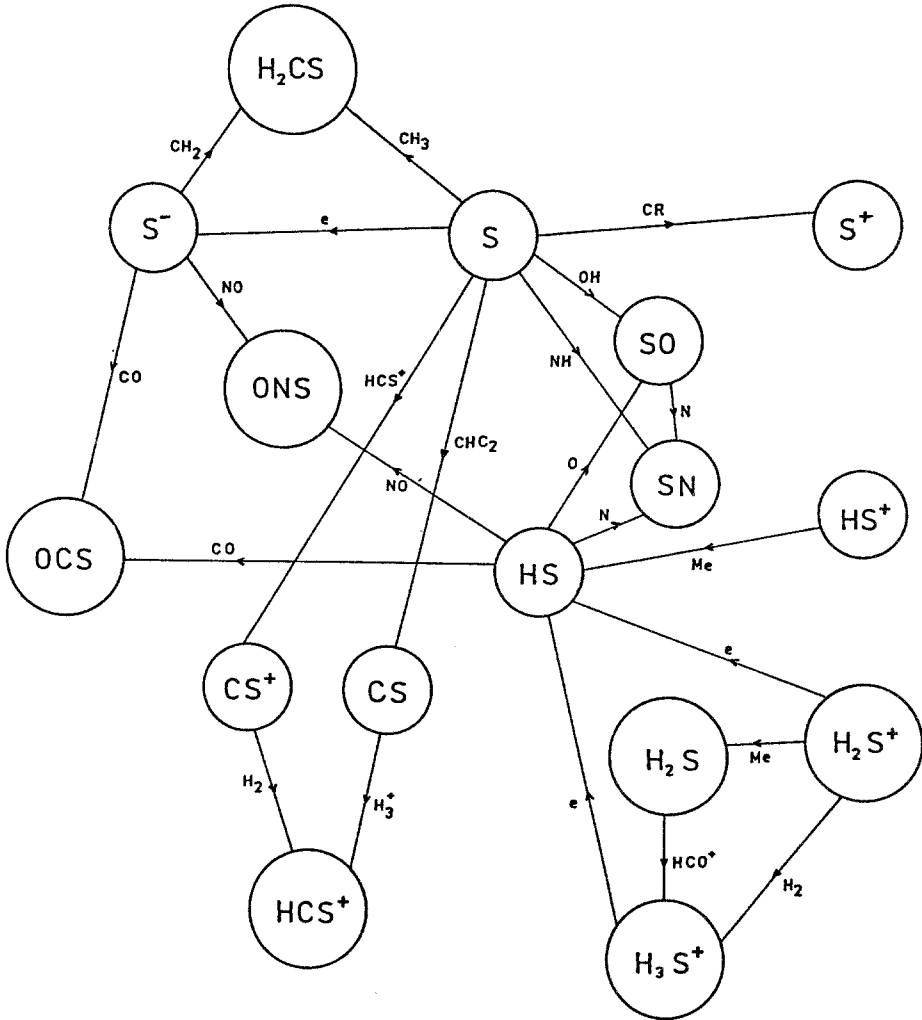


Fig. 8. The chemical network for sulphur family in the dense region.

1. Our value of CS in the density range $n = 10^5 - 10^7 \text{ cm}^{-3}$ is one order of magnitude greater than that observed for TMC-1 cloud and Orion ridge, or two orders of magnitude greater than that observed in Orion plateau.
2. The maximum fractional abundance of SO at a density of 10^5 cm^{-3} is in agreement with that observed in the compact region of the Orion cloud and is about one order of magnitude greater than that for the TMC-1 cloud and Orion ridge.
3. The maximum value of OCS the abundance of the molecule at a density of 10^5 cm^{-3} is in agreement with that observed for Orion plateau. This value also is about one order of magnitude greater than that observed for the TMC-1 cloud, and Orion ridge.

Comparing our results with those calculated by earlier authors, we note that:

1. The maximum value for CS agrees well with that of Nejad *et al.* (1990). This value is greater than that of Langer and Graedel (1989) by two orders of magnitude.
2. Our value for SO agrees with that given by Williams and Hartquist (1991). However it is about one order of magnitude greater than that reported by Caselli *et al.* (1993).
3. The maximum fractional abundance of SN at a density of 10^5 cm^{-3} is two orders of magnitude greater than those of Leung *et al.* (1984), and Hasegawa and Herbst (1993).
4. The maximum value for OCS is in agreement with those of Herbst and Leung (1989), and Hasegawa and Herbst (1993). This value is one order of magnitude greater than those of Nejad *et al.* (1990), and Williams and Hartquist (1991).

The molecules HS and H₂S require a high temperature to be formed by S and H₂ (Amin *et al.*, 1991). In this model, H₂S shows greater abundance than HS. The maximum abundance of H₂S agrees with that of Herbst and Leung (1989). The HS and H₂S molecules are formed by ion-molecular reactions and by negative-ion reactions (see Figure 8). The H₂CS molecule has the lowest abundance in this group. Comparison of the maximum fractional abundance of the sulphur family with the observed and theoretically calculated values. One can see that:

1. Our calculated value for H₂S at a density of 10^6 cm^{-3} is one or three orders of magnitude smaller than those observed in Orion ridge and Orion plateau, respectively.
2. The maximum fractional abundance of H₂CS at a density of 10^5 cm^{-3} is about four orders of magnitude smaller than that observed in Orion ridge.
3. The maximum fractional abundance of HS at a density of 10^7 cm^{-3} agrees well with those of Herbst and Leung (1986) and Hasegawa and Herbst (1993).
4. Our value for H₂S agrees with those of Herbst and Leung (1989), and Nejad *et al.* (1990).
5. The maximum value of H₂CS is about one or three orders of magnitude smaller than that given by Herbst and Leung (1986), and Langer and Graedel (1989).

3. Conclusion

The present model shows that CO, Cl⁺, HCl⁺ are the most abundant species in diffuse cloud. The time of chemical evolution was assumed equal to the time of contraction. Therefore, in diffuse region the time of contraction is smaller than the time required to reach steady state. Consequently the calculated abundances of CO and Cl⁺ are less than that observed in ζ Oph cloud. As the density increases to

intermediate values the abundances of the molecules CO, OH, O₂ and H₂O; HCl and H₂Cl; and SO, S, SN, HS and OCS increase relative to their values in the diffuse region, see Figures 3, 5 and 6, respectively. As the contraction proceeds to the dense region all molecules increase to their maximum values. Our chemical model produces fractional abundances of H₂CO, CO, OH, H₂O, SO and OCS which are in good agreement with the results of observations. On the other hand, the results of chlorine family are not in agreement with the results of previous theoretical studies. Furthermore, the calculated abundances of H₂CO, CO, OH, H₂O, SO, OCS and Cl⁺ are in agreement with the results of previous theoretical studies. As shown in Figures 3, 5 and 6, CO, H₂O, HCl, CS and SO are the most dominant molecules in dense region. In the following paper we will introduce the charge state distribution in interstellar clouds.

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