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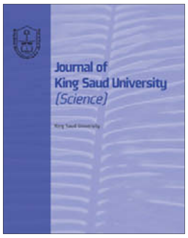

ORIGINAL ARTICLE

Deuterium-bearing molecules in cold and warm dense interstellar clouds

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Abstract We have studied the production of key observed deuterium species for TMC-1, Orion, L134N and W3IRS4 clouds, of densities 10^4, 10^4, 5×10^4, and 10^6 cm^{-3}, respectively, by using the pseudo-time dependent gas-phase chemistry. These clouds have temperatures in the range 10–70 K. The main results by using the more extensive chemical network with the most updating reaction rates show that the most of calculated fractional abundances are in agreement with observations, and suggest that triply-deuterated ammonia could be detectable in dark clouds. Also our models show that large abundance of NH_2D and NHD_2 can be produced in the interiors of cold dense clouds at steady state time.

1. Introduction

Because deuterium-bearing molecules used to: probes of the physics of interstellar clouds, study the relation of connection between interstellar and cometary ices and understand the formation mechanism of isotopic composition of interstellar molecules (Roberts and Millar, 2000a; Robets et al., 2002; Shah and Wotten, 2001; van der Tak et al., 2002). Therefore many theoretical and observational studies which have concerned on the formation of deuterated molecules in interstellar clouds.

In the last few years the studying of doubly-deuterated molecules in the interstellar medium has gained considerable attention. This is due to a large amount of doubly-deuterated formaldehyde, D_2CO, and ammonia, NHD_2, have been observed towards low mass protostar IRAS16293-2422 (Ceccarelli, 1998), Orion cloud (Turner, 1990), very young protostellar core 16293E (Loinard et al., 2001) and in the molecular cloud L1689N (Ceccarelli et al., 2002; Loinard et al., 2001). Also NHD_2 observed in the molecular cloud L134N (Roueff et al., 2000). While triply-deuterated ammonia, ND_3, observed in the low mass protostar NGC1333-IRAS4 (van der Tak et al., 2002), in the dark cloud B1 (Lis et al., 2002). But the methanol observed in the low mass protostar IRAS16293-2422 (Parise et al., 2002). All these observations suggest that deuteration of formaldehyde and methanol is produced during the cold and dense cloud (Ceccarelli et al., 2001).

There are two chemical networks for the formation of the deuterated molecules:

First, some deuterium-bearing molecules can be formed by the gas-phase reactions (Millar et al., 1989; Rodgers and

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Millar, 1996; Roberts and Millar, 2000a; Robets et al., 2002). At low temperatures 10–70 K, the H_2D^+ species is the key of gas-phase reaction to form DCO^+ and N_2D^+ (van der Tak et al., 2002). By gas-phase network, Lis et al. (2002) explained the observed abundance ratio of ND_3 in B1 cloud. Similarly, Tine et al. (2000) investigated the fractional abundance of NH_2D, which observed in L183 and TMC-1 clouds.

Second, the surface chemistry, in which deuterated molecules can be formed on dust grains. The high abundances of HDCO, D_2CO and CH_3OD in warm clouds are derived from the occurrence of grain surface chemistry during an earlier cold era followed by evaporation into the gas as temperature rise (Ceccarelli et al., 2001; Caselli et al., 2002; van der Tak et al., 2002; Parise et al., 2002). The formation of singly- and doubly-deuterated isotopomers of formaldehyde and singly-, doubly- and multiply-deuterated isotopomers of methanol on dust grain has been studied by Caselli et al. (2002), with a semi-empirical modified rate approach and Monte Carlo method in temperature range 10–20 K.

In the present work, we shall confine ourselves to calculate the chemical abundances of key observed deuterium species, in several different interstellar clouds and comparison with both available observation and other theoretical models which are given for justification. This paper is organized as follows, in Section 2, chemical models are given. Section 3 contains a brief description of our gas phase chemical models. The conclusions are given in Section 4.

2. Chemical models

In order to interpret the behavior of deuterium-bearing molecules on cold and warm interstellar clouds, we have carried a number of a pseudo-time dependent chemical models, which calculate the varying abundances of 408 species (130 of them containing deuterium) linked by 5320 reactions.

Our gas-phase model considers a standard gas-phase chemistry, in which we consider only reactions between gaseous species, with the exception that H_2 and HD forming on the grain surface, and we neglect the three body reactions.

Roberts and Millar (2000a,b) developed new models for the chemistry of deuterium, to investigate the fractionation of doubly-deuterated species, in interstellar molecular clouds. These models depend on a wide range of physical parameters including, density, temperature, elemental abundances and the freeze out of molecules on the dust grains. Our model is partially based on that part of gas-phase reactions of Roberts and Millar (2000a,b) for producing doubly-deuterated species. Our model extended the models of Roberts and Millar (2000a,b) to include multiply-deuterated ammonia.

The mono-deuterated reaction set is complete in the sense that for every reaction containing a hydrogen-bearing molecule there is an analogue reaction containing the equivalent mono-deuterated species. If more than one reaction product contains hydrogen atoms then uncertainly arises as to which will be the deuterium-bearing product. Due to lack of comprehensive experimental data, the usual approach is to assume statistical branching ratio between the various possibilities (Millar et al., 1989; Rodgers and Millar, 1996).

In this study we were interested in the chemistry of doubly-deuterated ammonia, NHD_2. We also interested with multiply-deuterated ammonia, which begin after the formation of NH_3, with deuterated ions XD^+. In this model the metals (Fe, Mg, Na and Si) play an important role in determining the ionization fraction.

Since the chemical structure of interstellar clouds depends on the temperature, the radiation field and density number, then we have adopted four models of initial elemental (see Table 1), to study the deuterium chemistry in TMC-1, Orion, L134N and W3 IRS4 clouds. We have neglected the chemistry of species of polycyclic aromatic hydrogen type and their reaction with smaller molecules. As Herbst and Leung (1986) we also neglected the effects of enhanced rate coefficient in ion-polar neutral reactions. The chemical scheme used here is based on that of the most recent UMIST rate file, RATE99 (Le Teuff et al., 2000), with updating the rate coefficients of some modifications by Chastaing et al. (2001). We have adopted the cosmic D/H ratio measured by Linsky et al. (1995). We used a constant ratio for C/O. We neglect the effect of X-ray ionization. The electron abundance is set equal to the sum of the ion abundances.

3. Results and discussion

We have followed a large number of runs for the four models listed in Table 1. Using a different initial elemental abundances and cosmic ray ionization rate, the best initial elemental abundances are given in Table 2.

The cosmic ray ionization rate of $1.3 \times 10^{-17}\ s^{-1}$ is used for models (1)–(3) and high cosmic ray ionization rate of $1.3 \times 10^{-16}\ s^{-1}$ is used for model (4). The reduction of the initial elemental abundances and a high cosmic ray ionization rate used in model (4) is in agreement with Amin (1999).

Tables 3–6 compare the molecular D/H ratios observed toward the above four clouds, with the results from our gas-phase models at both early (10^5 year) time and steady state (100 million year) time, and other theoretical calculations.

Table 1 Our models, where *n* is number density.

Model	*n* ($m^{-3)}$	*T* (K)	Average (mag.)	Clouds
1		10	10	TMC-1
2	1 (4)	70	10	Orion
3	1 (4)	10	15	L134N
4	5 (4)	55	30	W3 IRS4

Table 2 Initial fractional abundances.

Species	Model 1	Model 2	Model 3	Model 4
H_2	0.5	0.5	0.5	0.5
C^+	7.3 (−5)	7.3 (−5)	7.3 (−5)	4.0 (−6)
O	1.7 (−4)	1.7 (−4)	1.7 (−4)	8.0 (−6)
N	2.14 (−5)	2.14 (−5)	2.14 (−5)	5.1 (−6)
S	1.0 (−7)	1.0 (−7)	1.0 (−7)	6.0 (−8)
Si	2.0 (−8)	2.0 (−8)	2.0 (−8)	1.5 (−10)
Fe^+	1.0 (−8)	1.0 (−8)	1.0 (−8)	1.5 (−10)
Mg^+	1.0 (−8)	1.0 (−8)	1.0 (−8)	1.5 (−10)
Na^+	1.0 (−8)	1.0 (−8)	1.0 (−8)	1.5 (−10)
H^{3+}	1.0 (−11)	1.0 (−11)	1.0 (−11)	0.0
HD	1.6 (−5)	1.6 (−5)	3.2 (−5)	5.0 (−6)
He	0.14	0.14	0.14	0.14

Table 3 A comparison of abundance ratio measured in TMC-1 cloud with predictions from our model (1) and Roberts and Millar (2000a).

Species	Observation	Our cal. M1		RM 2000		Ref.
		Early	Steady	Early	Steady	
DCO^+/HCO^+	0.02	0.018	0.082	0.019	0.087	Tine et al. (2000)
NH_2D/NH_3	0.009–0.014	0.086	0.029	0.084	0.028	Tine et al. (2000)
$HDCO/H_2CO$	0.0059–0.11	0.043	0.056	0.042	0.055	Turner (2001)
DCN/HCN	0.023	0.006	0.022	0.009	0.025	Turner (2001)
DNC/HNC	0.015	0.015	0.015	0.015	0.015	Wootten (1987)
C_2D/C_2H	0.01	0.012	0.028	0.011	0.027	Millar et al. (1989)
C_4D/C_4H	0.004	0.004	0.027	0.004	0.029	Turner (1989)
N_2D^+/N_2H^+	0.08	0.03	0.058	0.025	0.025	Tine et al. (2000)
C_3HD/C_3H_2	0.08–0.16	0.007	0.027	0.006	0.02	Bell et al. (1988)
C_3H_3D/C_3H_4	0.054–0.065	0.082	0.098	0.083	0.099	Gerin et al. (1992)
DC_3N/HC_3N	0.03–0.1	0.008	0.026	0.007	0.026	Howe et al. (1994)
DC_5N/HC_5N	0.013	0.023	0.026	0.023	0.026	MacLeod et al. (1981)
$HDCS/H_2CS$	0.02	0.04	0.05	0.04	0.046	Minowa et al. (1997)

Table 4 A comparison of abundance ratio measured in Orion cloud with predictions from our model (2) and Millar et al. (1989).

Species	Observation	Our cal. M2	M1998	Ref.
DCO^+/HCO^+	0.002	0.002	8 (−4)–8 (−5)	Penzias (1979)
NH_2D/NH_3	0.003	0.0029	4 (−4)	Walmsley et al. (1987)
$HDCO/H_2CO$	0.02	0.019	0.004–0.005	Loren and Wootten (1985)
DCN/HCN	0.006	0.0058	0.001–4 (−4)	Wootten (1987)
DNC/HNC	0.01	0.043	9 (−4)–2 (−4)	Wootten (1987)
C_2D/C_2H	0.045	0.032	0.003	Combes et al. (1985), Vrtilek et al. (1985)
CH_3OD/CH_3OH	0.01–0.06	0.005	0.003–0.004	Mauersberger et al. (1988)
HDO/H_2O	>0.002	0.001	0.001–2 (−4)	Henkel et al. (1987)

Note: *a* (−*b*) stands for $a \times 10^{-b}$.

Table 5 A comparison of abundance ratio measured in L134N (Tine et al., 2000; Roueff et al., 2000) with predictions from our model (3) and Millar (2002).

Species	Observation	Our cal. M2		M2002	
		Early	Steady	Early	Steady
DCO^+/HCO^+	0.18	0.026	0.17	0.016	0.047
NH_2D/NH_3	0.1	0.006	0.1	0.0075	0.02
NHD_2/NH_3	5 (−3)	2.3 (−5)	5.1 (−3)	1.3 (−4)	8.4 (−5)
N_2D^+/N_2H^+	0.35	0.03	0.038	0.023	0.039

The most important primary reactions to extract deuterium from HD involve ion-neutral isotope exchange reactions:

$$H_3^+ + HD \rightarrow HD^+ + H_2, \tag{1}$$

$$CH_3^+ + HD \rightarrow CH_2D^+ + H_2, \tag{2}$$

$$C_2H_2^+ + HD \rightarrow C_2HD^+ + H_2, \tag{3}$$

where the reaction exoergicities although small – $\Delta E_1/k = 220$ K, $\Delta E_2/k = 375$ K, $\Delta E_3/k = 550$ K – are much larger than the temperatures of cold interstellar clouds. At low temperatures, the reverse reactions do not occur efficiently despite the large abundance of H_2. Once formed these deuterated ions can pass on their enhanced deuterium content to other species in chemical reactions (Millar, 2002). In addition to the forward and reverse reaction in (1), H_2D^+ can be destroyed by metals, by dissociative recombination with electron,

$$H_{2D}^+ + e \rightarrow H + H + D, \tag{4a}$$

$$H_2D^+ + e \rightarrow H_2 + D, \tag{4b}$$

$$H_2D^+ + e \rightarrow H + HD \tag{4c}$$

Table 6 A comparison of abundance ratio measured in W3IRS4 cloud by Helmich and van Dishock (1997) with predictions from our model (4).

Species	Observation	Our cal. M2
HDS/H_2S	<9.1 (−2)	1.0 (−3)
$HDCO/H_2CO$	<3.8 (−2)	0.02
DCN/HCN	<4.3 (−3)	0.001
DNC/HNC	7.1 (−3)	9 (−4)
C_2D/C_2H	0.045	0.032
CH_3OD/CH_3OH	<7.1 (−2)	0.006

Note: *a* (−*b*) stands for $a \times 10^{-b}$.

with total rate coefficient equal to $6\times10^{-8}(T/300)^{-0.5}$ cm^{-3} s^{-1} (Larsson et al., 1996) and by reaction with neutral molecules (CO, N_2, H_2D).

The reactions for CH_2D^+ and C_2HD^+ are similar to that of H_2D^+, except that each of these ions undergo a radiative association reaction with H_2 (Millar et al., 1989; Herbst et al., 1987)

$$CH_2D^+ + H_2 \rightarrow CH_4D^+ + \text{photon}, \tag{5}$$

$$C_2HD^+ + H_2 \rightarrow C_2H_3D^+ + \text{photon}. \tag{6}$$

Our calculated ratios for $H_2D^+/H_3, CH_2D^+/CH_3^+$ and $C_2HD^+/C_2H_2^+$ are all enhanced at low temperature, but H_2D^+ is responsible for D/H ratio other than the two molecules. At high temperature H_2D^+ is rapidly destroyed by H_2, so CH_2D^+ and C_2HD^+ are responsible for D/H ratio.

Our calculated ratio of C_2D/C_2H is in agreement with observations of TMC-1 at an early (10^5 year) time and higher at the steady state (10^8 year) time. This result is the same as that obtained by Roberts and Millar (2000a). The C_2D species is formed by:

$$C_2HD^+ + e \rightarrow C_2D + H, \tag{7}$$

$$C_2H + D \rightarrow C_2D + H + 580\ \text{K} \tag{8}$$

and is destroyed by

$$C_2D + H \rightarrow C_2H + D. \tag{9}$$

In model (2) with temperature of 70 K, the neutral–neutral rate coefficient of reaction (8) and dissociative recombination of C_2HD^+, become more competitive, and fractional abundance of C_2D increases. This result agrees with that of Herbst et al. (1987). Also C_2D is formed from cosmic ray induced photodissociation of C_2HD. At steady state time our calculated C_2D/C_2H ratio is in agreement with observations of Orion cloud and greater than that obtained by Millar et al. (1989).

As Millar et al. (1989) $C_2H_3D^+$ is precursor to C_2H_2D, so the reactions of C^+ with C_2H_2D transfer fractionation to C_3-bearing hydrocarbons via

$$C_2H_2D + C^+ \rightarrow C_3HD^+ + H \tag{10}$$

and subsequently to C_3D via dissociative recombination. The C_3H_2 molecule is not transferred easily to the C_3HD^+ and C_3HD is formed as (see Bell et al., 1988);

$$C_2HD + C^+ \rightarrow C_3D^+ + H, \tag{11}$$

$$C_3D^+ + H_2 \rightarrow C_3H_2D^+ + \text{photon}, \tag{12}$$

$$C_3H_2D^+ + e \rightarrow C_3HD + H. \tag{13}$$

Our calculated C_3HD/C_3H_2 ratios in both an early and the steady state times are not in agreement with observation of TMC-1 cloud.

In our model C + 3H_3D molecule is formed through the CH_2D^+ ion, by dissociative recombination of $CH_2DC_2H_2^+$ and $CH_2DC_3H_2^+$ ions, which are themselves formed from CH_2D^+ by ion-neutral reactions with small hydrocarbon species like methane or acetylene. C_3H_3D is destroyed by atomic and molecular ions, primarily H_3^+ and He^+. Our calculated C_3H_3D/C_3H_4 ratios at an early and the steady state time are greater than the lower and upper limit of observations of TMC-1 cloud. This results is the same as that of Roberts and Millar (2000a).

In our model C_4D species is formed by the following reactions:

$$C_4^+ + HD \rightarrow C_4D^+ + H, \tag{14}$$

$$C_4D^+ + H_2 \rightarrow C_4HD^+ + H, \tag{15}$$

$$C_3HD^+ + C \rightarrow C_4HD^+ + H, \tag{16}$$

$$C_4HD^+ + e \rightarrow C_4D + H \tag{17}$$

and is destroyed by

$$C_4D + O \rightarrow C_3D + CO, \tag{18a}$$

$$C_4D + H_3^+ \rightarrow C_4HD^+ + H_2, \tag{18b}$$

$$C_4D + HCO^+ \rightarrow C_4HD^+ + CO, \tag{18c}$$

$$7C_4D + H_3O^+ \rightarrow C_4HD + H_2. \tag{18d}$$

At an early time our calculated C_4D/C_4H ratio is in agreement with observations of TMC-1 clouds.

The D–N bond begins due to the lower proton (deuteron) affinity of H_2D^+, which reacts with N_2 to form N_2D^+ species,

$$H_2D^+ + N_2 \rightarrow N_2D^+ + H_2. \tag{19}$$

In addition to reaction (19), D atom can also react with N_2H^+ to form N_2D^+

$$N_2H^+ + D \rightarrow N_2D^+ + H. \tag{20}$$

Reaction (20) has an exothermicity of about 550 K (Adams and Smith, 1985). Due to the proton affinity of N_2 is very small, so that N_2D^+ reacts with CH_2D^+ and C_2HD^+.

IN our model N_2D^+/N_2H^+ ratios are less than the observations of TMC-1 and Orion clouds. This is because at dense clouds N_2D^+ condense onto grains, i.e. N_2 $D^+$is not easily predictable by gas-phase reactions and its value must be predicted through evaporation from the grain (Willacy and Millar, 1998; Millar et al., 1989; Millar, 2002).

After NH_3 is formed by the reaction sequence $N_2 \overset{He+}{\rightarrow} N^+ \overset{4H_2}{\rightarrow} NH_4^+ \overset{e}{\rightarrow} NH_3$, deuteron transfer reaction forms NH_3D^+ which can then recombine to give NH_2D as;

$$NH_3 + XD^+ + \rightarrow NH_3D^+ + XH, \tag{21}$$

$$NH_3^+ + e \rightarrow NH_2D + H, \tag{22}$$

where XD^+ represents all species capable of transferring a proton or deuteron to NH_3, principally H_3^+, N_2H^+, HCO^+ and their deuterated isotopomers. Successive deuteron transfer reaction can lead eventually to NHD_2 and ND_3 as

$$NH_2D + XD^+ \rightarrow NH_2D^+ + +X, \tag{23}$$

$$NH_2D_2^+ + e \rightarrow NHD_2 + H, \tag{24}$$

$$NHD_2 + XD^+ \rightarrow NHD_3^+ + X, \tag{25}$$

$$NHD_3^+ + e \rightarrow ND_3 + H, \tag{26}$$

$$NHD_3^+ + e \rightarrow NHD_2 + D. \tag{27}$$

From the last reactions (21)–(27) the relative fractional abundances depend on the XD^+/XH^+ and the branching ratio for dissociative recombination of the deuterated ions.

By assuming the rate coefficients of reactions (26) and (27) are equal, our calculated fractional abundances for ND_3 is about 2×10^{-11}. This value is greater than that obtained by Rodgers and Charnely (2001) by two times. The abundance of ND_3 in our model is in the same order of magnitude as given by Lis et al. (2002) for B1 cloud. From this result we can conclude that ND_3 can be detected in L134N cloud.

One species for which time dependence significant is DCO^+. The species DCO^+ is more readily observable than N_2D^+, because the abundance of CO is greater than that of

N_2 in interstellar clouds. So at low temperature the D–C band begins with the reaction:

$$H_2D^+ + CO \rightarrow DCO^+ + H_2 \tag{28}$$

at an early time. Also DCO^+ is formed by:

$$C^+ + HDO \rightarrow DCO^+ + H, \tag{29}$$

$$HCO^+ + D \rightarrow DCO^+ + H. \tag{30}$$

At the low temperature and density, the atomic deuterium is very abundant, so reaction (30) proceeds very rapidly and can further enhance the fractionation of DCO^+.

At high temperature the abundance of CH_4D^+ is greater than H_2D^+, then DCO^+ is formed by,

$$CH_4D^+ + CO \rightarrow DCO^+ + CH_4. \tag{31}$$

In addition to this reaction, there are significant contributions to DCO^+ formation in the reactions

$$CH_2D^+ + O \rightarrow DCO^+ + H_2, \tag{32}$$

$$C_2HD^+ + O \rightarrow DCO^+ + CH, \tag{33}$$

$$CD + O \rightarrow DCO^+ + e, \tag{34}$$

$$CH_2D^+ + O \rightarrow DCO^+ + H_2. \tag{35}$$

The primary of D in dark clouds is the dissociative recombination of DCO^+,

$$DCO^+ + e \rightarrow CO + D. \tag{36}$$

Our calculated DCO^+/HCO^+ ratio is in agreement with observations of TMC-1 cloud at an early time. At the steady state time it is in agreement with observations of Orion and L134N clouds. This result differs than that obtained by Millar et al. (1989) and Millar (2002).

The band between D–C–O begins by the formation of deuterated formaldehyde, HDCO, which is formed from two species derived from CH_2D^+, CH_4D^+ and CH_2D, via the reactions;

$$CH_4D^+ + O \rightarrow H_2DCO^+ + H_2 \tag{37}$$

followed by dissociative recombination

$$H_2DCO^+ + e \rightarrow HDCO + H \tag{38}$$

and

$$CH_2D^+ + O \rightarrow HDCO + H^+. \tag{39}$$

HDCO also reacts with H_3^+ to form H_2DCO^+ which will then recombine to HDCO. The calculated $HDCO/H_2CO$ ratio is in agreement with observations of TMC-1, Orion and W3IRS4 clouds.

Also the band between D–C–N begins by the formation of DCN, which is formed a derivative of CH_2D^+;

$$CH_2D^+ + e \rightarrow CHD + H, \tag{40}$$

$$CHD^+ + N \rightarrow DCN + H^+. \tag{41}$$

The main derives of DCN at high temperature is the neutral–neutral reactions;

$$DCO^+ + N \rightarrow DCN + O, \tag{42}$$

$$HCN^+ + D \rightarrow DCN + H. \tag{43}$$

We found that the reaction

$$H^+ + DCN \rightarrow HCN^+ + D \tag{44}$$

can cycle deuterium between the atomic D and the DCN molecule. This result is in agreement with that of Schilke et al. (1992) and Hatchell et al. (1998). As shown in Tables 3, 4 and 6 our calculated DCN/HCN is in agreement with observations of TMC-1, Orion and W3IRS4 clouds.

At the low temperature, the dominant route to deuterated cyanoacetylene, DC_3N, formation is thought to be

$$C_3H_2D^+ + N \rightarrow HDC_3N^+ + H \tag{45}$$

followed by

$$HDC_3N^+ + e \rightarrow DC_3N + H. \tag{46}$$

At the high temperature, the deuterated acetylene should form deuterated cyanoacetylene through

$$C_2HD + CN \rightarrow DC_3N + H. \tag{47}$$

DC_3N species is only observed in TMC-1 cloud, and our calculated its ratio is in agreement with observations at steady state time.

In our models we have assumed that the species CH_3OD is formed from the radiative association reaction

$$CH_3^+ + HDO \rightarrow CH_3OHD^+ + \text{photon} \tag{48}$$

and

$$CH_3OHD^+ + e \rightarrow CH_3OD + H. \tag{49}$$

The HDO species comes from the rapidly exothermic reaction

$$CH_2D^+ + H_2O \rightarrow CH_3 + HDO. \tag{50}$$

The calculated CH + 3OD/CH + 3OH ratio in our model differs from observations. This is because, at high densities most molecules condense onto grain; i.e. CH_3OH and CH_3OD is not easily predictable by gas-phase reaction and their values must be predicted through evaporation from the grains surface (Amin, 1999). Also our calculated ratio for HDO/H_2O is small, because the large value must be predicted by shock chemistry (Amin, 2001; Parise et al., 2002).

When we compare our predicted gas-phase abundances with those observed in TMC-1 and W3IRAS4 clouds, only HDCS is in agreement and other species HDS is smaller than observation. In our model after the formation of H_2S by the chain;

$$S^+ \xrightarrow{H2} HS^+ \xrightarrow{H2} H_3S^+ \xrightarrow{e} H_2S,$$

(By the last chain the calculated fractional abundance of H_2S is small) deuteron transfer reaction forms H_2DS^+ which then recombine to give HDS as:

$$H_2D^+ + H_2S \rightarrow H_2DS^+ + H_2, \tag{51}$$

$$H_2DS^+ + e \rightarrow HDS + H. \tag{52}$$

Also DCO^+ and H_2D^+ react with H_2CS to form HDCS as;

$$DCO^+ + H_2CS \rightarrow H_2DCS^+ + CO, \tag{53}$$

$$H_2D^+ + H_2CS \rightarrow H_2DCS^+ + CO, \tag{54}$$

$$H_2DCS^+ + e \rightarrow HDCS + H. \tag{55}$$

4. Conclusions

With a more extensive chemical network, we made a detailed study of a pseudo-time dependent chemical evolution of deuterium species in different interstellar clouds,TMC-1, Orion, L134N and W3IRS4, with different densities and temperatures. This has been done using different initial elemental abundances and without the temperature dependence of the ion–dipole molecule collisions. We have shown that large abundances of NH_2D and NHD_2 can be produced by gas phase chemistry in cold dense clouds. Ammonia is deuterated via deuteron transfer from species such as H_2D^+, DCO^+ and N_2D^+, followed by dissociative recombination. We predict the abundance of ND_3 is 2×10^{-11}, by a assuming the rate coefficients of reactions $NHD_3^+ + e \rightarrow ND_3 + H$, and $NHD_3^+ + e \rightarrow NHD_2 + D$ are equal. So we suggest that triply-deuterated ammonia could be detectable in L134N cloud. We have included the fractionation of sulphur-bearing molecules and found a good agreement with observation for HDCS. The very slow formation rates of HDS in cold gas make this molecule particularly useful in probing regions where grain surface chemistry may be important. Reduction of the initial elemental abundances and high cosmic ray ionization gave us good relative abundances for most of the observed deuterated species in W3IRS4.

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احتراق جزيئات الديوتريوم في السحب البين نجمية الكثيفة الباردة والدافئة

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ملخص البحث. حيث أن جزيئات الديوتريوم تستخدم في: 1- اختبار القوانين الفيزيائية لسحب ما بين النجوم. 2- دراسة علاقة الربط بين تكوين الثلج في مادة ما بين النجوم والمذنبات. 3- طريقة تكوين نظائر المركبات في مادة ما بين النجوم.

لهذا تقوم دراسات نظرية وعملية (عن طريق رصد السحب البين نجمية بطرق مختلفة)، لفهم عملية تكوين وتكوين مركبات الديوتريوم وحساب كمية الوفرة في سم^2 .

في هذا البحث نقوم بدراسة طريقة تكوين مركبات الديوتريوم وحساب كمية الوفرة في أربعة سحب بين نجمية ذات عوامل فيزيائية مختلفة وهي TMC-1 و Orion و L134N و W3IRS4 . وفي هذه الدراسة تم تسيد برنامج كيميائي يحتوي على 5340 تفاعل كيميائي لـ 408 مركب وعنصر كيميائي منهم 130 مركب للديوتريوم. وقد تم تحويل هذه التفاعلات إلى معادلات تفاضلية من الدرجة الأولى تحقق شرط stiff وحلها عدديا باستخدام طريقة الـ Gear. وقد تم الحصول على قيم متوافقة مع الأرصاد الفلكية باستخدام قيم بدائية مختلفة للعناصر الأساسية حسب الوضع الفيزيائي للسحابة المدروسة. وقد تم الحصول على قيم وفرة كبيرة لكل من NH_2D و NHD_2 في السحب الكثيفة الباردة عند حصول حالة الثبات في عملية التكوين والتكسير عند زمن قدرة مائة مليون سنة.