



Deuterium enrichment of the interstellar medium



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HIGHLIGHTS

- Despite of low D/H, our model shows several species could be heavily fractionated.
- Radial distribution of $\text{DCO}^+/\text{HCO}^+$ and $\text{N}_2\text{D}^+/\text{N}_2\text{H}^+$ are studied.
- Deuterated isotopomers of H_2CO & CH_3OH are mainly producing in ice phase.
- Computed column densities of deuterated species are compared with the observations.
- IR & sub-mm transitions of some deuterated species are calculated and are compared.

ARTICLE INFO

Article history:

Received 8 October 2013

Received in revised form 24 June 2014

Accepted 5 July 2014

Available online 16 July 2014

Communicated by D.B. Sanders

Keywords:

Astrochemistry

Spectra

ISM: molecules

ISM: abundances

ABSTRACT

Despite the low elemental abundance of atomic deuterium in the interstellar medium (ISM), observational evidence suggests that several species, both in the gas phase and in ices, could be heavily fractionated. We explore various aspects of deuterium enrichment by constructing a chemical evolution model in both gaseous and granular phases. Depending on various physical parameters, gases and grains are allowed to interact with each other through the exchange of their chemical species. It is known that HCO^+ and N_2H^+ are two abundant gas phase ions in the ISM and, their deuterium fractionation is generally used to predict the degree of ionization in the various regions of a molecular cloud. For a more accurate estimation, we consider the density profile of a collapsing cloud. The radial distributions of important interstellar molecules, along with their deuterated isotopomers, are presented. Quantum chemical simulations are computed to study the effects of isotopic substitution on the spectral properties of these interstellar species. We calculate the vibrational (harmonic) frequencies of the most important deuterated species (neutral and ions). The rotational and distortional constants of these molecules are also computed in order to predict the rotational transitions of these species. We compare vibrational (harmonic) and rotational transitions as computed by us with existing experimental and theoretical results. It is hope that our results will assist observers in detecting several hitherto unobserved deuterated species.

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1. Introduction

The study of deuterium enrichment received a major boost after the discovery of singly or multiply deuterated H_2CO and CH_3OH in the Interstellar Medium (ISM). Interestingly, the fractionation ratios of these deuterated species are often a cross elemental D/H ratio of the ISM ($\sim 1.5 \times 10^{-5}$, Linsky et al., 1995). Earlier work by Hasegawa et al. (1992), Chakrabarti et al. (2006a,b), Das et al. (2008a, 2010), Cuppen and Herbst (2007) and Das and Chakrabarti (2011) suggested that grain chemistry plays a crucial

role in the chemical composition of the ISM. The role of grain chemistry in deuterium enrichment has been also highlighted by various authors (Caselli, 2002a; Cazaux et al., 2010; Das et al., 2013a). In the gas phase, the basic reactions are followed by dominant ion-molecular reaction pathways. Around the cold, dense region of the cloud, CO and O are heavily depleted from the gas phase. A strong correlation between CO depletion and deuterium fractionation has been observed (Bacmann et al., 2003; Crapsi et al., 2005). Moreover, the ionization of the ISM could be traced by observing some deuterated ions, such as, DCO^+ and N_2D^+ (Caselli, 2002a). Deuterium chemistry is, therefore, extremely important for tracing the dynamic properties of a cloud.

Aikawa et al. (2005) and Das et al. (2008b, 2013b) have already discussed how the chemical composition of a cloud affects its

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dynamic parameters. Over the last two decades, several attempts have been made to differentiate the evolutionary stages of proto-stars. For example, Lada and Wilking (1984) defined three classes of proto-stars (Class I, Class II and Class III) which evolve progressively. André et al. (1993) defined another class of proto-stars, namely Class 0, which is the youngest among protostar classes. When Class 0 proto-stars reach a slightly more evolved stage, the source is considered to be a Class 0/I borderline object. These stages are defined by observing the variation in the spectral energy distribution of protostars. A number of studies have been carried out to attempt to find a connection between chemical species abundance and evolutionary stage (e.g., Smith, 1998; Myers et al., 1998). Several of these studies suggest that the deuterium fraction of some ions like N_2H^+ and HCO^+ could be used to define different evolutionary stages (Crapsi et al., 2005; Jørgensen et al., 2004). Recently, Majumdar et al. (2013) performed a quantum chemical calculation to obtain the spectral signatures (infrared and electronic absorption spectra) of the precursors of some biomolecules, such as adenine, alanine and glycine (Chakrabarti and Chakrabarti, 2000a,b; Majumdar et al., 2012). It was found that the spectral signatures of the gas phase significantly differ from those in the ice phase. Das et al. (2013a) discuss different properties of HCOCN and one of its isotopologues, DCOCN. These type of studies could also be carried out for other deuterated species, which could serve as benchmarks for observation.

In this paper, we have presented a systematic approach to determine the chemical evolution of some of the most important deuterated species, and given a complete spectral catalog for detecting these molecules around cold and dense regions of a molecular cloud. The outline of this paper is as follows. In Section 2 models and computational details are presented, the implications of our results are discussed in Section 3 and lastly in Section 4 the conclusions are outlined.

2. Chemical modeling

2.1. Gas phase chemical model

We prepared a large gas-grain chemical network to iteratively study the chemical processes in a molecular cloud. Our gas phase chemical network consists of 6149 reactions amongst 601 species. We mainly follow the UMIST-2006 database (Woodall et al., 2007) for the construction of our gas phase chemical network. Since, in the present context our motivation is to study the deuterium enrichment of the ISM, we use some of the important reactions from UMIST-2006 database and assume that these reactions would also be possible for the deuterated isotopomers. Reaction rates are calculated with the method used by Woodall et al. (2007). To avoid long computational times, as well as the complexity of handling a large chemical network, we identify some dominant pathways for deuterium enrichment and focus on them. This selection is based on the earlier studies of Albertsson et al. (2013), Roberts and Millar (2000) and Rodgers and Millar (1996a,b). We assume that gas and grains are coupled through accretion and thermal/cosmic ray evaporation processes. Details of these processes are already presented in Das and Chakrabarti (2011) and Das et al. (2013a,b).

2.2. Ice phase chemical model

2.2.1. Accretion

Gas phase species are depleted by their accretion onto interstellar ice. Following Hasegawa et al. (1992), the accretion rate of a gas phase species is given by:

$$k_{acc}(i) = s_i \sigma v(i) n(i) s^{-1},$$

where, s_i is the sticking coefficient, $n(i)$ is the gas phase concentration, $v(i)$ is the thermal velocity of the i th species and σ is the geometrical dust-grain cross section ($\sigma = 4\pi r^2$ where r is the radius of the grain ~ 1000 Å). In our simulation, we take $s_i = 1$ for all the neutrals, except H_2 and He. It is not certain whether atomic and molecular ions stick to the grain surfaces (Hasegawa et al., 1992; Watson, 1976), and here we consider $s_i = 0$ for the ions.

2.2.2. Binding energies

The chemical enrichment of the interstellar grain mantle solely depends on the binding energies of surface species (Das and Chakrabarti, 2013). The mobility of lighter species such as H, D, N and O mainly dictates the chemical composition of the interstellar grain mantle. The composition of the grain mantle, which depends on the mobility of H and O atoms, is already discussed in Das et al. (2008a, 2010) and Das and Chakrabarti (2011). We assume that the gas phase species are physisorbed onto dust grains (~ 0.1 μ m), having a grain number density of $1.33 \times 10^{-12} n_H$, where n_H is the concentration of H nuclei in all forms. The binding energies of deuterated species are assumed to be the same as their hydrogenated counterparts, because the binding energies of deuterated species are unknown. Several theoretical and experimental attempts to find out the diffusive behavior of atomic hydrogen have been made. According to a number of past studies, such as Allen and Robinson (1977), Tielens and Allamandola (1987), Hasegawa and Herbst (1993), Hasegawa et al. (1992) and Chakrabarti et al. (2006a,b), the binding energy for diffusion (E_b) of the H atom was found to be ~ 100 K, whereas for desorption (E_d) it was ~ 350 K. Following Hasegawa and Herbst (1993), for the H_2 molecule the desorption energy was determined to be ~ 450 K. According to Hasegawa and Herbst (1993), and references therein, the adsorption energy of N_2 is 1210 K. Caselli (2002a), and references therein, however, suggest that the adsorption energy of N_2 could be 787 K. In our simulation, we consider 787 K to be the adsorption energy for N_2 . Desorption energies (E_d) for all other species are taken from the study of Hasegawa and Herbst (1993). Following Tielens and Allamandola (1987) and Hasegawa et al. (1992), we assume $E_b = 0.3E_d$ for all other species except for the H atom. To show the importance of these binding energies towards the chemical complexity of the interstellar grain mantle, we construct three sets of binding energies. The first set consists of the binding energies mentioned above, and is labeled set 1. Unless otherwise stated, we always use the set 1 energy values. In set 2, we use results derived by Pirronello et al. (1997, 1999), Katz et al. (1999) for the binding energies (E_b and E_d) of H and H_2 with an olivine grain surface. The difference between set 1 and set 2 is that in set 2 we use different binding energies (both E_b and E_d) for H, H_2 , D, HD and D_2 . The binding energies of all other species are similar to those of set 1. Similarly, in set 3, the experimental findings of Pirronello et al. (1997, 1999) are used for the binding

Table 1
Various sets of binding energies.

Species	Set 1		Set 2		Set 3	
	E_b	E_d	E_b	E_d	E_b	E_d
H	100	350	287	373	511	657
H_2	135	450	95	315	163	542
D	100	350	287	373	511	657
HD	135	450	95	315	163	542
D_2	135	450	95	315	163	542
O	240	800	240	800	240	800
OH	378	1260	378	1260	378	1260
H_2O	558	1860	558	1860	558	1860
CO	363	1210	363	1210	363	1210
H_2CO	528	1760	528	1760	528	1760
CH_3OH	618	2060	618	2060	618	2060

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