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Study of the chemical evolution and spectral signatures of some interstellar precursor molecules of adenine, glycine & alanine

Liton Majumdar [a], Ankan Das [a,*], Sandip K. Chakrabarti [a,b], Sonali Chakrabarti [a,c]

[a] Indian Centre For Space Physics, 43 Chalantika, Garia Station Road, Kolkata 700084, India
[b] S.N. Bose National Center for Basic Sciences, JD-Block, Salt Lake, Kolkata 700098, India
[c] Maharaja Manindra Chandra College, 20 Ramakanto Bose Street, Kolkata 700003, India

HIGHLIGHTS

- Chemical evolution of the adenine, alanine and glycine along with its precursor molecules are shown.
- Spectral properties (IR & Electronic) of various pre-biotic molecules are explored.
- Spectral properties varies from the gas phase to the ice phase.
- We find that spectral signature is highly dependent upon the composition of ice.
- A comparison with experimentally obtained IR spectra of formamide is carried out.

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ABSTRACT

We carry out a quantum chemical calculation to obtain the infrared and electronic absorption spectra of several complex molecules of the interstellar medium (ISM). These molecules are the precursors of adenine, glycine & alanine. They could be produced in the gas phase as well as in the ice phase. We carried out a hydro-chemical simulation to predict the abundances of these species in the gas as well as in the ice phase. Gas and grains are assumed to be interacting through the accretion of various species from the gas phase onto the grain surface and desorption (thermal evaporation and photo-evaporation) from the grain surface to the gas phase. Depending on the physical properties of the cloud, the calculated abundances varies. The influence of ice on vibrational frequencies of different pre-biotic molecules was obtained using Polarizable Continuum Model (PCM) model with the integral equation formalism variant (IEFPCM) as default SCRF method with a dielectric constant of 78.5. Time dependent density functional theory (TDDFT) is used to study the electronic absorption spectrum of complex molecules which are biologically important such as, formamide and precursors of adenine, alanine and glycine. We notice a significant difference between the spectra of the gas and ice phase (water ice). The ice could be mixed instead of simple water ice. We have varied the ice composition to find out the effects of solvent on the spectrum. We expect that our study could set the guidelines for observing the precursor of some bio-molecules in the interstellar space.

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1. Introduction

Presence of interstellar dust towards the formation of complex interstellar molecules is taken for granted especially after the discovery of more than twenty molecules around the star forming region in the interstellar ice. Altogether, according to the CDMS catalog (http://www.astro.uni-koeln.de/cdms/molecules), one hundred and seventy molecules have been detected in the interstellar medium or circumstellar shells. To model the formation of complex molecules, and especially through interstellar grain chemistry, several attempts were made by various workers (Chakrabarti et al., 2006a,b; Das et al., 2008b, 2010; Cuppen and Herbst, 2007; Cuppen et al., 2009) over the years. Interstellar dust grains are thought to be consisting of amorphous silicate or carbonaceous core surrounded by molecular ice layer (Draine, 2003; Gibb et al., 2004). It has been clear from the experimental and observational results that almost 90% of the grain mantle is covered with H_2O, CH_3OH, CO_2 (Keane et al., 2001; Das and Chakrabarti, 2011 and references therein). Presence of HCN, CN, CS and H_2O in space were identified by anomalous absorption (Omont, 1993; Bujarrabal

* Corresponding author. Tel.: +91 3324366003; fax: +91 3324622153.
E-mail addresses: liton@csp.res.in (L. Majumdar), ankan.das@gmail.com, ankan@csp.res.in (A. Das), chakraba@bose.res.in (S.K. Chakrabarti), sonali@csp.res.in (S. Chakrabarti).

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et al., 1994). But a complete understanding of the chemical and physical processes which take place on a grain surface is still missing.

The origin of amino acids through the pre-biotic chemistry of the early earth has been a topic of long standing interest. However, complex pre-biotic molecules might also be formed due to very complex and rich chemical processes inside a molecular cloud. The production of amino acids, nucleobases, carbohydrates and other basic compounds can possibly start from the molecules like HCN, cyno compounds, aldehyde, and ketones (Orgel, 2004; Abelson, 1966), which could lead to the origin of life in the primitive earth conditions. However, even with the present observational tools, it is hard to confirm the presence of any bio-molecules in the ISM. So it may suffice, if we can identify a few precursor molecules which eventually form bio-molecules in the interstellar space. Quantum chemical simulations could be used to find out the spectral properties of these complex molecules. It is observed and experimentally verified that the spectral signature of a species significantly deviates between the gas phase and the ice phase. So a theoretical study of the spectral properties of the precursors of some important bio-molecules in both the gas and ice phases could serve as benchmarks for the observations.

In this Paper, we consider a large gas-grain network coupled with a hydrodynamic simulation to obtain the abundances of various complex molecules, which could lead to the formations of adenine, alanine & glycine. We also discuss the production of formamide which is an important precursor in the process of the abiotic synthesis of amino acids. In the literature, there are several observational studies on glycine (Kuan et al., 2003; Hollis et al., 2003; Snyder et al., 2005). But its existence in a molecular cloud, till date, is not verified without a reasonable doubt. In case of adenine, we find that though its abundance in our theoretical model is well under the observation limit, its precursor molecules are heavily abundant. It is also true for the alanine and glycine. These prompted us to find out the spectral signatures of the precursor molecules of these three molecules around the different astrophysical environment, from which one could roughly anticipate the abundances of adenine, glycine & alanine. All possible reaction pathways are included in the gas as well as in the grain phase network. Armed with the chemical abundances of these precursor molecules, we compute the infrared and electronic absorption spectra in the gas as well as for the icy grains.

The plan of this paper is the following. In Section 2, the models used and the computational details are presented. Implications of the results are discussed in Section 3. Finally, in Section 4, we draw our conclusions.

2. Computational details

2.1. Hydro-chemical model

The process of formation of complex molecules in the interstellar space is very much uncertain. There could be a number of pathways available for the formation of a complex molecule. However, depending on the chemical abundances of the reactive species and the reaction cross section, the rate of formation varies. Formation routes of several interstellar bio-molecules are already reported in Majumdar et al. (2012). They pointed out that despite of the huge abundances of the neutral species, radical-molecular/radical–radical reaction pathways dominates towards the formation of some pre-biotic species. Normally such reactions are barrier less and exothermic in nature. To study the chemical evolution of various complex radicals, ions, molecules which are very much important for the prebiotic synthesis of different bases of amino acids, we have constructed a hydro-chemical model to mimic the interstellar scenario.

The evolution of the chemical species is strongly dependent on the physical properties of the medium. So the dynamic nature of the medium at any particular instant could influence the chemical composition of the medium. Das et al. (2008b, 2010) considered a spherically symmetric isothermal (10 K) collapsing cloud, whose outer boundary was assumed to be located at one parsec and the inner boundary was assume to be located at 10^{-4} parsec. They used a finite difference Eulerian scheme (upwind scheme) to solve the Eulerian equations of hydrodynamics in spherical polar coordinates. Since they were interested in the spherical case, they only considered radial motion and ignored any dependency upon the θ & ϕ coordinates. By solving the hydrodynamic equations they studied fully time-dependent behaviour of the spherical flow.

To have a realistic condition, we have considered this density distribution as an input for our chemical model. The gas phase chemical network is mainly adopted from the UMIST 2006 database (Woodall et al., 2007). Here, we have chosen the initial elemental abundances according to the Woodall et al. (2007), these are the typical low-metal abundances often adopted for TMC-1 cloud. We add a few new reactions following Chakrabarti and Chakrabarti (2000a,b), Woon (2002), Quan and Herbst (2007), Woodall et al. (2007) and Rubalcava (1956) and references therein. Recently, Majumdar et al. (2012), calculated the rate coefficients for the reaction pathways described in Chakrabarti and Chakrabarti (2000a,b). They used Bates (1983) semi-empirical formula to find out the rate coefficients of any chemical reactions. Gupta et al. (2011) also followed the same prescription to find out the reaction rates for the adenine formation in interstellar space.

To show the importance of grains towards the chemical enrichment of the ISM, we have also included a detailed grain chemistry network following Hasegawa et al. (1992), Das et al. (2008a, 2010), Cuppen and Herbst (2007), Jones et al. (2011), Garrod et al. (2008) and Das and Chakrabarti (2011) into our reaction network. We therefore have the most updated chemical network to study the chemical evolution of several interstellar species. In order to perform a self-consistent study, we assume that the gas and the grains are coupled through the accretion and the thermal evaporation processes. We assume that the species are physisorbed onto the dust grain (classical size grain $\sim$1000 Å) having the grain number density $1.33 \times 10^{-12} n$, where n is the concentration of H nuclei in all forms. Thus, in principle, we have a complete interstellar model, which could be used to follow the hydro-chemical properties of a collapsing cloud.

2.2. Quantum chemical calculation

First of all, we have optimized the geometry of the molecules, which are the precursors of various bio-molecules in space. In order to have an idea for the stability of these molecules, B3LYP/6–311++G** level is used. Gas phase vibrational frequencies of these precursor molecules are also calculated by the B3LYP/6–311++G** level. Observational evidences suggest that grain mantles around the dense clouds are mainly covered by H_2O($>$ 60%), CH_3OH (2–30% with respect to solid water) and CO_2 (2–20% with respect to solid water). To find out the effects of the solvent on the spectrum, we have chosen three types of ice. (i) Unless otherwise stated, we use pure water ice. (ii) We use methanol ice also to mimic the ice composition around the methanol rich environment and finally, (iii) Based on the observational results, we construct an ice, which consists of 70% water 20% methanol and 10% carbon-di oxide and call is as the 'mixed ice'.

In order to find out the vibrational frequencies of these molecules in the ice phase, we have optimized the geometry of these molecules in ice at B3LYP/6–311++G** level. Here, the Polarizable

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