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Interstellar hydrogen bonding

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Abstract

This paper reports the first extensive study of the existence and effects of interstellar hydrogen bonding. The reactions that occur on the surface of the interstellar dust grains are the dominant processes by which interstellar molecules are formed. Water molecules constitute about 70% of the interstellar ice. These water molecules serve as the platform for hydrogen bonding. High level quantum chemical simulations for the hydrogen bond interaction between 20 interstellar molecules (known and possible) and water are carried out using different ab-intio methods. It is evident that if the formation of these species is mainly governed by the ice phase reactions, there is a direct correlation between the binding energies of these complexes and the gas phase abundances of these interstellar molecules. Interstellar hydrogen bonding may cause lower gas abundance of the complex organic molecules (COMs) at the low temperature. From these results, ketenes whose less stable isomers that are more strongly bonded to the surface of the interstellar dust grains have been observed are proposed as suitable candidates for astronomical observations.

Keywords: ISM; Abundance-ISM; Atoms-ISM; Molecules; Physical data and processes; Astrochemistry

1. Introduction

Gas phase chemical reactions and reactions that occur on the surfaces of interstellar dust particles are the dominant processes by which molecules can be synthesized from the precursor species. Of these two processes, reactions that occur on the surfaces of interstellar dust particles have been invoked for the formation of molecular hydrogen (Biham et al., 2001; Chakrabarti et al., 2006); as well as for the synthesis of larger interstellar molecules (Das et al., 2010; Das and Chakrabarti, 2011; Das et al., 2016). Dust grains and ice play an indisputable role for the synthesis of interstellar species. Whereas in the gas phase, reactions relying on three-body collisions are very rare, species residing on the solid surfaces can roam around the surfaces until a reaction occurs, thus forming new species. These surfaces therefore serve as reaction sites for chemical processes that would either being very slow or not occur at all. From spectroscopic observations, the composition of the interstellar ice is dominated by water which accounts for 60–70% (Das and Chakrabarti, 2011; Das et al., 2016) of the ice in most lines of sight. Other spectroscopically observed species include methanol, carbon monoxide and carbon dioxide, as well as smaller abundances of other species (Tielens, 2013; Fraser et al., 2002; Draine, 2003; van Dishoeck, 2004; Gibb et al., 2000; Gibb et al., 2004; Whittet, 2003). The composition of the interstellar ice causes most of the molecules formed on the surface of the interstellar dust to form hydrogen bonding with the components of the ice most

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predominantly, water. This causes a greater part of these molecules to be attached to the surface of the interstellar dust grains, thus reducing its interstellar gas phase abundance.

Weak intermolecular interactions are very vital in the elucidation of structures and properties of many important biological molecules like water, DNA, protein etc. Among these weak intermolecular interactions, hydrogen bonding is well recognized, studied and understood to a great extent because of its overwhelming impacts in different systems and phenomena. It is responsible for the unique properties of water essential to life; it serves as a vital force in determining the basic structure of large bio-molecules such as DNA, RNA, proteins etc (Park and Lee, 2007). The binding energy of the hydrogen bonded complex gives information about the strength of the bonding. This binding energy can be determined both experimentally and theoretically. With the advances in quantum chemical calculations, on a careful choice of method (level of theory) and basis set, it is now possible to theoretically estimate binding energy that is in good agreement with the experimentally measured value.

As useful as the DFT method is, it has a number of drawbacks (especially for large systems); insufficient description of van der Waals interaction, inaccurate estimation of polarizabilities of large π-conjugate molecules. It has also been shown to underestimate the binding energy of complexes in comparison with the MP2 to MP4(SQD) methods. This underestimation is said to arise from the insufficient description of electron correlation effects. Among the available ab initio methods, the Møller-Plesset second order method (MP2) has been shown to be effective and accurate in investigating hydrogen-bonded systems; the use of the smallest augmented correlation consistent basis set (aug-cc-pVDZ) for hydrogen-bonded complexes is strongly recommended (Park and Lee, 2007; Ikeda et al., 2007; Møller and Plesset, 1943; Head-Gordon et al., 1988; Frisch et al., 1990).

The formation of interstellar species essentially depends on their formation pathways not on the thermodynamic parameters. However, some correlation between the observed molecules and thermodynamic parameters really exists wherever reaction pathway does not appear to influence. For example, recently, Etim et al. (2016) had shown that the detectability of the odd numbered carbon chains could be correlated due to the fact that they are more stable than the corresponding even numbered carbon chains. Some more studies by Etim et al. (2017) investigated the possibility of detecting most suitable isomer in the C5H9N isomeric group. However, it is not true always. For example, Sil et al. (2017) investigated the possibility of detecting certain amines and aldimines, Gorai et al. (2017) investigated the possibility of detecting some complex thiols in the ISM based on various relevant parameters. They found that most stable species should not be considered as the most potential candidate always because interstellar chemistry is far away from the equilibrium. We also have noticed some deviations from the fact that most stable isomer is observed among some of the groups considered; the conspicuous abundance of a less stable isomer (methyl formate) over the most stable one (acetic acid) and the non-detection of some of the most stable isomers whose less stable counterparts have been detected.

In the present study, we discuss that if the formation/destruction of some species are not influenced by their gas phase pathways and completely controlled by means of the grain surface reactions, gas phase abundances of these species will be strongly influenced by the binding energies. The binding energy of simple interstellar species like H_2, CO, N_2, CO_2, CH_3OH, CH_4, NH_3, H_2CO, etc. are well known but for the complex species, it is mostly unknown. Very recently, Wakelam et al. (2017) extensively studied the binding energy of simple as well as some complex interstellar species by using quantum chemical calculations. They considered a single water monomer as an adsorbent. Initially, they calculated the binding energy of 16 stable species and calibrated their values with the experimentally available BE. We have extracted their fitted values and found that if we use following relation then there values for the 16 stable species can be explained.

$$\text{Scaled BE} = \text{A0} + \text{A1} \times \text{Calculated BE},$$

where A0 = 289.019 and A1 = 1.65174. From KIDA database it can be seen that uncertainties of their estimated values are mentioned to be ~30% even after using the scaling factor. So, we think that after appropriate scaling our proposed BE values of the complex species would certainly help the community to build astrochemical model with an educated estimation rather than considering a blind guess.

We aim to account for these variations and try to correlate the difficulty in the astronomical observation of sugars and want to propose suitable candidates for astronomical observation within the range of our molecules under consideration. For the present study, 20 interstellar molecules (known and possible) which are suitable in achieving the aims of the present study stated above are considered. The strength of their hydrogen bonded complexes with water is investigated by estimating their binding energies at different levels of theory and basis sets. After describing the computational methods used here, the results obtained are presented and discussed.

2. Computational details

All the calculations reported in this work are performed using the Gaussian 09 suite of programs (Frisch et al., 2009). The geometry optimization of all the monomers, water and the corresponding hydrogen bonded complexes have been carried out using the Møller-Plesset second order perturbation theory; MP2(full) with the 6-311++G(d,p) and aug-cc-pVDZ basis sets, the G4 composite method and the Weizmann theory (W1U) (Møller and Plesset, 1943; Martin and de Oliveira, 1999; Parthiban and Martin, 2001; Curtiss et al., 1998; Curtiss et al., 2007a,b).

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