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EDITORIAL
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Editorial: Understanding the Astrophysical Molecular Complexity: Theoretical and Experimental Investigations

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Editorial on the Research Topic

Investigation into the Astrophysical Molecular Complexity: Observational, Theoretical and Experimental Aspects

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The interstellar medium (ISM) is the site of a rich chemistry that evolves from simple to complex organic molecules. To date, a large number of molecular species (more than 220) have been detected in the ISM. The formation and decomposition routes of the different species must be quantitatively understood in order to interpret the observed spectra in terms of local physical conditions. Such studies are very challenging due to the possibility of multiple processes including gas phase reactions as well as crucial catalytic effects of ices and dust grains in a highly dilute environment.

It is also very important to look for spectral signatures of species in different wavelength ranges in order to explore a wide variety of physical and chemical conditions of the environment and possibly identify new species. For this purpose, Far Infrared Spectroscopy (FIR), in close relation with the observations, is an important tool for two reasons. First, the wavelength is large enough relative to the size of the interstellar dust grains to be little affected by interstellar extinction. Second, FIR spectra contain many fine structures of naturally abundant ions and atoms, and several low-level rotational transitions of abundant light hydrides. Since these lines are optically thin, they are excellent probes for the physical conditions of the ISM. All papers included in the present collection fully contribute to a better "understanding of the astrophysical molecular complexity."

When considering the chemistry occurring in the ISM, laboratory experiments often do not accurately reproduce the relevant physical conditions and only one experimental parameter is considered. In a paper presented in this volume, N. J. Mason et al. propose a global approach based on systems science in which the influence of several parameters is studied simultaneously. Such an approach has already been used to great effect in prebiotic chemistry and origins-of-life studies, and its extension to laboratory astrochemistry would thus be of great interest and may reveal hitherto unmined data.

The other contributions to this collection are all theoretical and computational. First, two papers deal with the identification of new species that could enrich the understanding of the chemistry of the ISM. From high level ab initio quantum studies, Doerksen and Fortenberry determine the bond strength of H_mX-YH_n type molecules containing double and triple X-Y bonds, X an Y being all atoms between Li and Cl across periods 2 and 3. The results allow the prediction of a different chemistry (inorganic or organic) depending on the percentage of

hydrogen present in the observed regions. On the other hand, Al-Mogren and Senent present important results on the spectroscopic parameters and far infrared spectra of the D, ^{15}N and ^{13}C monosubstituted isotopes of methylamine. The methods used are very innovative as they allow to treat the strong interactions between bending and wagging modes. Methylamine has been observed in different astrophysical environments and a possible detection of deuterated methylamine has been mentioned. This molecule plays an important role in the gas-phase chemistry of the ISM and some recent studies consider it as a precursor for the formation of glycine in outer space.

The three following papers tackle chemical reactivity studies. Szabo et al. present two different methods to describe the formation by radiative association (RA) of BeH^+ and BeD^+. In their work, it is shown that due to the important role of resonances in the RA cross sections, quantum methods cannot represent the very fine resonances as a result of the large number of populated quasi-bound states at high energies. The Breit-Wigner method is then more appropriate. The data may be used in the modelling of BeH^+ abundance in the ISM as well as its production in thermonuclear fusion reactors on Earth.

Understanding the mechanisms of solid phase reactivity, especially on icy grain surfaces, is a major challenge for the physical chemistry of ISM. Very often, the reactions take place in several steps and the results are strongly dependent on the ice model, crystalline or amorphous and on the presence of other species on the surface. The kinetic isotope effects (KIE) of hydrogen and deuterium diffusion on water ice surfaces are studied by G. Nyman. The method consists in determining the transition state rates of H or D atoms hopping between two adjacent minima on the surface of the grain. Both types of ice are modelled. The results are compared to recent experiments by Kuwahata et al., 2015 and show that KIEs on amorphous ice are well reproduced by transition state theory, while tunnelling scattering contributes significantly on crystalline ice.

The Langmuir-Hinshelwood (LH) and Eley Rideal (ER) mechanisms of H_2 molecule formation on a formaldehyde-doped amorphous ice surface are studied by Kerkeni et al. The ice surface is computed with Molecular Dynamics techniques and reflects the observed density. QM/MM calculations have led to the reaction paths for both mechanisms. Sophisticated semi-classical transition state theory rate constants show that the LH mechanism is faster than the ER. Quantum effects are important in the range 15–200 K.

The works presented in this collection demonstrate the great vitality of the different activities aimed at understanding the origin of the molecular complexity of the interstellar medium. This is a very active field, which is progressively oriented towards the study of prebiotic molecules, with the ultimate ambition of understanding the origin of life on Earth. Many progresses are expected in relation with the forthcoming unprecedented high spatial and spectral resolution observations in the coming years.

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BK: has written parts of the text DD: has improved some statements in the text NF: has provided a first draft of the contribution.

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