



Editorial: Exploring the Chemical Universe

Ankan Das¹*, Luca Bizzocchi²* and Piero Ugliengo³*

¹Indian Centre for Space Physics, Kolkata, India, ²University of Bologna, Bologna, Italy, ³Department of Chemistry, University of Turin, Turin, Italy

Keywords: astrochemistry, interstellar medium (ISM), quantum-chemical calculations, astrochemical modeling, experimental astrochemistry, radio observation, spectroscopy

Editorial on the Research Topic

Exploring the Chemical Universe

The role of molecules in astronomy is now so convincing that we may now use the term "Molecular Universe" to describe a significant fraction of the stellar region. In interstellar space, a wide variety of molecules has already been identified.

OPEN ACCESS

Edited by:

Sven Thorwirth, University of Cologne, Germany

Reviewed by:

Ashraf Ali, University of Maryland, United States

*Correspondence:

Ankan Das ankan.das@gmail.com Luca Bizzocchi luca.bizzocchi@unibo.it Piero Ugliengo piero.ugliengo@unito.it

Specialty section:

This article was submitted to Astrochemistry, a section of the journal Frontiers in Astronomy and Space Sciences

Received: 19 December 2021 Accepted: 28 February 2022 Published: 21 March 2022

Citation:

Das A, Bizzocchi L and Ugliengo P (2022) Editorial: Exploring the Chemical Universe. Front. Astron. Space Sci. 9:839076. doi: 10.3389/fspas.2022.839076 Since the physics and chemistry of the star-forming regions are interrelated, tracing the evolutionary history of these molecules would broaden our understanding of the various stages of star formation. Our knowledge of this development would also expand once we can identify more interstellar species in diverse regions of the Interstellar Medium (ISM). Fortunately, over the last few decades, Astrochemistry has witnessed some dramatic changes due to some notable advances in observational, experimental and computational techniques. There is now evidence that observational findings on molecular cloud cores, simulations and experiments related to the chemical evolution of star-forming regions are beginning to corroborate each other. We are now on the threshold of a new data and simulation-rich era. The following body of work comprises nine articles describing some state-of-the-art investigation at the forefront of Astrochemical research (see Figure 1 for a graphic table of contents).

Several critical aspects of interstellar ice are yet to be fully explored. Our work shows the extensive effort being made to address some of these issues. In the denser molecular cloud region, the dust is covered with a wide variety of chemical species. Moreover, the coating of dust grains is predominantly negatively charged, as described by Rimola et al., and could play a crucial role in the neutralization process of gas phase cations. The consequences of the interaction of these cations with the negatively charged grains give us an improved understanding of the chemical composition of the Universe. Miniscule (<1 nm diameter) spinning dust grains can produce anomalous microwave emission (AME), as reported by Guiu et al., which is likely to be affected by the formation of water ice mantles. The binding energies of interstellar species are key to controlling both the final composition of the interstellar grain mantle as well as species presence in the gas phase due to desorption processes. A realistic estimation of the binding energies is therefore essential for astrochemical modelling. Furthermore, the values of binding energy are sensitive to the grain adsorption sites. Some theoretical studies (see Duflot et al. and Das et al.) have been presented that report classical molecular dynamics and electronic structure methods for finding the binding energies of various interstellar species and include some of the principal constituents of interstellar ice. The values reported warrant the use of astrochemical modelling to estimate the abundances of interstellar species. These computational studies, coupled with the JWST infrared observations will provide further insights on dust and its physical and chemical processes.

1



A drawback for constructing a realistic astrochemical model, however, is the lack of knowledge about the reactivity of the radical cations. Experimental and theoretical studies are needed to address this issue, as shown in the work by Richardson et al.

The recently launched James Webb Space Telescope (JWST) is opening up an extraordinarily detailed view on the infrared Universe and will become a powerful astrochemical tool. With improvements in the sensitivity of the orders of magnitude and spatial resolution compared with previous and other existing technology, it is expected to bring about a revolution in the study of the chemical inventories of gases and solids in many extra-terrestrial environments such as star-forming regions, disks, nuclei of starburst galaxies as well as atmospheres of giant exoplanets. For the useful interpretation of such a wealth of cutting edge data, support from laboratory experiments is crucial. Infrared spectra of molecules are complex and the lack of accurate and comprehensive spectroscopic information can negatively affect the pace of discoveries, hampering both the identification of new species and the quantitative modelling of the features produced by widespread tracers. Detailed studies devoted to the rovibrational spectrum of suitable astrochemical species, such as that reported by Jiang et al., provide very accurate quantitative knowledge of their infrared band structure and spectral profiles thus fully exploiting JWST observations.

Unidentified infrared (UIR) emission bands are observed in various astronomical objects. The collective emissions of PAHs may be responsible for these UIR emissions. However, a single PAH among the Research Topic of these PAHs is yet to be individually identified in space. Monocyclic aromatic hydrocarbons are believed to play an essential role in the formation of such PAHs. They could likely be present in the water-ice-dominated mantle. Laboratory studies (Salter et al.) of these simple aromatic hydrocarbons in the presence of water ice are thus required to assist future identification. Interstellar ice could be processed by various forms of interstellar radiation. UV/VUV and IR absorption spectra are needed to understand the changes in the icy structure as addressed in the work by Lo et al.

The Orion molecular cloud is a stellar nursery and many chemical species have been detected there. This source is well

studied and hosts a variety of high and low mass star-forming regions as revealed by Sahu et al. As a case study, millimetre observations of the Orion molecular cloud could unfold the physical and chemical conditions related to the giant molecular cloud complex.

This Research Topic, then, addresses the above-mentioned issues and will undoubtedly form a useful contribution towards progress in the field of astrochemical research.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's Note: All claims expressed in this article are solely those of the authors and do not necessarily represent those of their affiliated organizations, or those of the publisher, the editors and the reviewers. Any product that may be evaluated in this article, or claim that may be made by its manufacturer, is not guaranteed or endorsed by the publisher.

Copyright © 2022 Das, Bizzocchi and Ugliengo. This is an open-access article distributed under the terms of the Creative Commons Attribution License (CC BY). The use, distribution or reproduction in other forums is permitted, provided the original author(s) and the copyright owner(s) are credited and that the original publication in this journal is cited, in accordance with accepted academic practice. No use, distribution or reproduction is permitted which does not comply with these terms.