frontiers in Astronomy and Space Sciences

EDITORIAL
published: 28 March 2022
doi: 10.3389/fspas.2022.845241

Editorial: Theoretical Characterization of Astrophysical Species

Malgorzata Biczysko[1]*, *Roberto Linguerri*[2] *and Majdi Hochlaf*[2]

[1]International Centre for Quantum and Molecular Structures, Department of Physics, College of Sciences, Shanghai University, Shanghai, China, [2]COSYS/LISIS, Université Gustave Eiffel, Champs sur Marne, France

Keywords: diatomics, complex organic molecules, anharmonic, vibrational, rotational, electronic, spectra, big data

Editorial on the Research Topic

Theoretical Characterization of Astrophysical Species

A deep understanding of the structure, spectroscopic properties and reactivity of astrophysical molecular species is crucial to enlighten the complex processes governing the physical chemistry of the astrophysical media (Biczysko et al., 2017; Hochlaf, 2020; Puzzarini and Barone, 2020; Sandford et al., 2020; Widicus Weaver and Fortenberry, 2021). The Research Topic "Theoretical Characterization of Astrophysical Species" gathers seven contributions highlighting the most recent advances in the theoretical approaches and their applications for the characterization of astrophysical molecules. Indeed, it includes the description of new theoretical methodologies for accurate simulations of molecular systems in the gas phase, or their extension and use for the study of complex organic molecules (COMs) or exotic molecular species. For instance, Yang et al. discussed the performance of density functional theory coupled to generalized second order vibrational perturbation theory for the generation of the patterns and intensities of the IR bands of molecules ranging in size from water to naphthalene and glycine. Through these benchmarks, they concluded that DFT/VPT2 represents a reliable and cost/effective model for the analysis of vibrational spectra of medium- to large-size molecules, whereas flexible molecules should be treated with care because of the presence of large amplitude motions. Similarly, Zapata Trujillo et al. presented computational IR spectroscopic studies of 958 phosphorus-bearing molecules, which could be detected spectroscopically in planetary atmospheres. Again, these authors adopted a DFT/VPT2 scheme, whose accuracy for predicting both band positions and intensities was discussed. They also showed that such big data spectral analysis of P-bearing compounds may be used for future machine learning applications. Besides, the case of DNA bases and their cations was considered by Zhao et al. through the treatment of structures and the spectroscopy of the ground state neutral and cationic thymine. These authors deduced anharmonic wavenumbers for both species again at the DFT/VPT2 level. These data were used to assign the mid- to near-infrared spectrum of thymine and its cation, as well to simulate vibrationally-resolved photoelectron spectrum of thymine in the VUV 8.7–9.4 eV range.

For small molecules, advanced post Hartree-Fock methodologies can be used for electronic structure computations in order to generate their potential energy surfaces (PESs). These include standard and explicitly correlated coupled-cluster methods for ground state species and the CASSCF and MRCI approaches for electronic excited states computations. For better accuracy it was shown that large basis sets are needed, where extrapolation to the complete basis set limit is highly recommended. For instance, Tschöpe et al. and Dallas et al. treated ketenimine and ethynol COMs, where they used either a rovibrational configuration interaction variational approach or perturbation theory to generate rigorous anharmonic spectral data of both species in the IR and microwave regions. Such data are mostly lacking in the literature limiting the possibility of their detections in

OPEN ACCESS

Edited and reviewed by:
Ryan C. Fortenberry,
University of Mississippi, United States

***Correspondence:**
Malgorzata Biczysko
biczysko@i.shu.edu.cn

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

Received: *29 December 2021*
Accepted: *28 February 2022*
Published: *28 March 2022*

Citation:
Biczysko M, Linguerri R and Hochlaf M (2022) Editorial: Theoretical Characterization of Astrophysical Species. Front. Astron. Space Sci. 9:845241. doi: 10.3389/fspas.2022.845241

astrophysical media. In particular, these authors showed the need of special treatments of anharmonic resonances such as Fermi resonances.

This themed collection contains also two articles treating molecules in their electronic excited states, in addition to ground state computations. Indeed, Montes de Oca-Estévez and Prosmiti computed the potential energy curves of noble gas hydride cations, NgH^+ (Ng = He, Ne, Ar). They derived the vibrational levels and molecular spectroscopic constants for all known stable isotopologues of ground state NgH^+ cations. Also, Jarraya et al. characterized the isomers of thionitroxyl radical (H_2NS) in their ground and lowest electronic states. They computed their one-dimensional PESs cuts along the internal coordinates. These cuts allowed for discussion of the photochemistry and assigning of the deep blue glow observed after reactions between "active nitrogen" and H_2S at the beginning of the XXth century.

In sum, the treated molecular systems range from diatomics to medium-sized molecules up to ~15 atoms, including species that are already detected or suspected of being present in astrophysical media. These works focused on the accurate determinations of their stable structures and vibrational fingerprints. They targeted the identification of the best electronic structure methods to be used for the studies of larger molecules, which may exhibit complex PES topologies and resonance patterns. They also considered the isomeric forms and discussed their possible formation in astrophysical media. For some of them, IR intensities were computed to facilitate their detection states, and computations on the ground and electronic excited were carried out to understand their reactivity. Besides, these contributions showed the need of development of new theoretical approaches. Indeed, the already well-established approaches for di- or tri- atomic molecules cannot be transposed to larger systems because of the excessively large number of degrees of freedom. Furthermore, these works enlighten the potential contributions of such data to help the identification of COMs by the new missions and support laboratory experimental results.

AUTHOR CONTRIBUTIONS

MH prepared the original draft. MB, MH, and RL reviewed and edited the final manuscript.

REFERENCES

Biczysko, M., Bloino, J., and Puzzarini, C. (2017). Computational Challenges in Astrochemistry. *Wires Comput. Mol. Sci.* 8. doi:10.1002/wcms.1349

Hochlaf, M. (2020). *In-Silico* Astrochemistry of Life's Building Blocks. *Phys. Life Rev.* 32, 101–103. doi:10.1016/j.plrev.2019.08.008

Puzzarini, C., and Barone, V. (2020). A Never-Ending Story in the Sky: The Secrets of Chemical Evolution. *Phys. Life Rev.* 32, 59–94. doi:10.1016/j.plrev.2019.07.001

Sandford, S. A., Nuevo, M., Bera, P. P., and Lee, T. J. (2020). Prebiotic Astrochemistry and the Formation of Molecules of Astrobiological Interest in Interstellar Clouds and Protostellar Disks. *Chem. Rev.* 120, 4616–4659. doi:10.1021/acs.chemrev.9b00560

Widicus Weaver, S. L., and Fortenberry, R. C. (2021). Space is the Future: Interdisciplinary Research in Astrochemistry and Planetary Science Leads to Innovations that Impact All of Chemistry. *Acc. Chem. Res.* 54, 1309–1310. doi:10.1021/acs.accounts.1c00105

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.