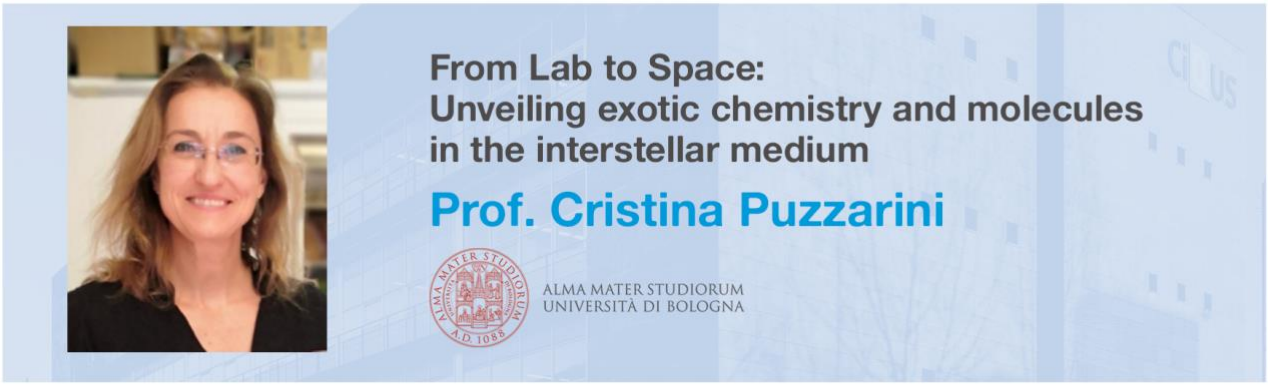
CiQUS Lecture



Thursday, September 19, 2024

12:15 p.m. - CiQUS Seminar Room

Prof. Cristina Puzzarini
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Abstract

The development of a comprehensive understanding of the chemistry that led to the formation of hundreds (likely thousands) of molecules in space is a challenging but fundamental goal of astrochemistry.[1,2] In the last couple of years, we have witnessed spectacular achievements in the discovery of molecular species in terms of number and chemical complexity. The interstellar medium (ISM) is a hostile environment, characterized by extremely low density and temperature, which is however characterized by a rich chemistry. Several are the open questions: Can we explain how the detected molecules were formed? How far does chemical complexity go? How many molecules are still escaping detection?

The starting point for the development of any astrochemical model is the knowledge of the molecular census of the astrophysical object under consideration, together with the corresponding molecular abundances. In this scenario, rotational spectroscopy plays a crucial role because most of the molecular species have been detected by radioastronomy owing to their rotational signatures.[3] The subsequent step is to understand how the detected molecules were formed and how they can further react. In this respect, accurate computational approaches play a fundamental role.[4-6]

In this seminar, by means of a few selected examples taken from the work done at the ROT&Comp Lab, I will address how state-of-the-art computational approaches can derive plausible formation routes able to explain the presence in the ISM of detected molecules and suggests potential candidates for new detections.

References

1. E. F. van Dishoeck. Astrochemistry: overview and challenges. Proc. Int. Astron. Union, 2017, 13, 3.
2. C. Puzzarini. Grand Challenges in Astrochemistry. Front. Astron. Space Sci. 2020, 7, 19.
4. C. Puzzarini, S. Alessandrini, L. Bizzocchi, M. Melosso, V.M. Rivilla. From the laboratory to the interstellar medium: a strategy to search for exotic molecules in space. Front. Astron. Space Sci. 2023, 10, 1211784.
3. H. Ye, S. Alessandrini, C. Puzzarini. Gas-phase formation route for trans -HC(O)SH and its isomers under interstellar conditions: a state-of-the-art quantum-chemical study. MNRAS 2023, 525, 1158.

4. H. Ye, S. Alessandrini, C. Puzzarini. On the General Mechanism for the Gas-phase Reaction of Methanimine with a Radical Species in the Interstellar Medium: Some Failures and an Important Success. Astrophys. J. 2024, 962, 32.
5. J.G. de la Concepción, C. Cavallotti, V. Barone, C. Puzzarini, I. Jiménez-Serra, I. Relevance of the P+O2 Reaction for PO Formation in Astrochemical Environments: Electronic Structure Calculations and Kinetic Simulations. Astrophys. J. 2024, 963, 142.

Biosketch

Cristina Puzzarini is full professor of Physical Chemistry at the University of Bologna. Head of the ROT&Comp lab at the Department of Chemistry ''Giacomo Ciamician''. After a PhD in Theoretical Chemistry (1997), in 2000 she moved back to the Millimeter/Submillimeter wave Spectroscopy lab, where in 1993 she got her MSc degree in Chemistry. Her research activity spans from computational chemistry and spectroscopy to experimental rotational spectroscopy. Her main research interest is astrochemistry: laboratory spectroscopic studies in support of astronomical observations as well as investigation of interstellar chemistry and chemical evolution.