

Astrochemical challenges: the role of quantum chemistry

Cristina Puzzarini

University of Bologna, Department of Chemistry “Giacomo Ciamician”, Bologna, 40126, Italy.

Email: cristina.puzzarini@unibo.it

Understanding the chemical evolution of the universe is one of the main aims of Astrochemistry, with the starting point being the knowledge whether a molecule is present in the astronomical environment under consideration and, if so, its abundance [1]. In this context, rotational spectroscopy plays the central role. The astronomical observation of the spectroscopic features of a given molecule is the definitive, unequivocal proof of its presence in the astronomical environment under consideration, with the overwhelming majority of gas-phase chemical species being discovered via their rotational signatures [1].

Among the goals of astrochemistry, the detection of prebiotic COMs in astrophysical environments is fundamental in view of possibly understanding the origin of life. While the evidence for molecular complexity in the universe is undisputed, there is still much to be understood about what prebiotic molecules are present and how they are formed in the typically cold and (largely) collision free environment of the interstellar medium [1].

By means of selected examples, it will be shown that: (i) theory in the field of rotational spectroscopy plays a crucial role in supporting the identification of new molecules [2,3]; (ii) state-of-the-art computational approaches allow for deriving formation pathways able to explain the molecular abundances derived from astronomical observations [4,5] as well as explaining the products formed in reactions studied via molecular-beam techniques [6].

References

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