Rotational Spectroscopy Meets Quantum Chemistry for Elucidating Astrochemical Challenges

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Cosmic evolution is the tale of progressive transition from simplicity to complexity. The newborn universe starts with the simplest atoms formed after the Big Bang and proceeds toward "astronomical complex organic molecules" (aCOMs). 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. In this context, molecular spectroscopy plays the central role: because of the tremendous distances involved, there is no chance to do direct experiments on astrochemical processes, and detection via interaction of molecules with radiation is the only viable route of investigation. 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 [1-3]. However, the interpretation of astronomical detections and the identification of molecules are not all straightforward.
Among the goals of astrochemistry, the detection of prebiotic aCOMs in astrophysical environments, and in particular in star forming regions, is fundamental in view of possibly understanding the origin of life. While, nowadays, 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. By means of selected examples [4-7], it will be shown that: (*i*) state-of the-art computational approaches are required to derive structures, energies, spectroscopic properties, and thermochemical data for an accurate characterization of the prebiotic aCOMs under consideration and their potential precursors [3,8]; (*ii*) crucial challenges in astrochemistry can be successfully overcome by combining state-of-the-art computational spectroscopy approaches [9] with experiment in the field of rotational spectroscopy.

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