ASTROCHEMICAL CHALLENGES: THE ROLE OF ROTATIONAL SPECTROSCOPY

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Understanding the chemical evolution of the universe is one of the main aims of Astrochemistry, with the starting point being the census of the molecules present in the astronomical environment under consideration and their abundance. 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. Therefore, the detection of a molecular species requires an accurate laboratory investigation.

This contribution presents the strategy developed at the ROT&Comp lab (https://site.unibo.it/rotational-computational-spectroscopy/en)[1,2] and its application to illustrative systems.[3,4,5] The strategy starts from the interplay of experiment and theory: state-of-the-art quantum-chemical calculations are used to predict the relevant spectroscopic information required to guide the spectral recording, analysis and assignment. Rotational spectra measurements are then performed in the millimeter-/submillimeter-wave region. Subsequently, the spectral analysis leads to accurate spectroscopic parameters, which are then used for setting up accurate line catalogs for astronomical searches and detections. The last step is the derivation of the molecular abundance within the local thermodynamic equilibrium (LTE) approximation by exploiting the rotational diagram method. However, going beyond the LTE approximation might be needed, thus requiring the knowledge of their collisional coefficients for the most abundant perturbing species.[6,7]

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