Astronomical complex organic molecules in space: the crucial frequency information from rotational spectroscopy

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Understanding the chemical evolution of interstellar clouds and star-forming regions is a central problem in astrophysics and astrochemistry. The starting point is the identification of the chemical species through their spectroscopic signatures: the frequency information in fact provides the unequivocal proof of the presence of a chemical species. Such identification requires the direct comparison of the frequencies retrieved from the astronomical observations with those obtained in the laboratory, with gas-phase species being mostly discovered via their rotational signatures (with frequencies going from the millimeter-wave region to far-infrared).

The systematic observation of a given astronomical source at all wavelengths leads to line surveys that in principle provide a complete census of the molecular content. The assignment of these line surveys allows for an unbiased picture of the chemical composition that in turn can also be used to infer information on physical conditions (such as temperature and density). The new powerful astronomical facilities (like ALMA, Herschel and SOFIA, just to mention a few examples) opened up to unprecedented resolution and sensitivity as well as frequency coverage, thus offering unique opportunities to extend the chemical inventory, in particular to organic species of increasing complexity (the so-called astronomical complex organic molecules). On the other hand, sensitivity and resolution increase the line confusion in spectral observations, thus requiring a large effort to be taken in laboratory measurements (from both an experimental and computational point of view) to help in unravelling it.

Furthermore, to interpret and analyze the astronomical observations, an important piece of information is provided by the collisional excitation rates of the molecules with the predominant collision partners (like H_2 and He); these rates can be calculated using quantum-chemical methods or measured in the laboratory.

In this contribution, the role played by laboratory (experimental and computational) rotational spectroscopy in the field of astronomical observations and in the investigation of astronomical complex organic molecules will be illustrated through a number of examples and case studies.