From lab to space: An integrated rotational spectroscopy–quantum chemistry strategy

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Understanding the chemical evolution of the interstellar medium is one of the main aims of astrochemistry, and one of the biggest challenges (see Figure 1). The starting point for the development of astrochemical models is the knowledge whether a molecule is present in the astronomical environment considered and, if so, its abundance [1]. In this scenario, rotational spectroscopy plays a crucial role because most of the molecular species have been detected thanks to their rotational signatures. These, in turn, are accurately obtained from laboratory spectroscopy studies that are increasingly assisted by quantum-chemical calculations, also in the derivation of molecular abundances [2-6]. The subsequent step is understanding the chemical evolution: how the detected molecules were formed and how they can further react [1]. Accurate computational approaches play a fundamental role in this respect [7-10].

In this presentation, by means of a few selected examples taken from the work done in my laboratory, I will address: (*i*) the interplay of experiment and theory in the field of rotational spectroscopy in support of astronomical observations; (*ii*) the exploitation of state-of-the-art computational approaches to derive non-LTE molecular abundances and formation pathways able to explain molecular detections.

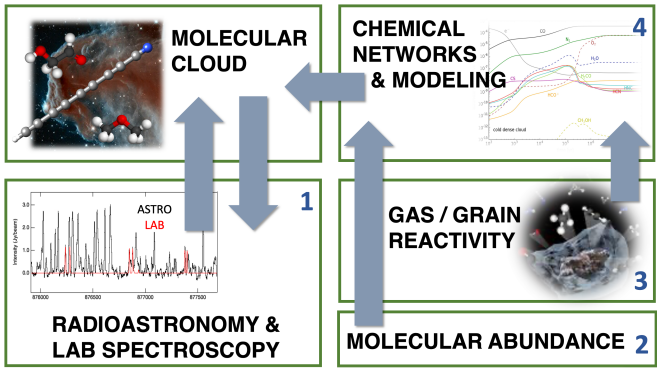

Figure 1: Chemical evolution – the required steps for the chemical characterization of a molecular cloud.

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