AstroDySp

Dynamics and spectroscopy of small and medium sized astrophysical molecules

Abstract

If we want to make sense of the place we occupy in the universe, we must go back to its origin and understand the formation mechanisms and processes of the stars, planets and exoplanets in the interstellar medium (MIS). In the interstellar medium of our Milky Way (the medium between the stars), space is not really empty but filled with gas and dust, it is the reservoir of future stars. In the interstellar clouds, the list of molecules, atoms and ions detected, where particular conditions prevail has since ceased to grow. Indeed, understanding the way in which molecules form and become more complex provides an ample insight into how we end up with the formation of a planet like the Earth carrying life. This medium is often out of thermodynamic equilibrium, because of the extremely low densities (diffuse cloud $n\sim10^1$ to 10^2 per cm^3 and dense cloud $n\sim10^4$ to 10^8 per cm^3) compared to the terrestrial atmospheric density ($n\sim10^{19}$ per cm^3). In order to be able to decipher this environment carefully, it is interesting to determine the populations of molecular energy levels in the MIS. This requires detailed knowledge of the molecular spin-rovibronic spectra and the collision rates of the inelastic collisional settlement processes that occur more frequently.

In the first part of this project we will characterize spectroscopically important astrophysical molecular species such as carbon-chain molecules and their ions which represent ~ 40% of the interstellar molecular species detected to date. During this project the potential energy surfaces of these molecules will be incorporated into nuclear motion treatment to determine their spin-rovibronic spectra.

In the ISM, the populations of the molecular rovibrational levels are not only controlled by the temperature of the interstellar gas and the radiative processes but also by the collisional processes governing the excitations and de-excitations of the molecular energy levels. The interstellar medium, which occupies about 10% of the mass of our galaxy, is essentially composed of 90% of hydrogen in atomic or molecular form and of 10% of helium, the other elements are present only in traces. Therefore, the study of the collision dynamics of abundant molecules in the ISM with H_2 and He are of great interest for astrophysical diagnosis. Contrary to the radiative phenomena, collisional excitation phenomena are not easy to measure in laboratory. Thus, in order to understand the physico-chemical conditions of the astrophysical environments that we want to probe, it is essential to know with sufficient precision these collisional processes, which are characterized by a transition probability from one energy state to another for a given temperature: the collision rates. The second part of this project concerns thus the determination of the collision rates of the small and medium sized molecular systems investigated spectroscopically in collision with He and H_2, where we will generate their intermonomer potential energy surfaces followed by full quantum treatment of nuclear motions.

The proposed research consists of providing the astrophysical community with very accurate spectroscopic properties and collision rates essential to model the observed lines, especially after the implementation of new observation tools such as the ALMA interferometer or JWST. This project will also show the impact of the use of very precise quantum nuclear dynamical methods and mD-PESs computed with the most recent quantum chemistry methods on the collision rates and spectroscopic properties.