

Theoretical study of the vibrational energy redistribution in CO and CO:N₂ aggregates

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In the coldest regions (≈ 10 K) of the interstellar medium (ISM), most molecular species apart from H₂ accrete on dust grains to form ice mantles, acting as particularly rich molecular reservoirs. Nevertheless, large amounts of gas phase species are also detected in these regions and their existence can be explained by desorption processes at the ice surface. Among these processes, the desorption induced by UV radiations, known as UV photodesorption, has been the subject of several experimental studies on different compounds, such as CO^{1,2}, the second most abundant species in the interstellar medium. It has been shown that the UV photodesorption in pure CO and mixed CO:N₂ ices follows an indirect "Desorption Induced by Electronic Transition" (DIET) mechanism.³ In this astrochemical context, the theoretical work presented here aims to understand, at the molecular level, the vibrational energy redistribution mechanism in pure CO and binary CO:N₂ ices. The chosen approach is the molecular dynamics one, either *ab initio* (AIMD) with the VASP software or based on classical force fields.⁴ In particular, the focus is on the end of the DIET mechanism where the electronic energy of the excited molecule, redistributed on some high vibrational states of its electronic ground state, is transferred to neighbouring molecules inducing or not a desorption. To do this, an aggregate approach is used to model the amorphous structure of the simulated ice. These aggregates, initially created, optimised, and then thermalised at temperatures similar to those of the ISM, are then used in molecular dynamics simulations in which a randomly selected CO or N₂ molecule is excited at given vibrational levels (from $v=5$ to 40). The energy redistribution in translational, rotational, and vibrational modes taking place in the aggregate, after a single molecule vibrational excitation, is analysed and compared for the two molecular dynamics approaches used in this study.

Références

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