CO_2 on interstellar iced grains: insights into adsorption and spectral features

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Dust grains covered by thick water-dominated ice mantles are present in the coldest and densest parts of the interstellar medium (ISM) and in protoplanetary disks during different stages of planetary formation. Until 2021 almost 300 species have been identified in the gas phase in the ISM, while only a fraction of these species has been detected in ices [1]. Since, observations of ices require a background-illuminating source for absorption, the available lines of sight for investigation are constrained. Further challenges arise when observations are compared with laboratory spectra, which is due to the influence of temperature, ice structure and the presence of other species. Some of these issues can be solved by employing quantum chemical calculations to simulate the infrared (IR) spectra. While, James Webb Telescope (JWST) has been already proven to be an excellent tool for detecting the chemical components of the icy mantles by means of IR spectroscopy, it requires precise spectral references [2]. In my work I use the ACO-FROST procedure to address the adsorption and IR spectral signature of CO_2, a third most abundant and astrochemically relevant icy species, on a model of an iced grain [3]. I will discuss the binding energy distribution and the IR spectral features of CO_2 in the context of experimental spectra and the findings from the JWST.

References

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