Crystallization of CO2 ice at astronomical conditions

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Authors	Escribano, R M*, Molecular Physics, Inst. Estructura de la Materia, IEM-CSIC, Madri Munoz-Caro, G, Centro de Astrobiología (CAB), INTA-CSIC, Madrid, Spain Cruz-Diaz, G, Centro de Astrobiología (CAB), INTA-CSIC, Madrid, Spain Mate, B, Molecular Physics, Inst. Estructura de la Materia, IEM-CSIC, Madrid, Spain Rodriguez-Lazcano, Y, Molecular Physics, Inst. Estructura de la Materia, IEM-CSIC,
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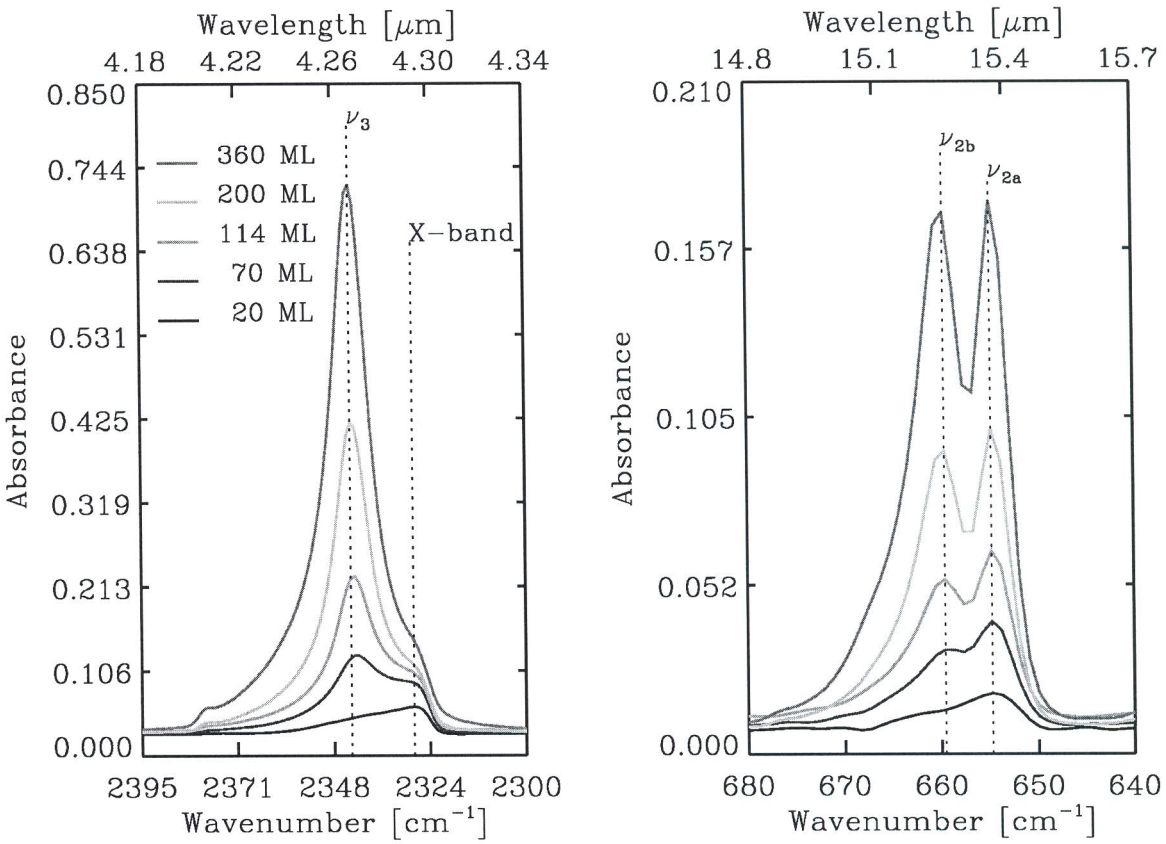
Abstract

Carbon dioxide is, after water and comparable to carbon monoxide, one of the most abundant frozen molecular species observed in the lines of sight towards many astrophysical media. We present here an experimental and theoretical investigation on carbon dioxide ices, generated in the lab in a range of temperature, density, amorphicity, and growing conditions (1), and simulated via high level theoretical calculations. Amorphous CO2 ice was generated at CAB by deposition onto a CsI substrate at 8 K under ultrahigh vacuum conditions in the 10-11 mbar range. The pressure increase used for the deposition of CO2 was very low, 10-9 mbar, to enable the formation of highly amorphous CO2 ice, at very low deposition rate. The transmittance infrared spectra, collected at several stages of sample growth, from 20 to 360 monolayers, are shown in the Figure. In a different set of experiments performed at IEM, the morphology of the amorphous CO2 ice has been studied using reflexion-absorption infrared (RAIR) spectroscopy. Calculated spectra of amorphous CO2 ice are obtained using the SIESTA code (2). In a first step, crystalline structures are processed by molecular dynamics to generate amorphous samples, which are subsequently relaxed until an equilibrium configuration is reached. The vibrational spectra of the amorphous solids are then calculated. The spectra of amorphous ice can change significantly depending on the density of the sample. An IR band, red-shifted with respect to v3, has been identified as a witness of pure and amorphous CO2 ice. It vanishes when the sample becomes crystalline, either by temperature increase or by accumulation of increasing number of layers. The absence of this band in the observed spectra of solid CO2 is an indication that there is no pure and amorphous CO2 ice in inter- and circumstellar mantles

References 1. Escribano, R., Muñoz Caro, G., Cruz-Díaz, G.A. Rodríguez-Lazcano, Y. and Maté, B., PNAS, accepted for publication, July 2013.. 2. Ordejón, P., Artacho, E., Soler, J.M., Phys. Rev. B, 53, R10441 (1996).



Transmission spectra of CO2 ice samples deposited at 8 K, for increasing thickness expressed as monolayer coverage. Spectral regions of v3 (stretching mode) and v2 (bending mode), are shown on the left- and right-hand panels, respectively.

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