Theoretical models for the spectroscopy of methane/ethane ice mixtures

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In a recent work [1], we have determined the optical constants and band strengths of methane/ethane ice mixtures in the near- and mid-infrared ranges. We present here recent calculations on models for these mixtures. Methane and ethane are constituents of planetary ices in our Solar System. Methane has been detected in outer solar system bodies like Titan, Pluto, Charon, Triton, or other TNO's [2]. Ethane has also been identified in some of those objects [2]. The motivation of this work was to provide new laboratory data that may contribute to the understanding of those systems, in the new era of TNO's knowledge opened up by the New Horizons mission [3].

The models are designed to match the composition and density of the mixtures studied in our laboratories. The calculations include several steps: first, the amorphous samples are generated, via a Metropolis Montecarlo procedure (see Fig. 1); next, the amorphous structures are relaxed to reach a minimum in the potential energy surface; at this point, the harmonic vibrational spectrum is predicted. Finally, the relaxed structures are processed by molecular dynamics with the final aim of obtaining an anharmonic prediction of the spectra, which includes the near-infrared region. Both the harmonic and anharmonic spectra are compared to the experimental measurements in the mid- and near-infrared regions (see Fig.2), respectively.

All calculations are carried out by means of Materials Studio software, using the Density Functional Theory method, with GGA-PBE approximations.

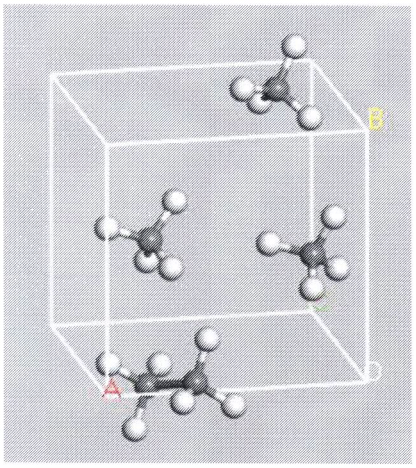

Fig.1. Schematic representation of an amorphous mixture with three methane and one ethane molecules.

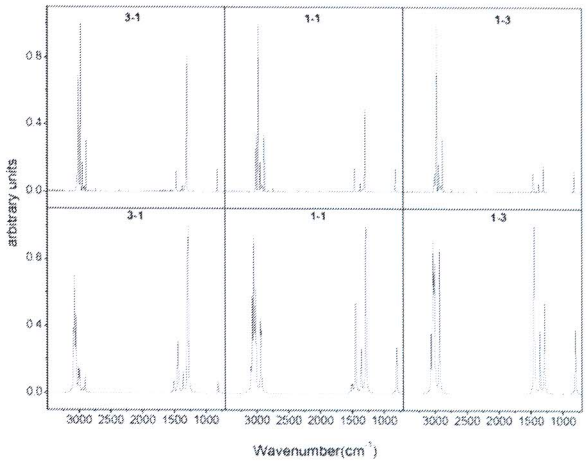

Fig. 2. Comparison of experimental (top) and calculated spectra in the mid-IR for three of the mixtures studied in this work with the indicated CH_4:C_2H_6 ratio

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