Infrared spectra of ice mixtures: Methane/Ethylene

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Ethylene, a product of energetic processing of methane ices [1] is known to be an astromolecule present in our solar system [2]. In addition, methane is thought to be the most abundant of hydrocarbons among those present in the surface of transneptunian objects (TNOs) [3]. Recently, the New Horizons mission has provided abundant data of Pluto's surface, and assignment of several spectroscopic features associated with planetary ices is required.

In the present work, the second of a series dedicated to astrophysical relevant mixtures[4], a full set of spectroscopic data from 6000 cm^{-1} (1.6μm) to 800 cm^{-1} (12.5μm) has been obtained of ice mixtures at 30K of CH_4/C_2H_4 in several proportions, namely 100/0, 75/25, 50/50, 25/75 and 0/100. Band displacements, band strengths and imaginary and real components of the complex refractive index have been determined for these materials in the spectral window under consideration. Along with the spectroscopic features, density and visible refractive index of these ices have also been measured.

For the study of the subtle spectroscopic effects arising from the mixtures with respect to the pure species, we have built several theoretical models at the DFT level using the CASTEP code [5]. Simulation cells are randomly built using Montecarlo simulations and then, molecules in the cell are relaxed until a minimum in the potential energy surface of the system is reached. Infrared spectra are computed at this minimum.

From our experiments we observe a deviation in several factors such as band positions and band strengths with respect to the pure species, as expected from previous works [6]. Band displacements follow the trend expected for methane, in which a dilution in a non polar environment displaces the methane vibrations to lower wavenumbers with an increase in the wavenumbers of the second molecule. An abrupt decrease of the density of ethylene in comparison with previous diffractometric measurements has also been observed [7]. Band strengths for methane also behave as in our previous work, leading to decays in the total band strength with the dilution. However, for ethylene, strengthening and weakening have been observed for different bands, leading to a complex interpretation in which atomistic calculations play an important role.

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