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DIFFUSION AND INFRARED PROPERTIES OF MOLECULES IN ICE MANTLES

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Within dense molecular clouds the formation of frozen icy mantles on interstellar dust grains is thought to be the result of various growth processes. The molecules, which make up the ice mantles are probably completely mixed. To study the physical properties of such ice mixtures we performed experiments on the evaporation processes and on the spectroscopic properties of CO, CO_2 and CH_4 in water rich ices.

The decrease in concentration of volatile molecules in ice samples deposited at 10 K and subsequently heated is found to occurs essentialy in two steps. The first one, corresponding to an evaporation of part of the volatile molecules, starts at about 25 K for CO, 32 K for CH_4 and 70 K for CO_2. During the crystallization of H_2O ice at T > 120 K a second evaporation occurs leading to the complete disappearance of the volatile molecules in the solid phase. The rates of disappearance are closely connected with the crystallization rates of H_2O ice. These crystallization rates have been measured between 125 and 150 K and the activation energy of the amorphous to cubic transition has been determined.

We show that when CO is trapped in water rich ice mixtures at 10 K the 2137 cm^{-1} (4.68 μm) absorption undergoes an initial irreversible change in shape upon warmup. Subsequent changes in intensity with temperature are reversible. These phenomena can be understood by considering two different interactions between CO and H_2O. The formation of a quite strong hydrogen bond between the carbon atom and a hydrogen atom explains the existence of the 2152 cm^{-1} (4.64 μm) CO satellite. Rearrangement of the water hydrogen bonding network during warmup explains its disappearance. The thermal reversibility of the CO 2137 cm^{-1} line intensity suggests either the involvement of a localized mode or dipolar interactions between CO and H_2O molecules.

The main astrophysical implications of the diffusion and spectroscopic behaviors are presented. We focus on the possible effects of a heating source on the fraction of volatile molecules, such as CO, trapped in grain mantles observed towards protostars. Furthermore, we explain how the spectroscopic effects observed have important implications on the use of laboratory spectra in the interpretation of column densities, temperature and thermal history of interstellar grain mantles.