

Hydrogen Defect Vibrations in Various Phase Deuterium Ices.

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The inelastic incoherent neutron scattering spectra of mixed D₂O with a very small amount of H₂O (<5%) in the high density amorphous (hda) ice, ice VIII and ice II have been measured recently at Rutherford Appleton Laboratory (UK). The hydrogen atom in D₂O ice lattice has three distinguished vibrations. The lower frequency of two bending vibrations and a stretching frequency have been recognised. For the different phases of ice these frequencies are slightly different. It was found that the lower bending frequency is at ~100 meV for hda ice, ~94 meV for ice VIII and ~95 meV for ice II and they are all lower than the value 105 meV for ice Ih (J.C. Li, J. Chem. Phys. 105 (1996) 6733). It was also found that ice VIII stretching frequencies are at ~320 meV for the O-D vibrations and 430 meV for the O-H vibrations respectively and they are significantly higher than the values of ~305 meV and ~410 meV for ice Ih, indicating that the inter-molecule interactions is weakened by the increase of O-O separation distance in ice VIII which is consistent with the Infrared Absorption results (B.M. Sukarova, W.F. Sherman and G.R. Wilkinson, Spectrochim Acta A 41 (1985) 315).