Ordering of Hydrogen Bonds in High-pressure Low-temperature Ices

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We have studied the near *K*-edge structure of oxygen in liquid water and ices III, II, and IX at 0.25 GPa and several low temperatures down to 4 K using inelastic x-ray scattering at 9884.7 eV with a total energy resolution of 305 and 175 meV [1]. It is found that the ordering of the oxygen network from the liquid phase to ice III causes only a small decrease of the preedge intensity, whereas the ordering of the hydrogen bonds in the proton-ordered lattice of ices II and IX dramatically reduces the preedge intensity, which is interpreted as a result of the diminishing number of uncoordinated hydrogen bonds in ices II and IX. Some preedge intensity remains, however, in the latter phases unexpectedly according to previous first principles calculations [2]. Our density functional theory calculations of the near-edge X-ray absorption spectrum for ice IX indicate that the remaining intensity may be due to the influence of the local electronic structure by the Madelung potential of the crystal lattice. Substantial changes of the near *K*-edge spectra from ice IX have also been observed below 50 K.

[1] Cai Y.Q., et al., *Phys. Rev. Lett.*, 2005, **94**, 025502. [2] Myneni S., et al., *J. Phys. : Condens. Matter*, 2002, **15**, L213.

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