

The Local Structure of Ice VII Determined by Neutron Total Scattering

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The structural characterization of the local geometry of the H-bond network in Ice VII has been a long-standing problem in ice physics. Rietveld refinements of neutron powder-diffraction data have revealed an apparently short molecular O-D bond-length [1,2] in the average structure. The assumption that the real bond-length is close to that found in the (ordered) ice VIII structure has led to the proposal of site disorder of the oxygen atom in ice VII. By converting the neutron-diffraction pattern of ice VII into a total structure factor, thereby retaining the information content of the diffuse scattering, we have been able to make a direct measurement of the molecular bond-length, demonstrating that it is indeed identical to that found in ice VIII. Additionally, we observe clear differences in the radial-distribution function from 1.5 - 2.0 Å, potentially indicating differences in the O...D separation between the two phases and, thus, H-bond geometry.

These results should have interesting implications for the interpretation of inelastic studies of the hydrogen-bond dynamics and may shed light onto the mechanism of bond centering at higher pressures.

[1] Kuhs W.F., et al., *J. Chem Phys.*, 1984, **81**, 3612. [2] Nelmes R.J., et al., *Phys. Rev. Lett.*, 1998, **81**, 2719.

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