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The structure of ice VII on the approach to symmetrisation MALCOLM GUTHRIE, REINHARD BOEHLER, Geophysical Laboratory, Washington, DC, USA, CHRISTOPHER TULK, ANTONIO MOREIRA DOS SANTOS, Neutron Sciences Directorate, ORNL, Oak Ridge, TN, USA, KUO LI, Geophysical Laboratory, Washington, DC, USA, JAMIE MOLAISON, Neutron Sciences Directorate, ORNL, Oak Ridge, TN, USA, RUSSELL HEMLEY, Geophysical Laboratory, Washington, DC, USA — The symmetrisation of the H-bonds in water was first predicted almost 60 years ago [1]. In subsequent decades, the formation of symmetric ice X has been extensively studied. Neutron-diffraction studies of D_2O ice [2,3] are particularly useful in characterising the structure, providing the only direct measurements of the proton (deuteron) density distribution. However, to date, a limited maximum pressure (of <30 GPa) for these studies has confined them to a regime where the water molecule geometry remains essentially unchanged from ambient pressure [3]. We will present an implementation of diamond-anvil-cell techniques for neutron powder diffraction at the SNS, Oak Ridge TN. This new capability permits neutron structural measurements up to at least 70 GPa. We will show data on crystalline D_2O up to these pressures, which approach those of the symmetrisation transition.

[1] B. Kamb & B.L. Davis PNAS **52** 1433 (1964);
[2] W.F. Kuhs J. Chem. Phys. **81** 3612 (1984);
[3] R.J. Nelmes et al Phys. Rev. Lett. **81** 2719 (1998).

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