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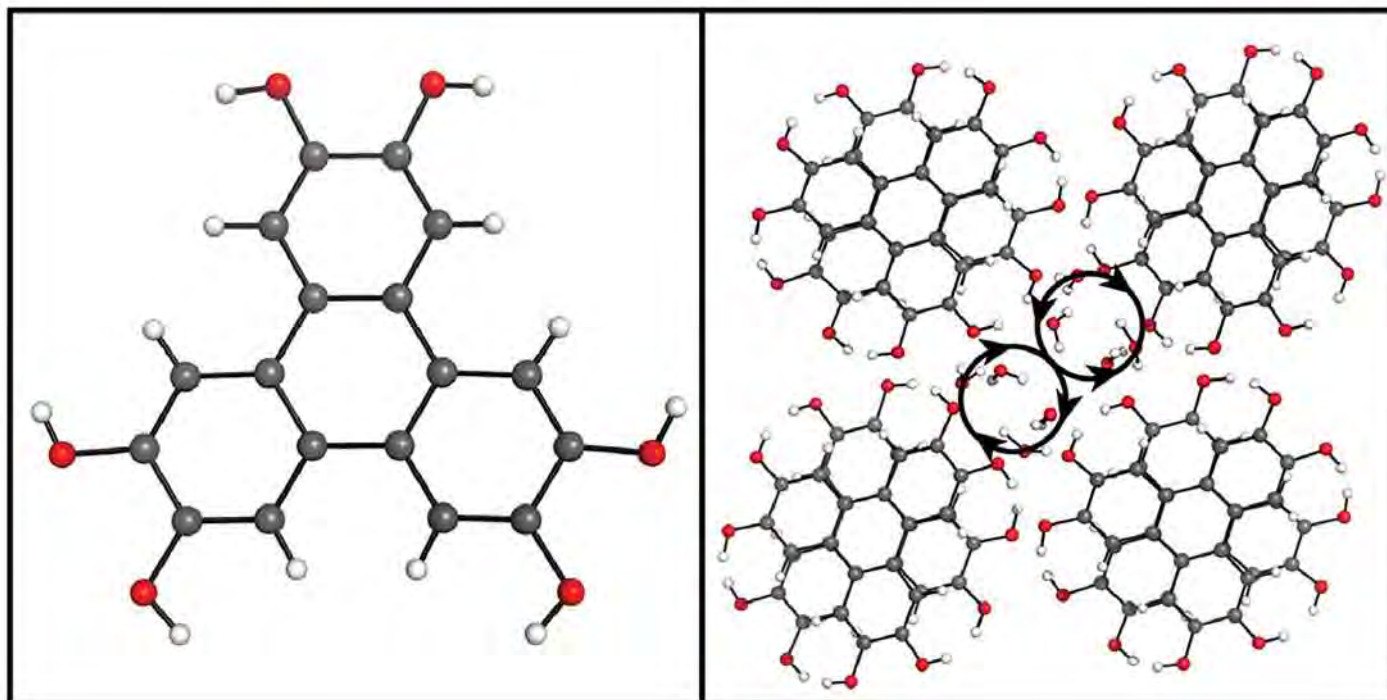
Hydrogen bond order/disorder in a polar one-dimensional confined ice

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Ice is one of the most well-studied substances yet forming a polar, bulk phase, where the water molecule dipoles are all aligned, has proved to be challenging. One approach is to confine the water in nanotubes, such that the molecules are restricted in orientation [1], however this hinders their use as ferroelectric devices – the primary application of polar ices. An alternative is to exploit the voids in nanoporous crystalline hosts but there are, as yet, no reported confined ice systems where the water molecules are able to switch between paraelectric and ferroelectric states whilst retaining a crystalline structure. One such porous system is 2,3,6,7,10,11-hexahydroxytriphenylene (HHTP) tetrahydrate, where columnar stacks of the HHTP molecules are arranged in a pseudo-square arrangement and the water molecules occupy the pores, forming one-dimensional, meso-helical chains. The structure, determined previously [2], crystallises in Pbcn, however this places inversion centres within the water chains leading to unphysical intermolecular H...H contacts. A variable-temperature single-crystal X-ray diffraction investigation is described where careful consideration of the data shows how long-range dipole ordering within and between the water chains is induced, by varying temperature, transforming the crystal structure to the polar Pna21 space group [3]. Subsequent reassessment of the ambient temperature structure reveals a superposition of opposing polarisation states.

[1] K. Koga, G. T. Gao, H. Tanaka and X. C. Zeng, *Nature*, (2001), 412, 802-805, [2] F. Thébault, L. Öhrström and M. Haukka, *Acta Cryst.*, (2011), C67, o143-o145, [3] J. Adamson, N. P. Funnell, A. L. Thompson and A. L. Goodwin, *Phys. Chem. Chem. Phys.*, (2014), 16, 2654-2659



Keywords: Hydrogen bonding, Confined ice, Disorder