

## Quantum behaviour of ultraconfined water in minerals

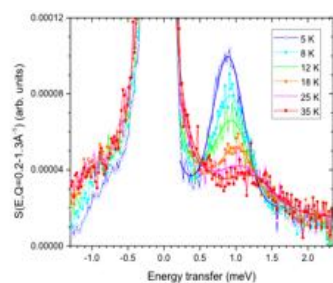
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Recently, using inelastic neutron scattering (INS), we observed quantum tunnelling of type-I water confined in  $\sim 5.1$  Å diameter channels of mineral beryl (hcp structure) oriented with its dipole perpendicular to the c-axis [1]. The study revealed that, at low temperatures, water does not have hydrogen bonds to the surrounding structure and its protons tunnel between the 6-fold equivalent positions in the ab-plane. No evidence of tunneling has, however, been observed in the related, but lower-symmetry, cordierite structure or in alkali-rich beryl with type-II water oriented with its dipole parallel to the c-axis. Basanite ( $\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$ , monoclinic I121 [2]), has a structure with channels formed by  $\text{CaO}_8$  and  $\text{CaO}_6$  polyhedra with water molecules in the channels occupying two positions. INS spectra measured with wide range of energy transfers, showed that, at low temperatures ( $T=5$  K), intramolecular O-H stretching modes of water are at high energy, around 445 meV (compared to 410 meV in ice-Ih), and the intermolecular librational band is at significantly low energies, 35 – 90 meV (65 – 125 meV in ice-Ih), indicating weak hydrogen bonds acting on water molecules. At lower energies, we observed a peak at  $\sim 1$  meV that shows tunneling behaviour (see Fig. 1): its intensity decreases with increasing temperature (from 5 to 35 K) and increases as a function of neutron momentum transfer (thus it is a nonmagnetic peak). In addition, two peaks were observed at  $\sim 4.5$  and 5.5 meV. The intensity of the first



grows with temperature faster than it should be due to the Bose population factor, while the second decreases. Therefore, a possible phase transition or a change in water position in the basanite channels occurs around 15 K.

Figure 1. Temperature dependence of the dynamical structure factor  $S(E,Q)$  for basanite measured with  $E_i=4$  meV. [1] Kolesnikov, A.I. et al. Phys. Rev. Lett., 2016, 116, 167802. [2] Bezou, C. et al. J. Sol. State Chem., 1995, 117, 165.

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