Concerted proton tunnelling in ordinary ice

L.E. Bove[1], S. Klotz[1], A. Paciaroni[2], F. Sacchetti[2]

[1] *IMPMC, CNRS- Université P. et M. Curie, F-75252 Paris, France.*
[2] *CNR-INFM CRS-Soft, c/o Dipartimento di Fisica, Università di Perugia, I-06123 Perugia, Italy.*

We present high-resolution, incoherent quasielastic neutron scattering measurements on ice *Ih* (ordinary ice) and *Ic* (cubic ice) which show the existence of an anomalous, non-harmonic motion of hydrogen at low temperatures. We show that this dynamics is localized, non-vibrational, and related to the hydrogen disorder since it is absent in the hydrogen-ordered phase, ice VIII (see figure). A main jump distance of 0.75 Angstrom is identified, i.e. close to the distance between the two possible proton sites along the oxygen-oxygen bond. The motion is non-Arhenius, has a large time rate of 2.7 $x10^{11}$ s^{-1}, and affects only a few percent of the total number of hydrogen atoms in the crystal [1]. A partial (20%) deuteration of the sample, assuring, statistically, a breaking of the symmetry of the *ordered hexagonal rings* [2], hinders the observed dynamics.

These results give evidence for the existence of concerted proton tunnelling in these ice phases.

[1] L.E. Bove et al., Phys. Rev. Lett. , in press October 2009.
[2] L. Pauling, J. Am. Chem Soc. 57, 2680, 1935.

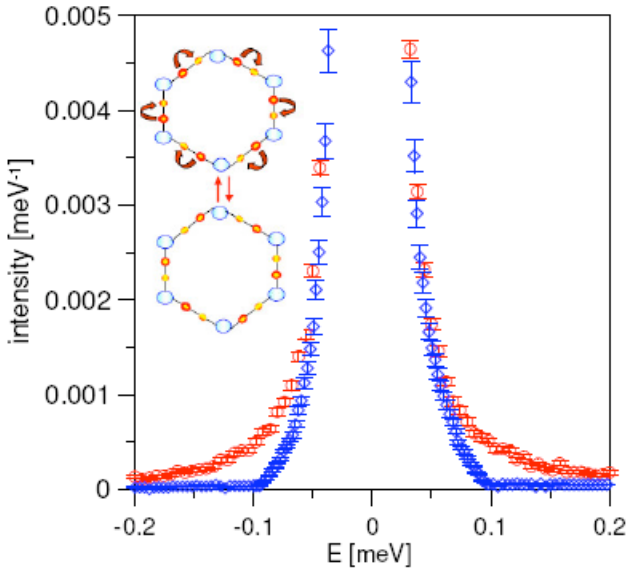

Figure 1: Quasi-elastic contribution in ice Ih (red circles) compared with ice VIII (blue rhombus) at 5 K. The ice VIII spectrum is coincident with the measured instrument energy resolution. Insert: a sketch of the proposed concerted tunnelling of the hydrogen atoms in the *hexagonal ordered loops*.