Structure of Liquid Water up to 6.5 GPa and 672 K

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The local structure of liquid water has been and still is the subject of discussion [1 and references therein]: (i) many of the theoretical concepts of water base upon two-state models, (ii) local inhomogeneities in the liquid phase have been proposed and (iii) the relationship between the amorphous ice phases and the liquid remains unclear. We have extended the pressure range of previous diffraction studies by more than a factor four. Our study along the melting line of ice VII reveals pronounced structural changes induced by pressure. We discuss details on the experimental aspects [2] and on the method of *Empirical Potential Structural Refinement* (EPSR) [3], which allowed us to extract partial and angular averages from a single neutron scattering experiment without isotope substitution. Our experimental findings are compared to classical and *ab-initio* molecular dynamics calculations [4] and preliminary conclusions are drawn.

[1] P.G. Debenedetti et al., Physics Today, June 2003, 40.

[2] Y. Le Godec et al., High Pressure Research 2004, 24, 205.

[3] A.K. Soper, Chem.Phys. 1996, 202, 295.

[4] E. Schwegler et al., Phys.Rev.Lett. 2000, 83, 2429.