ESRF	**Experiment title:** Hydrogen bonding in liquid water	**Experiment number:** CH-1664
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Report:

Isotropic Compton profiles of liquid and solid water have been measured at different temperatures, ranging from -30 to 90 °C. The incident photon energy was 56 keV and the scattered radiation was measured using a 13-element solid-state detector at a scattering angle of 157°. The momentum resolution was about 0.64 a.u. while the statistical accuracy was about 10^{-2} % of $J(0)$ at the peak for each temperature.

The aim of the experiment was to study the breaking of hydrogen bonds in water as a function of temperature, a subject that is still under debate [1-3]. In the Compton profile the breaking of hydrogen bonds in water is observed as a small oscillating modulation of the monomer profile [4]. Due to the small size of the effect, an excellent statistical accuracy is crucial.

The amplitude of the above mentioned modulation of the Compton profile depends primarily on the elongation of the hydrogen bonds. Therefore we observe the change in the bond-length distribution, rather than breaking of the individual bonds.

In figure 1 the temperature-dependent changes in the liquid water Compton profiles are shown, in comparison with a model based on experimental bond-length distributions [1]. A manuscript is in preparation.

[1] K. Modig et al., Phys. Rev. Lett. **90**, 075502 (2003).
[2] Ph. Wernet et al., Science **304**, 995 (2004).
[3] B. Hetenyi et al., J. Chem. Phys. **120**, 8632 (2004).
[4] M. Hakala et al., Phys. Rev. B (2004), in press.

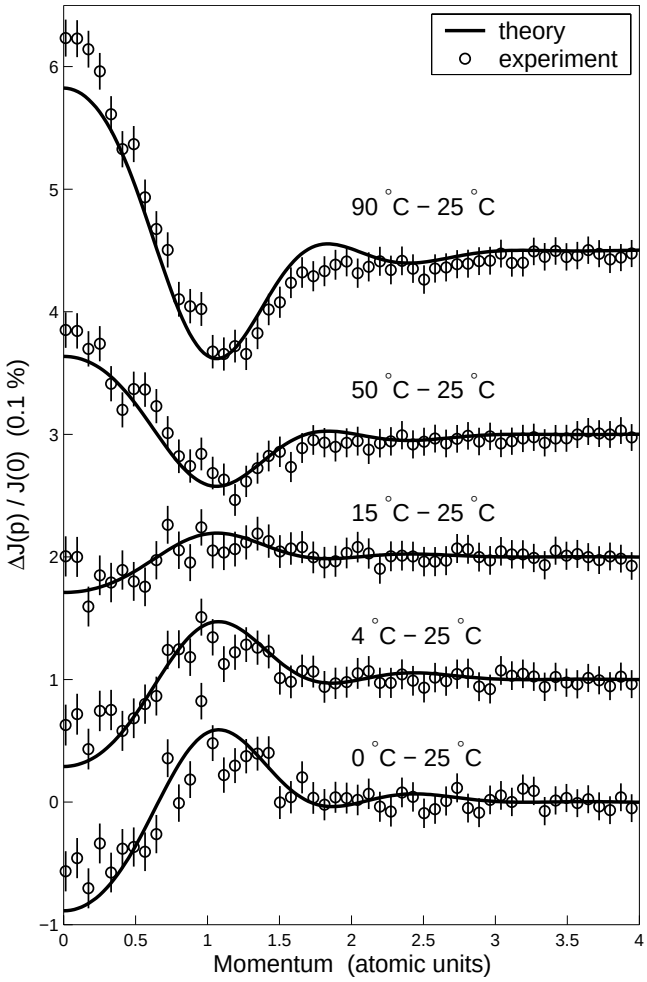

Figure 1. Temperature-dependent change in the liquid water Compton profile. The computation based on density-functional theory assumes experimental bond-length distributions [1].