ESRF	**Experiment title:** Stabilizing hydrogen bonds: Compton scattering study on water-TMAO mixtures	**Experiment number**: SC-3718
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Report:

The structure of liquid water is one of the unsolved problems in condensed matter physics [1]. In aqueous solutions the hydrogen bond network is typically disturbed, however, mathylamines such as trimethylamine N-oxide (TMAO) are suggested to strengthen the water's hydrogen bond [2], but experimental data are rare.

In experiment SC-3718 we measured Compton profiles of a water-TMAO mixture (2M TMAO) in the temperature range between 273 K and 313 K. We used the standard Compton scattering set-up of ID15B. The custom made sample cell including a temperature control via a chiller and heating foils was holding a glass capillary (sample thickness around 2 mm) and placed onto the sample stage. The 13-element Ge solid state detector was mounted at a scattering angle of about 160°. To keep a constant flux, we used a wedge shaped absorber in front of the sample. The formation of ice was controlled by x-ray diffraction patterns measured at least every 60 min during a Compton measurement run. The Compton scattering data was stored every 10 minutes and checked afterwards for consistency. During the analysis, the data was corrected for background scattering, relativistic cross section and absorption, before summing up, see [3] for details.

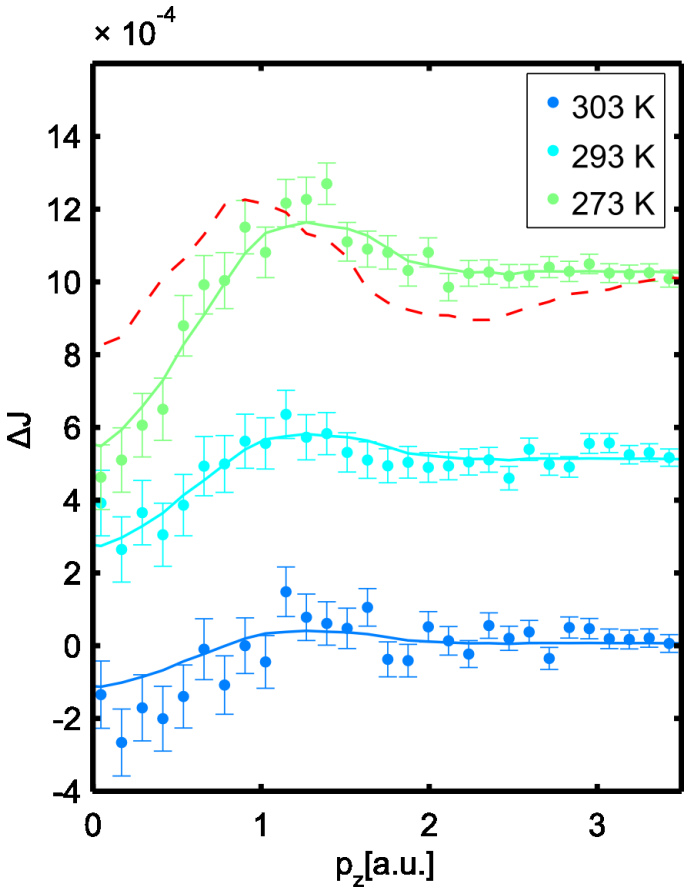

Figure 1: Compton profile differences for a water-TMAO mixture as function as temperature with respect to 313 K. The dashed red line represent a typical water difference for ΔT=40 K.

First Compton profile differences are shown in Fig. 1. Here, the profile measured at 313 K was chosen as reference and subtracted from the other ones as indicated in the legend. In addition, a scaled water difference representing the pure temperature effect on the water hydrogen bond is shown as dashed line for ΔT=40 K (see experimental report HD-614). Surprisingly, addition of TMAO affects the bond network strongly, the pure temperature effect is superposed by additional contributions. In a next step we will compare the experimental data to DFT calculation to obtain qualitative results such as bond length changes that may reveal the additional contributions originated by TMAO addition.

[1] A. Nilsson and L.G.M. Pettersson; Chem. Phys. 389,1 (2011).
[2] A. Panuszko et al. J. Chem. Phys. 113, 14797 (2009). M. Schroer et al. Angew. Chem. Int. Ed. 50, 11413 (2011).
[3] F. Lehmkühler et al. J. Phys. Chem. Lett. 1, 2832 (2010); F. Lehmkühler et al. J. Phys. Chem. C 115, 21009 (2011) and references therein.