ESRF	**Experiment title:** The effect of Guanidinium Chloride on the structure of water	**Experiment number**: SC-3910
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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, methylamines such as trimethylamine N-oxide (TMAO) are suggested to strengthen the water's hydrogen bond [2]. In the previous experiment SC-3718 we studied the influence of TMAO on the bond network by means of Compton scattering. This study was extended by comparing those results to aqueous solutions of guanidinium chloride (GdCl) which is suggested to disturb the hydrogen bond network [3].

In experiment SC-3910 we measured Compton profiles of a water-GdCl solution at concentrations of 2M, 4M and 6M GdCl in the temperature range between 273 K and 323 K. We used the standard Compton scattering set-up of ID15B at an x-ray energy of 87.2 keV. 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 152°. To keep a constant flux, we used a wedge shaped absorber in front of the sample. The sample structure 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 [4] for details.

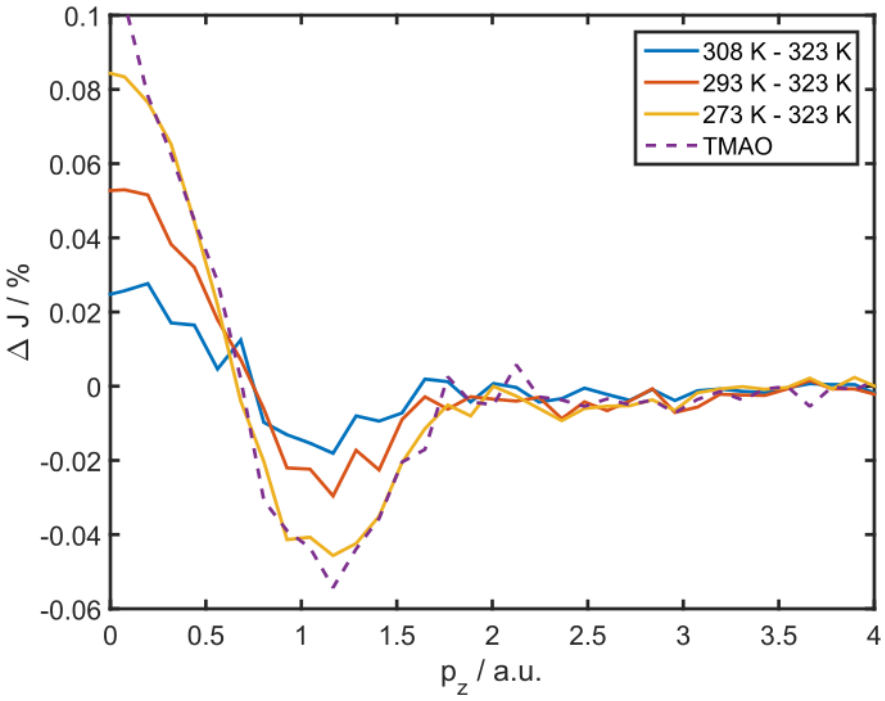

Figure 1: Compton profile difference of 2M GdCl solution compared to a scaled difference of 2M TMAO solution.

First Compton profile differences are shown in Fig. 1 for 2M GdCl. Here, the profile measured at 323 K was chosen as reference and subtracted from the other ones as indicated in the legend. The observed differences resemble the well-known temperature effect on the hydrogen bond network in water-based sample systems [4]. In addition, a difference of a 2M TMAO solution at different temperatures scaled to $\Delta T = 50$ K is shown as dashed line. Surprisingly, there is no significant difference to the GdCl data. In a next step we will compare the experimental data to pure water and the other solutions quantitatively and to DFT calculations modeling different effects on the liquids' structure.

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