ESRF	**Experiment title:** Gas-phase dimerisation of acetic acid via hydrogen bonding	**Experiment number:** CH-3898
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Report:

We performed an inelastic X-ray scattering (IXS) experiment to study the dimerization of acetic acid (AA, CH_3COOH) in solid, liquid, and gaseous phases. The aim was to elucidate the underlying mechanism of changes in the electronic structure due to the complex formation of a hydrogen bond (HB) in a simple molecule. The dimerisation of AA has been studied previosly with various techniques [1-5], and there has been discussion on the presence of the dimers in different conditions.

The IXS spectra were obtained with the X-ray Raman Scattering spectrometer of the beamline ID20. The incident beam was monochromatized with a Si(111) premonochromator and a Si(311) channel-cut monochromator, and the spectra were recorded using the 72 bent Si(660) analyzer crystals and two dimensional detectors.

For the gas-phase measurements a novel sample chamber setup was constructed. The actual chamber was a quartz capillary, which was oriented parallel to the incident beam to maximize the probed sample volume and thus the scattering signal. The capillary was in turn connected by glueing to the rest of the setup, including a container for liquid acid, a pressure gauge, and a pressure regulator. After loading the AA liquid to the sample chamber setup, it was evacuated to remove contribution of air. The liquid container was heated using a resistive heating element, thus vaporizing some of the liquid and allowing control of the pressure of the gas. To control the temperature of the probed volume of the gas, the capillary was covered with a copper tube, which was heated by resistive elements.

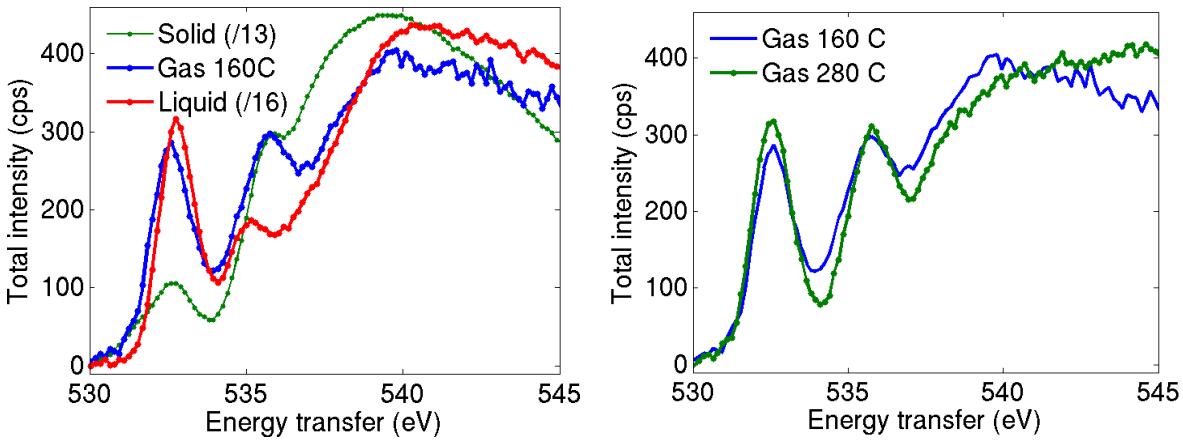

Figure 1: IXS spectra from oxygen K-edge of different phases of AA (left panel), and from gaseous AA at different temperatures (right panel).

For the liquid phase measurements the AA was loaded directly to the capillary. For the solid phase measurements a nitrogen flow from a cryostream sample cooler was used to lower the sample temperature to -40 °C.

The preliminary results of the measurements from the oxygen K-edge of different phases of AA are shown in the left panel of Fig. 1. This comparison shows the sensitivity of the spectrum to the phase. The spectra from gaseous AA at different temperatures in the right panel show no clear signs of the dimer formation, contrary to what was expected based on the model of Ref. 5. The data analysis is in progress, which is focused to the examination of the effect of the H-bonding to the spectra. The publication based on this experiment is in course of preparation.

References:

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