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S-XANES of $CuSO_4x5H_2O$ and $CuSO_4$
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Beamline(s): X19A

Introduction: X-ray absorption spectroscopy is not only highly element specific, but also very sensitive to the oxidation state and local symmetry. It is well-known that the Cu K-edge in $CuSO_4$ depends on the content of water in the lattice. $CuSO_4$ is highly hygroscopic and is better described as $CuSO_4x5H_2O$ in its normal state. This compound has a dark, blue color, while dry $CuSO_4$ is better described as brownish-white. 4 water-molecules are attached to the Cu while one is bound to the sulfate. It is obvious that 4 water-ligands have a significant effect on the energy of the Cu K-edge in moist $CuSO_4$, but the change in the S K-edge is much less since the central S^{6+}-ion is shielded by 4 O^{2-}-ions from the water-ligand. The idea of this experiment is to study the effect of the water ligands.

Methods and Materials: The experiment was performed at beamline X19a. The sample was ground to fine powder and spread on scotch-tape in a thin layer. In order to obtain dry $CuSO_4$, the powder was heated in an over to 270°C for 2 days. The absorption was measured by tuning the incident energy through the absorption edge and measuring the total fluorescence yield of the sample. To investigate self-absorption effects, the same samples were measured with a total electron-yield detector. These measurements showed that only the white line is reduced in height by about 20%. Structures in the pre-edge region and above the white line are not affected by self-absorption effects.

Results: The experimental results are shown in the figure. Differences are obvious: a small additional peak at 2477.5eV in the dried sample, and more structure between 2485eV and 2500eV. Model calculations are planned to investigate the causes for the different line-shapes and peaks.

Conclusions: High-resolution XANES at the S K-edge in $CuSO_4x5H_2O$ and $CuSO_4$ shows significant differences, which show the high sensitivity of XANES even to the ligands.

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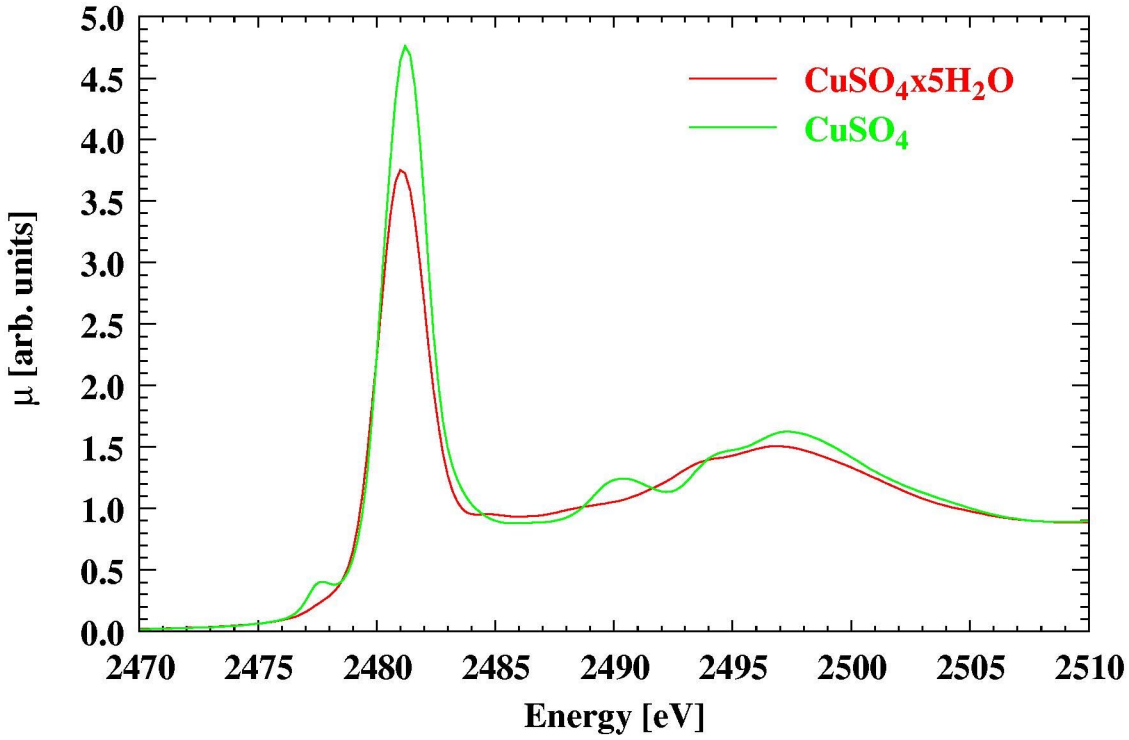

Figure 1: S K-edge in coppersulfate.