ESRF	**Experiment title:** Understanding the methyl-group dynamics in Li-acetate dihydrate	**Experiment number:** HS 3763
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Report:
We planned to study changes in the lattice dynamics of Lithium Acetate Dihydrate at low temperatures. Prior to the IXS experiments we had shown by low temperature specific heat measurements and by low temperature ultrasound spectroscopy that fully protonated LiAc undergoes a structural phase transition at about 11 K. This is in variance with published data, where a phase transition was believed to occur only in the deuterated compounds [1,2].

We planned to determine the lattice dynamics at 5 K and at 20 K, and, from a comparison, deduce the mechanism of the phase transformation. We grew large perfect single crystals by slow evaporation of a solution, and produced oriented and polished samples of an appropriate size (a few mm edge lengths) for the experiments. Prior to the experiments, we computed the lattice dynamics of a fully ordered structure with density functional perturbation theory based model calculations. This approach allows for very efficient measurements, as the DFPT data can be employed to predict optimal measureing conditions. These calculations were performed with a programme provided by A. Bosak.

The sample alignment on the spectrometer was straightforward due to the provision of oriented samples. The first cryostat employed was defective and had to be exchanged prior to the first measurement.

We then began the measurements for several directions in reciprocal space. The overall good agreement between the predicted values and the measure values are obvious from Fig. 1.

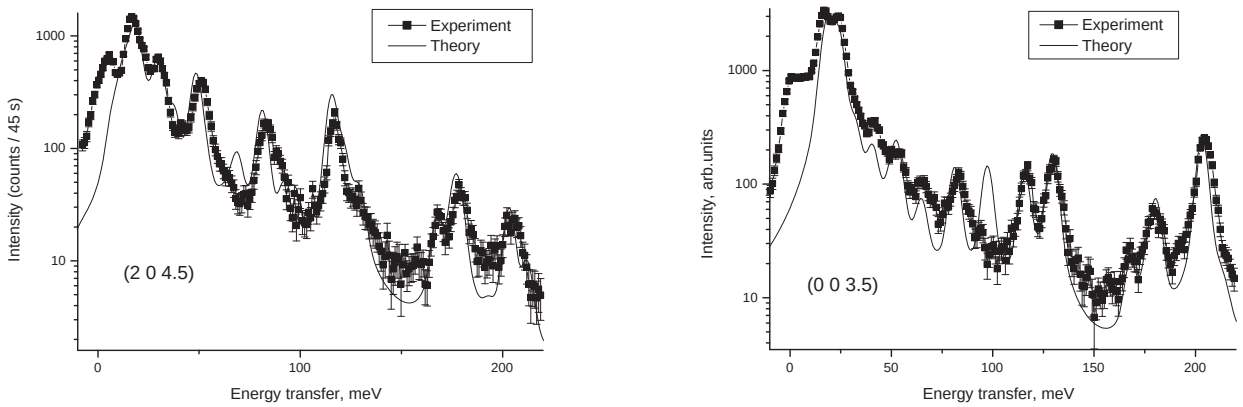

Fig. 1. Predicted (lines) and measured (points) inelastic spectra of Lithium Acetate Dihydrate. The model corresponds to a presumed fully ordered low temperature structure. The experimental data were collected at 140 K.

The overall agreement between the model and the measurements indicates that the lattice dynamics are correctly described by the model. This was expected. The two distinct deviations (6 meV mode in high temperature experimental data is absent in low temperature theoretical data, 75 - 100 meV mode in theoretical data absent in experimental data) are probably due to the change in the lattice dynamics across the phase transition.

However, as the cryogenic system was not able to cool the sample down to below the phase transition temperature, we were unable to verify this theory.

[1] Schiebel et al., J. Chem. Phys., 108, 2375-2382 (1998)
[2] Nicolai et al., Chem. Phys., 290, 101-120 (2003)