ESRF	**Experiment title:** Structure of the Unknown High Pressure Polymorph of Sodium Oxalate	**Experiment number:** **HS-1239**
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Report:

The effect of hydrostatic pressure on the crystal structure of sodium oxalate was studied at BM1A using a MAR345-detector. Two types of diamond anvil cells were used (a Merrill-Bassett cell, and a cell without Be from one side, which avoids the absorption corrections for the powder-line intensities and allowed to collect data without secondary Be-background from diamond reflections), and two different pressure-transmitting media (neon and methanol/ethanol/water) were used, in order to check if pressure-transmitting medium has any effect on the phase transition.

Effect of pressure on the structure of sodium oxalate was the same in neon and in the methanol/ethanol mixture. Anisotropic structural distortion was observed at pressures up to 3.4 GPa. At 3.4 GPa the first reflections of the high-pressure phase were observed. We have measured consequently a series of diffraction patterns at the same pressure at different time intervals. In about 12 hours the reflections of the low-pressure phase disappeared and there was only the high-pressure phase present in the sample. We have increased pressure further on up to 7 GPa. The high-pressure polymorph was shown to be less compressible, than the low-pressure one. The polymorph transition was reversible, although with a very small hysteresis, and after pressure decreased, we have got the ambient pressure polymorph again.

The quality of the data makes it possible to hope that we can not only index the diffraction pattern, but also suggest a structural model for the high-pressure polymorph, which can be refined using the experimental data. This work is presently in progress. Simultaneously with processing the experimental diffraction data, we are using the atom-atom potentials method to predict the structural distortions and possible polymorph transitions in sodium oxalate with pressure. The predictions of the computer simulations will be compared with the results of the experiments.