



Contribution ID: 169

Type: **Talk**

“Diffraction Spectroscopy” - Refinement of Anomalous Dispersion

Tuesday, 15 March 2022 09:40 (20 minutes)

The presentation reports on our results of the inclusion of anomalous dispersion refinement into crystal structure determinations. Synchrotron experiments were carried out at different energies around the K-edge of Molybdenum. A very good correlation between the absorption spectrum of a given element and the refined dispersion values is achieved. The structure model remains unchanged before, after and even at the absorption edge.

Primary authors: MEURER, Florian (Universität Regensburg); Dr HENNIG, Christoph (European Synchrotron Radiation Facility); Dr BODENSTEINER, Michael (Universität Regensburg)

Co-authors: Dr DOLOMANOV, Oleg V. (OlexSys Ltd); Prof. PEYERIMHOFF, Norbert (Durham University); Dr KLEEMISS, Florian (Universität Regensburg); Prof. PUSCHMANN, Horst (OlexSys Ltd)

Presenter: Dr BODENSTEINER, Michael (Universität Regensburg)

Session Classification: Advanced Structure Analysis I

Track Classification: Main conference: Theory, simulation, modeling, computational crystallography