Oral presentation

Anomalous dispersion - versatile and useful

Michael Bodensteiner[1], Florian Meurer[1,2], Christoph Hennig[2,3]

[1]University of Regensburg, Universitaetsstr. 31, 93053 Regensburg, Germany, [2] Institute of Resource Ecology, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany, [3]Rossendorf Beamline (BM20-CRG) European Synchrotron (ESRF), Grenoble, France

michael.bodensteiner@ur.de

Many different applications of resonant scattering or anomalous dispersion have been reported in recent decades. When determining the X-ray structure of small molecules in single crystals, it is usually only used to distinguish the absolute structure. To this day, almost exclusively tabulated values are used for the correction of anomalous dispersion, and the accuracy of these thirty-year-old tables is practically never questioned, although the three most common ones differ considerably in some cases [1]. However, there is so much more to it than many people realize. Now that the measurements have reached an unprecedented quality and quantum crystallographic models can describe the electron density at the highest level, artifacts of other effects appear, which may originate from the poor anomalous dispersion correction [2].

Figure 1 shows the effect of an incorrect correction on the example compound $Mo(CO)_6$, where other elements at the metal position can lead to even better structural models. This presentation shows the benefits of anomalous dispersion refinement (ADR), i.e., the consideration of the variability of the values in the least squares refinement [3]. This not only improves the structural models, but also allows conclusions to be drawn about the chemical properties, such as oxidation states.

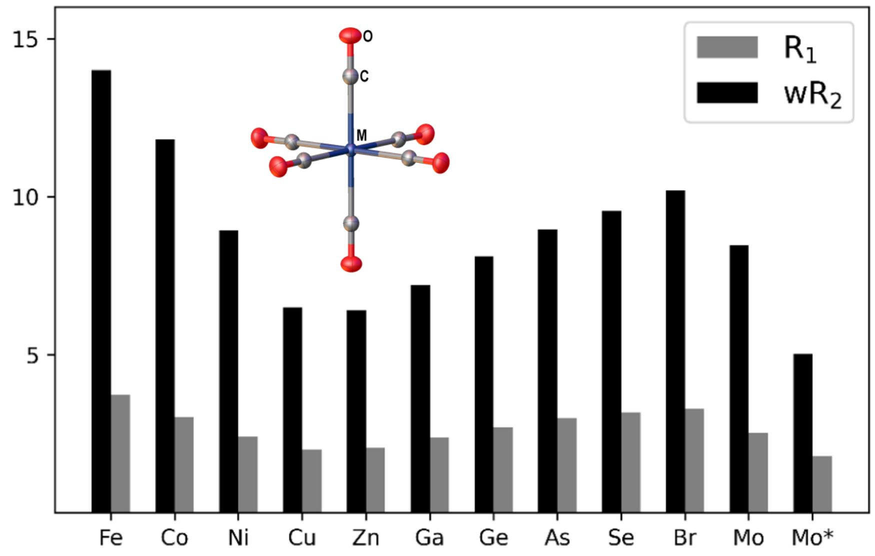

Figure 1. Effects on R factors of placing different elements at the metal position in Mo(CO)6 using tabulated anomalous dispersion values[1] versus using ADR (Mo*)[3].

[1] a) Henke, E., Gullikson, M. & Davis, J. C. (1993). *At. Data Nucl. Data Tables*, **54**, 181–342; b) Brennan, S. & Cowan, P. L. (1992). *Rev. Sci. Instrum.*, **63**, 850–853; c) Sasaki, S. (1989). *KEK Report*, **88**, 1–136.

[2] Grabowsky, S., Genoni, A. & Buergi, H.-B. (2017). *Chem. Sci.*, **8**, 4159–4176.

[3] Meurer, F., Dolomanov, O. V., Hennig, C., Peyerimhoff, N., Kleemiss, F., Puschmann, H. & Bodensteiner M. (2022) *IUCrJ*, **9**, 604–609.

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