MS24 3D electron diffraction

MS24-1-6 Crystal Structure Study of Xenon Compounds Using 3D Electron Diffraction #MS24-1-6

K. Gurung ¹, P. Brázda ¹, L. Palatinus ¹ ¹Czech Academy of Sciences - Prague (Czech Republic)

Abstract

The low stability of the xenon compounds in the atmosphere and under the electron beam makes it quite a challenge for their crystal-structure studies using electron diffraction. At the same time, some of these compounds are difficult to crystallize in large crystals, and electron diffraction is the only way to elucidate their structure. Recent progress in 3D electron diffraction (3D ED) makes it a promising technique for studying the crystal structures of these largely unexplored compounds. To verify the feasibility of the application of 3D ED to these compounds, we investigated XeF2 and [XeF][TaF6]. Sample loading was achieved by the use of a glovebox and a homemade construct that utilized liquid nitrogen, preventing the exposure of the sample to moisture. Energy-dispersive X-ray spectroscopy (EDS) confirmed the presence of xenon and fluorine in the loaded sample. The electron diffraction on XeF2 confirmed the presence of this phase. However, the crystal quality was not sufficient to obtain a full single crystal 3D ED data set. However, the compound turned out to be sufficiently stable under the electron beam to potentially permit a 3D ED data collection. These results, albeit preliminary, demonstrate that it is possible to investigate nanocrystalline xenon-containing compounds as well as other air-sensitive and reactive materials by 3D ED.

References

[1] Hargittai, I. Neil Bartlett and the First Noble-Gas Compound. Struct. Chem. 2009, 20 (6), 953.
[2] Levy H., Agron P. The Crystal and Molecular Structure of Xenon Difluoride by Neutron Diffraction, J. Am. Chem. Soc, 1963, 85, 241-242