MS24-1-2 On the Cutting Edge of Electron Diffraction Quality
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Abstract
Electron diffraction (3D ED) has recently emerged as a powerful tool for structure determina-tion on crystallites in the nanometre range, as it allows to bypass the common bottleneck of growing single crystals, big enough for X-ray diffraction. 3D-ED, using both the continuous rota-tion method and software as we know from X-ray crystallography, is gaining a lot of attention in all fields of research from organic and inorganic molecules, over polymorphism, geological sciences, natural products, biomolecules, material sciences to energy-storage materials and many others.

Here we showcase results from our electron diffractometer, the first entirely dedicated device for 3D ED, on representative case studies dealing with challenging organic compounds to demonstrate the benefits over TEM-based MicroED experiments. Pioneers in the field of electron diffraction already agree that a dedicated device is of great advantage for all fields of nano-crystallography.

As a benchmark and to show the capabilities of a dedicated electron diffractometer, we recently performed 3D ED experiments on Metaxalone, $C_{12}H_{15}NO_3$. Sold as Skelaxin, it is a muscle relaxant, but its exact mechanism of action is still not known. Metaxalone exhibits various polymorphic forms with substantial effects on e.g. solubility and bioavailability, one of which could only be obtained[1] as nanometre-sized needles and thus required electron diffraction for accurate structure elucidation.

The data quality obtained is clearly superior to previously reported[1], despite room-temperature data collection, indicating a higher performance of a dedicated diffractometer compared to equipment commonly used until today.

References
[1] V. Hamilton et al., Cryst. Growth Des., 20, 7, 4731–4739 (2020)

Fig.1 Metaxalone from nano-crystal