MS25 3D electron diffraction for structure solution of organics and proteins

MS25-05
Electron diffraction as a tool to study novel organometallic complexes
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Abstract
3D electron diffraction (3DED) is a technique that is sparking huge interest within the chemistry community as a tool to rapidly determine the structures of newly synthesised compounds. At the York Structural Biology Laboratory (YSBL) we collected our first 3DED data in late 2019 from paracetamol using a T12 microscope with a retrofitted Ceta camera. This was a manual and laborious process. Since April 2021 we have been using our Glacios microscope with Ceta-D camera to collect 3DED data from hundreds of crystals of small molecule compounds and have determined multiple structures. Our focus is on applying 3DED to determine structures of novel and challenging samples, in particular air-sensitive organometallic compounds, synthesised by our colleagues at the University of York. This has enabled us to characterise materials that were precluded from earlier structure determination by X-ray crystallography. I will describe our workflow for collecting and processing 3DED data from small molecule complexes, highlight our recent results from an air-sensitive σ-alkane complex[1] and illustrate how 3DED can be incorporated into a pipeline for synthetic chemists to accelerate research.

References
1 L. R. Doyle, E. A. Thompson, A. L. Burnage, A. C. Whitwood, H. T. Jenkins, S. A. Macgregor and A. S. Weller, Dalt. Trans., 2022, **51**, 3661–3665.

Electron diffraction from organometallic crystals

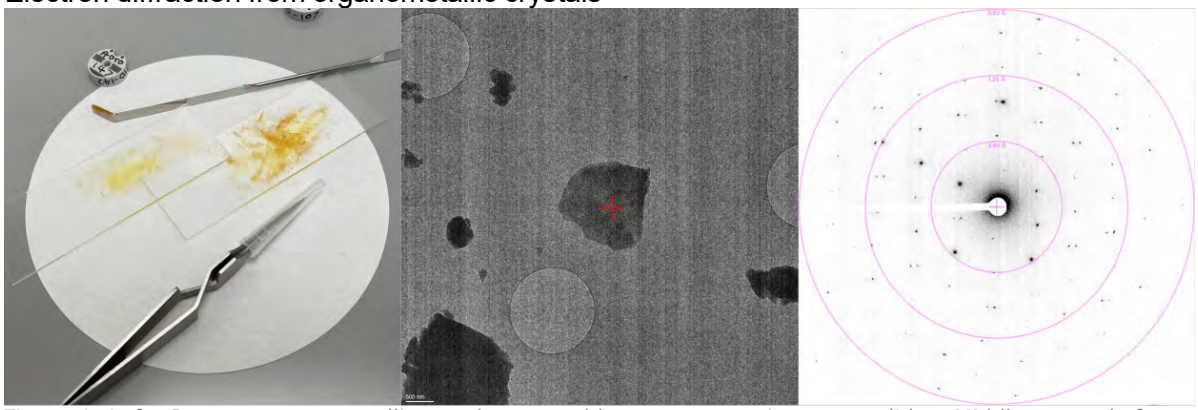

Figure 1. Left: Orange organometallic powder ground between two microscope slides. Middle: crystals from orange powder deposited on a TEM grid. Right: representative electron diffraction pattern from a single crystal.