

MS24-2-5 The XtaLAB Synergy-ED: progress and latest results
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Abstract

Recognizing the potential of Single-Crystal Electron Diffraction (SC-ED), also known as 3DED and MicroED, Rigaku and JEOL announced a collaboration in 2020 to develop a product designed in a fashion that will make it easy for any crystallographer to use. The resulting product, the XtaLAB Synergy-ED[1], a new and fully integrated electron diffractometer, was released around one year later in May 2021. Many materials only form nanosized crystals or are challenging to produce in large quantities. Before the development of the SC-ED technique, synthetic chemists were forced to rely on other techniques, such as NMR, often in combination with each other, to postulate 3D structure. Unfortunately, the NMR results can be difficult to interpret for complicated molecules such as natural products. SC-ED has become a revolutionary technique for the advancement of structural science. The XtaLAB Synergy-ED is an electron diffractometer operated via CrysAlisPro for a seamless workflow from data collection to structure determination of three-dimensional molecular structures from nanocrystals.

Since its launch, our demo lab XtaLAB Synergy-ED has generated over 160 structures of various samples, see Figure 1, from organics to MOFs, with a range of compositions and cell dimensions. In this presentation, we will provide an overview of the capabilities of the Synergy-ED and review some of more interesting structures that have been determined since May of 2021.

References

[1] Ito, S.; White, F.J.; Okunishi, E.; Aoyama, Y.; Yamano, A.; Sato, H.; Ferrara, J.D.; Jasnowski, M.; Meyer, M; CrystEngComm 2021, 23, 8622-8630