Applications of X-ray diffraction for microcrystalline sample using the latest single crystal laboratory systems.

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Molecular structure determination plays an important role both in fundamental and applied sciences such as organic chemistry, inorganic chemistry, biochemistry, drug discovery, and material chemistry, etc.

A number of analytical methods are routinely used to determine molecular structure: nuclear magnetic resonance (NMR), mass spectrometry (MS), infrared absorption spectroscopy (IR), X-ray diffractometry (XRD), and so on. In particular, single-crystal X-ray structure (SC-XRD) analysis is the most effective method to obtain a detailed and overall three-dimensional molecular structure of a molecule. However, it is generally believed that single crystal analysis takes a relatively long time, and requires a large crystal and information of elemental composition.

A combination of "PhotonJet-R (rotating anode X-ray generator + newly designed optic)" and "HyPix-6000HE (Hybrid Photon Counting detector)" has achieved high brightness and noise-free shutterless data collection in an in-house instrument for the latest SC-XRD analysis.

By the recent progress of the elemental technology, we came to be able to get structure of a single crystal in the order of a few μm in an in-house instrument. Furthermore, evolution of the software enabled automatic measurement and analysis without any expertise.

We determined precise crystal structure of agrochemical products microcrystalline powders using “What is this?” (WIT) experiment without any elemental information[1]. The WIT combined with the latest SC-XRD system provides the best way to obtain unambiguous structural information from microcrystalline powders (Fig. 1).

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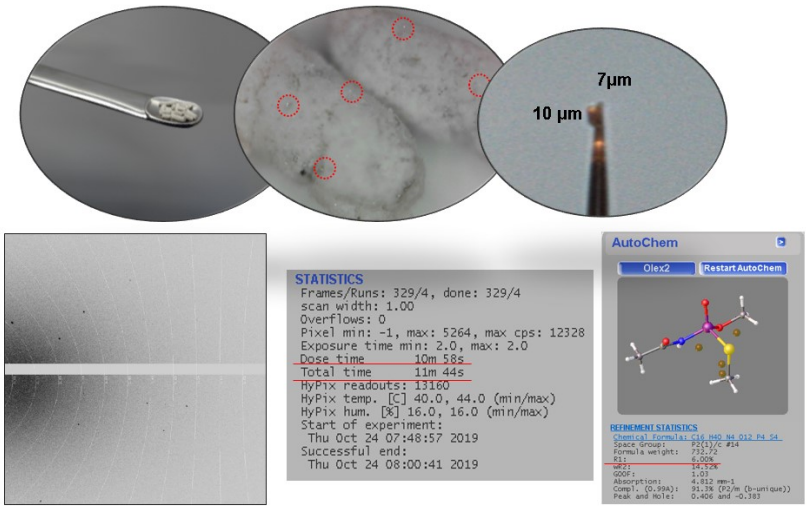

Figure 1. Structure identification of a polychlorine agrochemical metabolite by the CS method.

[1] Matsumoto, T., Yamano, A., Sato, T., Joseph, D. F., Fraser J. W., Mathias, M., . (2020). *J. Chem. Crystallography* **51***, 438.*

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