MS25-P01 | Electron Crystallography for Studying MOF-Intercalated Guests

samperisi, laura (Stockholm University, Stockholm, SWE)

Immobilization of target molecules in MOFs has allowed interesting structures to be determined using X-ray single crystal diffraction [1;2]. However, one of the most important parameters that determine the data quality is the ratio of guest to host, which is strongly influenced by the concentration of the target molecule in the crystal and the dimensions of the crystalline host [1]. Electrons interact with matter $10^4\times$ more strongly than X-rays. Thus, electron diffraction can be used to study crystals $10^8\times$ smaller by volume than X-ray diffraction. Electron microscopy is the only method capable of acquiring imaging and diffraction data from the same sample volume. Moreover, the development of continuous rotation electron diffraction (cRED) has enabled very fast data collection, allowing multiple datasets to be rapidly collected from a large number of crystals. For these reasons we expect that electron crystallography can be used to solve structures of MOF-intercalated guests present in small quantities in the host complex. Working toward this goal, we prepared a Zn-based MOF that has already been used for target molecule immobilization [1], $[(ZnI_2)_3$(2,4,6-tris(4-pyridyl)triazine$)_2\cdot$x(solvent)$]_n$, and solved and refined its structure using cRED and standard X-ray crystallographic software (XDS, SHELX). Data were collected on a JEOL2100 LaB_6 under cryogenic conditions using an ASI Timepix hybrid detector. An atomic model of the structure is presented.

[1] Hoshino, M. et al. (2016). IUCrJ, 3, 139–151
[2] Lee, S. et al. (2016). Science 353 (6301), 808-811