MS30-2-2 Structure determination of a highly disordered 2D MOF by continuous rotation electron diffraction method
#MS30-2-2

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Abstract
As a combination of metal-organic frameworks and 2D materials, 2D MOFs have garnered increasing attention due to the uniformed porosity, tunable structures, exfoliation property. These features make 2D MOFs exhibit in potential application catalysis, gas storage, gas separation, luminescence, et al. However, the structure determination is challenging for conventional X-ray diffraction technology. Data collection is hindered by the small size of the crystals (< 1 μm) and data processing, structure refinement often suffers from disorders caused by displacement of the layers.
Herein, we present the successful structure determination of a novel 2D MOF with Zr12 as node and 2,2'-Bipyridine-5,5'-dicarboxylic acid as linker based on continuous rotation electron diffraction method[1]. The data set suffers from the ambiguous value of c axis length caused by the interlayer disorders (Figure 1b, 1b). We first refine the structure with c axis equals to 28.75 Å. The double-layered hxl net can be nicely refined (Figure 2a), while interlayer structure can not be solved. The inter layer distance is 15 Å, longer than the ligand. There remain obvious residues between the layers which can not be assigned. These residues look just like the Zr12 cluster. By using cryo-holder, the data quality has been improved slightly still showing severe disorders. By adjusting XDS parameters[2], the c axis can be confirmed to be 15.92 Å and the interlayer structures thus can be solved.

References
1. J. Appl. Cryst. (2018). 51, 1094-1101.
2. J. Appl. Cryst. (1988). 21, 67-72.

Figure 1

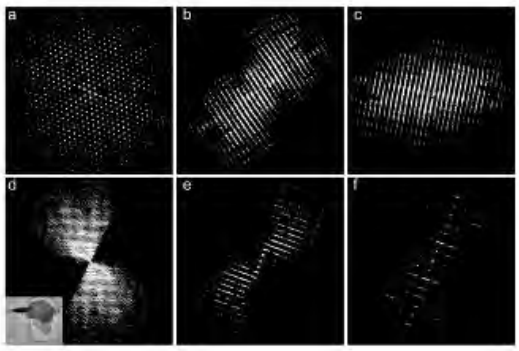

Figure 2