On the Completeness of Three-Dimensional Electron Diffraction Data for Structural Analysis of Metal-Organic Frameworks

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Three-dimensional electron diffraction (3DED) has been proven as an effective and accurate method for structure determination of nano-sized crystals. In the past decade, the crystal structures of various new complex metal-organic frameworks (MOFs) have been revealed by 3DED, which have been the key to understand their properties. One drawback of 3DED experiments is the limited tilt range of goniometer in transmission electron microscopes (TEMs), which often leads to incomplete 3DED data, particularly when the crystal symmetry is low. This drawback can be overcome by high throughput data collection using continuous rotation electron diffraction (cRED), where data from a large number of crystals can be collected and merged. Here we investigate the effects of data completeness on structural analysis of MOFs using a zinc zeolitic imidazolate framework (ZIF), denoted ZIF-EC1(Zn), as an example. ZIF-EC1 crystallizes in a monoclinic system with a plate-like morphology. cRED data of ZIF-EC1 with different completeness and resolution were analyzed. The data completeness increased to 92.0% by merging ten datasets. We show the structures could be solved from individual datasets with a completeness as low as 32.5% and refined to a high precession (better than 0.04 Å). We demonstrate that a high data completeness could improve the structural model, especially the electrostatic potential map. We further discuss the strategy adopted during data merging.