Crystals structure of CFA-1, a metal organic framework (MOF) by micro electron diffraction (microED)

Nicole Hoefer[1]

[1]The Ohio State University

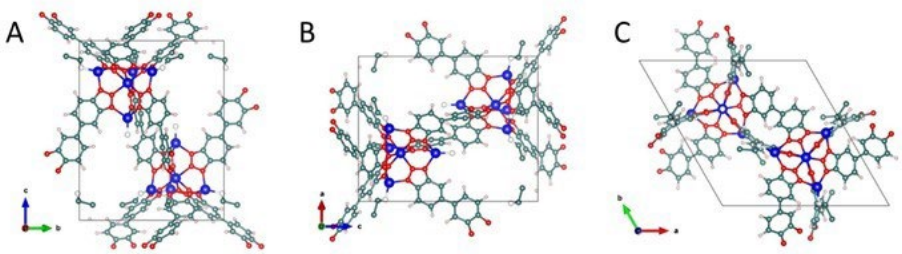
hoefernicole07@gmail.com

Metal-organic frameworks (MOFs) are crystalline organic-inorganic hybrid porous materials that offer unique structural properties such as tunable pore structures, large surface areas, and adjustable chemical functionality. MOFs for which large crystals cannot be obtained, may still have there structures determined via microED by utilizing nanometer- and micrometer-sized crystals. MicroED is performed in the transmission electron microscope (TEM), and data are collected at cryogenic temperatures. Data are obtained by continuously tilting the crystal in the cryo-TEM while recording diffraction information. Electron diffraction data are very similar to X-ray diffraction data and can be processed similarly, in many cases using the same software.

In the present work, we applied the microED technique to the MOF CFA-1 (coordination framework Augsburg-1), a chiral coordination framework of the Kuratowski type consisting of a chiral penta-nuclear structural building unit. CFA-1 is formed from 1H,1′H-5,5′-bibenzo[d][1,2,3]triazole (H2-bibta), a skewed ligand. This introduces dissymmetry into the MOF and leads to helical channels.

CFA-1 crystallized in space group P321 with unit cell dimensions a = 17.750 Å c = 19.192 Å, consistent with X-ray diffraction. Multiple CFA-1 data sets were collected and many of them had a completeness of 90% or greater due to the relatively high symmetry of the nano-crystals. The datasets sets were solved by direct methods using ShelxT. The structure obtained in this work agrees well with the published x-ray structure. In addition, crystals with both left and right handed channels could be observed.

The authors gratefully acknowledge funding from the Foundation For A Better World (https://www.forabetterworldfoundation.org/) and the Kickstart Facility grant from the Institute for Materials Research (IMR) at The Ohio State University.



Model of CFA-1 shown in the unit cell along axis a (A), b (B), and c (C). Atoms are labeled as follows; blue – zinc, red – nitrogen, green – carbon, white – hydrogen.

Figure 1