Structure Determination of Nanocrystalline Metal-Organic Frameworks by MicroED

Dr. Christian Jandl[1], Dr. Johannes Merkelbach[1], Dr. Gunther Steinfeld[1], Danny Stam[1], Dr. Sebastian Schegk[1], Dr. Eric Hovestreydt[1]
[1]ELDICO Scientific AG
jandl@eldico.ch

MicroED (microcrystal electron diffraction) is emerging as a powerful technique for the structural elucidation of challenging compounds as it bypasses the main limitation of growing crystals of suitable size for single-crystal X-ray diffraction. Applications range from natural products and pharmacology to geological sciences, advanced materials, nanotechnology, and many more.
Metal-Organic Frameworks (MOFs) are porous materials, which are commonly obtained from solvothermal synthesis and therefore cannot be recrystallised. Structure elucidation is thus limited to the as synthesised material. Being able to work with nanocrystalline powders makes microED the ideal tool to tackle this challenge and determine structures from crystals that are too small even for synchrotron facilities.
We show a range of examples including both nanocrystalline samples of known MOFs and new materials, all measured in continuous rotation mode on a dedicated electron diffractometer. High quality data also allow the study of molecular motion in the crystals and the identification of changes of the structures by solvent removal from the pores. The results illustrate the potential of this technique in the field of porous coordination networks and the benefits of dedicated instrumentation that has become available in recent years.

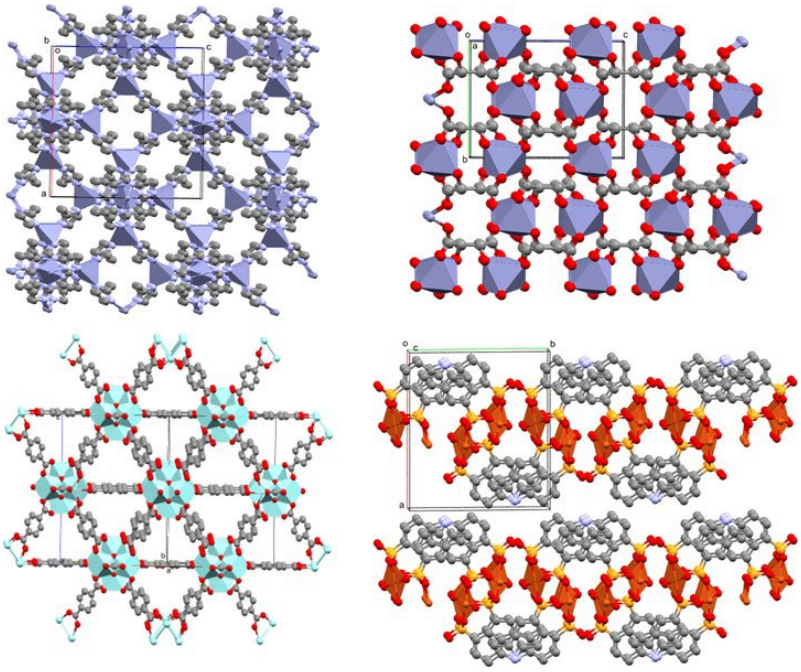

Figure 1