MOF Glasses for Gas Separation: Structural Information from Laboratory Pair Distribution Function Analysis

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Metal-Organic Frameworks (MOFs) are a class of materials forming porous structures thanks to their network of interconnected inorganic building units and organic linker molecules.[1] The use of MOFs for carbon capture and storage (CCS) has been extensively investigated, however water is often preferentially absorbed over CO2. Thus, the use of MOFs for direct capture of CO2 from a flue-gas stream is likely to be limited.

Applying suitable thermal treatment and subsequent cooling to the MOF ZIF-62, a so-called MOF glass may be obtained.[2] MOF glasses demonstrate a remarkable microporosity, the accessibility of which to small molecules depends on the exact procedure used to prepare the MOF glass.[3] It thus foreseeable that with appropriate changes to the vitrification process, it may be possible to develop a MOF glass to help solve the problem of CO2 separation in CCS. Moreover, MOF glasses may be processed into monoliths following similar approaches to their inorganic counterparts, simplifying the process of commercialisation.

Understanding the pore network of a MOF glass is clearly crucial for the application of these materials. Pair Distribution Function (PDF) analysis is well suited to the analysis of amorphous materials and can easily be performed on a laboratory instrument such as a Bruker D8 ADVANCE. Using high energy radiation (e.g. Mo-Kα or Ag-Kα) and a focussing Goebel mirror with a modern detector, such as the EIGER2 R 500K, a PDF of a MOF glass can be collected in a matter of hours. Here we use the combined software solution of PDF processing in DIFFRAC.EVA and fitting in DIFFRAC.TOPAS to extract structural details of both the parent ZIF-62 material and its MOF glass, to demonstrate the utility of laboratory PDF for understanding the structures of these important materials.

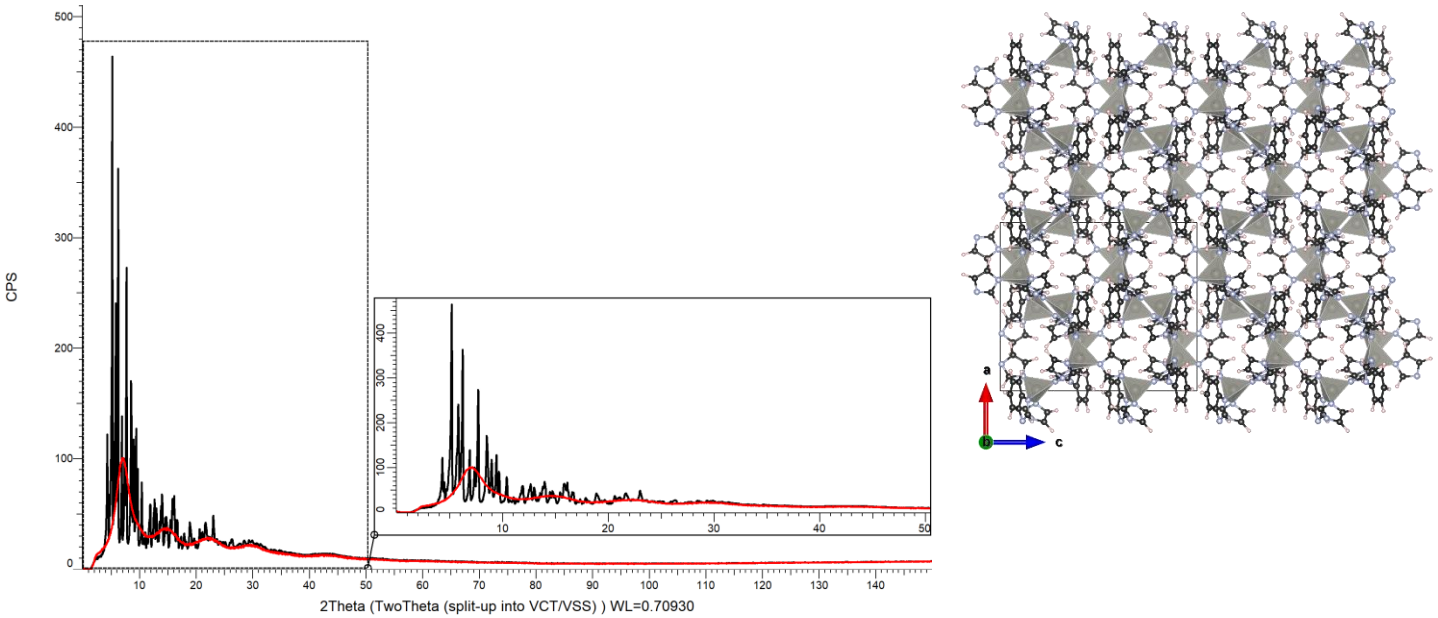


Figure 1. *Diffraction patterns of ZIF-62 (crystalline - black) and a_g-ZIF-62 (glass - red), measured on Bruker D8 ADVANCE laboratory diffractometer using Mo-Kα radiation. Right:structure of crystalline ZIF-62.*

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[2] L. Frentzel-Beyme et al., J. Am. Chem. Soc. (2019), 141, 12362-12371
[3] O. Smirnova et al., Nat. Mater. (2024), 23, 262-270