MS33-P03 | Heterocyclic Ligands for Water Sorption in Metal–Organic Frameworks: A Structural Study Using the Rietveld Method

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The application of metal-organic frameworks (MOFs) as water sorbents for de-/humidification and water production applications has grown in popularity in recent years. MOFs constructed from high-valence metals, such as Zr^{4+} or Cr^{3+}, have demonstrated good stability under operating conditions (i.e. repeated ad-/desorption cycles under hydrothermal conditions), with a number of Al^{3+}-based MOFs showing even better stability and water sorption performances. For instance, aluminium isophthalate [$Al(OH)(O_2C\text{-}C_6H_4\text{-}CO_2)$], also known as CAU-10 (CAU=Christian-Albrechts-Universität),[1] has achieved at least 10,000 water sorption cycles [2]. By replacing the isophthalate unit with structurally similar heterocyclic linker molecules (i.e. 2,6- and 3,5-pyridinedicarboxylic acids or furandicarboxylic acid), three new coordination compounds were obtained, the structures of which were refined by the Rietveld method [3,4]. Two of these have extended 3d-networks and demonstrate promising water sorption properties: CAU-10-pydc and MIL-160 (MIL=Materiaux Institut Lavoisier) [5]. Interestingly both compounds show a displacive phase transition on ad-/desorption of water, which has also been fully characterised. For MIL-160, DFT calculations were used to confirm the locations of water molecules determined during Rietveld refinement. DFT and Rietveld derived sites are in excellent agreement.

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