Synthesis and structural characterization of triptycene based MOF

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The structural diversity of metal-organic frameworks (MOFs) has found a large variety of physical and chemical properties leading to various applications. MOFs are extended crystalline architecture where metal ions or their clusters interconnected by multifunctional organic ligands/linkers forming infinite arrays of one-, two-, or three-dimensional networks. The striking feature of such crystalline material is high porosity, very low density, and hence enormously large surface area per unit mass. The use of a variety of metal ions, organic ligands with different functional groups have resulted into the formation of an astronomical number of MOFs having variety of applications like gas adsorption and storage, gas separation, drug delivery and imaging, sensing application, optoelectronic applications etc. They can be used as hosts for a range of guest molecules with adjustable pore sizes and functionalities. The pore sizes can be manipulated by altering the distance between the active functional groups in the selected organic linkers. Different metal ions and organic ligands/linkers can be used to synthesize MOFs by many types of chemical reactions and reaction conditions, leading to extraordinary structural diversity and porosity. The characteristics of the metals and linkers, such as properties and coordination preferences, play the leading role in determining the structure and its properties out of the resulting framework. Thus, the desired character of the target network makes the choice of metal and linker. Carboxylate based linkers are commonly use to synthesis MOFs. The universal use of transition metal ions in MOF synthesis stems from their well-known coordination behaviour with carboxylate based linkers, thus facilitating design strategies. In our laboratory, we have used triptycene as starting material for the first time to synthesize large, 3D ligands with six carboxylate sites for metal coordination. A MOF has been made by solvo-thermal method using Cu(II) as the metal ion to produce a cubic (a = 48.0573(5)Å, space group = Fm-3m) MOF having volume of 110989 cubic Å. The crystals were found to be poorly diffracting and hence three different X-ray facilities were used to collect data on the sample. A comparison of crystal data collected using three sources will be presented.


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