

## Unusual porosity behavior in a new zinc-based MOF with the heptanodal topology

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Currently, the design and synthesis of metal-organic frameworks (MOFs) attract broad attention because of the interesting structural architectures and topological features which have a key role in the final behavior of their application [1]. In order to construct porous compound networks, the common strategy is employed based on the suited selection of organic linkers and metal ions that affect the final topology of the clustered networks [2, 3].

In this work, to obtain a new topological structure of a zinc-1,3,5-benzentricarboxylate (Zn-BTC) MOF, we choose the various synthetic methods in the presence of different solvents and ratios of the Zn:BTC reagents. Herein, we report the synthesis and characterization of a new Zn-BTC MOF (**FUM-181**) with the heptanodal topology. The single-crystal X-ray diffraction (SCXRD) reveals that **FUM-181** crystallizes in the monoclinic space group  $P2_1/c$ . The crystal structure of **FUM-181** consists of seven independent  $\text{Zn}^{2+}$  centers, four topologically different kinds of  $\text{BTC}^{3-}$  groups (BTC-1, BTC-2, BTC-3, and BTC-4), four  $\text{H}_2\text{O}$ , two -OH groups, and three coordinated DMF molecules in the asymmetric unit. A precise examination of **FUM-181** demonstrates that it is a three-dimensional network with complicated and unusual pore structures. Furthermore, a detailed theoretical study has been carried out on the adsorption of  $\text{CO}_2$  and  $\text{CH}_4$  in this MOF at 298, 303, 318, and 333 K and 1-50 bar. The theoretical gas adsorption measurement predicts that **FUM-181** has a superior performance in  $\text{CH}_4$  gas adsorption compared to  $\text{CO}_2$ . It is worth mentioning, Hong et. al have recently reported a new hexanodal zinc-BTC MOF with high  $\text{CO}_2$  gas adsorption [4]. Interestingly, the changing gas adsorption behavior can be observed in our reported Zn-BTC MOF by changing the hexanodal to heptanodal topology.

**Keywords:** Zn-BTC Metal-Organic Frameworks, The heptanodal MOF Topology, Sorption behavior

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