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A new self-penetrating amine-decorated microporous metal-organic

framework: crystal structure, adsorption selectivity, and

luminescence properties

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ABSTRACT

A new microporous metal–organic framework, $[Cd(bpdc)_{0.5}(atz)(DMF)]\cdot 0.5DMF$ (1) (H₂bpdc = 4,4'-biphenyldicarboxylic acid, Hatz = 3-amino-1,2,4-triazole, DMF = N,N-dimethylformamide) has been solvothermally synthesized by employing the mixed H₂bpdc and Hatz ligands. 1 is a 3D pillared-layer framework, consisting of Cd-triazolate layer and dicarboxylate pillar, which exhibits a 6-connected (4⁶·6⁸·8) self-penetrating net. Because of the pores system functionalized by amino groups and open metal sites, this material shows high CO₂ adsorption selectivity over H₂ and N₂. In addition, 1 exhibits blue emission at ambient temperature.

Keywords: Metal-organic framework, Self-penetrating, Sorption, Luminescence

Porous metal–organic frameworks (MOFs) have gained great interests due to their fascinating topologies and promising applications as materials [1]. Particularly, MOFs have been extensively studied for selective CO_2 capture in recent years due to their advantages such as high porosity, modifiable pore surface, and flexible structures [2]. Commonly, the interactions between the framework and adsorbate play a primary role for enhancing the MOF's sorption affinity and capacity, especially in low pressure. Thus, some strategies, including generation of open metal sites, control of pore size, and incorporation of specific polar functional groups (-NH₂, -CF₃, -OH, etc.) on the ligands, have been investigated to augment the CO_2 adsorptive affinity and selectivity [3]. Grafting of amines onto the pore surfaces of MOFs not only allows for the increase of polarity but also could adjust the pore size, which has been investigated to augment the CO_2 adsorptive affinity and selectivity [4].

On the other hand, Self-penetration, in contrast to interpenetrating nets, features a single network having the peculiarity that the smallest topological circuits from the same network are catenated with each other. Compared to the fruitful productions of interpenetrating networks,

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