Supporting information

for

Change in synthetic strategy for MOF fabrication: From 2D non porous to 3D porous architecture and its sorption and emission property studies

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General information

All the chemicals used for synthesis are of analytical grade and commercially available. 3,3′,5,5′-tetramethyl-4,4′-bipyrazole (BPz) was synthesized according to the reported method [1]. IR spectrum was measured on a Thermo Nicolet Nexus FTIR spectrophotometer with KBr pellet. Powder X-ray diffraction (PXRD) spectrum was recorded on a Rigaku D/Max-2500

diffractometer at 40 kV, 100 mA for a Cu-target tube and a graphite monochromator. Thermogravimetric (TG) analyses were carried out on a Rigaku standard TG-DTA analyzer with a heating rate of 10°C min^{-1} from ambient temperature to 800°C, an empty Al_2O_3 crucible was used as reference.

X-ray crystallography

X-ray single crystal diffraction data for **1** was collected on a Bruker Apex diffractometer at room temperature with Mo Kα radiation (λ = 0.71073 Å) by ω scan mode. The program SAINT [2] was used for integration of the diffraction profiles. The structure was solved by direct methods using the SHELXS 97 [3] program of the SHELXTL package and refined by full-matrix least-squares methods with SHELXL 97 (semiempirical absorption corrections were applied using SADABS program) [4]. All the atoms in the complex were located from the Fourier map and refined with anisotropic thermal parameters on F^2. Bond distances and angles are given in Table S1.

CCDC 1431335 contains the supplementary crystallographic data for **1**. The data can be obtained free of charge *via* http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK, fax: (+44) 1223-336-033, or e-mail: deposit@ccdc.cam.ac.uk.

Gas and Vapor adsorption study of 1

Gas and vapor adsorption measurements were performed using BELSORP MAX and BELSORP AQUA (BEL JAPAN) adsorption analyzers. Before every measurement, samples were pretreated for 12 h at 373 K under 10−2 kPa continuous vacuum.

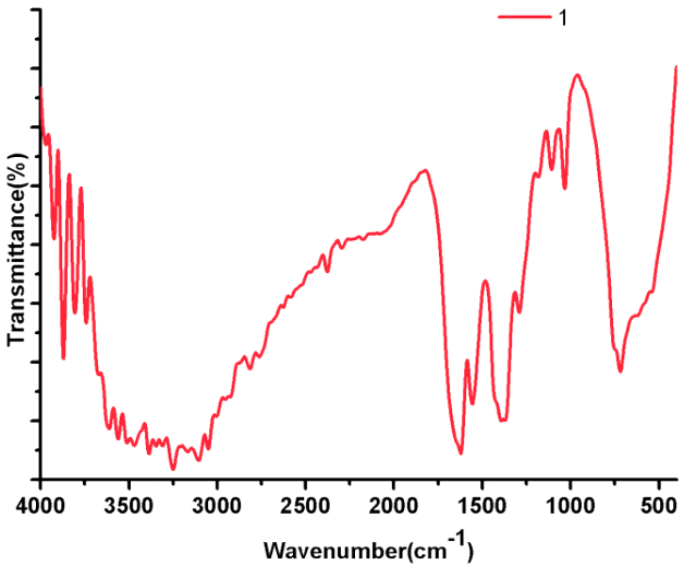

Fig. S1 Infrared spectrum of **1**.

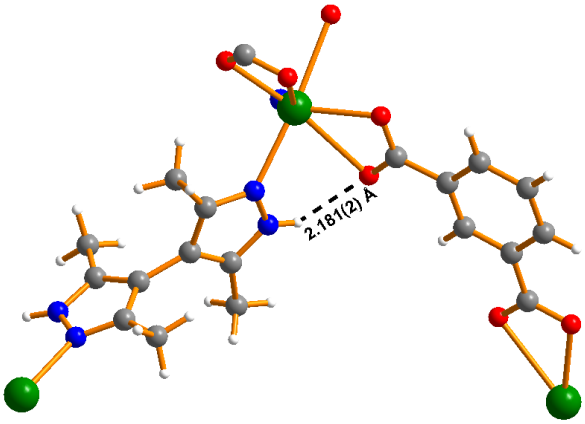

Fig. S2 N-H···O type hydrogen bonding in **1**.

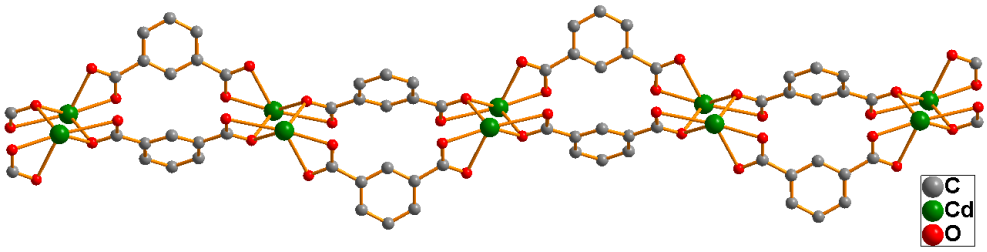

Fig. S3 Infinite double chain structure of $[Cd\text{-}BDC]_n$ in **1**.

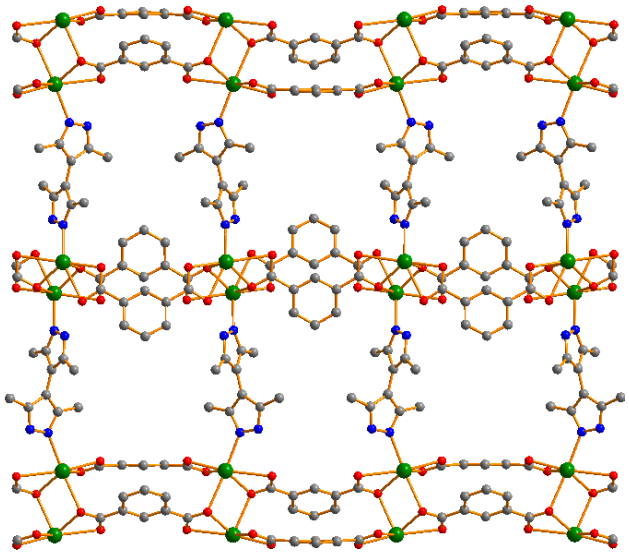

Fig. S4 A portion of 2D sheet structure in **1**.

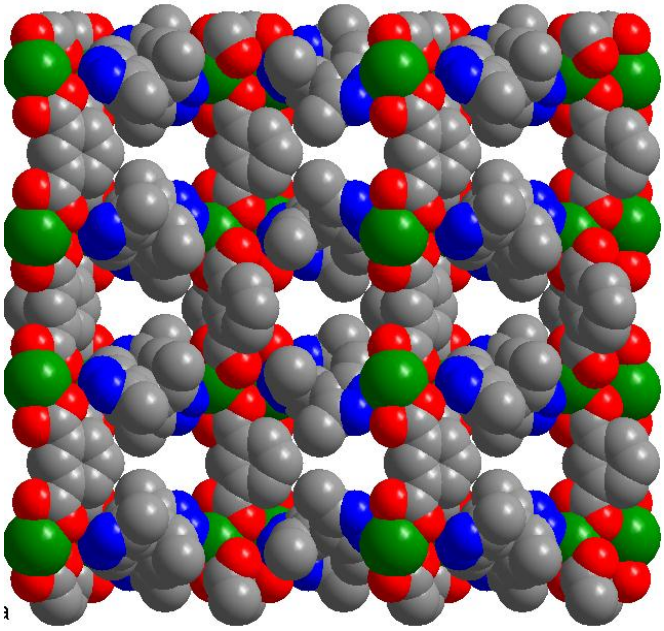

Fig. S5 Space fill model of 3D packing of **1**.

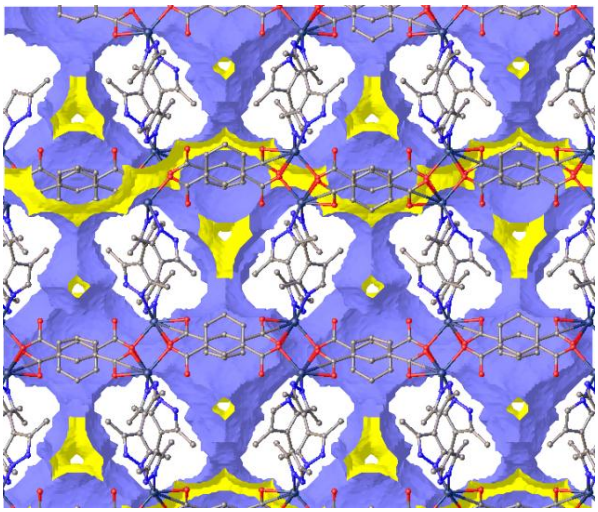

Fig. S6 Shape of solvent accessible void volume in the framework of **1**.

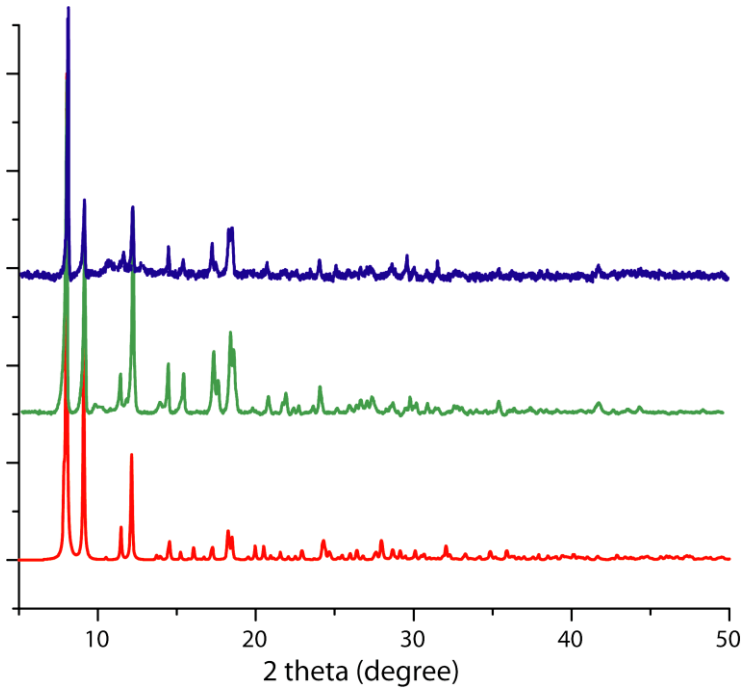

Fig. S7 Powder XRD of the simulated (in red), as synthesized (in green), and after activation (in blue) sample of **1**.

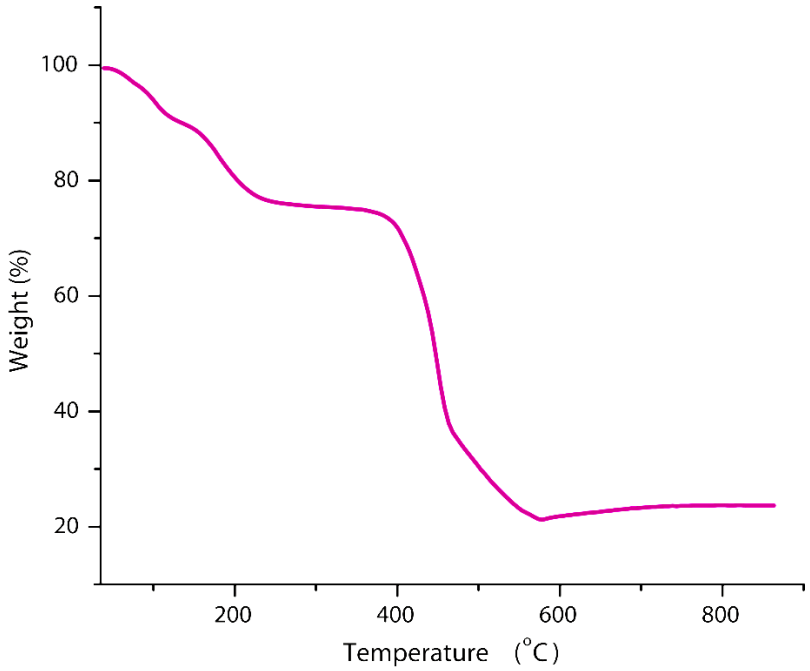

Fig. S8 Plot of TG analysis of **1**.

Table S1 Bond distances and angles:

{[Cd(BDC)(BPz)]·H_2O·2DMF}$_n$ **(1)**			
Bond Distances (Å)			
Cd1-O1	2.268(2)	Cd1-N1	2.327(3)
Cd1-N3^i	2.280(4)	Cd1-O3	2.524(3)
Cd1-O4	2.275(3)		
Bond Angles (°)			
O1—Cd1—N3^i	115.95(10)	O1—Cd1—N1	108.96(10)
O1—Cd1—O4	131.19(9)	N3^i—Cd1—N1	93.23(12)

N3—Cd1—O4	102.78(9)	O4—Cd1—N1	96.69(11)
O1—Cd1—O1^{ii}	78.44(8)	N3—Cd1—O1^{i}	77.96(8)
O4—Cd1—O1^{ii}	82.20(8)	N1—Cd1—O1^{i}	170.81(8)

Symmetry codes:
(i) 0.5-x, 1-y, -0.5+z; (ii) -x, 1-y, -z

References:

1. I. Boldog, E. B. Rusanov, A. N. Chernega, J. Sieler, and K. V. Domasevitch, Acentric extended solids by self assembly of 4,4'-bipyrazolyls, Angew. Chem., Int. Ed. 18 (2001) 40.
2. SMART and SAINT; Bruker AXS Inc.: Madison, WI, 1998.
3. G. M. Sheldrick, SHELXS-97, Program for solution of crystal structures; University of Göttingen: Germany, 1997.
4. G. M. Sheldrick, SHELXL-97, Program for refinement of crystal structures; University of Göttingen: Germany, 1997.