Electronic Supplementary Material (ESI) for Dalton Transactions
This journal is © The Royal Society of Chemistry 2013

Electronic Supplementary Information

Photoluminescence and Gas Sorption Properties of Three Cd(II) MOFs based on 1,3,5-benzenetribenzoate with $–NH_2$ or –OH groups

Hong-Ru Fu, Fei Wang and Jian Zhang*

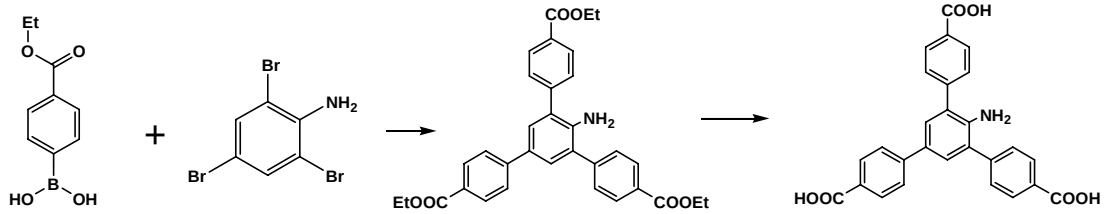
State Key Laboratory of Structural Chemistry
Fujian Institute of Research on the Structure of Matter
Chinese Academy of Sciences
Fuzhou
Fujian 350002
P. R. China.

** Corresponding Author*
E-mail: zhj@fjirsm.ac.cn
Fax: +86-591-83715030
Tel: +86-591-83715030

This journal is © The Royal Society of Chemistry 2013

General methods

Commercially available reagents were purchased used without further purification. 1,3,5-(tri-benzoic acid)aniline and 1,3,5-(tri-benzoic acid) phenol) were syntheized via suzuki reaction



A mixture of 2,4,6-Tribromoaniline (2.5 g, 7.5 mmol), p-ethoxycarbonylphenyl boronic acid (6 g, 30.0 mmol), Na_2CO_3 (4.0 g, 40 mmol), and $Pd(PPh_3)_4$ (0.7 g, 0.5 mmol) was added into degassed toluene–methanol–water (80/40/40 mL) under an argon atmosphere. The resulting reaction mixture was stirred for 24 h under reflux. After removal of the solvent, the residue was extracted with dichloromethane (80×3 mL), washed with brine (80 mL), dried over anhydrous $MgSO_4$ and concentrated in vacuum. The residue was purified by silica gel column chromatography (petroleumether/dichloromethane¼1/5) to give 1,3,5-tri(p-methoxycarbonyl-phenyl)aniline (2.56 g, 73%), which was hydrolyzed with 6 M NaOH to afford the title compound. 1H NMR (DMSO-d 6 , 400 MHz) d (ppm): 13.04 (s, 3H), 8.10 (s, 3H), 8.0 6 (s, 12H); 13 C NMR (DMSO-d6 , 150 MHz) d (ppm): 167.11, 143.81, 140.72, 130.02, 129.88, 127.39, 125.54; FT-IR (KBr, cm┐ 1): 3382, 3014, 2660, 2538, 1697, 1608, 1569, 1512, 14 47, 1416, 1393, 1317, 1286, 1241, 1181, 1016, 847, 76 4; MS (ESI) (m/z) calcd for C27N1H20O6 : 451.1, found: 451.6.

X-Ray Crystallography Supporting Information

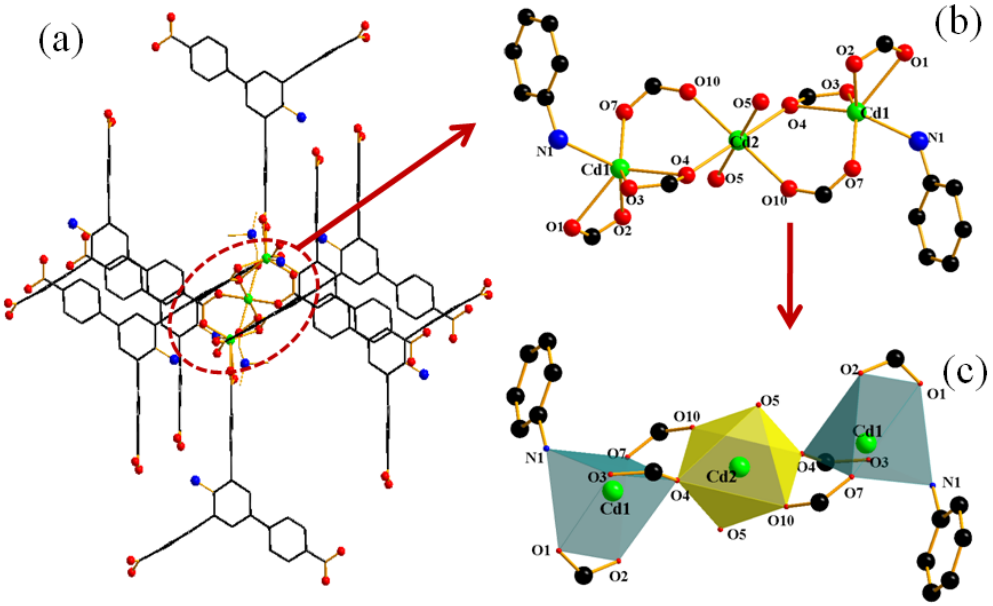


Fig. S1 The coordination environment of three nuclear cadmium in **3**: (a) the wire style of three nuclear cadmium and ligands; (b) the amine group of ligand coordinate the two cadmium ions; (c)the centralsymmetrical structure of the three nuclear cadmium , it can be simplied one octahedron and two triangular prism .

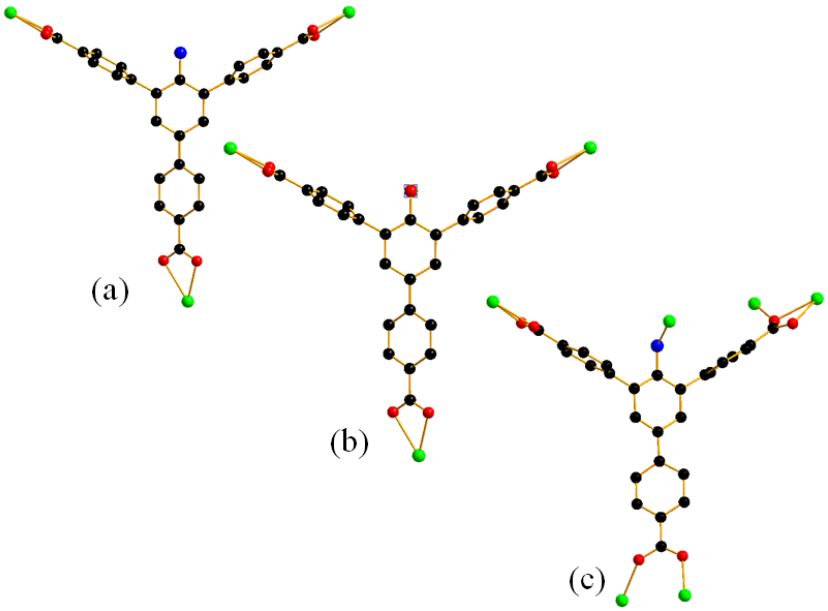


Fig. S2 The coordination environment of the ligands: (a)in **1**; (a)in **2**; (a)in **3** (solvent molecules are shown as large blue spheres for clarity).

Powder X-ray Diffraction Studies

X-ray powder diffraction (XPD) patterns of 1-3 were collected on a MiniFlex-II diffractometer X-ray powder diffraction (XPD) patterns of 1-3 were collected on a MiniFlex-II diffractometer

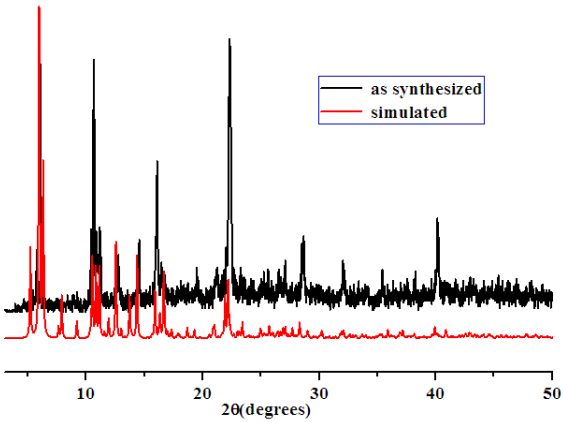


Fig. S3 For **1**, comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and the as-synthesized product.

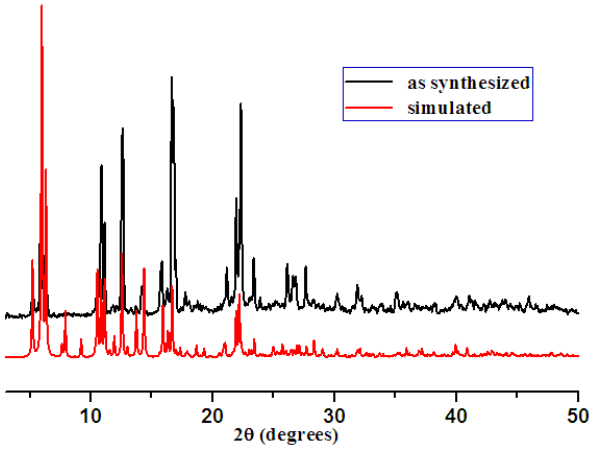


Fig. S4 For **2,** comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and the as-synthesized product.

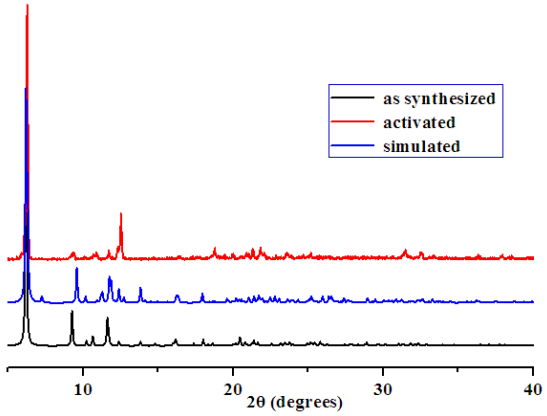


Fig. S5 For **3,** comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and the as-synthesized product.

Themogravimetric Analysis of MOFs

Thermal Gravimetric Analysis (TGA) was carried out using a NETSCHZ STA-449C simultaneous TG-DSC thermoanalyzer, under a constant stream of dry nitrogen gas (flow rate 20 mL min^{-1}) over the temperature range of 30 to 800 °C and at a heating rate of 10 °C min^{-1}.

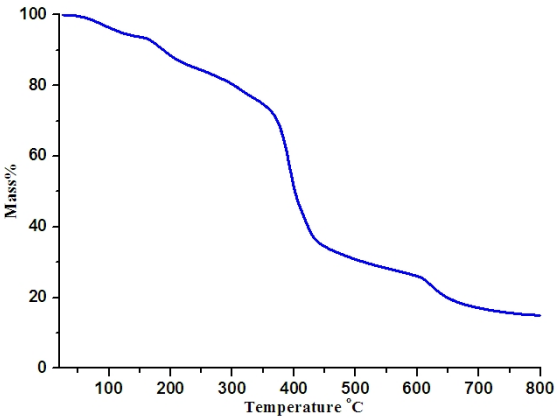


Fig. S6 TGA curve of compound **1** under N_2 atmosphere.

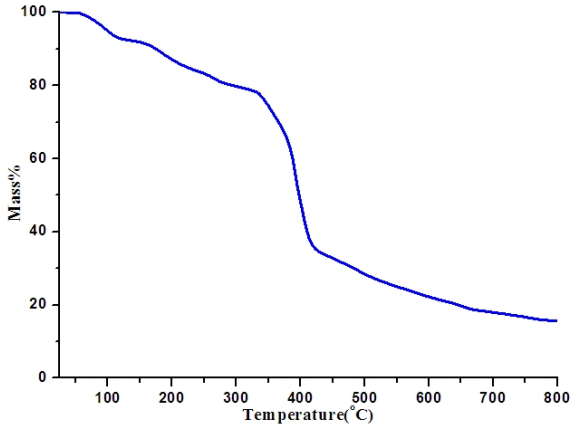


Fig. S7 TGA curve of compound **2** under N_2 atmosphere.

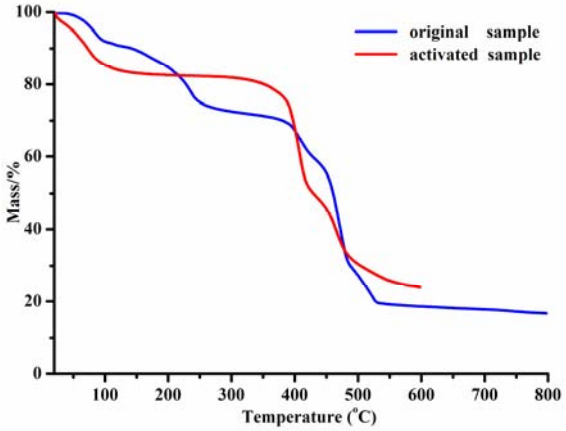


Fig. S8 TGA curves of compound **3** under N_2 atmosphere.

The adsorption equilibrium selectivity α_{12} between components 1 and 2 is defined as where component 1 is the stronger adsorbate and 2 is the weaker adsorbate. X_1 and X_2 are the molar fractions of components 1 and 2 on the adsorbent surface (or in the adsorbed phase), Y_1 and Y_2 are the molar fractions of components 1 and 2 in the gas phase. q_{m1} and q_{m2} and b_1 and b_2 are the Langmuir equation constants for components 1 and 2. K_1 and K_2 are the Henry's constants for components 1 and 2.

$$\alpha_{12} = \frac{X_1}{X_2} * \frac{Y_2}{Y_1} = \frac{K_1}{K_2} = \frac{q_{m1} b_1}{q_{m2} b_2}$$