Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

Metal-Organic Framework Architecture with Polyhedron-in-Polyhedron and Further Polyhedral Assembly

Ting-Ting Lian,[a,b] Shu-Mei Chen,*[a,b] Fei Wang[b] and Jian Zhang[b]

[a]College of Chemistry & Chemical Engineering, Fuzhou University, Fuzhou, Fujian 350108, P. R. China and [b]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. E-mail: csm@fzu.edu.cn

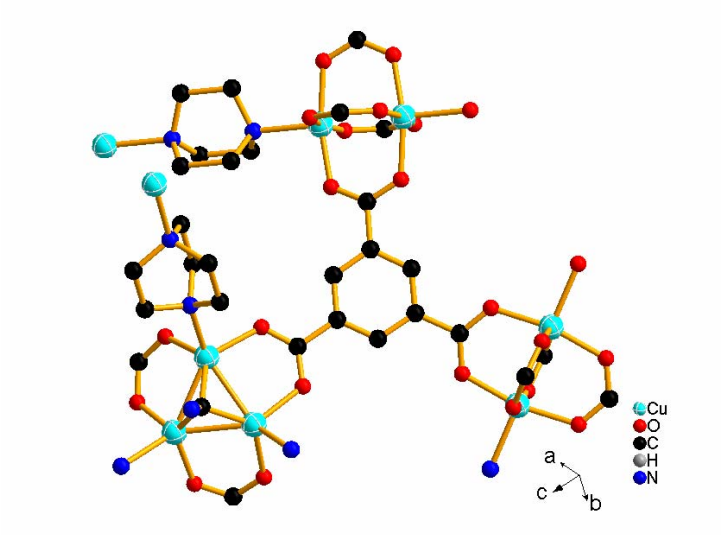

Figure S1. The crystal structure of **1**.

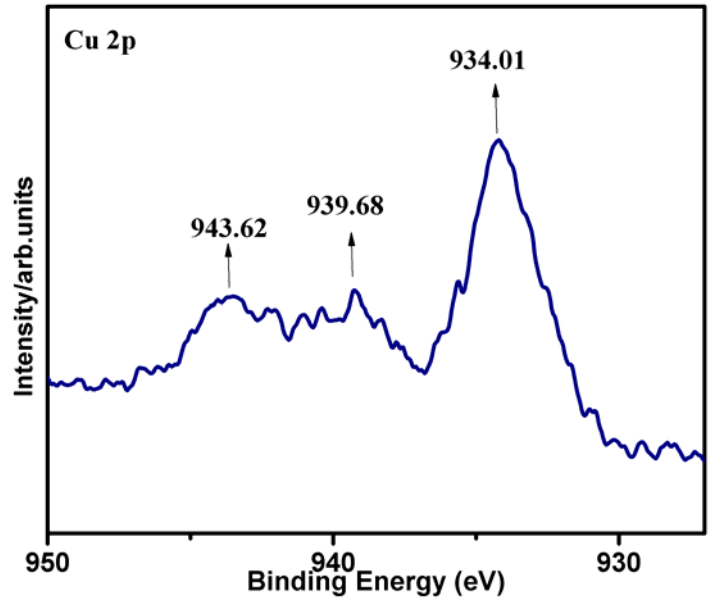

Figure S2. Cu_{2p} spectra of **1** shown that the main component peak at higher BE (↑ 934.01eV) is assigned to Cu^{2+} ions. Observation of the satellite (939.68-943.62eV) structure also is consistent with a copper oxidation state of +2.

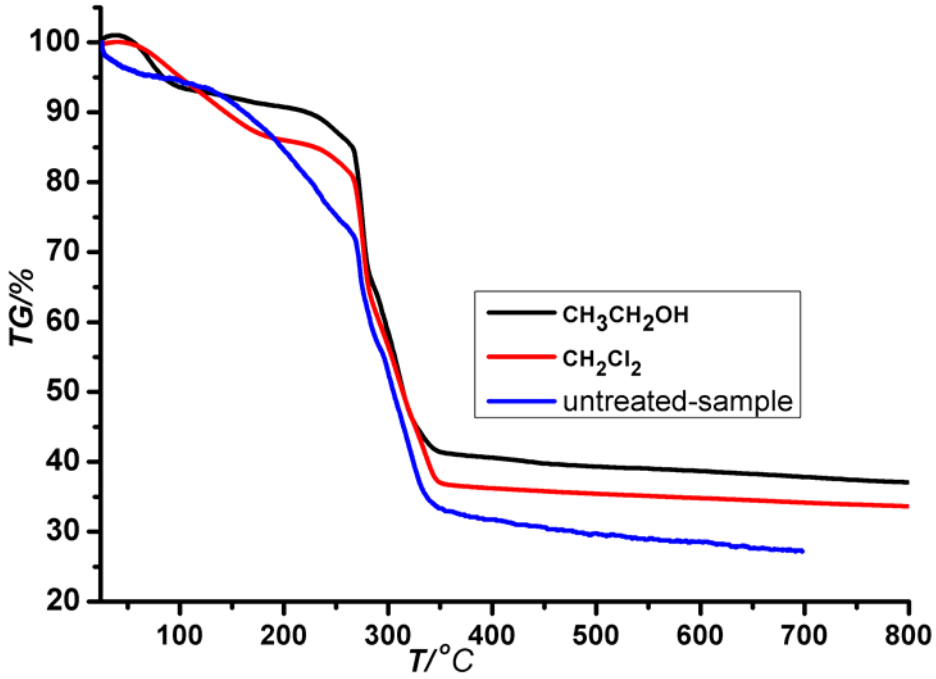

Figure S3. The TG plots of **1**, ethanol-exchanged sample **1** and CH_2Cl_2-exchanged sample **1**.

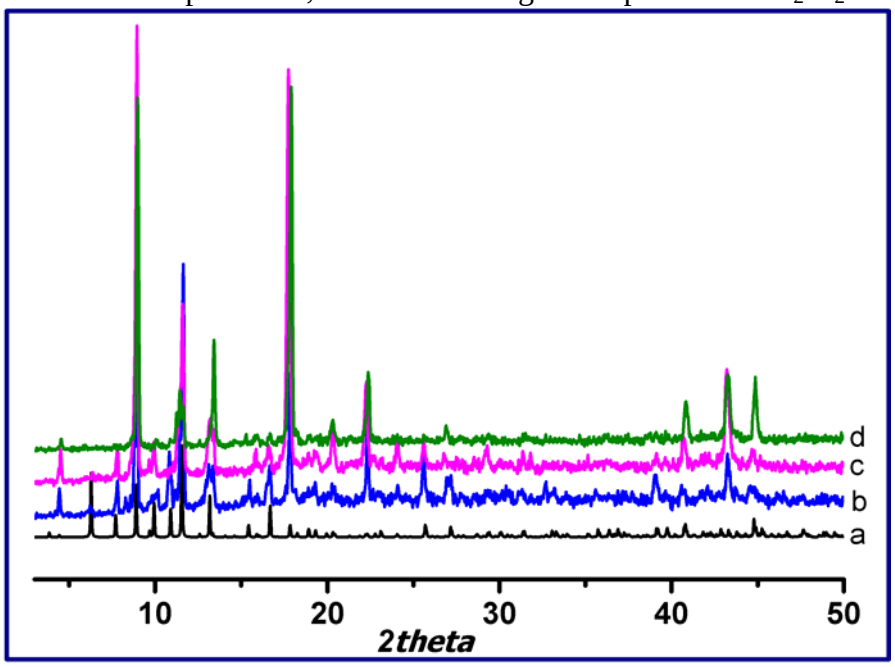

Figure S4. Powder XRD patterns: (a) simulated one, (b) after removal of the guests, (c) ethanol-exchanged one, (d) dichloromethane –exchanged one.

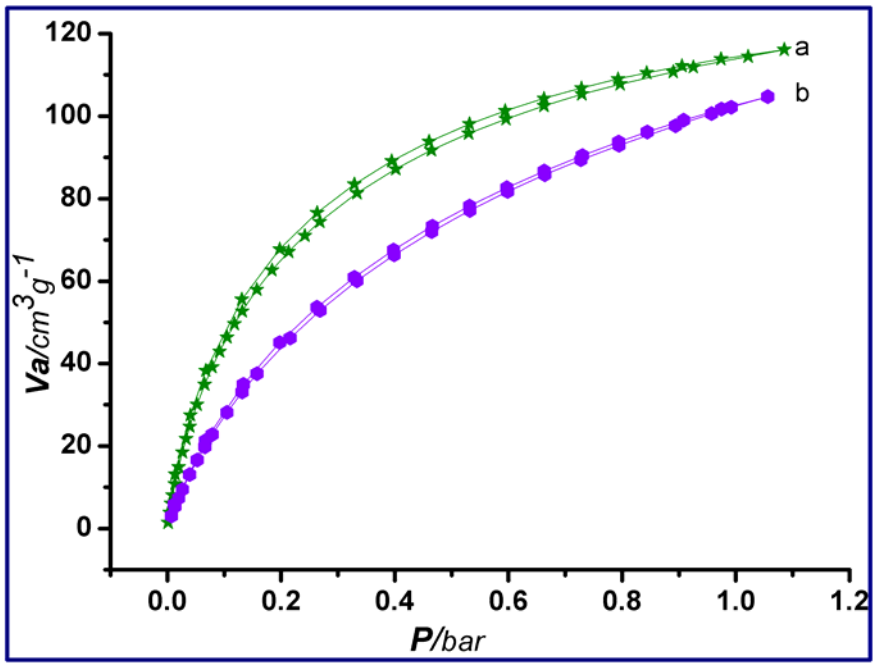

Figure S5. H_2 adsorption isotherms of **1**: (a) H_2 at 77K; (b)H_2 at 87 K**.**

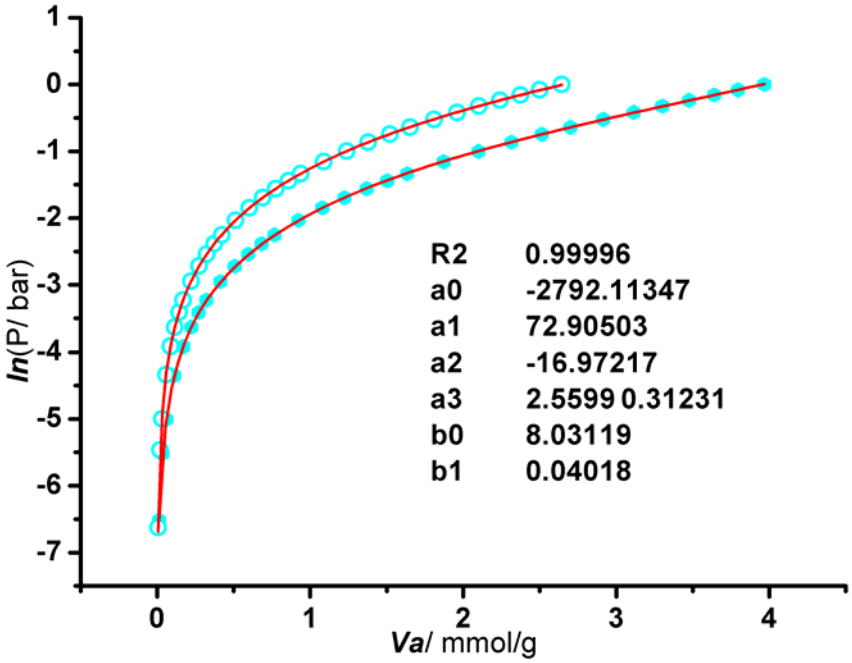

Figure S6. CO_2 adsorption isotherms for **1** fitting by virial method.

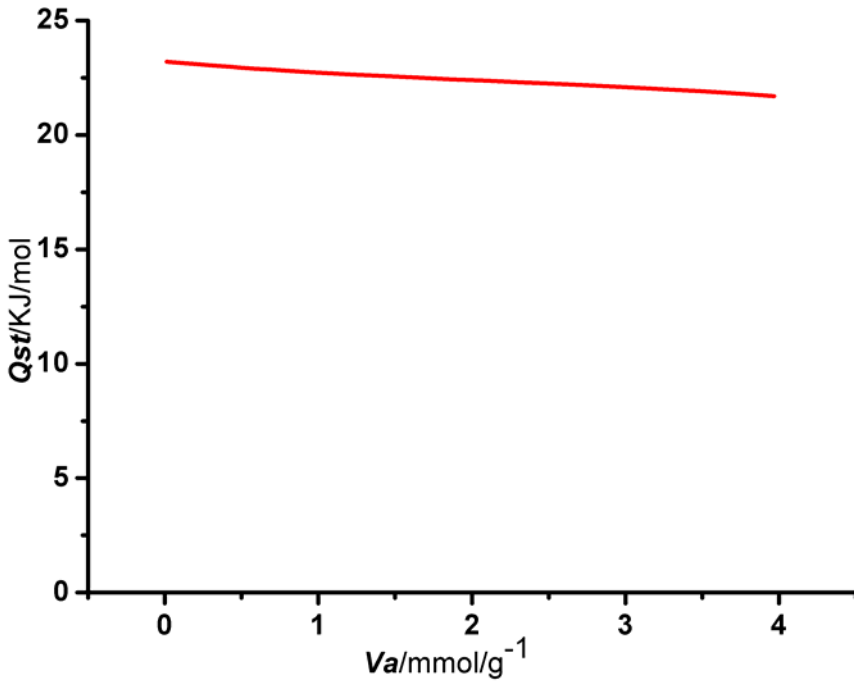

Figure S7. The isosteric heat of CO_2 adsorption for **1** estimated by the virial equation.

Adsorption selectivity of CO_2/N_2 calculation:

The CO_2 and H_2 sorption data for **1** measured up to 1 bar at different temperature were fitted by the virial equation (Figure S5, S6, S7).

$$\ln(P) = \ln(Va)+(a0+a1*Va+a2*Va^2+a3*Va^3)/T+(b0+b1*Va) \quad (1)$$

Where ***P*** is pressure, ***Va*** is amount adsorbed, ***T*** is temperature, and **a0**, **a1**, **a2**, **a3** and **b0**, **b1** are temperature independent empirical parameters.

References:

(a) R. Banerjee, A. Phan, B. Wang, C. Knobler, H. Furukawa, M. O'Keeffe, and O. M. Yaghi, High-throughput synthesis of zeolitic imidazolate frameworks and application to CO_2 capture, Science 319 (2008) 939-943;

(b) B. Wang, A. P. Côté, H. Furukawa, M. O'Keeffe, and O. M. Yaghi, Colossal cages in zeolitic imidazolate frameworks as selective carbon dioxide reservoirs, Nature 453 (2008) 207-212;

(c) H. Kim, Y. Kim, M. Yoon, S. Lim, S. M. Park, G. Seo and K. Kim, Highly Selective Carbon Dioxide Sorption in an Organic Molecular Porous Materials, J. Am. Chem. Soc. 132 (2010) 12200-12202.

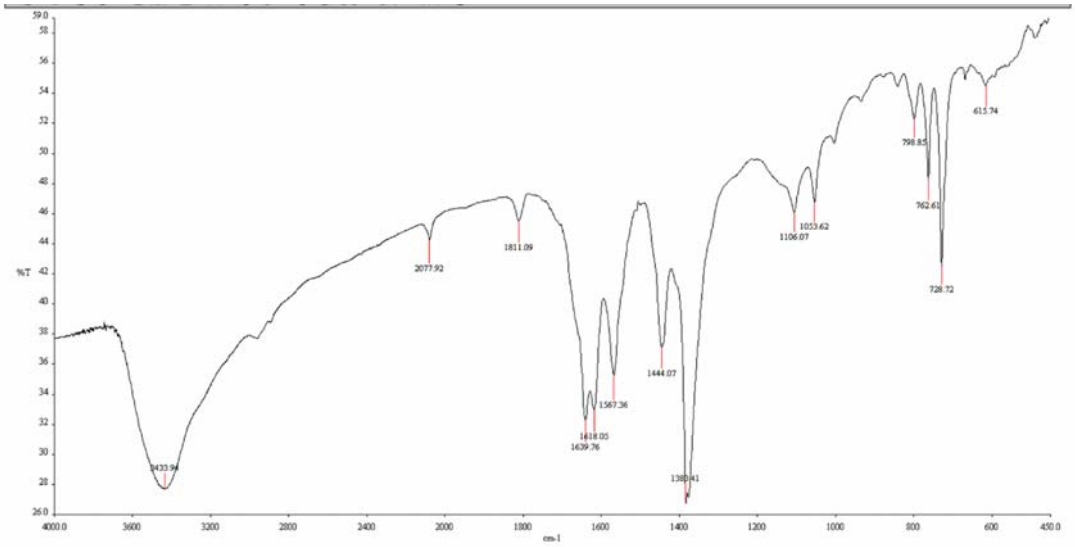

Figure S8. The FT-IR spectrum of **1**.