Electronic supplementary information

A zinc(II) metal−organic framework with high affinity for CO_2 based on triazole and tetrazolyl benzene carboxylic acid

Donghai Sheng,* Ying Zhang,* Yang Han, Guang Xu, Qingxiang Song, Yanping Hu, Xiangyun Liu, Dongming Shan and Achao Cheng

The State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Changping District, Beijing 102249, P. R. China. Tel:+8610-89733200, E-mail addresses: shengdonghai120@163.com. (Sheng, D. H.); y.zhang@cup.edu.cn (Zhang, Y.).

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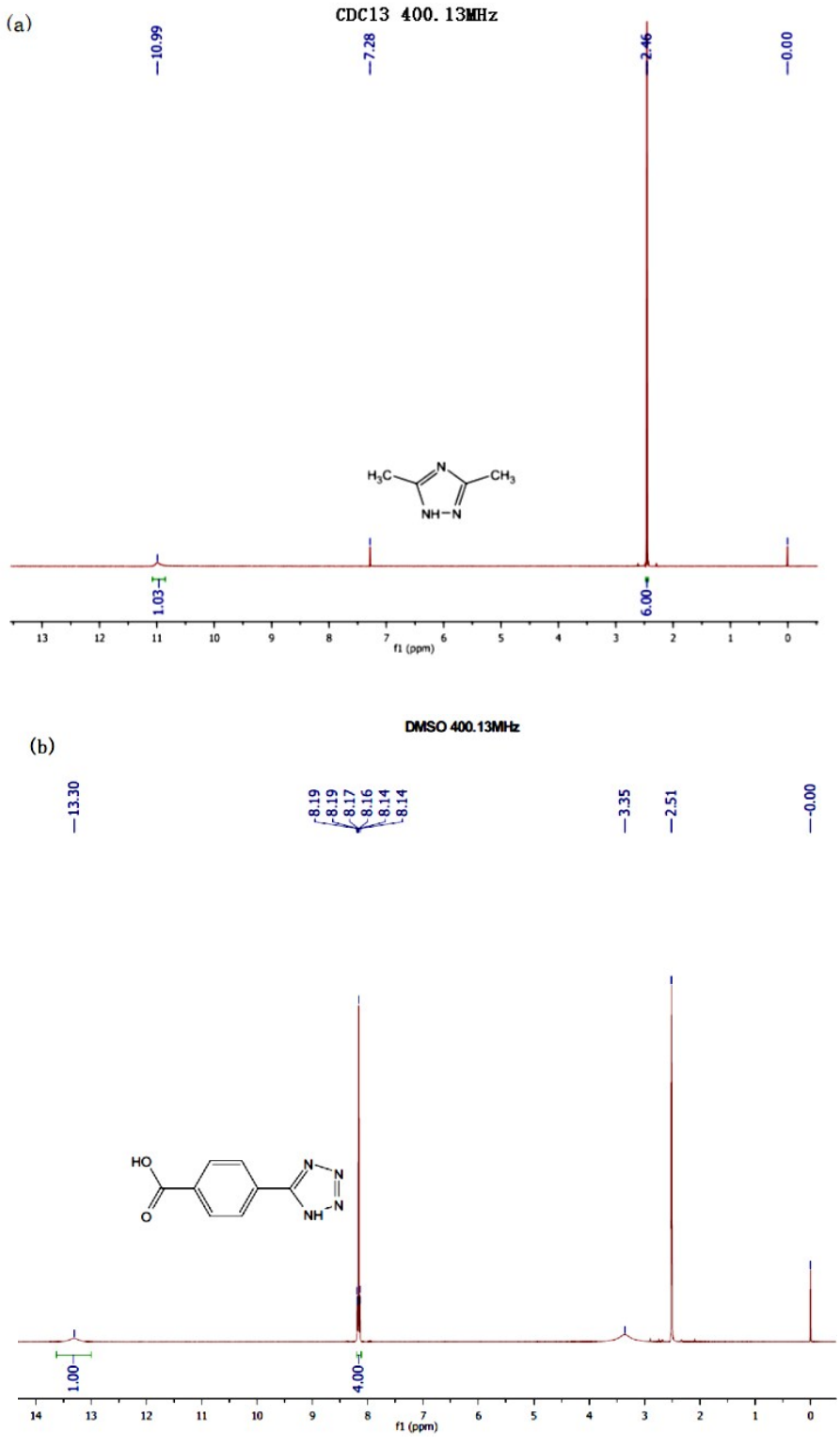

Fig. S1. (a) HNMR of 3,5-dimethyl-4H-1,2,4-triazole (Hdmtrz). (b) HNMR of 4-(1H-tetrazol-5-yl)benzoic acid (H_2tzba).

Table S1. Selected bond lengths [Å] and angles [°] for 1.

Zn(1)-O(1)	2.032(3)	Zn(2)-N(1)^{ii}	1.982(3)
Zn(1)-O(1)^{v}	2.032(3)	Zn(2)-N(1)^{iii}	1.982(3)
Zn(1)-N(5)	2.033(4)	Zn(2)-N(6)^{iv}	1.994(3)
Zn(1)-O(2)^{i}	2.061(3)	Zn(2)-N(6)^{v}	1.389(6)
Zn(1)-O(2)^{vi}	2.061(3)		
Zn(1)-O(1)^{v}-O(1)	90.5(2)	Zn(2)–N(6)^{iv}-N(1)^{iii}	110.9(1)
Zn(1)-N(5)-O(1)	103.7(1)	Zn(2)-N(6)^{iv}-N(1)^{iii}	107.8(1)
Zn(1)-O(2)^{i}-O(1)^{v}	86.7(1)	Zn(2)-N(1)^{iii}-N(1)^{ii}	109.0(2)
Zn(1)-O(2)^{vi}-O(1)^{v}	157.2(1)	Zn(2)-N(6)-N(1)^{iii}	107.8(1)
Zn(1)-O(2)^{i}-N(5)	98.87(1)	Zn(2)-N(6)-N(6)^{iv}	110.2(1)

Symmetry codes used for **1**: i=-x+1, -y+1, -z+2; ii=-x+1/2, -y+1/2, -z+2; iii=x+1/2, -y+1/2, z+1; iv=-x+1, y, -z+3; v=x, -y+1, z; vi= -x+1, y, -z+2.

Table S2. Isothermal adsorption data and calculated value of Q_{st}.

T_1	T_2	P_1	P_2	Amount(cm^3/g)	Q_{st}(KJ/mol)
195	273	0.00118	6.87	12.50	49.19
195	273	0.10	12.35	25.01	27.33
195	273	0.50	20.48	37.50	21.07
195	273	1.25	39.56	50.12	19.60
195	273	2.25	54.57	62.53	18.09
195	273	4.23	87.71	75.62	17.16
195	273	6.87	106.16	87.53	16.64
195	273	9.53	140.26	100.07	16.32
195	298	0.00118	20.00	12.53	45.67
195	298	0.10	25.16	25.14	25.93
195	298	0.50	69.42	37.57	23.14
195	298	1.25	114.29	50.31	21.18
195	298	2.25	171.53	62.53	20.32
195	298	4.23	243.61	75.06	18.97
195	298	6.87	306.96	87.53	17.81
195	298	9.53	359.34	100.14	17.02

Table S3. Fitting parameters of DSLF model for CH_4 and CO_2 at 298K.

Adsorbent	Temperature / K	q_c / mmol/g	q_i / mmol/g	K_c	K_i	R^2
CO_2	298	0.0274	7.1574	-0.0426	0.0263	0.9999
CH_4	298	0.0085	0.4769	-0.0426	0.0081	0.9999
N_2	298	0.0086	1.5853	0.0019	0.0085	0.9999

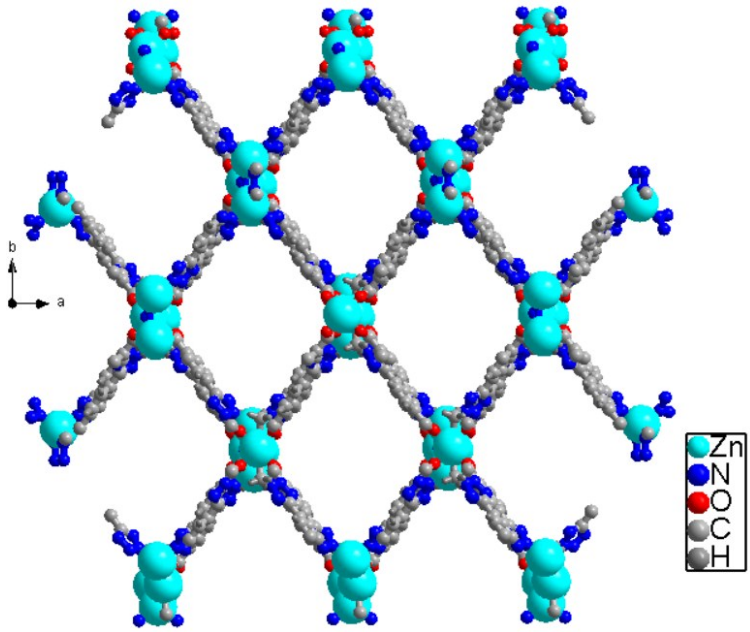

Fig. S2. The 1 with channels in the plane of [1 1 0] and this diffraction plane gives the diffraction peak at 2θ = 7.0°.

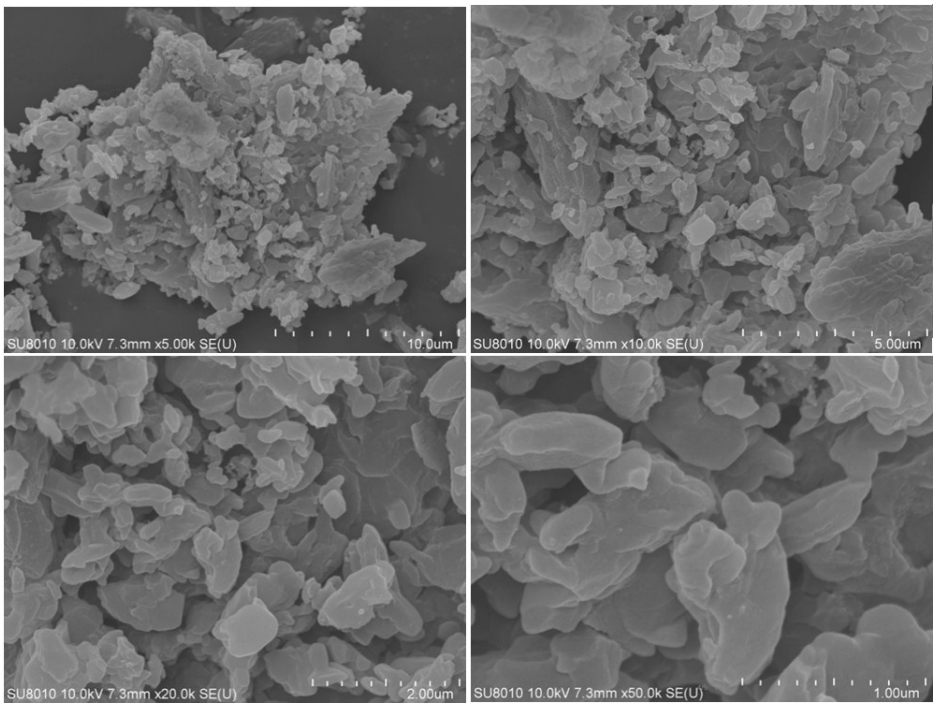

Fig. S3. SEM images of **1** with different magnifications.

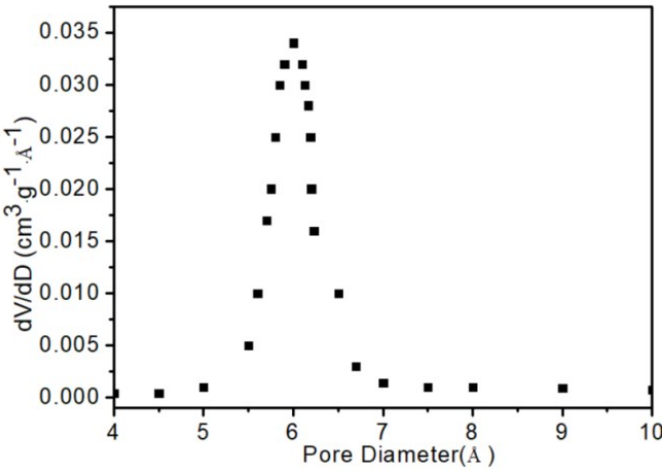

Fig. S4. The pore sizedistribution of **1**.

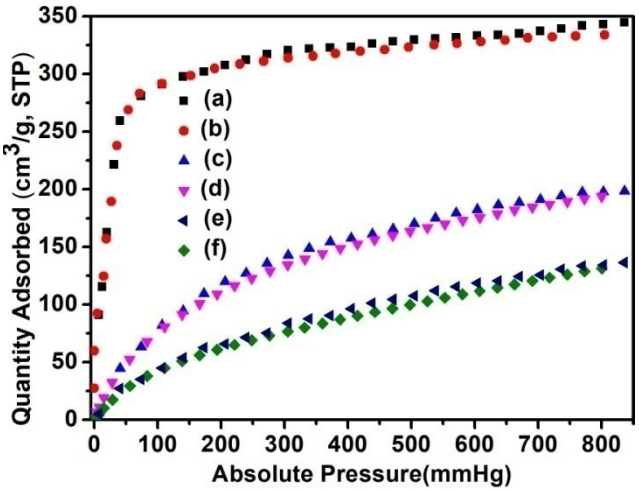

Fig. S5. CO_2 adsorption isotherms based on GCMC and experiments at 195K, 273K and 298 K. (a) Simulated ads. CO_2 at 195K. (b) Experimental ads. CO_2 at 195K. (c) Simulated ads. CO_2 at 273K. (d) Experimental ads. CO_2 at 273K. (e) Simulated ads. CO_2 at 298K. (f) Experimental ads. CO_2 at 298K.