SUPPORTING INFORMATION

A Carbonate Based Zeolitic Imidazolate Framework for Highly Selective CO_2 capture

Sajani A. Basnayake[‡], *Jie Su*[†], *Xiadong Zou*[†], *Kenneth J. Balkus Jr.*[‡]*

[‡]Department of Chemistry, University of Texas at Dallas, 800 West Campbell Road, Richardson, TX 75080-3021, USA

[†]Inorganic and Structural Chemistry and Berzelli Centre EXSELENT on Porous Materials, Stockholm University, SE-10691, Stockholm, Sweden

Table S1. Selected bond lengths and angles for ZIF-CO_3-1[a]

Atoms 1,2	d 1,2 [Å]	Atoms 1,2	d 1,2 [Å]
Zn1 – N2	1.972(5)	C4 – N3	1.376(9)
Zn1 – N3	1.970(5)	C5 – N2	1.381(8)
Zn1 – O2	1.982(3)	C4 – C5^{ii}	1.344(10)
Zn1 – O1^{i}	1.988(4)	C1 – C6	1.487(8)
C1 – N3	1.328(7)	O1 – C7	1.247(5)
C1 – N2^{ii}	1.349(6)	O2 – C7	1.338(9)
Atoms 1,2,3	Angle 1,2,3 [^{o}]	Atoms 1,2,3	Angle 1,2,3 [^{o}]
N2 – Zn1 – N3	119.9(2)	C1 – N3 – C4	105.4(5)
N2 – Zn1 – O2	109.63(16)	N3 – C4 – C5^{ii}	109.6(6)
N2 – Zn1 – O1^{i}	108.00(18)	N2 – C5 – C4^{iii}	107.3(6)
N3 – Zn1 – O2	111.60(15)	N3 – C1 – C6	123.9(5)
N3 – Zn1 – O1^{i}	107.26(18)	N2^{ii} – C1 – C6	124.4(5)
O2 – Zn1 – O1^{i}	98.11(18)	O1 – C7 – O1^{iv}	128.6(7)
N2^{ii} – C1 – N3	111.7(5)	O1 – C7 – O2	115.7(4)
C1^{iii} – N2 – C5	106.0(5)		

a Symmetry transformations used to generate equivalent atoms: (i) x, y, -1+z; (ii) 0.5+x, 0.5-y, z; (iii) -0.5+x, 0.5-y, z; (iv) -x, -y, z.

Calculation of the amount of CO_2 released from ZIF-CO_3-1

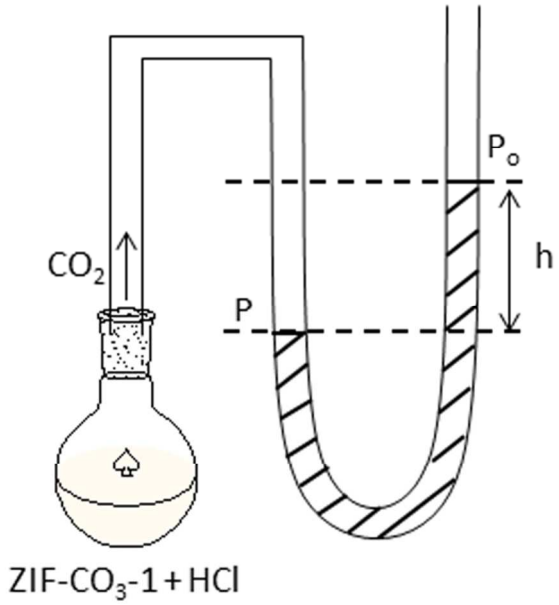

Figure S1. The manometer set up used for the calculation of amount of CO_2 released from ZIF-CO_3-1

The pressure applied by released CO_2:

$P = P_o + h\rho g$

Where P_o = atmospheric pressure (101325 Pa)

ρ = density of the manometer fluid (water, 997.8 $kg \cdot m^{-3}$ at 22 ^oC)

g = acceleration of gravity (9.81 $m \cdot s^{-2}$)

Volume of CO_2 released:

$VCO_2 = \pi \cdot r^2 \cdot h$

Where r = radius of the manometer tube (1.59 mm)

Number of moles of CO_2 released:

$nCO_2 = PVCO_2/RT$

Where R = universal gas constant (8.314 $J \cdot K^{-1} \cdot mol^{-1}$)

T = temperature (22 ^oC)

For triplicate trials using 3.04 mg ZIF-CO_3-1;

Average displacement of fluid, h = 2.62 cm

Thus, average moles of CO_2 released $nCO_2 = 2.71\times10^{-3}$ mol·g^{-1}

The percent weight of released CO_2 was calculated using nCO_2 and the mass of ZIF-CO_3-1 used.

Gas adsorption data for ZIF-CO_3-1

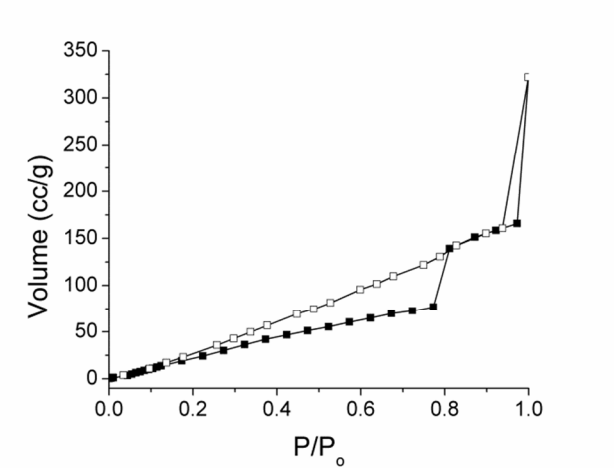

Figure S2. The N_2 adsorption isotherm of ZIF-CO_3-1. The adsorption and desorption are represented by black filled squares and open squares respectively.

The crystallinity of ZIF-CO_3-1 after regeneration

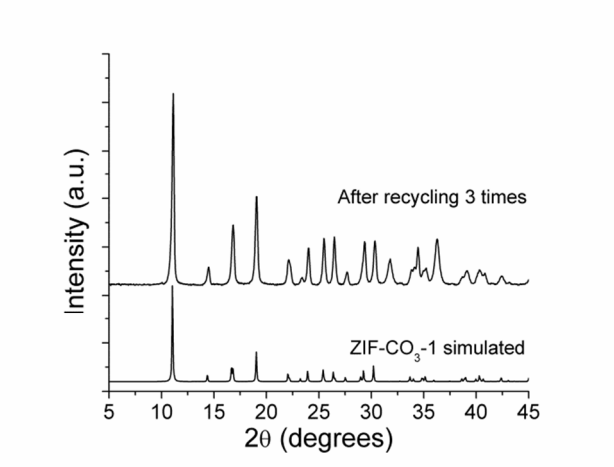

Figure S3. PXRD pattern of ZIF-CO_3-1 after 3 cycles of release and regeneration as compared to simulated PXRD pattern