Sol–Gel Synthesis of High-Density Zeolitic Imidazolate Framework Monoliths via Ligand Assisted Methods: Exceptional Porosity, Hydrophobicity, and Applications in Vapor Adsorption

Elwin Hunter-Sellars, Paola A. Saenz-Cavazos, Anthony R. Houghton, Sean R. McIntyre, Ivan P. Parkin, and Daryl R. Williams*

In the original published version of this article, the bulk densities of the powder ZIF-8 and ZIF-67 were quoted as 0.96 g/cm³ and 0.94 g/cm³ respectively. However, the values for the powder samples' true density were quoted in error. The correct bulk densities, used for calculating volume-relative capacities and surface areas, were 0.39 g/cm³ and 0.38 g/cm³ for ZIF-8 and ZIF-67, respectively. As this affects the calculated 'volume-relative' quantities, corrected tables and graphs are included below.

The authors apologise for any inconvenience or confusion this error may have caused.

Corrected tables

Corrected values will be written and underlined in red.

Table 1. Physical characteristics of ZIF samples. Surface areas and porosities expressed in mass-relative and volume-relative terms. $T_{pycometry} = 25 \text{ °C}$. $T_{gas adsorption} = -196 \text{ °C}$.

Adsorbent	Density [g/cm ³]	BETSu	rface Area	Micropore volume		Total pore volume	
		[m²/g]	[m ² /cm ³] ^{a)}	[cm ³ /g]	[cm ³ /cm ³] ^{a)}	[cm ³ /g]	[cm ³ /cm ³] ^{a)}
ZIF-8	<u>0.39</u>	1801	<u>702</u>	0.506	<u>0.197</u>	1.665	0.649
ZIF-8 (NB)	1.17	1597	1869	0.334	0.390	1.177	1.377
ZIF-8 (ML)	1.25	9	11	_b)	_b)	0.004	0.005
ZIF-67	<u>0.38</u>	1753	<u>666</u>	0.583	0.222	1.779	<u>0.676</u>
ZIF-67 (NB)	1.11	1731	1922	0.391	0.434	1.647	1.828
ZIF-67 (ML)	1.28	1458	1866	0.515	0.660	0.643	0.823

^{a)}Volume-relative quantities calculated by multiplying bulk density by mass-relative quantity; ^{b)}Due to lack of micropores within sample, micropore volume could not be determined.

Table 3. Summary of low concentration dynamic adsorption experiments. All measurements carried out at a toluene partial pressure of 0.00026, and a temperature of 25 °C.

Adsorbent	Capacit	ty [mg/g]	Capacity [mg/cm ³]		Useability [%] ^{a)}
	Useable	Total	Useable	Total	
ZIF-8	56.3	93.7	22.0	<u>36.5</u>	60.1
ZIF-8 (NB)	34.3	76.8	40.2	89.8	44.7
ZIF-67	54.4	97.2	<u>20.7</u>	<u>36.9</u>	56
ZIF-67 (NB)	44.7	92.1	49.6	102.3	48.5
ZIF-67 (ML)	39.4	95.9	50.5	122.8	41.1

^{a)}Calculated by dividing capacity when toluene is first detected by the capacity when the inlet and outlet concentrations of toluene are equal.

Table 4. Estimated mass-relative and volume-relative toluene vapour capture productivities for adsorbents. Calculated using gravimetric toluene adsorption data at a partial pressure of 0.1 and a temperature of 25 °C.

Sample	Capacity [mg/g]	Time [min] ^{a)}	Produ	Productivity	
			[kg/ kg h]	[kg/ m ³ h]	
ZIF-8	321.8	274	0.0705	27.5	
ZIF-8 (NB)	298.6	293	0.0611	71.5	
ZIF-67	323.9	285	0.0682	25.9	
ZIF-67 (NB)	329.4	270	0.0732	81.3	
ZIF-67 (ML)	299.7	300	0.0599	76.7	

^{a)}Time taken to reach a mass gradient value of 0.00075% dry mass per minute.

Corrected main text figures

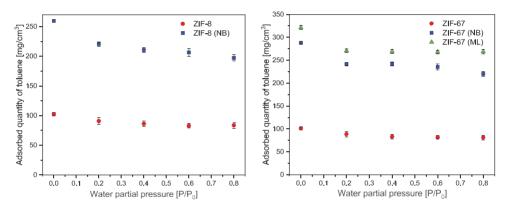


Figure 6. Co-sorption volume-relative toluene vapour capacities as a function of process humidity, for zinc (left) and cobalt (right) ZIF samples. Partial pressure of toluene in all measurements, $P/P_0 = 0.005$, while water vapour partial pressure varied. All measurements carried out at 25 °C.

Corrected supplementary information figures

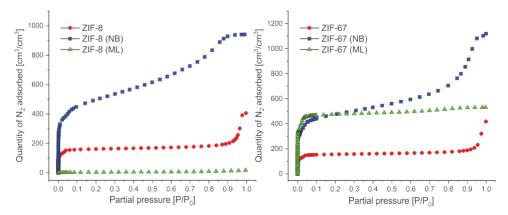


Figure S4. Volume-relative nitrogen adsorption isotherms for zinc (left) and cobalt (right) samples. Temperature in all experiments is -196 °C.

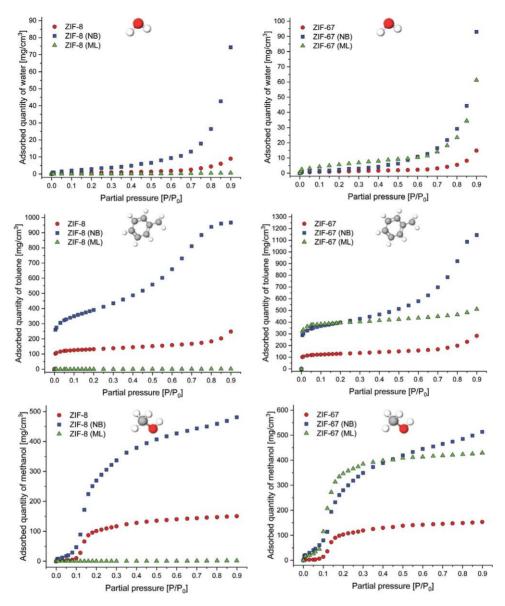


Figure S5. Volume-relative adsorption isotherms for zinc (left) and cobalt (right) samples: water (top), toluene (middle), methanol (bottom). Temperature in all experiments is 25 °C.