SUPPLEMENTARY MATERIAL

Two Coordination Polymers Constructed from Pentanuclear Zinc Clusters with Triazolate and Benzenecarboxylate Ligands: Selective Gas Adsorption

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Scheme S1. Coordination modes of the organic ligands in 1 and 2.
Fig. S1 TGA curves for 1 and 2.
IAST calculations of adsorption selectivity

In order to determine the adsorption selectivities of CO$_2$ with respect to CH$_4$ and N$_2$, binary mixture adsorption equilibrium was determined using the Ideal Adsorbed Solution Theory (IAST)
of Myers and Prausnitz.\(^1\) The IAST was used to predict mixed gas behavior from experimentally measured single-component isotherms. The experimental isotherm data for pure CO\(_2\), CH\(_4\) and N\(_2\) (measured at 273 K) were fitted using a Langmuir-Freundlich (L-F) model (eqn 1).

\[
q = \frac{a \times b \times p^c}{1 + b \times p^c} \quad (1)
\]

Where \(q\) and \(p\) are adsorbed amounts and pressures of component \(i\), respectively.

Using the Langmuir-Freundlich fits, the adsorption selectivity factor, \(S_{\text{ads}}\), is defined by (eqn 2)

\[
S_{\text{ads}} = \frac{q_i}{q_j} / \frac{p_i}{p_j} \quad (2)
\]

Where \(q_i\) is the amount of \(i\) adsorbed and \(p_i\) is the partial pressure of \(i\) in the mixture.