# SUPPLEMENTARY MATERIAL

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

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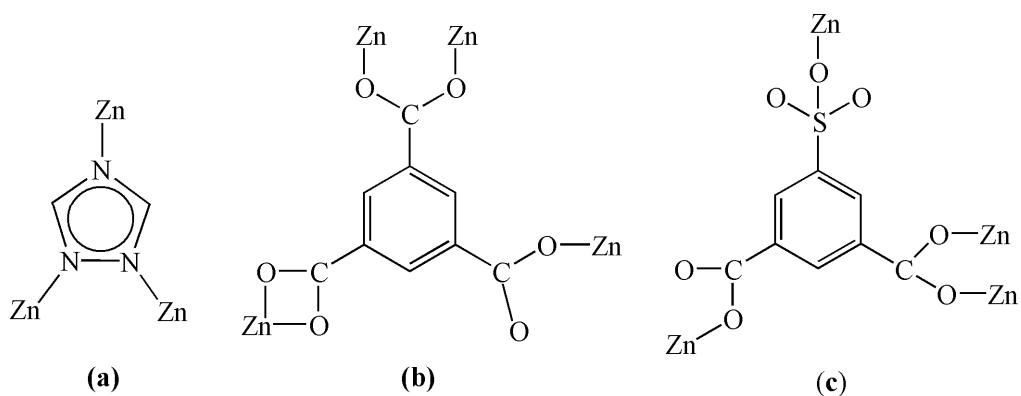
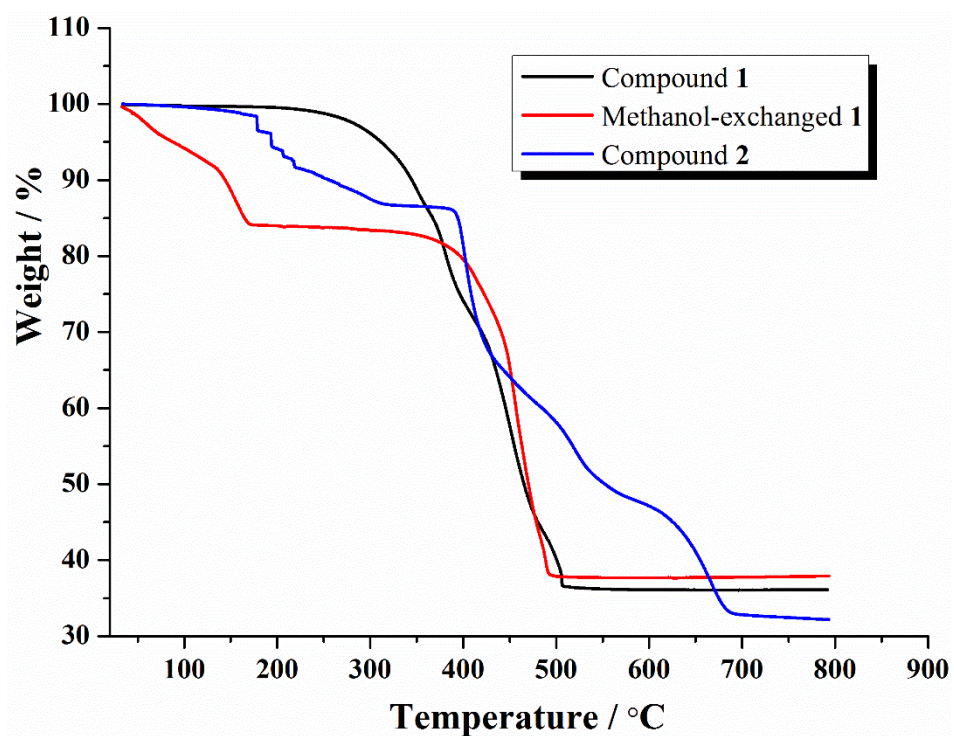**Scheme S1.** Coordination modes of the organic ligands in **1** and **2**.
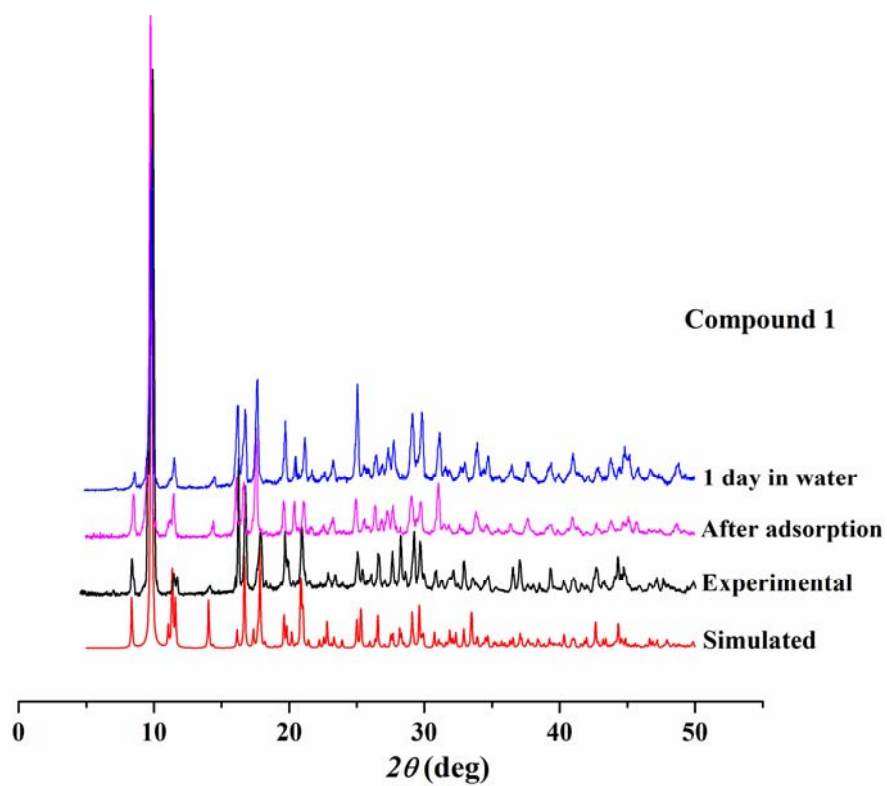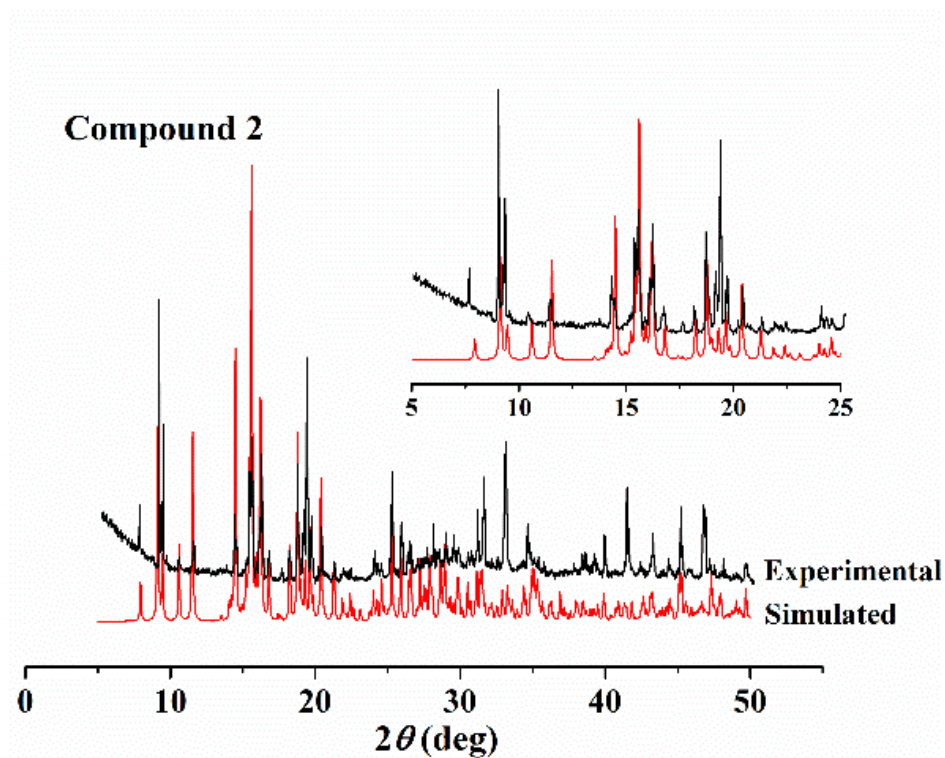
Fig. S1 TGA curves for **1** and **2**.

Fig. S2 Simulated and experimental powder X-ray diffraction patterns for **1** and **2**.
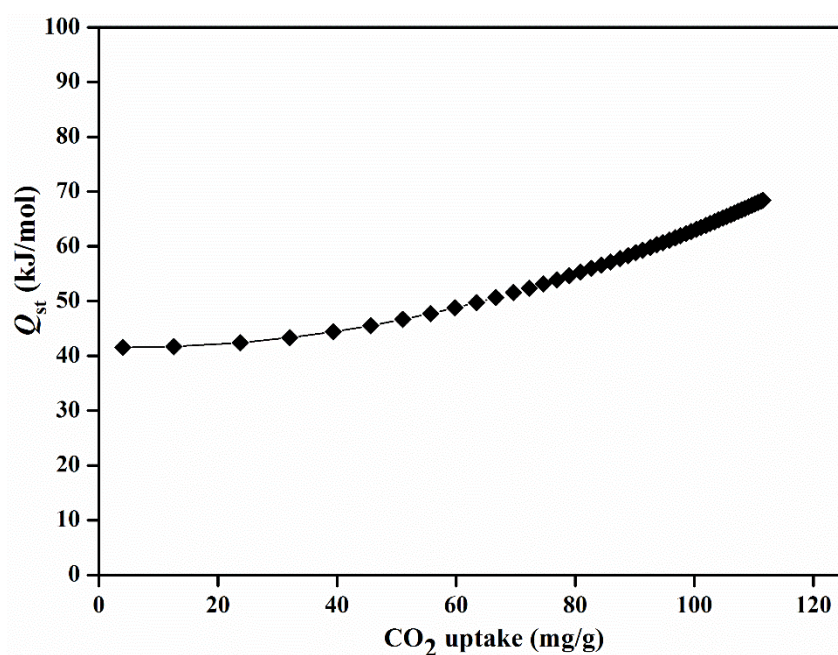

Fig. S3 The CO_2 adsorption enthalpy for **1** calculated from the CO_2 adsorption isotherms at 273 K and 293 K.

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).

$$q = (a \times b \times p^c)/(1 + b \times p^c) \quad (1)$$

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

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

$$S_{ads} = (q_i/q_j)/(p_i/p_j) \quad (2)$$

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