Supporting Information

New amine-functionalized cobalt cluster-based frameworks with open metal sites and suitable pore sizes: multipoint interactions enhanced CO_2 sorption

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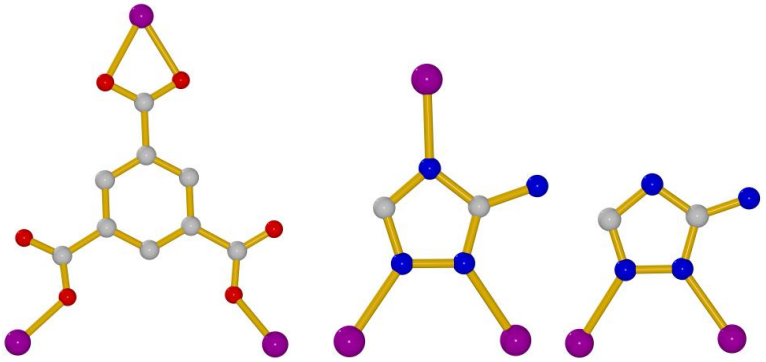


Figure S1. The coordination modes of the btc^{3-} (a), atz^{-} (b) and Hatz (c) in **1**.

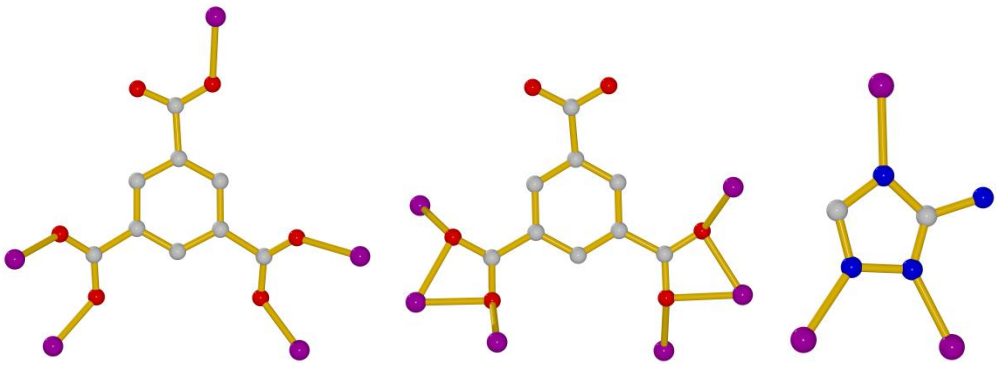
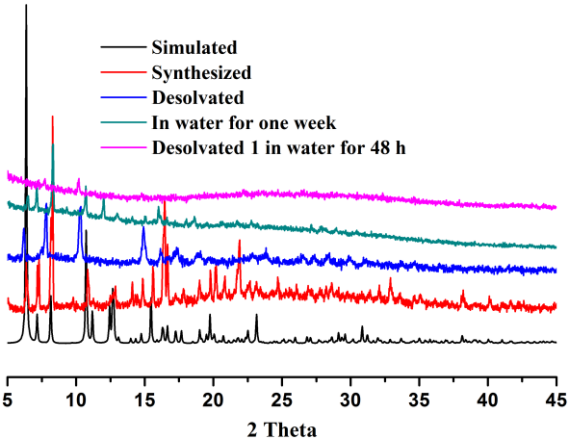
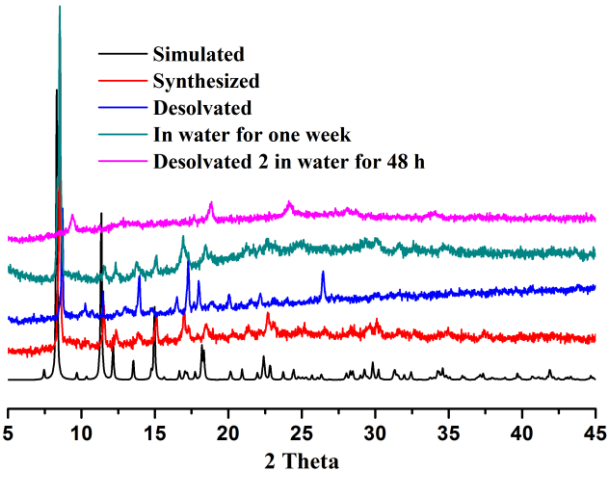


Figure S2. The coordination modes of the btc^{3-} (a), $Hbtc^{2-}$ (b) and atz^{-} (c) in **2**.

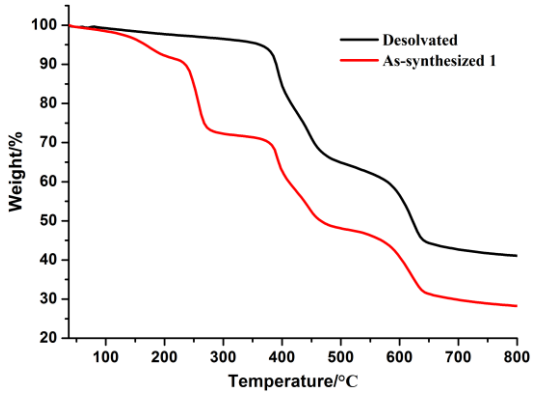


(a)

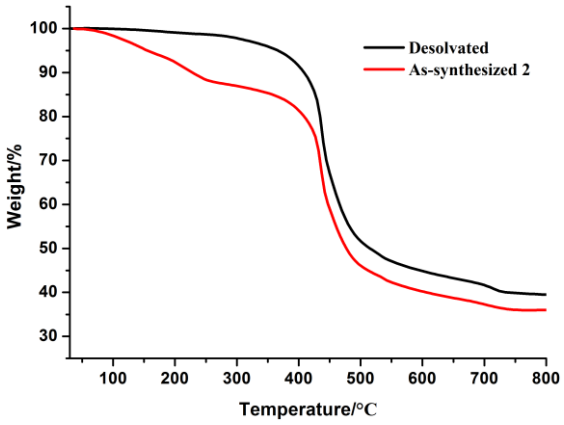


(b)

Figure S3. PXRD patterns of **1** (a) and **2** (b) after different treatments.

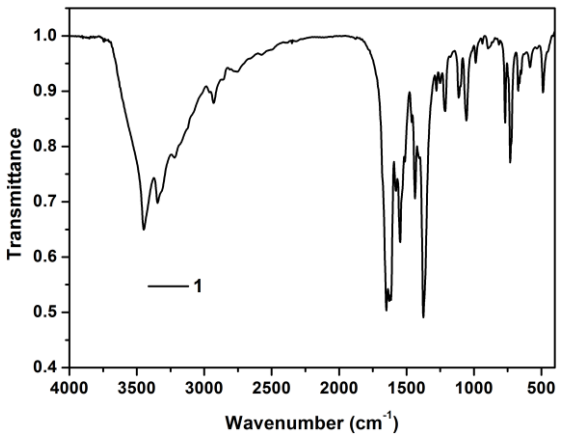


(a)

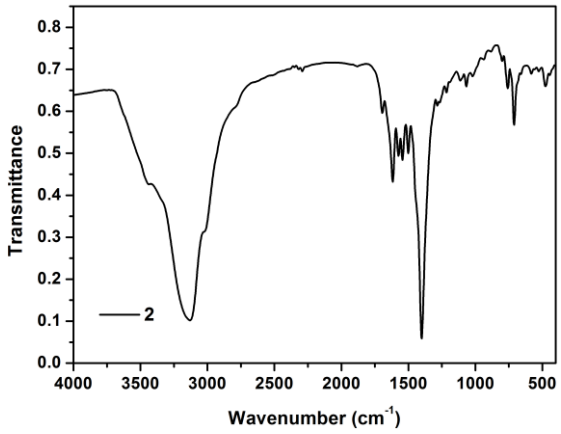


(b)

Figure S4. TGA curves of **1** (a), **2** (b), desolvated **1** and **2**.



(a)



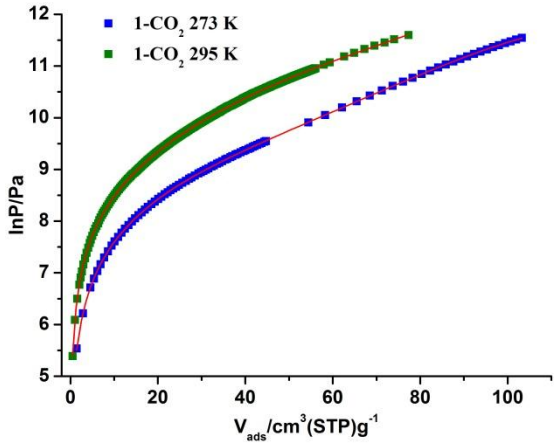
(b)

Figure S5. IR spectra of **1**(a) and **2** (b).

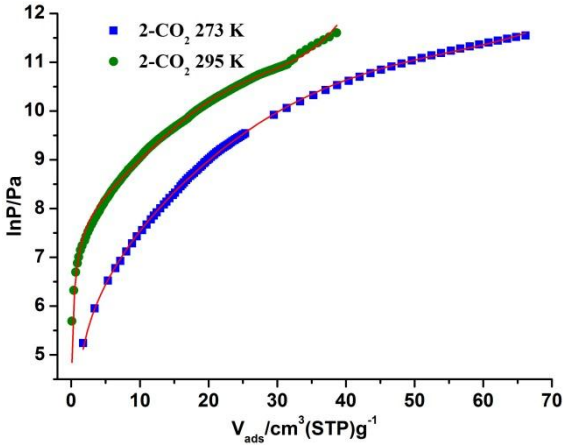
Calculation of sorption heat for CO_2 uptake using Virial 2 model

$$\ln P = \ln N + 1/T \sum_{i=0}^{m} aiN^i + \sum_{i=0}^{n} biN^i \qquad Q_{st} = -R\sum_{i=0}^{m} aiN^i$$

The above equation was applied to fit the combined CO_2 isotherm data for desolvated **1** and **2** at 273 and 295 K, where P is the pressure, N is the adsorbed amount, T is the temperature, *ai* and *bi* are virial coefficients, and m and n are the number of coefficients used to describe the isotherms. Q_{st} is the coverage-dependent enthalpy of adsorption and R is the universal gas constant.



(a)



(b)

Figure S6. (a) CO_2 adsorption isotherms for desolvated **1** with fitting by Virial 2 model. Fitting results: a0 = -3595.44147, a1 = 51.05360, a2 = 7.89771, a3 = 11. 48727, a4 = -8.60000 $\times 10^{-6}$, b0 = 18.28262, b1= -0.16620, b2 = -0.02931, b3 = -0.04207. Chi^2 = 0.00003, R^2 = 0.99997. (b) CO_2 adsorption isotherms for desolvated **2** with fitting by Virial 2 model. Fitting results: a0 = -3678.84498, a1 = 53.10015, a2 = 8.09084, a3 = 11. 47996, a4 = 1.03215 $\times 10^{-4}$, b0 = 17.9306, b1= -0.14128, b2 = -0.02860, b3 = -0.04210. Chi^2 = 0.00340, R^2 = 0.99718.