Supporting information:

Porous Coordination Polymers Based on Azamacrocyclic Complex: Syntheses, Solvent-induced Reversible Crystal-to-Crystal Transformation and Gas Sorption Properties

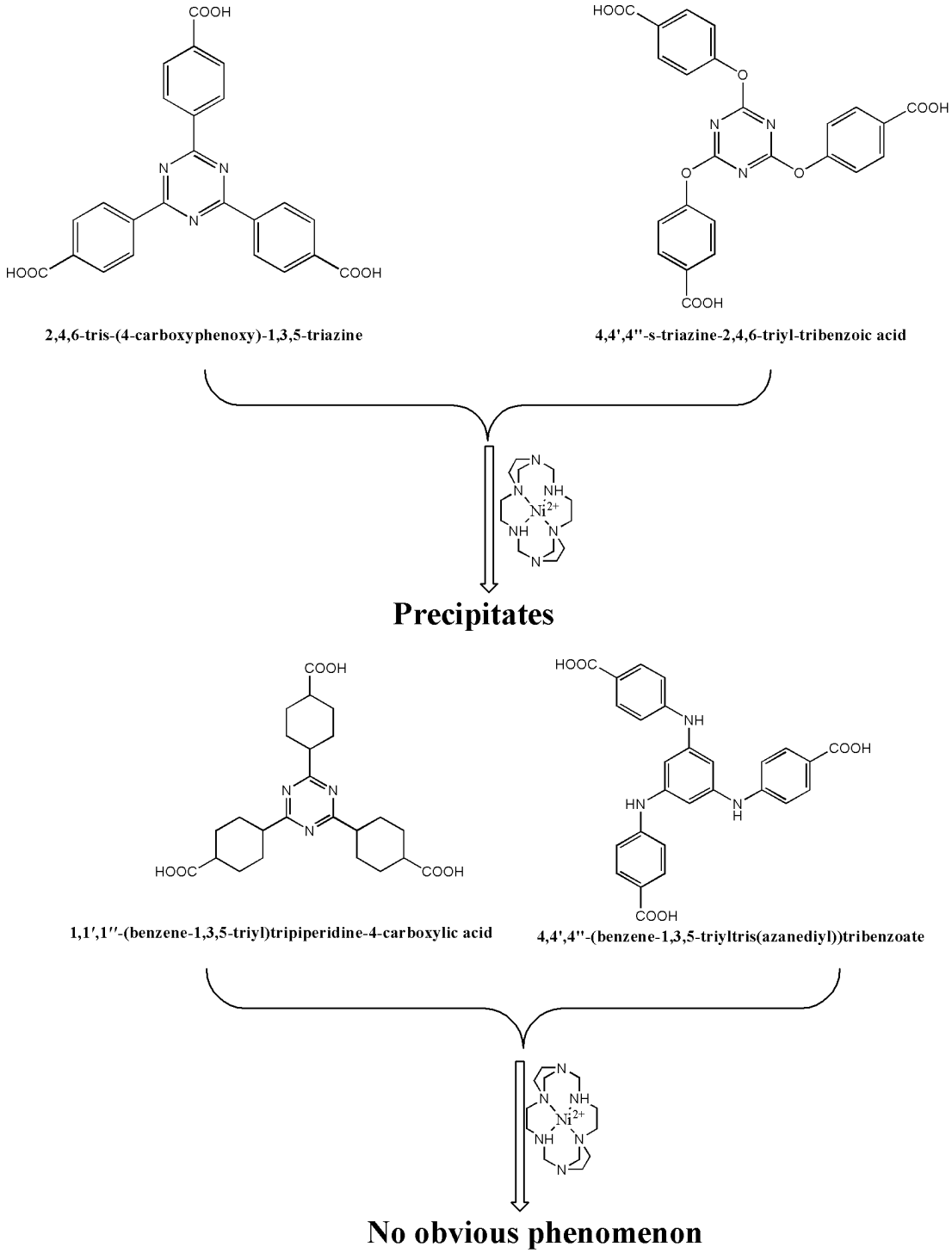


Figure S1, Other used analogous tripodal carboxylate ligands in experiments.

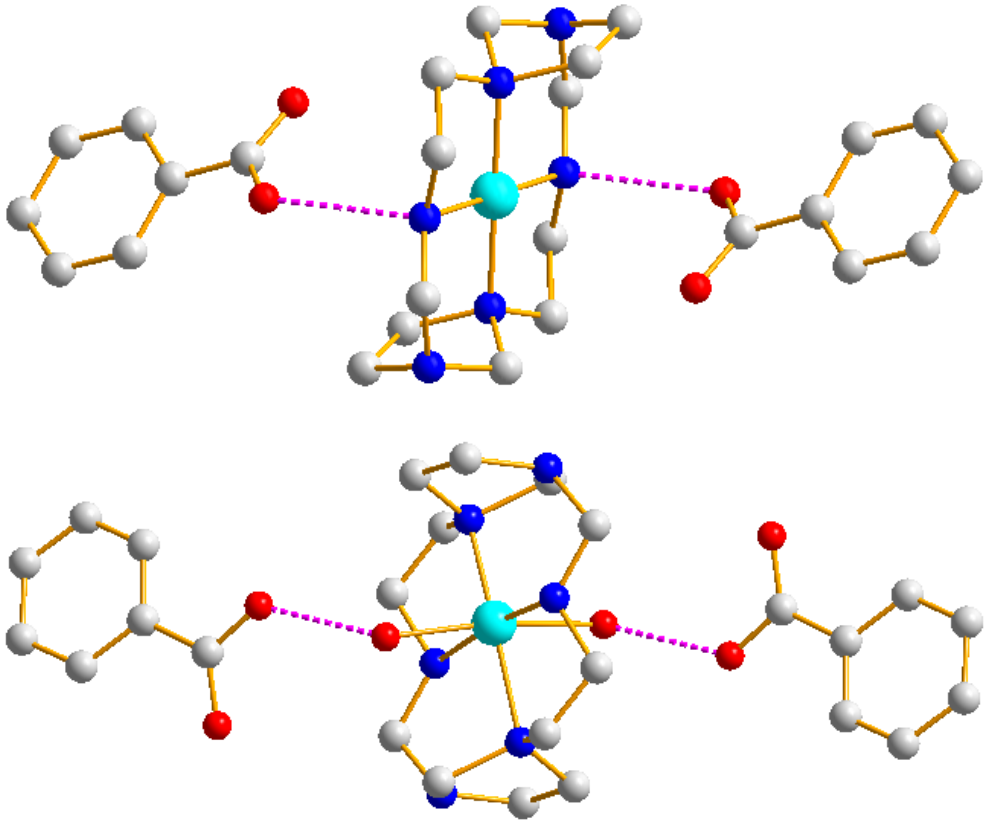


Figure S2, hydrogen bonds around $[NiL]^{2+}$ in compound **1**.

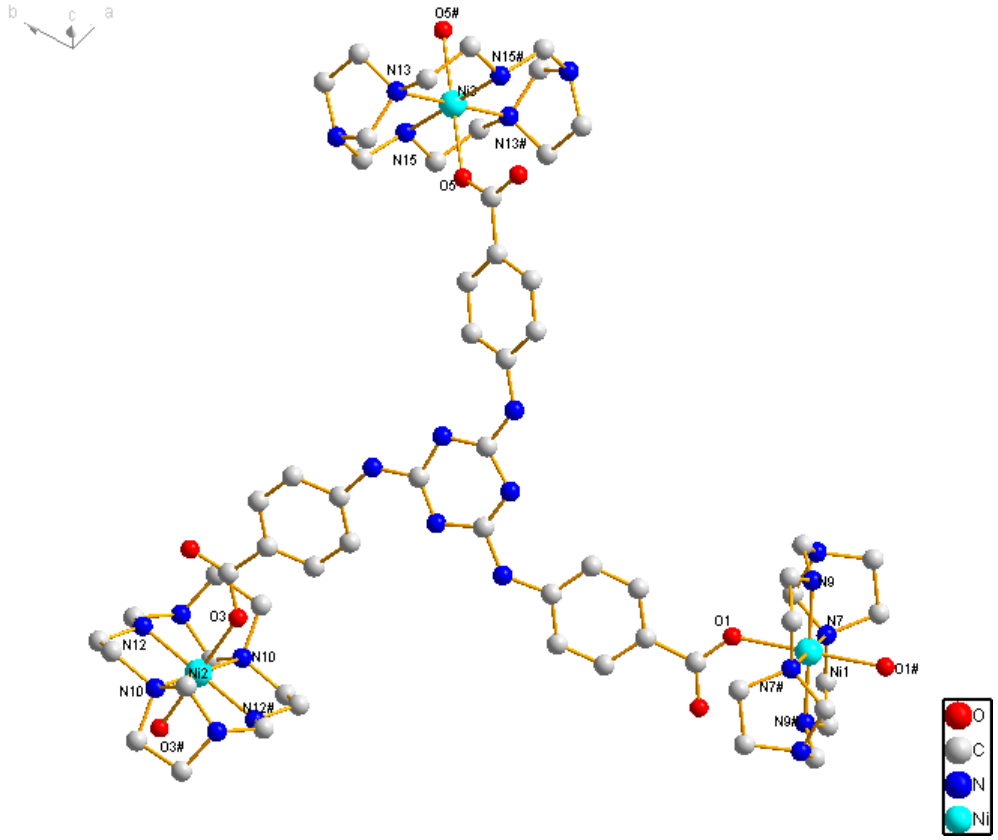


Figure S3: ORTEP of compound **2.** #: 0.5-x,1.5-y,-z;

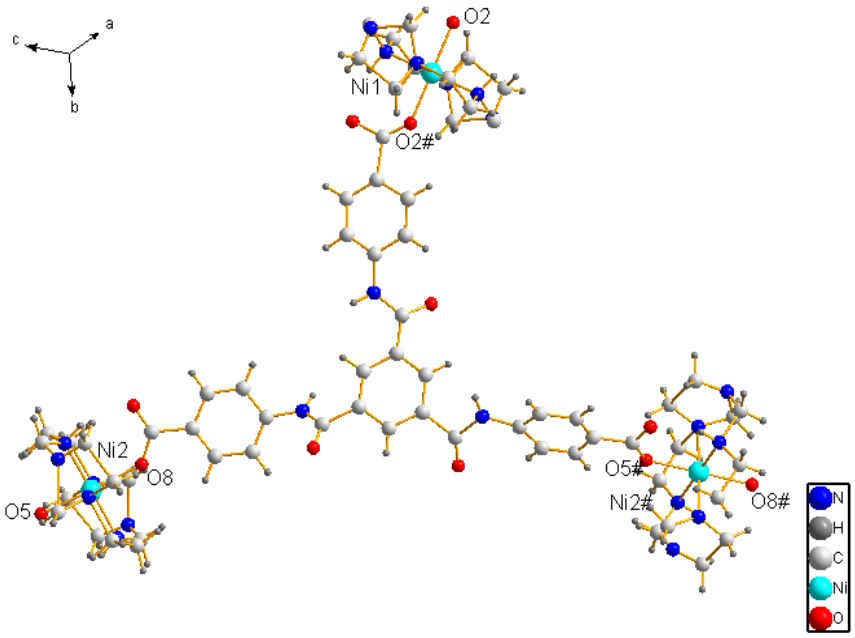


Figure S4, ORTEP of compound **3**. #:1-x, 1.5+y, -0.5-z

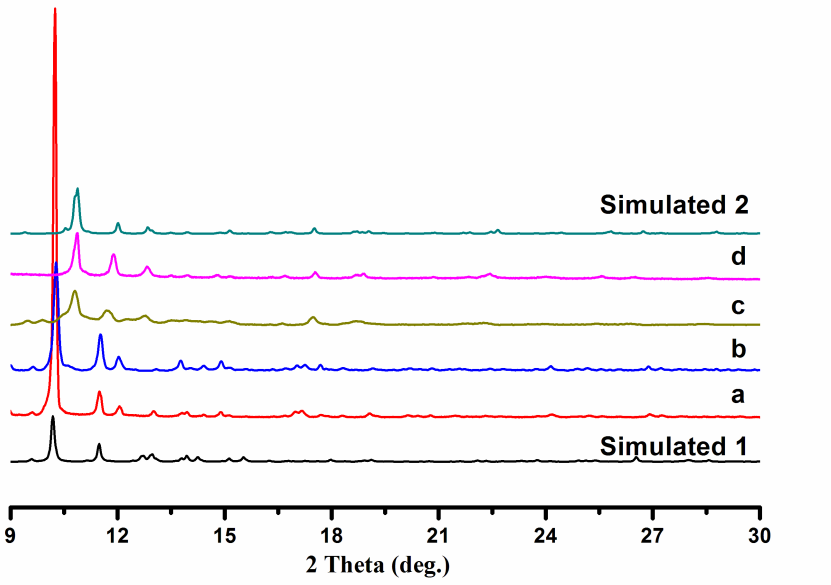


Figure S5. PXRD of those bulk samples. a: as-synthesized of **1**; b: isolated of solid samples after immersion of **2** in H_2O solution for 1 min; c: isolated of solid samples after immersion of **1** in DMF solution for 1min; d: as-synthesized of **2**.

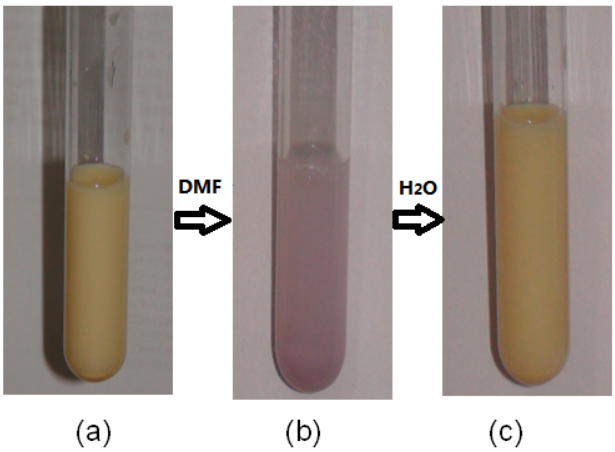


Figure S6: Reversible solvatochromic behavior of compound **1** and **2**. (a): immersion of **1** in H_2O solution for 1 min; (b) immersion of **1** in DMF solution for 1 min; (c) immersion of **2** in H_2O solution for 1 min

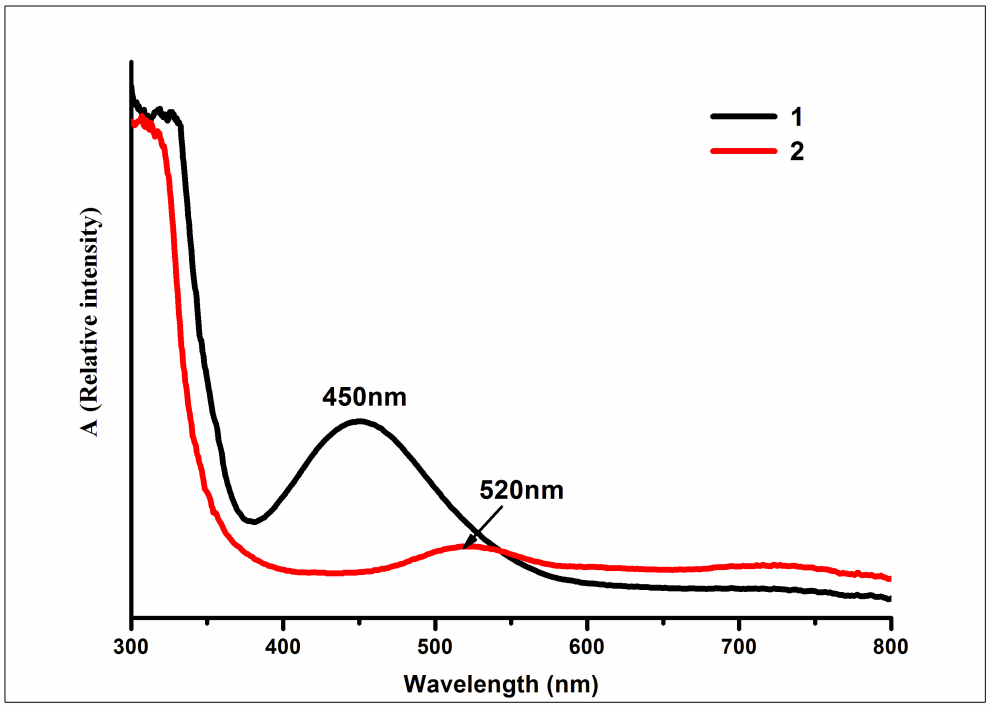


Figure S7, The solid state UV-Vis of **1** and **2**.

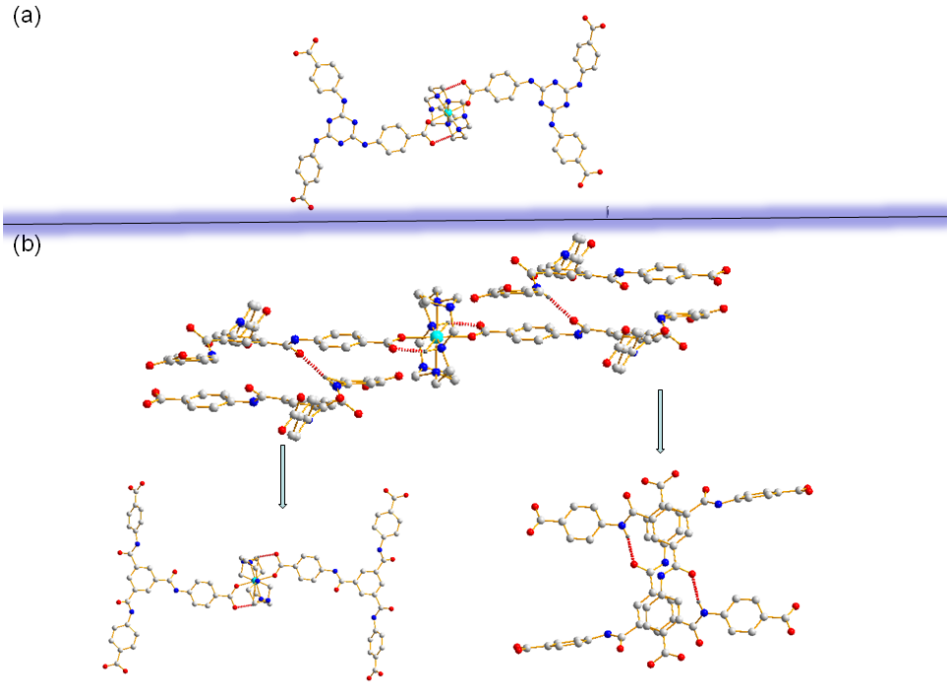


Figure S8, The hydrogen bonding (red dash line) interactions observed in **2**(a) and **3**(b).

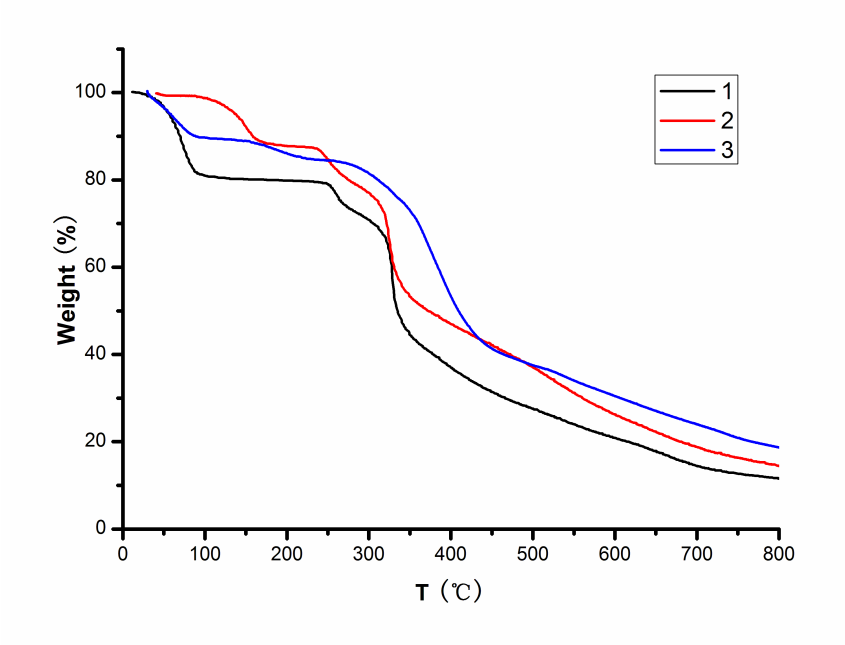
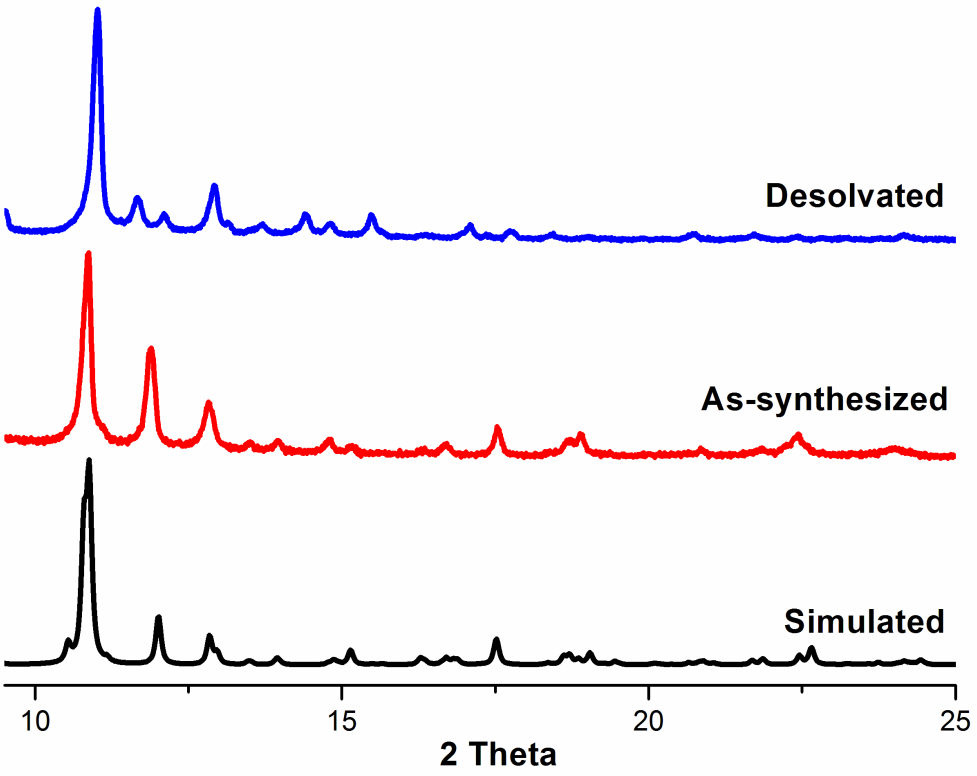
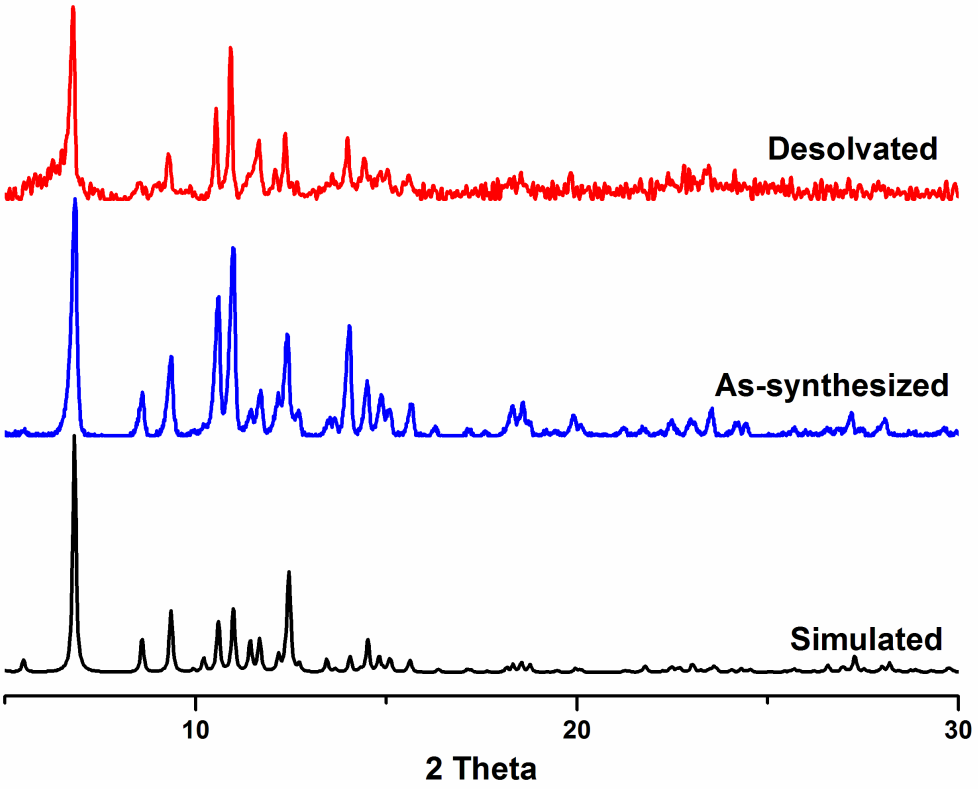


Figure S9, TGA of compounds 1-3.



(a)



(b)

Figure S10, The powder XRD patterns of compounds **2** (a) and **3** (b).

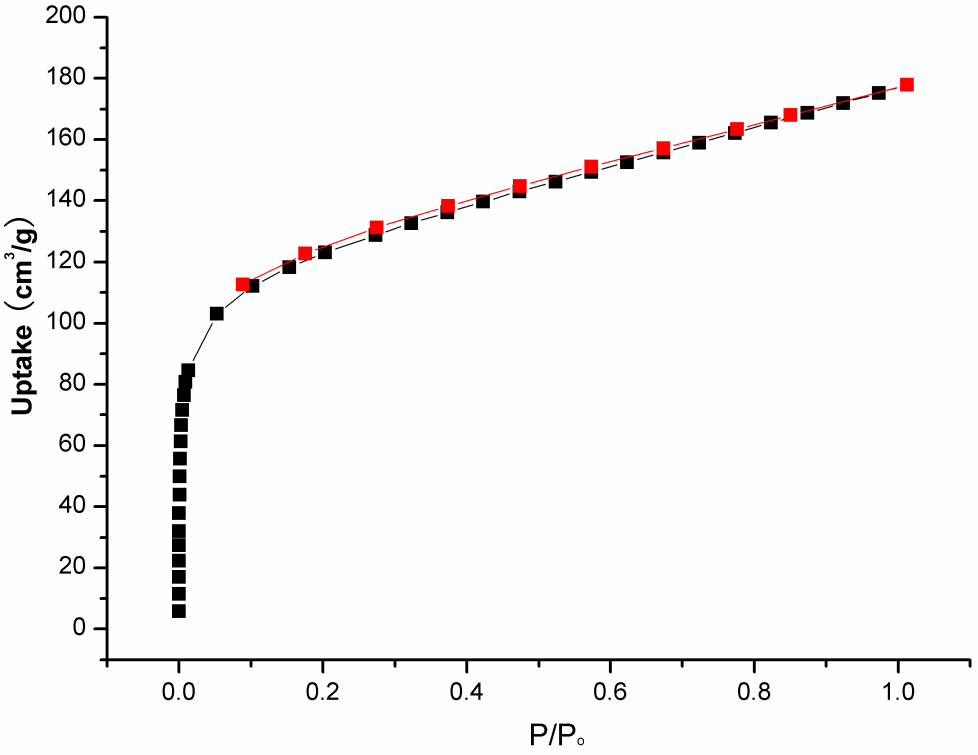


Figure S11, Gas sorption curves of CO_2 for **3** at 195K.

Calculation of sorption heat for CO_2 uptake using Virial 2 model

$$lnP = lnN + 1/T\sum_{i=0}^{m} a_i N^i + \sum_{i=0}^{n} b_i N^i \qquad Qst = -R\sum_{i=0}^{m} a_i N^i$$

The above virial expression was used to fit the combined isotherm data for **3** at 273 and 293 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. Qst is the coverage-dependent enthalpy of adsorption and R is the universal gas constant.

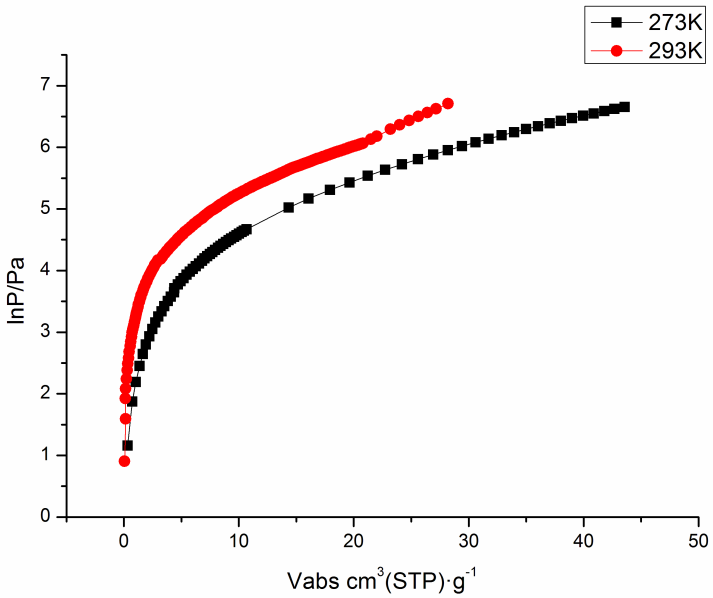


Figure S12, CO_2 adsorption isotherms for **3** with fitting by Virial 2 model. Fitting results: a0 = -4636.47999, a1 = 298.18290, a2 = -3.57734, a3 = -0.41588, a4 = 0.01072, a5 = -9.76186976433046E-5, b0 = 19.34017, b1= -1.22335, b2 = 0.03770; R^2 = 0.99693.