Supporting Information

Solvent/Temperature and Dipyridyl Ligands Induced Diverse Coordination Polymers Based on 3-(2',5'-dicarboxylphenyl)pyridine

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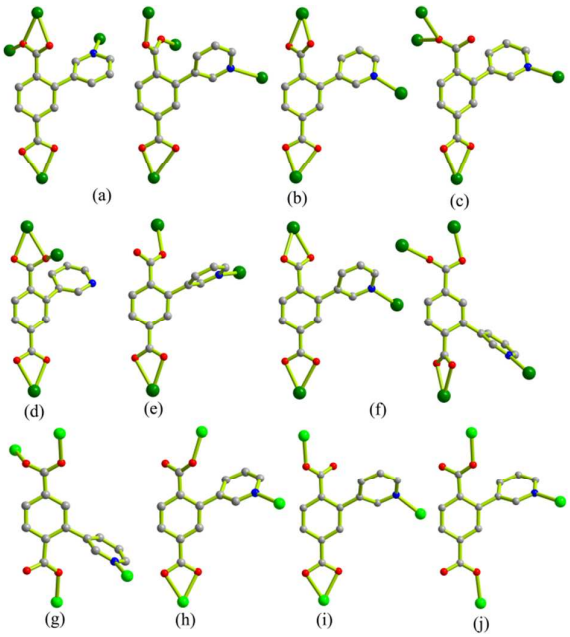


Scheme S1. The different bridging fashions of $dcpy^{2-}$ in **1**−**11**.

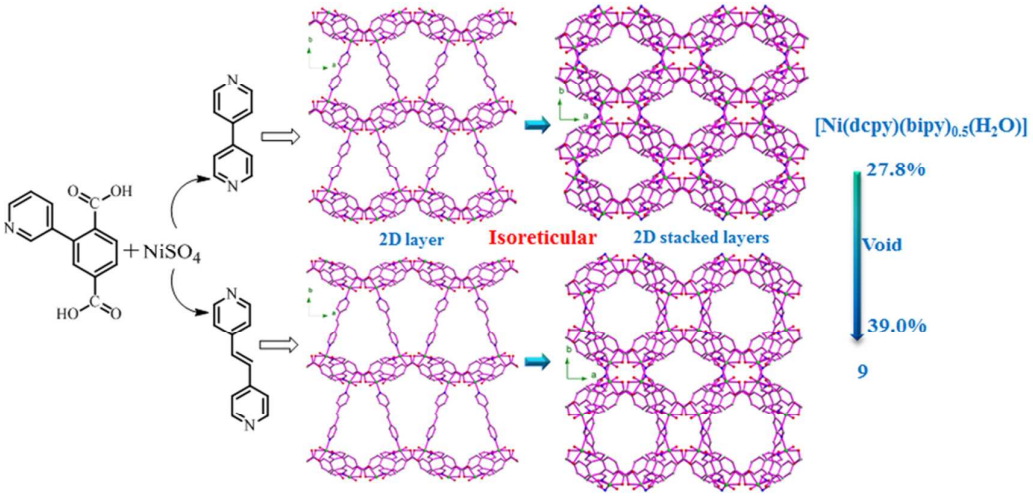
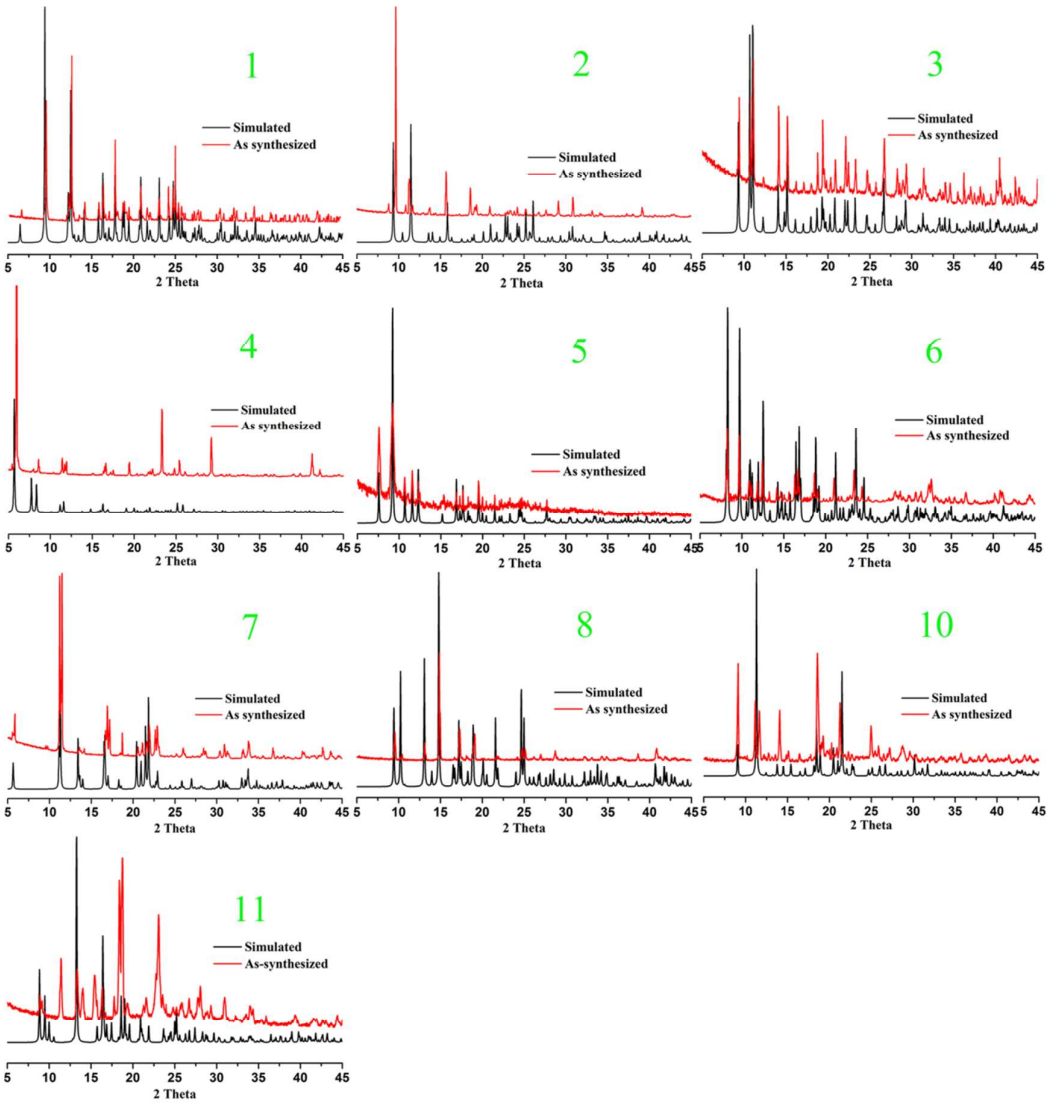
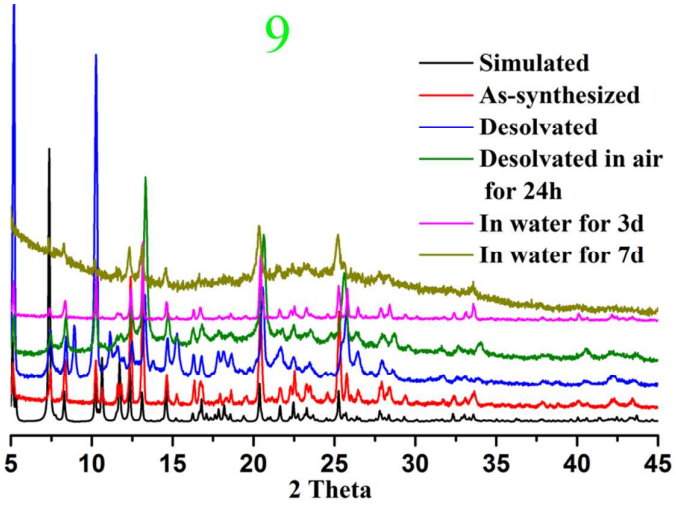


Figure S1. The structures of **9** and $[Ni(dcpy)(bipy)_{0.5}(H_2O)]$, and their void volume.

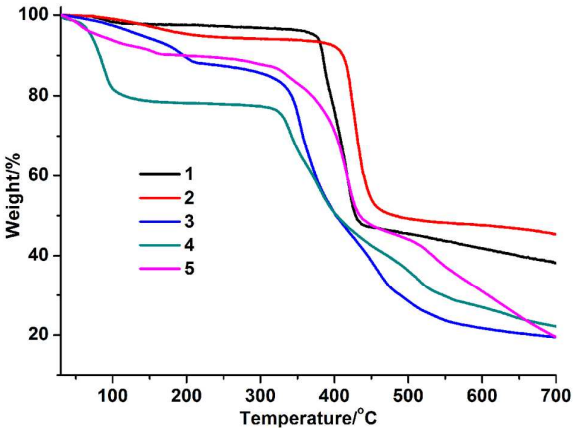

1
Simulated
As synthesized
2 Theta
2
Simulated
As synthesized
2 Theta
3
Simulated
As synthesized
2 Theta
4
Simulated
As synthesized
2 Theta
5
Simulated
As synthesized
2 Theta
6
Simulated
As synthesized
2 Theta
7
Simulated
As synthesized
2 Theta
8
Simulated
As synthesized
2 Theta
10
Simulated
As synthesized
2 Theta
11
Simulated
As-synthesized
2 Theta

(a)

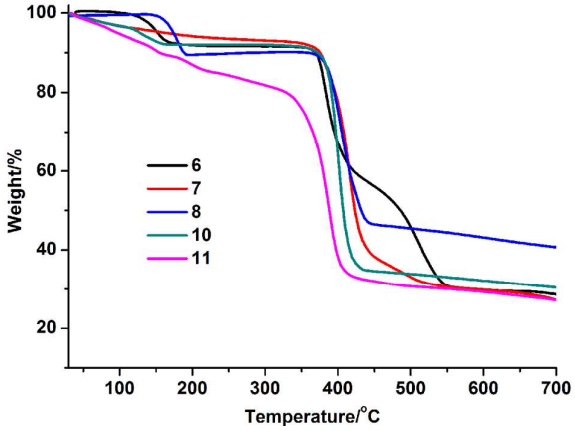

9
Simulated
As-synthesized
Desolvated
Desolvated in air
for 24h
In water for 3d
In water for 7d
2 Theta

(b)

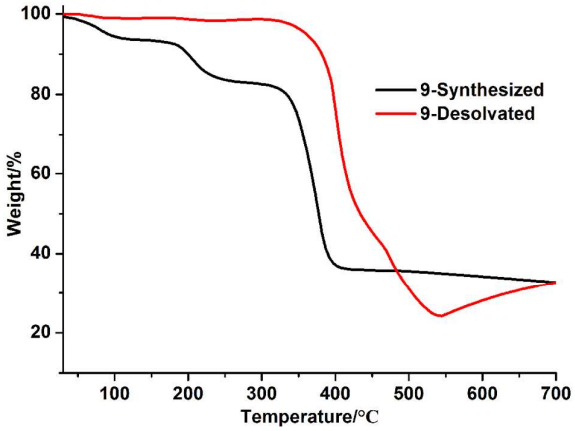
Figure S2. The PXRD patterns of **1**−**8**, **10** and **11** (Simulated: black; as-synthesized: blue) (a); PXRD patterns for **9** in different state (b).



(a)



(b)



(c)

Figure S3. TGA plots of the synthesized samples of **1**−**5** (a), **6**−**8**, **10** and **11** (b), and the synthesized and desolvated samples of **9** (c).

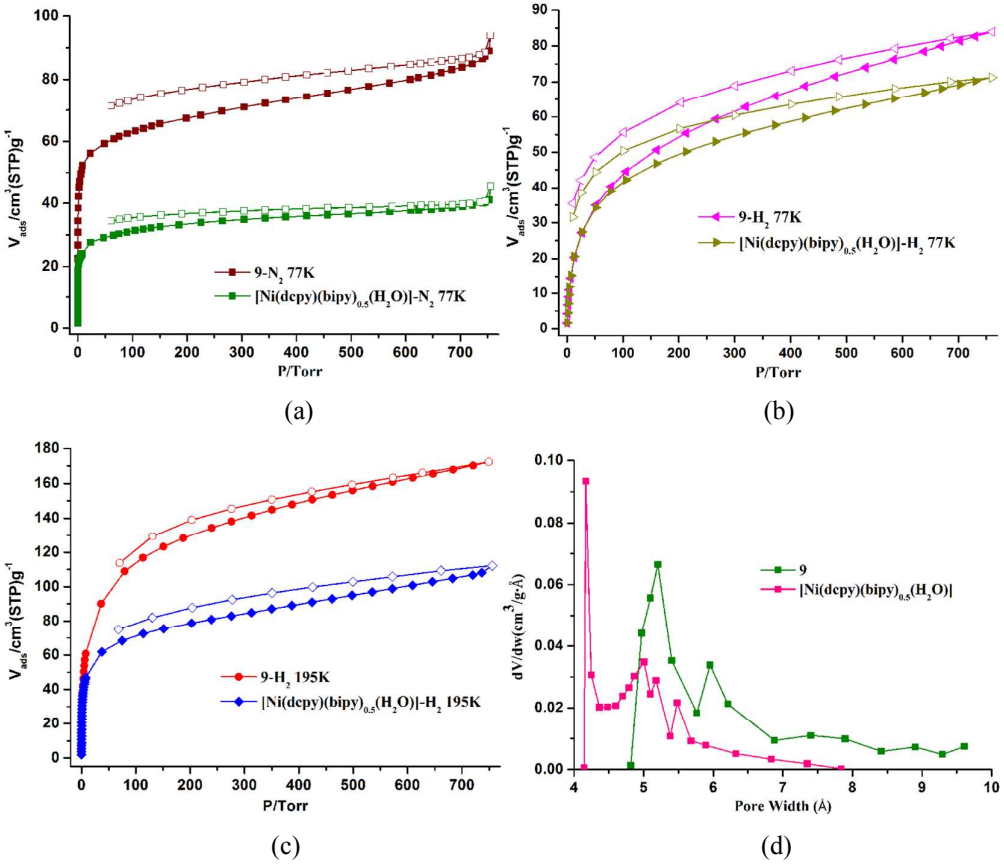


Figure S4. Gas sorption isotherms of **9** and [Ni(dcpy)(bipy)$_{0.5}$(H_2O)] for N_2 (77 K) (a), H_2 (77 K) (b) and CO_2 (195 K) (c), and differential pore volume as a function of pore width calculated from the adsorption isotherm of N_2 at 77 K using the Horvath-Kawazoe model (d).

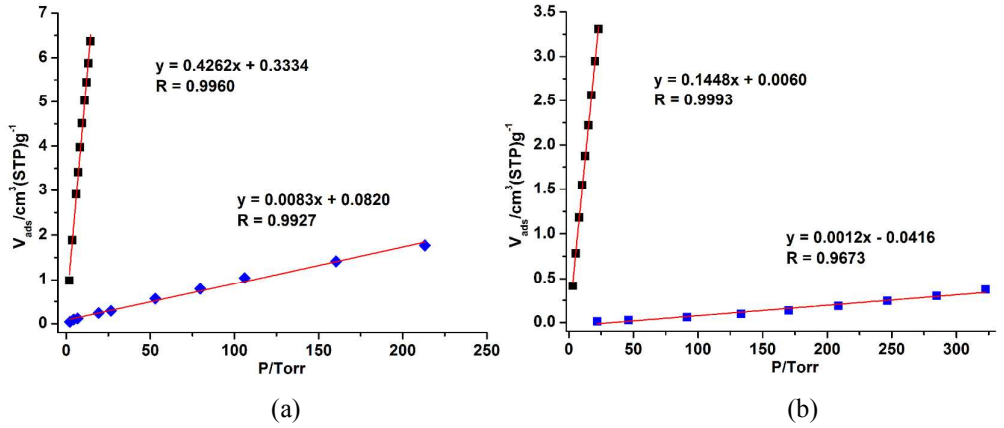


Figure S5. Initial slope calculation for CO_2 and N_2 isotherms collected at 273K (a) and 298 K (b). (CO_2: black squares; N_2: blue squares).

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 **9** at 273 and 298 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.

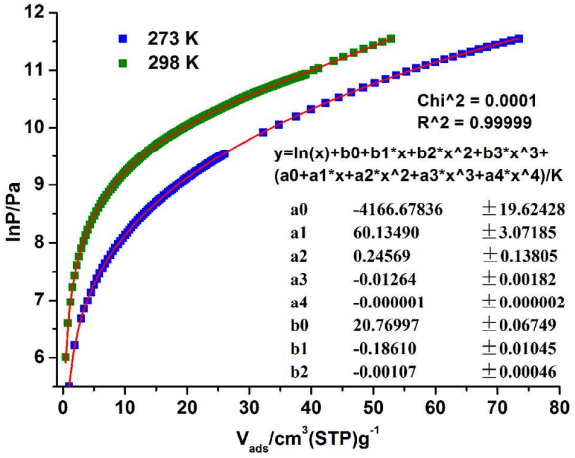
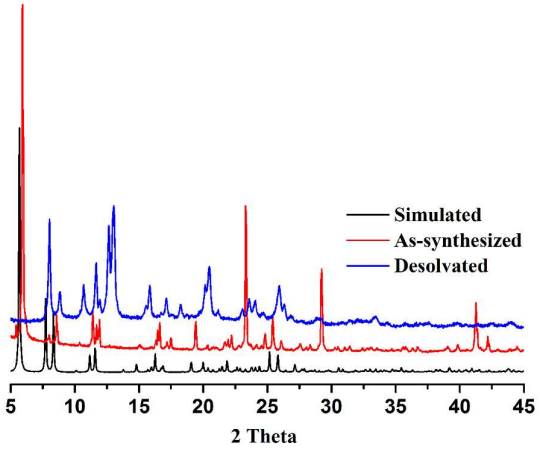
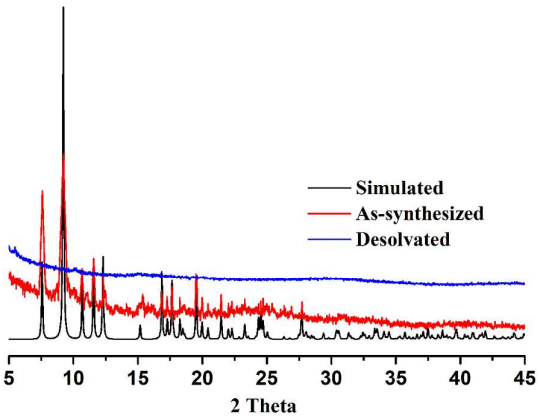


Figure S6. Virial analysis of the CO_2 sorption datas (273 and 298 K at 1 bar) for **9**.

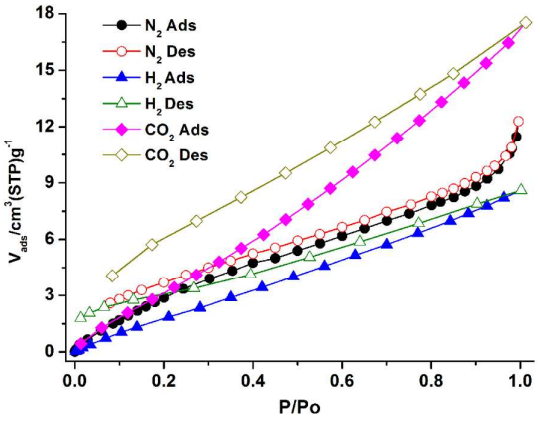


(a)

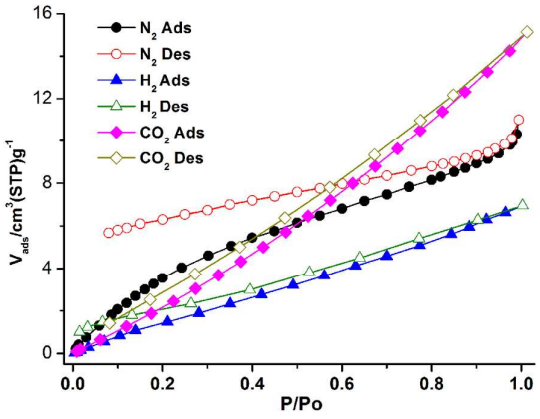


(b)

Figure S7. PXRD patterns of **4** (a) and **5** (b) simulated from the X-ray single-crystal structure, as-synthesized and desolvated samples.



(a)



(b)

Figure S8. N_2 (77 K), H_2 (77 K) and CO_2 (195 K) gas sorption isotherms of **4** (a) and **5** (b).

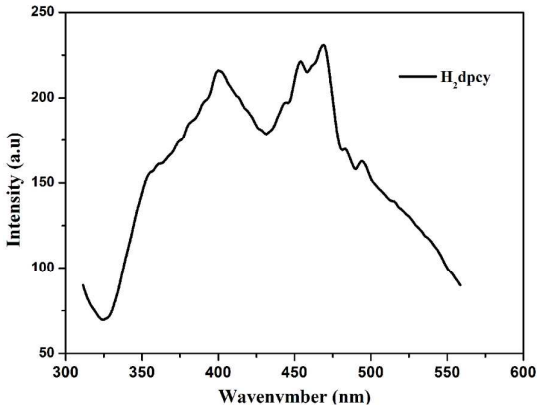


Figure S9. The emission spectra of the solid-state H_2dcpy ligand.