Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Materials

Cobalt(II) coordination polymers constructed from bis(N-pyrid-3-ylmethyl)adipoamide and polycarboxylic acids: reversible structural transformation upon proton delivery and removal

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Fig. S1. (a) Simulated and (b) experimental PXRD patterns of **1**.

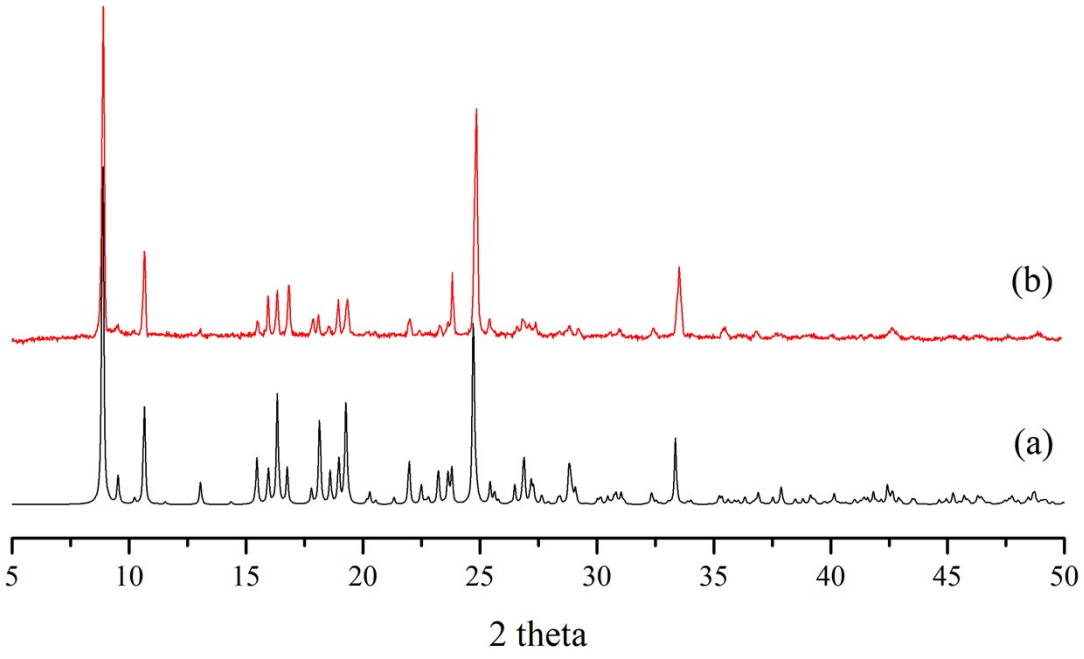

Fig. S2. (a) Simulated and (b) experimental PXRD patterns of **2**.

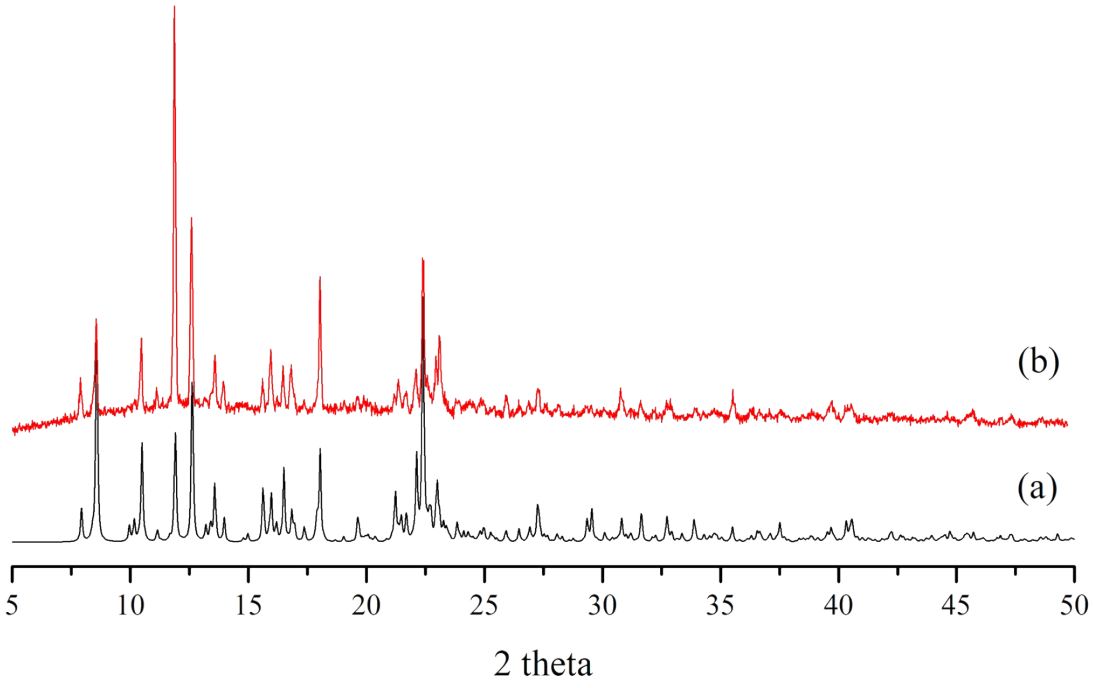

Fig. S3. (a) Simulated and (b) experimental PXRD patterns of **3**.

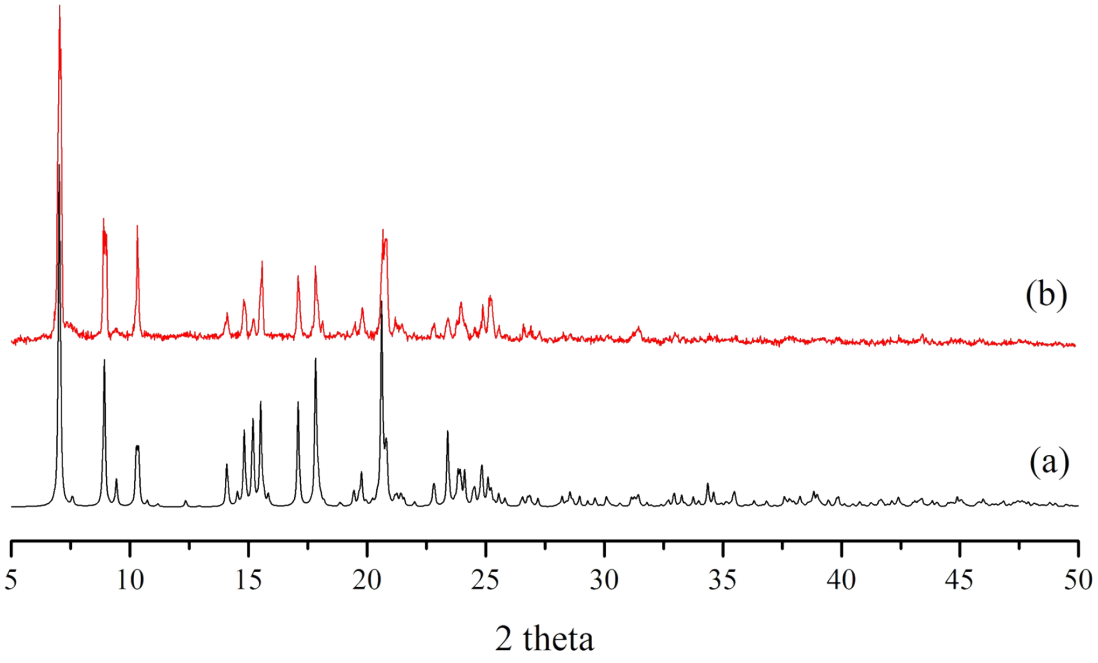

Fig. S4. (a) Simulated and (b) experimental PXRD patterns of **4**.

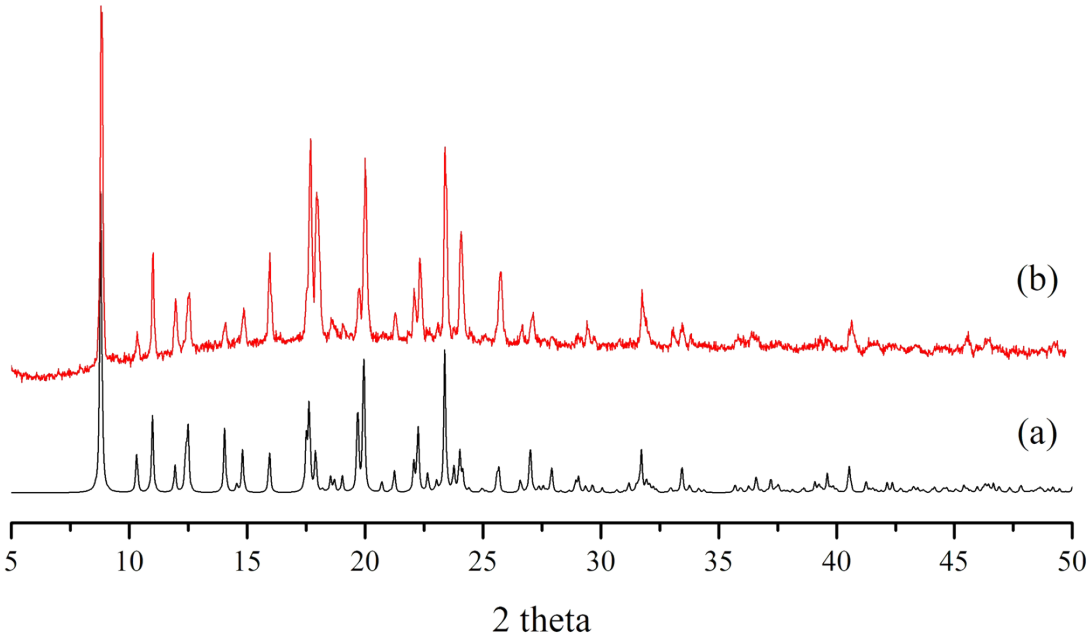

Table S1. H---O distances (Å) of hydrogen bonds with angles (°) in parenthesis for **1** – **4**.

Complex	**1**	**2**	**3**	**4**
[a]N-H---O	2.23 (175)	2.48 (138)	2.16 (175)	2.01 (176)
			2.40 (141)	
[b]N-H---O		2.10 (151)		
		2.07 (156)		
[c]N-H---O				2.41 (112)
				2.56 (158)
[d]N-H---O				2.29 (158)
[e]O-H---O	2.38 (170)	1.90 (147)	1.83 (151)	
		1.82 (162)	2.43 (123)	
		2.00 (130)	1.79 (165)	
[f]O-H---O	2.02 (177)	1.98 (156)	1.98 (177)	
		2.00 (166)		
[g]O-H---O	2.21 (152)	1.85 (173)		2.56 (157)
	2.66 (122)	2.02 (165)		
[h]O-H---O	1.92 (171)	1.97 (161)		1.88 (162)
		2.28 (160)		
[i]O-H---O	1.80 (165)			
[j]O-H---O		1.87 (157)		
		2.16 (129)		
		1.96 (143)		
[k]O-H---O		2.09 (174)		
[l]O-H---O		2.44 (131)		
		1.69 (169)		

a from the amine hydrogen atoms of **L** to the carboxylate oxygen atoms;

b from the amine hydrogen atoms of **L** to the cocrystallized water oxygen atoms;

c from the amine hydrogen atoms of 5-NH_2-IPA^{2-} to the carboxylate oxygen atoms;

d from the amine hydrogen atoms of 5-NH_2-IPA^{2-} to the cocrystallized water oxygen atoms;

e from the coordinated water molecules to the carboxylate oxygen atoms

f from the coordinated water molecules to the amide oxygen atoms

g from the cocrystallized water molecules to the carboxylate oxygen atoms

h from the cocrystallized water molecules to the amide oxygen atoms

i from the carboxylate oxygen atoms to the cocrystallized water molecules

j from the coordinated water molecules to the cocrystallized water molecules

k from the cocrystallized water molecules to the coordinated water molecules

l from the cocrystallized water molecules to the cocrystallized water molecules

Fig. S5. Hydrogen bonds of complex **1**.

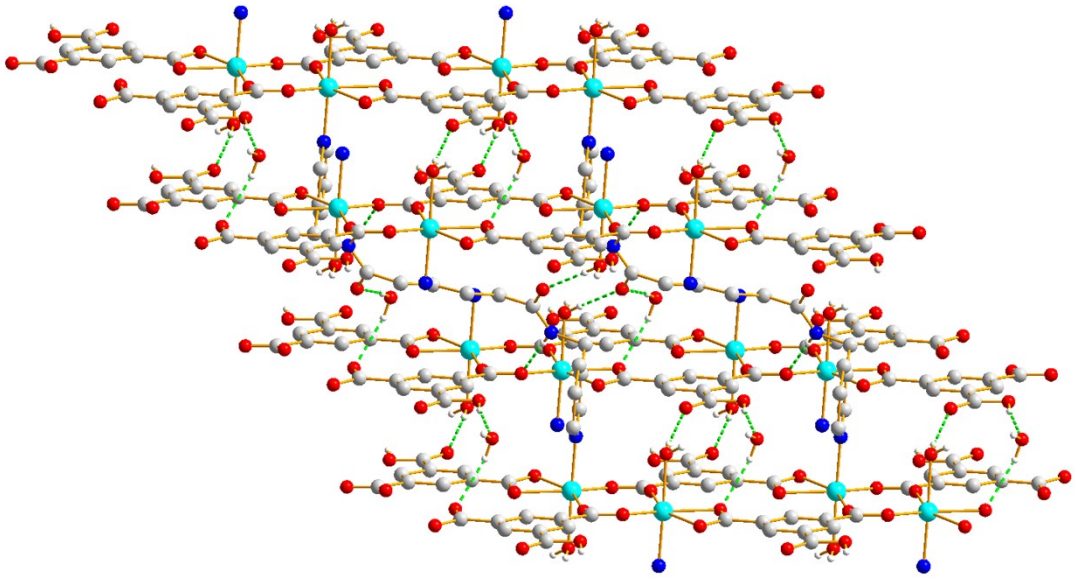

Fig. S6. Hydrogen bonds of complex **2**.

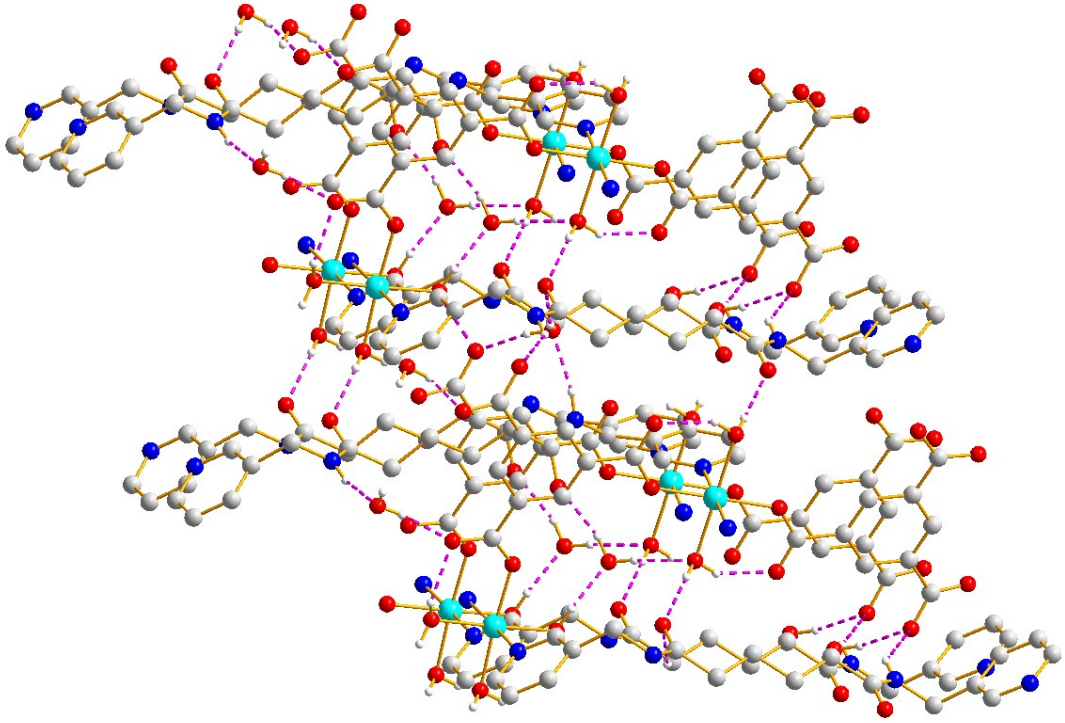

Fig. S7. Hydrogen bonds of complex **3**.

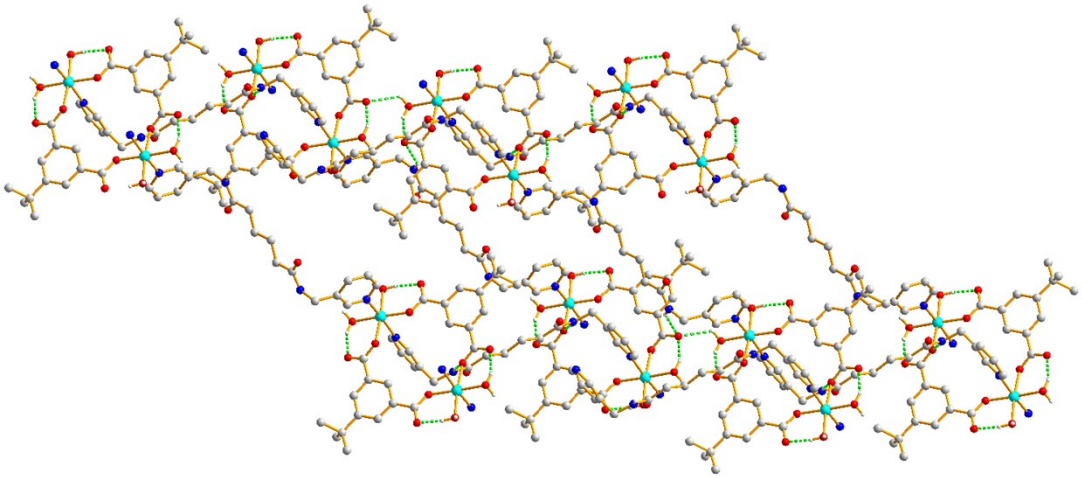

Fig. S8. Hydrogen bonds of complex **4**.

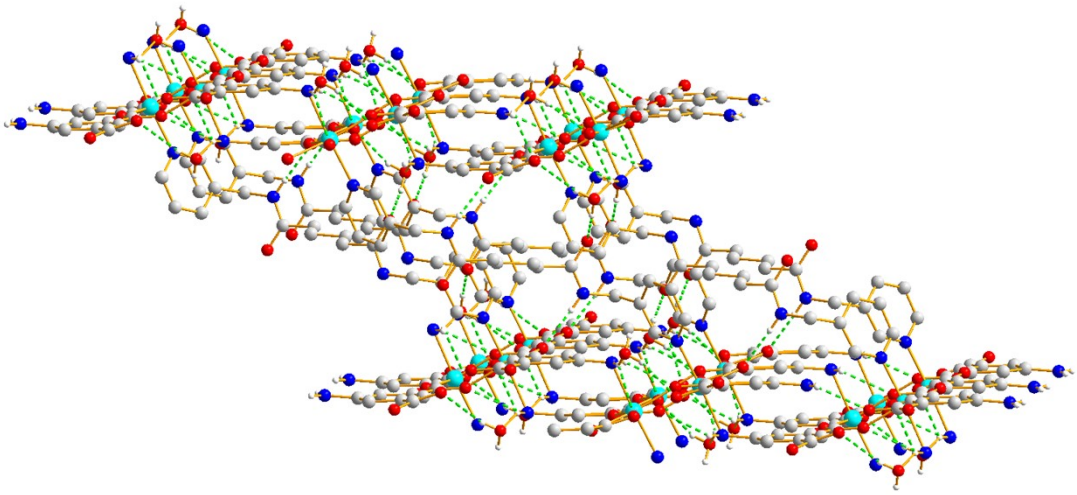

Fig. S9. The high resolution XPS spectra of Co 2p regions of (a) $Co(CH_3COO)_2 \cdot 4H_2O$, (b) complex **1** and (c) complex **2**.

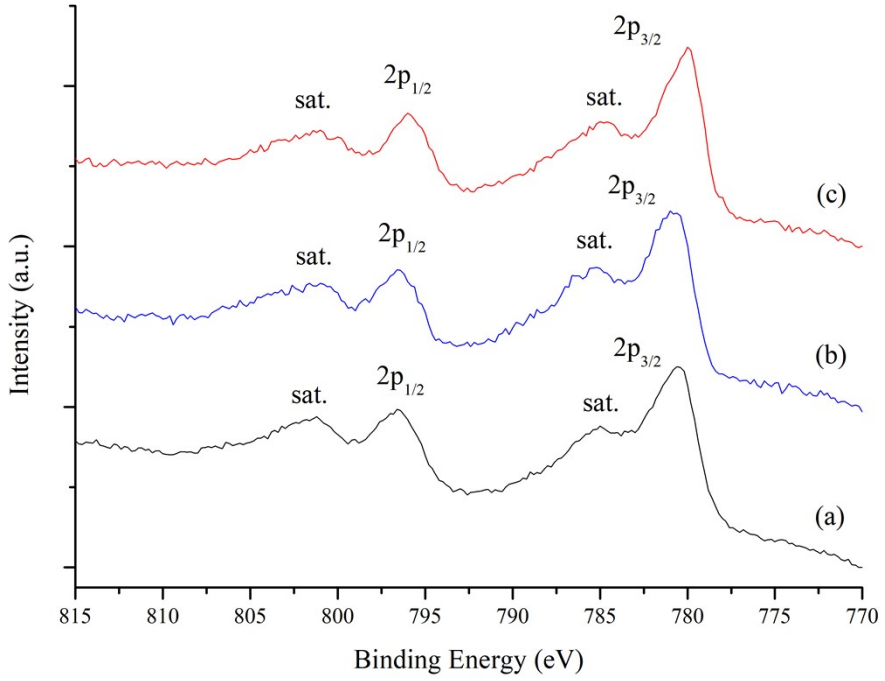

Table S2. Thermal properties of complexes **1** - **4.**

Complex	Weight loss of solvent ^{o}C (calc/found), %	Weight loss of ligand ^{o}C (calc/found), %
1	2 H_2O 130 ~ 175 (7.92/7.45)	0.5 **L** + 1,3,5-$HBTC^{2-}$ 275 - 740 (79.57/79.81)
2	8 H_2O ~ 120 (15.51/15.31)	1.5 **L** + 1,3,5-BTC^{3-} 250 - 600 (74.90/73.25)
3	2 H_2O 105 ~ 190 (5.61/5.56)	**L** + 5-tert-IPA^{2-} 275 - 695 (84.86/84.68)
4	H_2O ~ 200 (4.29/2.56)	**L** + 5-NH_2-IPA^{2-} 380 - 700 (81.65/82.58)

Fig. S10. The TGA curve for complex **1**.

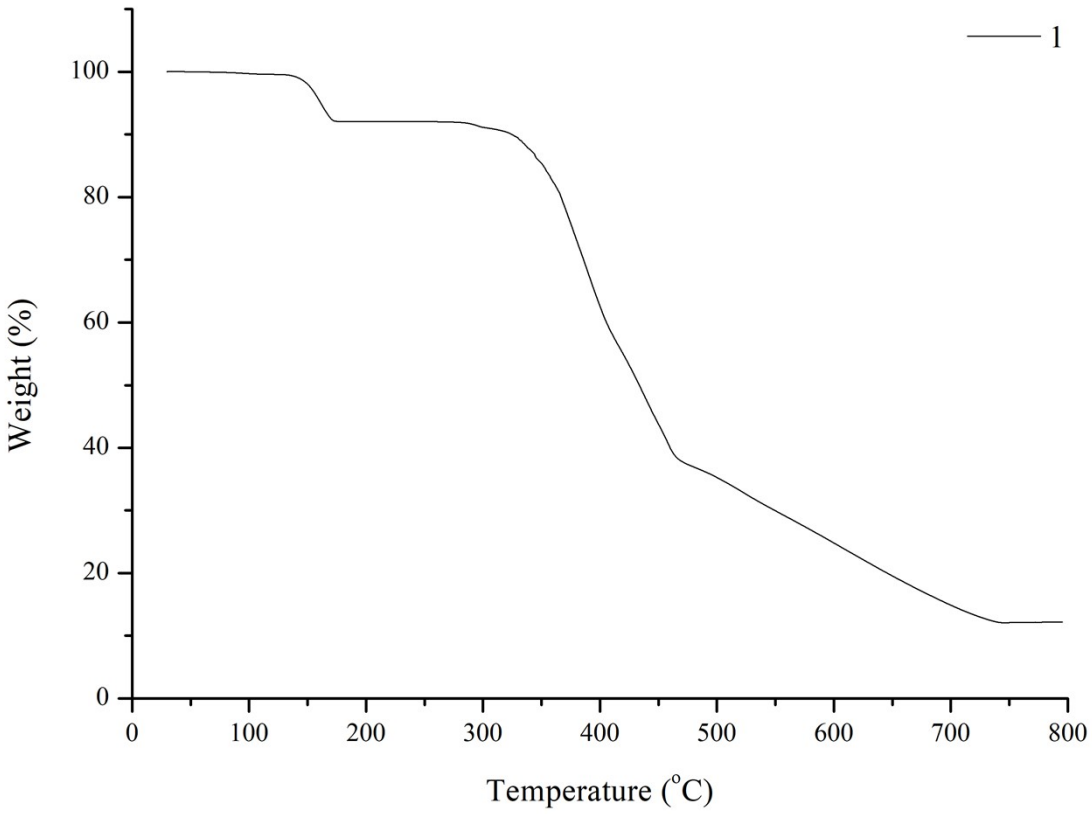

Fig. S11. The TGA curve for complex **2**.

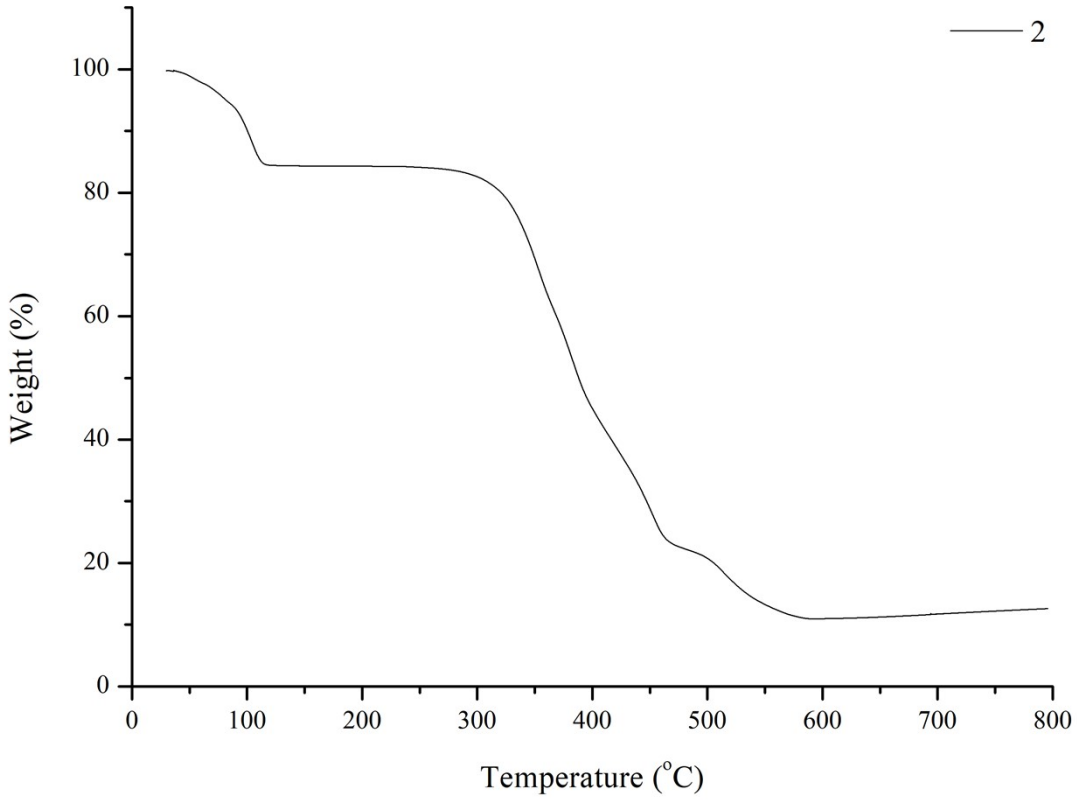

Fig. S12. The TGA curve for complex **3**.

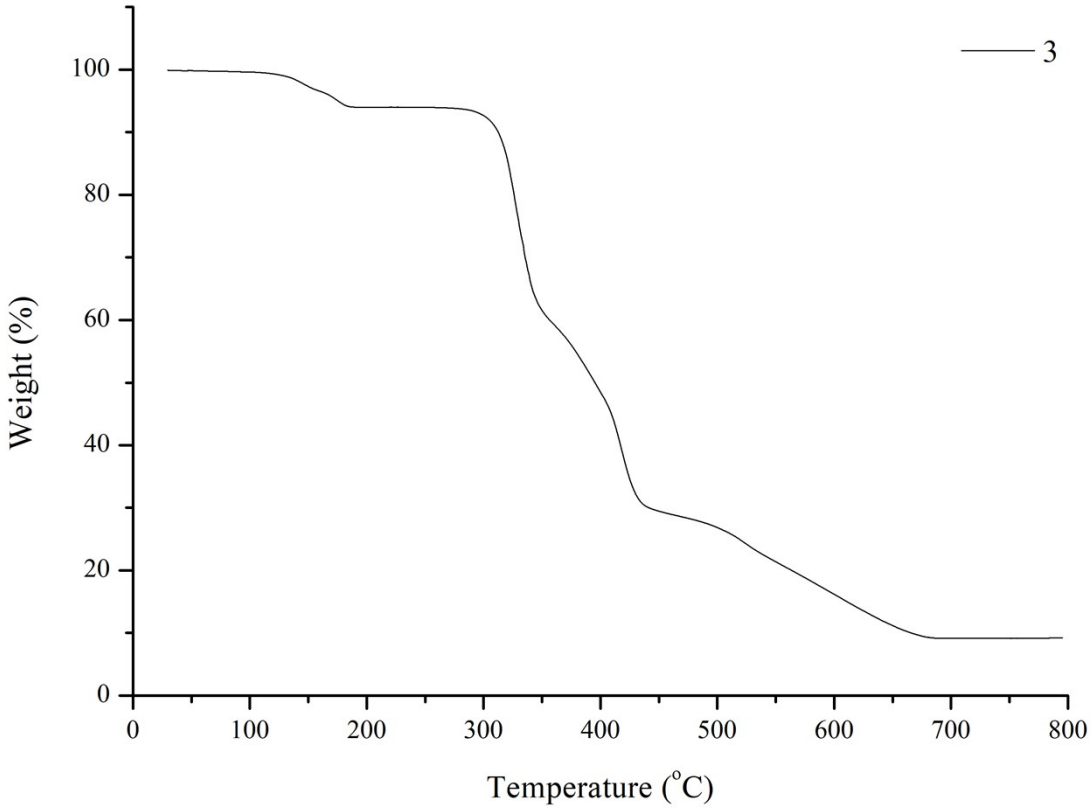

Fig. S13. The TGA curve for complex **4**.

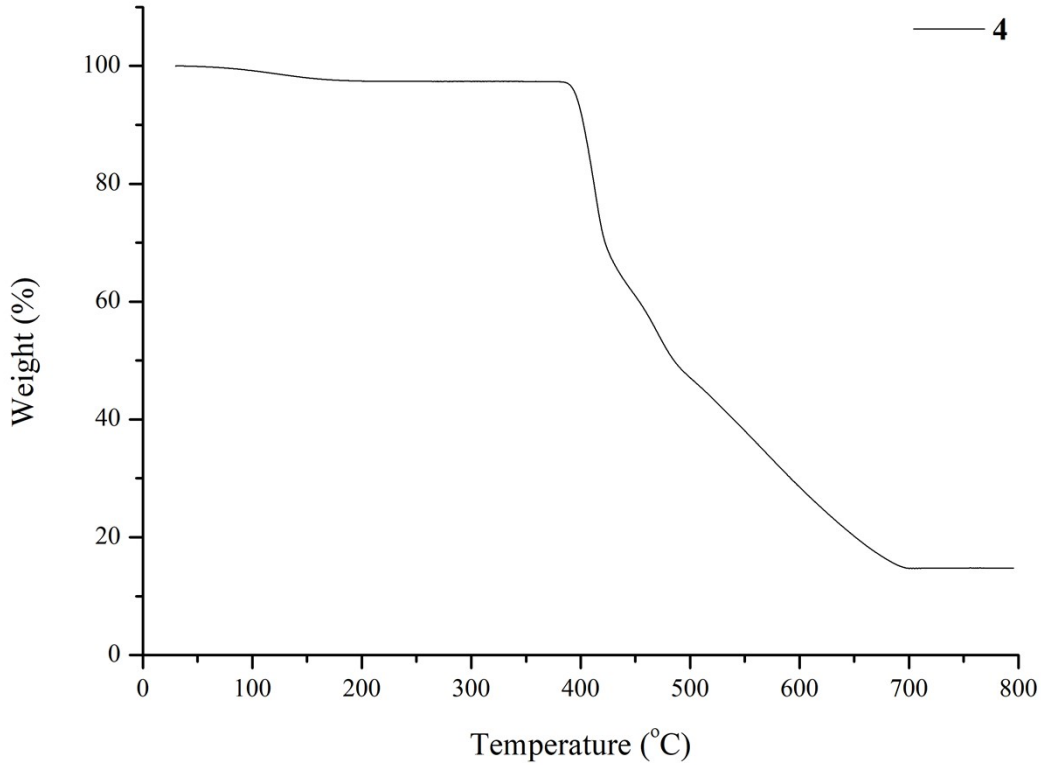

Fig. S14. PXRD patterns of complex **1** immersed in aqueous solutions with different pH values.

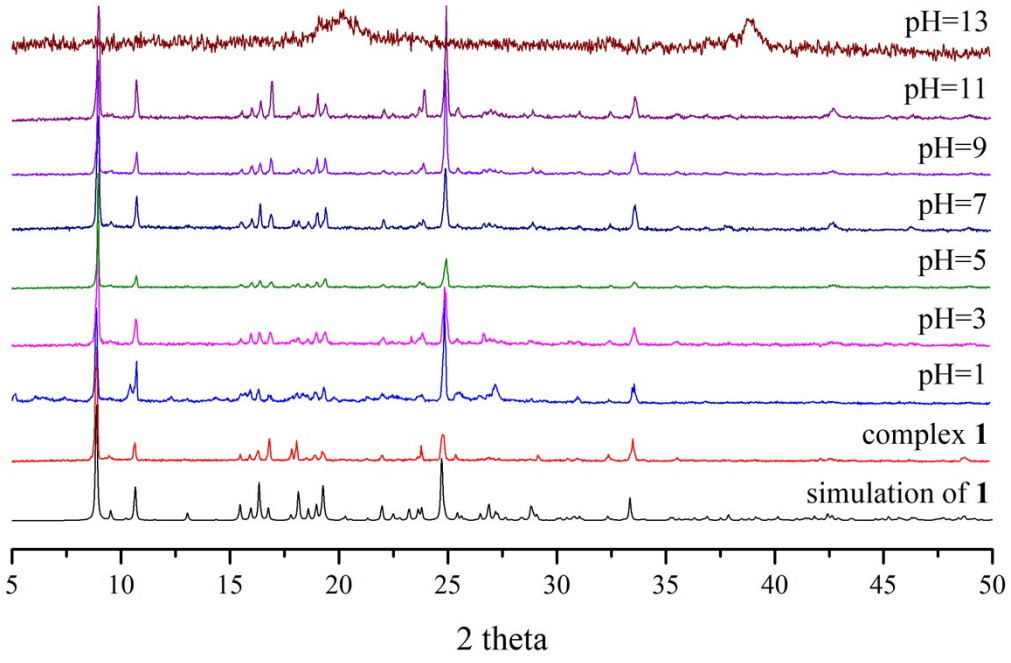

Fig. S15. PXRD patterns of complex **2** immersed in aqueous solutions with different pH values.

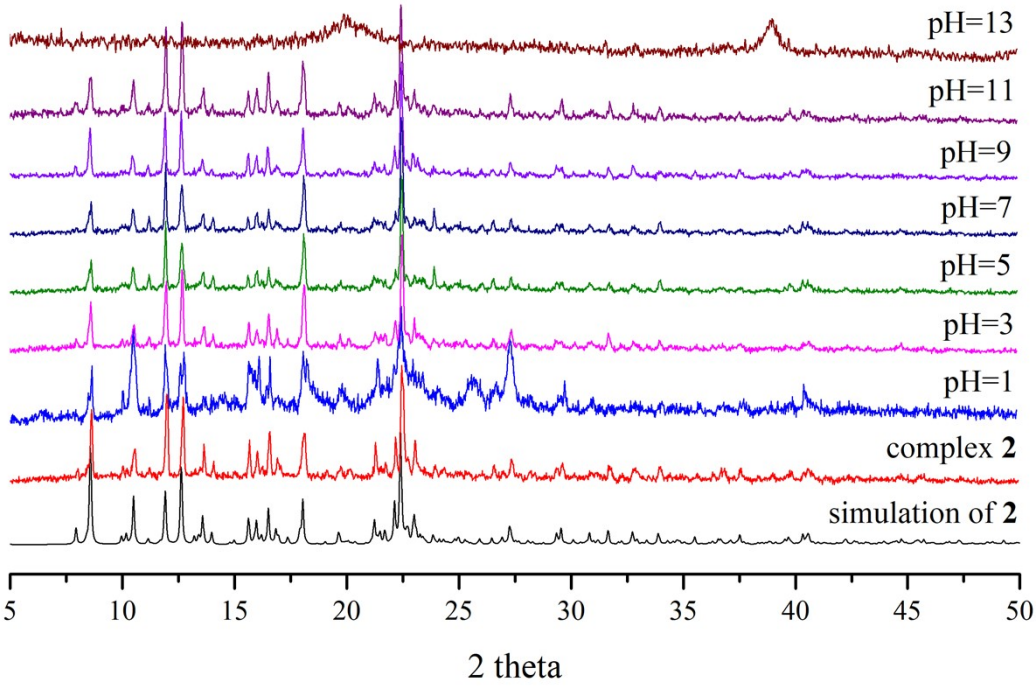

Fig. S16. PXRD patterns of complex **1**. (a) simulation, (b) as-synthesized and (c) heated at 175 ℃ for 1 h.

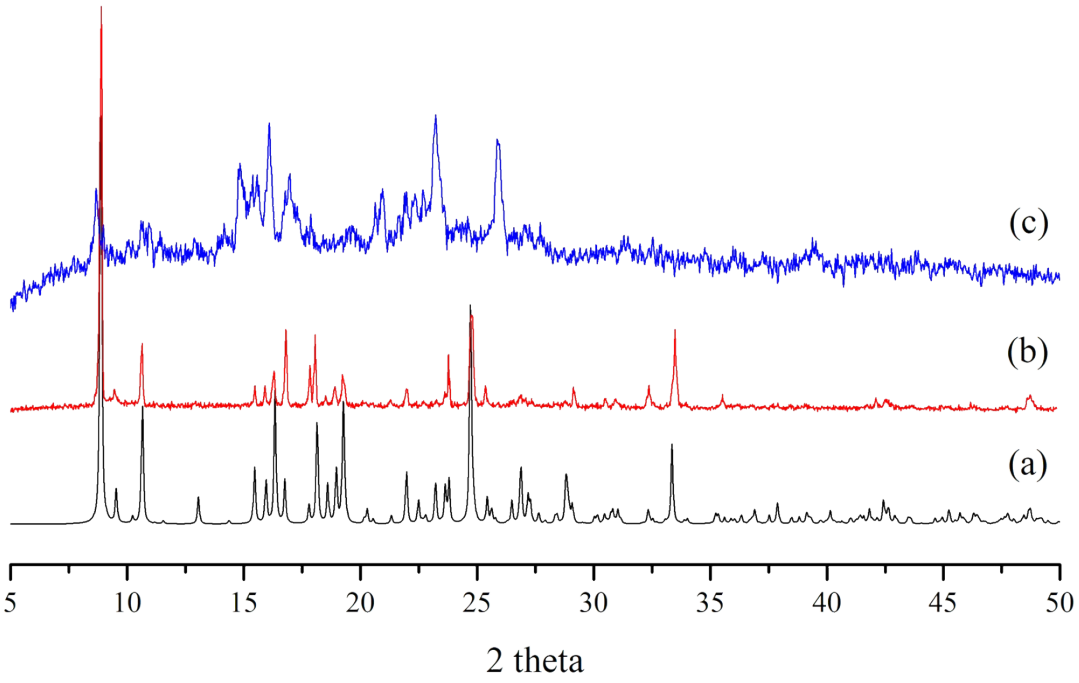

Fig. S17. PXRD patterns of complex **2**. (a) simulation, (b) as-synthesized and (c) heated at 120 ℃ for 1 h.

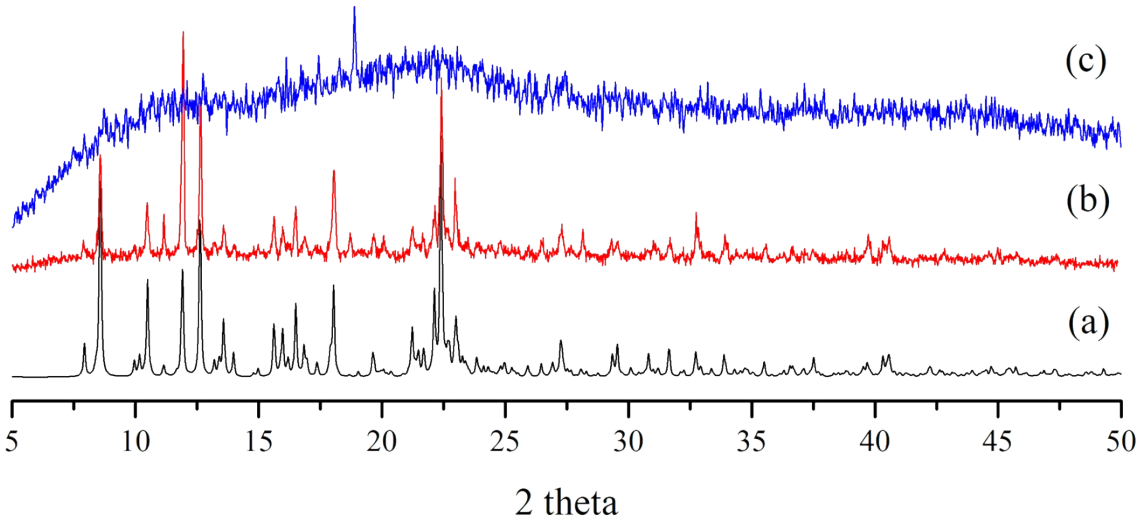

Fig. S18. PXRD patterns of complex **1**. (a) simulation, (b) as-synthesized, (c) heated at 175 ℃ for 1 h and then immersed in (d) water, (e) MeOH, (f) EtOH, (g) THF and (h) DMF.

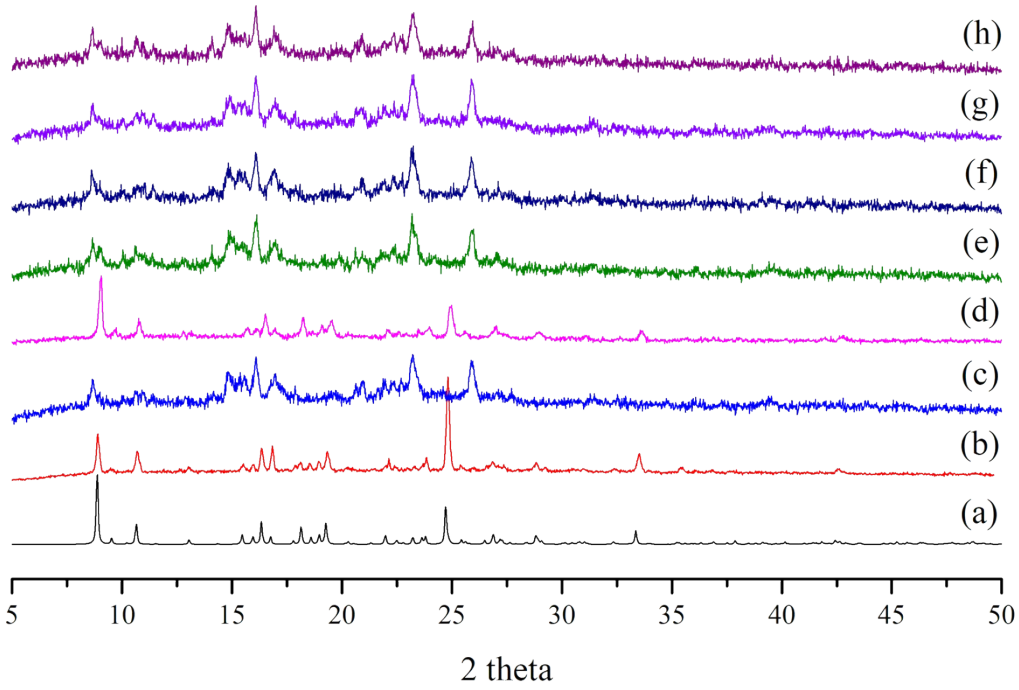

Fig. S19. PXRD patterns of complex **2**. (a) simulation, (b) as-synthesized, (c) heated at 120 ℃ for 1 h and then immersed in (d) water, (e) MeOH, (f) EtOH, (g) THF and (h) DMF.

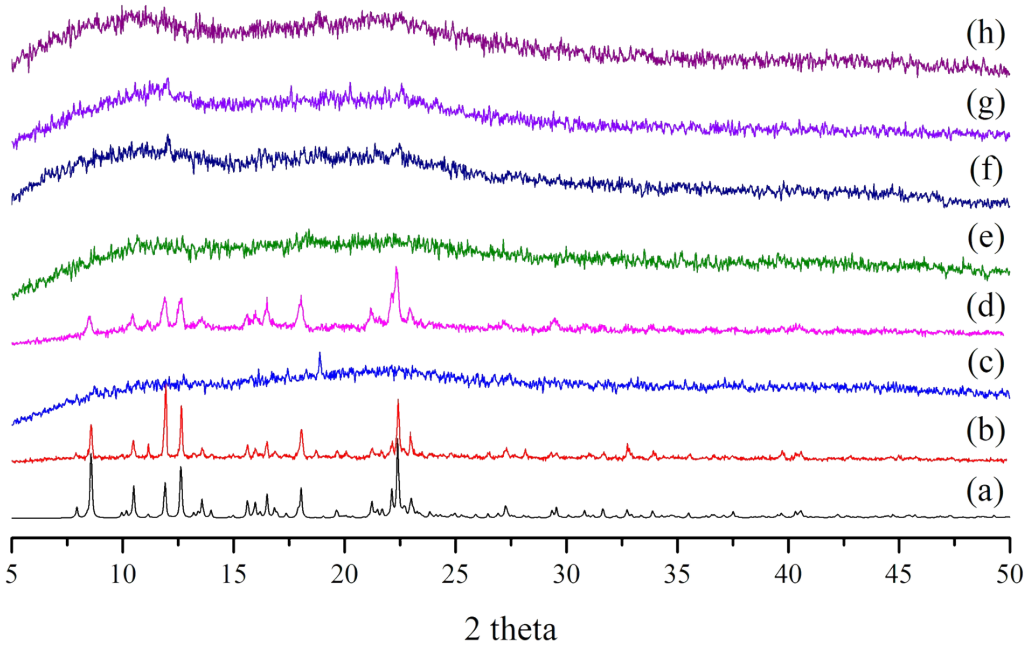

Fig. S20. PXRD patterns of complex **1** immersed in a variety of organic solvents.

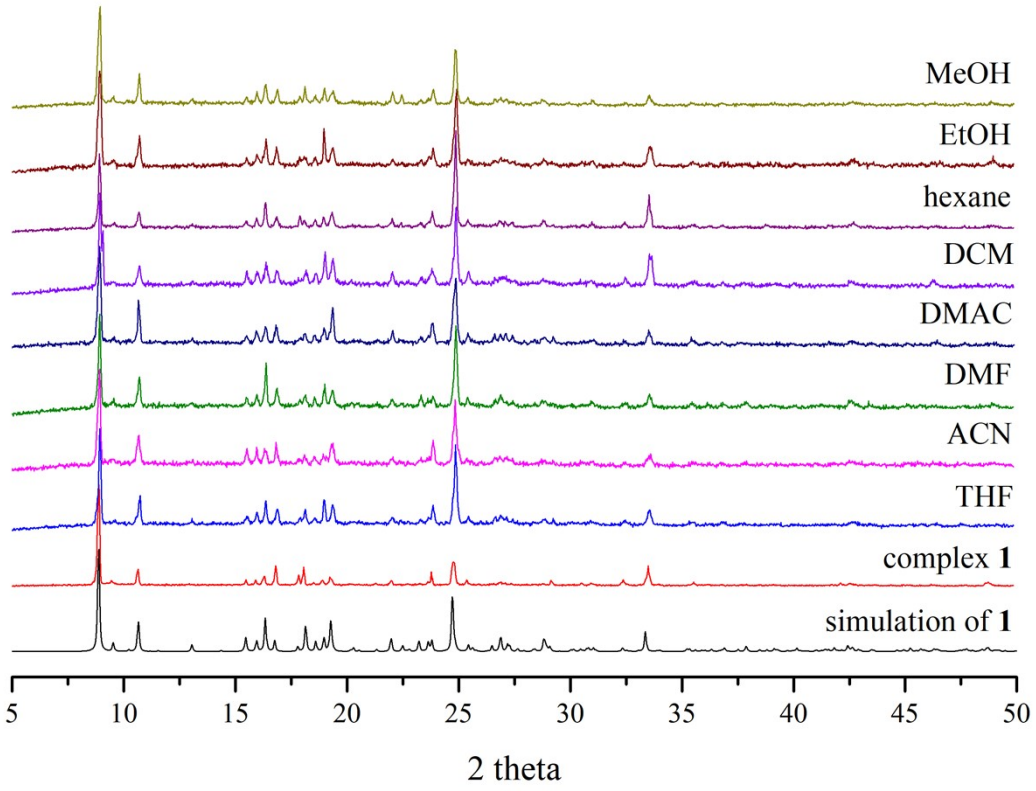

Fig. S21. PXRD patterns of complex **2** immersed in a variety of organic solvents.

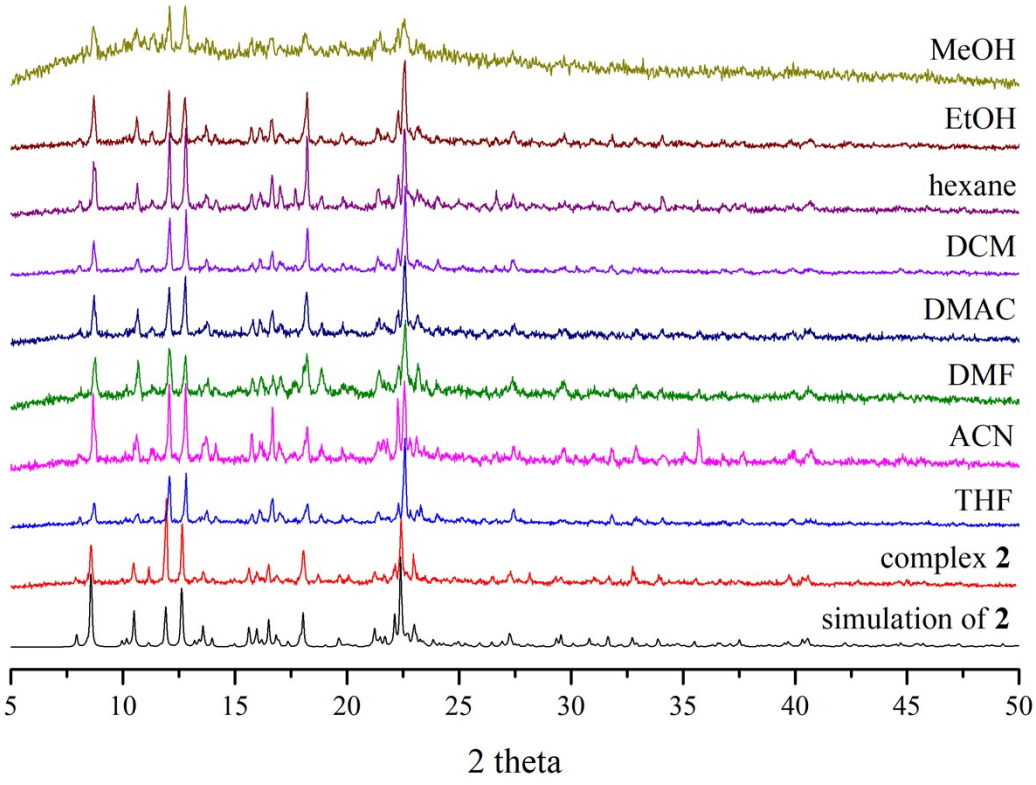

Fig. S22. PXRD patterns for **2**. (a) simulation, (b) as-synthesized, (c) heated in water at 120 ℃ for 2 days and (d) simulation of **1**.

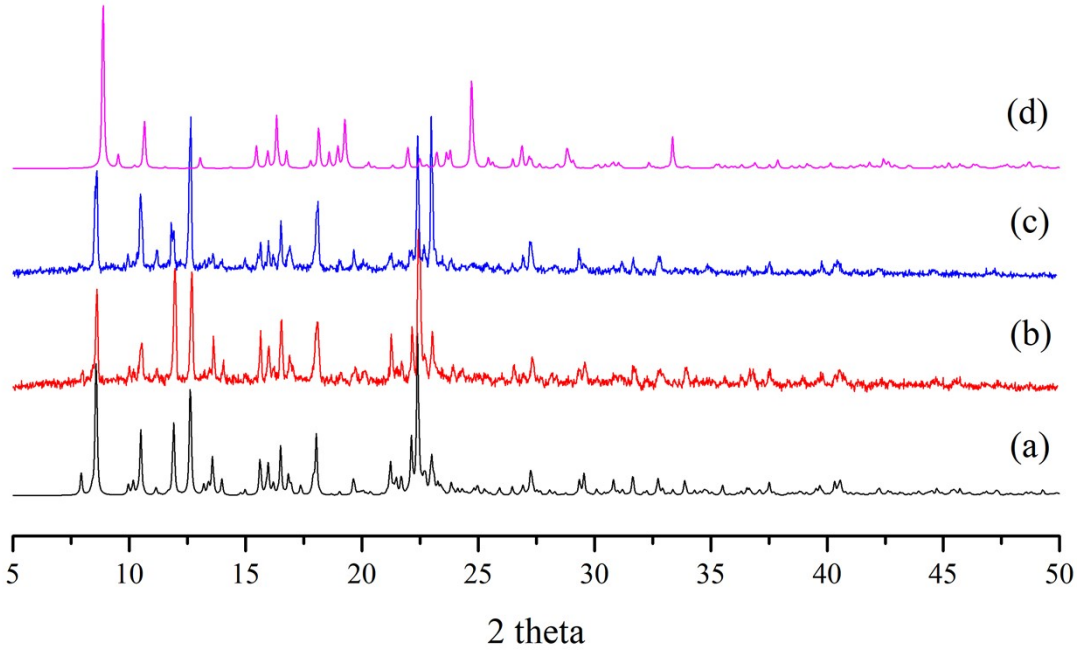

Fig. S23. PXRD patterns of **2**. (a) simulation, (b) as-synthesized and heated at 120 ℃ for 2 days in HCl solutions with pH values of (c) 1, (d) 3 and (e) 5 and (f) simulation of **1**.