Electronic supplementary information

Seven novel coordination polymers constructed by rigid 4-(4-carboxyphenyl)-terpyridine ligands: synthesis, structural diversity, luminescence and magnetic property

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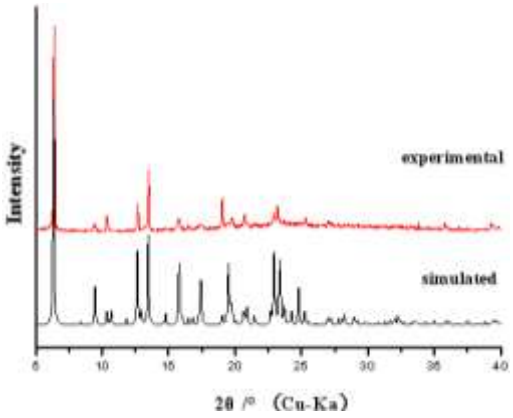
Table S1. Selected bond distances (Å) and angles (°) for complexes 1–7[a]

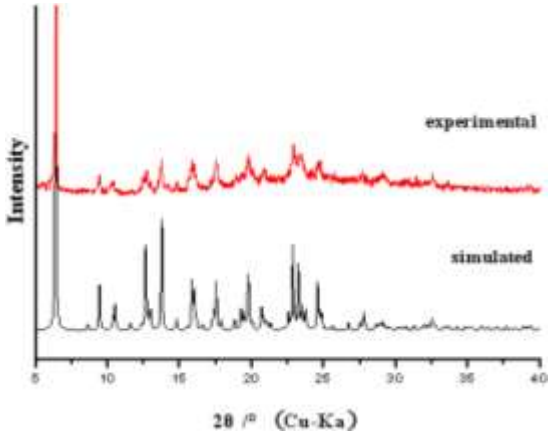
		1			
Mn(1)–O(1)#2	2.115(2)	Mn(1)–O(2)#1	2.066(3)	Mn(1)–N(1)	2.298(3)
Mn(1)–O(3)#3	2.189(2)	Mn(1)–O(4)#3	2.426(3)	Mn(1)–N(4)	2.238(3)
O(2)#1–Mn(1)–O(3)#3	142.78(10)	O(1)#2–Mn(1)–O(4)#3	151.75(10)	N(4)–Mn(1)–N(1)	174.25(11)
O(1)#2–Mn(1)–N(1)	89.75(11)	O(1)#2–Mn(1)–O(3)#3	96.65(10)	N(4)–Mn(1)–O(4)#3	90.49(10)
O(2)#1–Mn(1)–O(1)#2	120.22(9)	O(1)#2–Mn(1)–N(4)	86.66(10)	N(1)–Mn(1)–O(4)#3	94.78(11)
O(2)#1–Mn(1)–N(4)	90.45(11)	O(3)#3–Mn(1)–O(4)#3	55.81(9)	O(3)#3–Mn(1)–N(1)	87.79(11)
O(2)#1–Mn(1)–O(4)#3	87.87(10)	O(2)#1–Mn(1)–N(1)	87.48(11)	O(3)#3–Mn(1)–N(4)	97.07(10)
		2			
Co(1)–O(1)#3	2.126(2)	Co(1)–O(2)#3	2.318(2)	Co(1)–N(1)	2.133(2)
Co(1)–O(3)#2	2.032(2)	Co(1)–O(4)#1	1.991(2)	Co(1)–N(4)	2.173(2)
O(4)#1–Co(1)–O(1)#3	146.47(7)	O(3)#2–Co(1)–O(2)#3	154.74(7)	N(1)–Co(1)–N(4)	178.15(8)
		3			
Mn(1)–O(1)	2.076(6)	Mn(3)–O(2)	2.108(5)	Mn(2)–O(7)	2.132(4)
Mn(1)–O(3)	2.211(4)	Mn(3)–O(3)	2.312(4)	Mn(2)–O(10)	2.120(5)
Mn(1)–O(5)	2.125(5)	Mn(3)–O(6)	2.105(5)	Mn(2)–O(12)	2.009(5)
Mn(1)–O(1W)	2.233(6)	Mn(3)–O(7)	2.380(5)	Mn(2)–N(2)	2.225(6)
Mn(1)–N(14)	2.307(6)	Mn(3)–O(9)	2.138(5)	Mn(2)–N(8)	2.284(6)
Mn(1)–N(17)	2.281(5)	Mn(3)–O(11)	2.164(6)		
O(5)–Mn(1)–O(1W)	171.1(2)	O(6)–Mn(3)–O(9)	174.4(2)	O(7)–Mn(2)–N(8)	175.4(2)
O(1)–Mn(1)–N(17)	164.8(2)	O(2)–Mn(3)–O(11)	170.9(2)	N(2)–Mn(2)–N(8)	86.6(2)
O(3)–Mn(1)–N(14)	174.09(18)	O(3)–Mn(3)–O(7)	175.21(15)	O(10)–Mn(2)–O(12)	137.4(2)
		4			
Co(1)–O(1)	2.035(5)	Co(1)–N(3)#1	2.110(5)	Co(1)–O(3)#2	2.143(4)
Co(1)–N(1)	2.112(5)	Co(1)–O(4)#2	2.199(4)	Co(1)–O(1W)	2.195(4)
N(1)–Co(1)–O(3)#2	156.12(19)	N(3)#1–Co(1)–O(4)#2	152.95(18)	O(1)–Co(1)–O(1W)	176.89(18)
		5			
Zn(1)–Cl(1)	2.2174(12)	Zn(1)–N(1)	2.058(3)	Zn(1)–Cl(1)#1	2.2174(12)
Zn(2)–Cl(2)	2.2228(16)	Zn(2)–N(2)	2.062(3)	Zn(2)–Cl(2)#2	2.2228(16)
Zn(1)–N(1)#1	2.058(3)	Zn(2)–N(2)#2	2.062(3)		
N(1)–Zn(1)–Cl(1)	105.26(9)	N(1)#1–Zn(1)–N(1)	101.15(17)	N(1)#1–Zn(1)–Cl(1)	110.31(10)
N(1)–Zn(1)–Cl(1)#1	110.31(10)	N(1)#1–Zn(1)–Cl(1)#1	105.26(9)	Cl(1)–Zn(1)–Cl(1)#1	122.56(8)
N(2)–Zn(2)–N(2)#2	97.64(18)	N(2)–Zn(2)–-Cl(2)	112.20(12)	N(2)#2–Zn(2)–Cl(2)	104.08(11)
N(2)–Zn(2)–Cl(2)#2	104.08(11)	N(2)#2–Zn(2)–Cl(2)#2	112.20(12)	Cl(2)–Zn(2)–Cl(2)#2	123.71(10)

		6			
Co(1)–O(1)	2.048(2)	Co(1)–O(15)	2.083(2)	Co(1)–N(5)	2.176(2)
Co(1)–O(3)	2.053(2)	Co(1)–O(2W)	2.199(2)	Co(1)–N(6)	2.201(2)
Co(2)–O(2)	2.060(2)	Co(2)–O(2W)	2.192(2)	Co(2)–N(4)	2.183(2)
Co(2)–O(4)	2.032(2)	Co(2)–O(17)	2.096(2)	Co(2)–N(7)	2.209(2)
Co(3)–O(6)	2.078(2)	Co(3)–O(1W)	2.175(2)	Co(3)–N(3)	2.162(2)
Co(3)–O(8)	2.036(2)	Co(3)–O(14)	2.091(2)	Co(3)–N(8)	2.250(2)
Co(4)–O(5)	2.022(2)	Co(4)–O(1W)	2.165(2)	Co(4)–N(1)	2.164(2)
Co(4)–O(7)	2.077(2)	Co(4)–O(12)	2.094(2)	Co(4)–N(2)	2.238(2)
O(1)–Co(1)–O(15)	172.14(8)	O(3)–Co(1)–N(6)	175.09(8)	O(2W)–Co(1)-N(5)	173.56(7)
O(4)–Co(2)–O(17)	173.12(8)	O(2W)–Co(2)–N(4)	174.69(7)	O(2)–Co(2)–N(7)	174.12(8)
O(8)–Co(3)–O(14)	170.50(9)	O(1W)–Co(3)–N(3)	174.43(7)	O(6)–Co(3)–N(8)	173.73(7)
O(5)–Co(4)–O(12)	172.42(8)	O(1W)–Co(4)–N(1)	175.16(8)	O(7)–Co(4)–N(2)	172.95(7)
Co(1)–O(2W)–Co(2)	114.89(9)	Co(3)–O(1W)–Co(4)	114.71(9)		
		7			
Mn(1)–O(1)	2.195(3)	Mn(1)–O(3)	2.186(3)	Mn(1)–N(1)	2.319(4)
Mn(1)–O(2)	2.196(3)	Mn(1)–O(4)	2.167(3)	Mn(1)–N(2)	2.308(4)
O(1)–Mn(1)–O(4)	176.25(11)	O(2)–Mn(1)–O(3)	172.92(13)	N(1)–Mn(1)–N(2)	175.17(12)

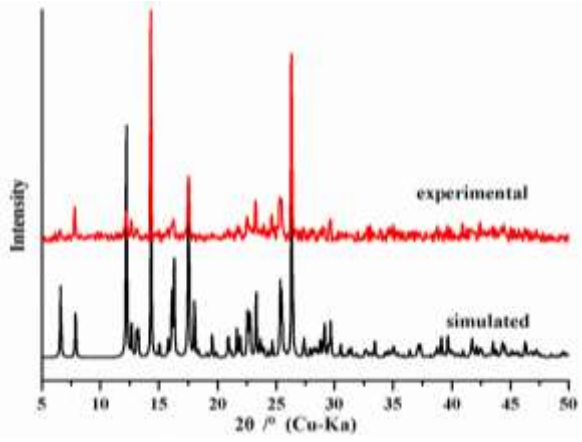
[a] Symmetry transformations used to generate equivalent atoms. For **1**: #1 –x+3/2, y–1/2, –z+3/2; #2 x–1/2, –y+1/2, z+1/2; #3 –x–1/2, y+1/2, –z+3/2. For **2**: #1 –x+3/2, y–1/2, –z+3/2; #2 x–1/2, –y+1/2, z+1/2; #3 –x–1/2, y+1/2, –z+3/2. For **4**: #1 x–1, y, z–1; #2 –x+1/2, y+1/2, –z+1/2. For **5**: #1 –x+1/2, –y+1, z. #2 –x+1/2, –y, z.



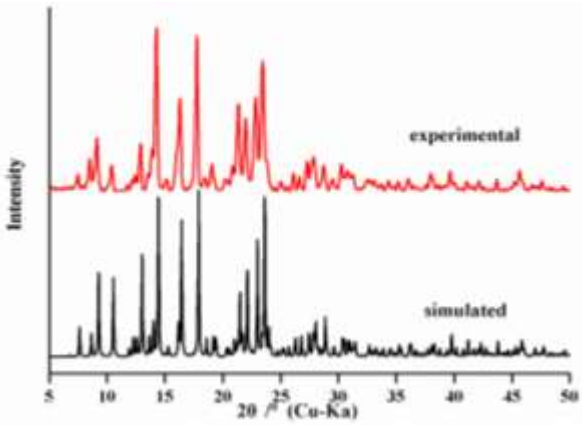
$[Mn(4\text{-cptpy})_2]_n$ (**1**)



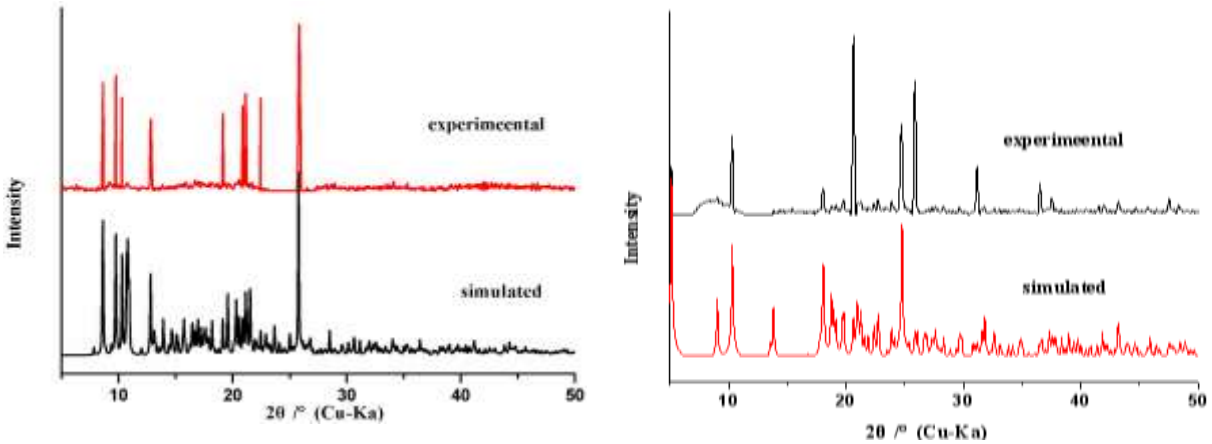
$[Co(4\text{-cptpy})_2]_n$ (**2**)



$[Co(4\text{-cptpy})(HCOO)(H_2O)]_n \cdot n$DMF (**4**)



$[Zn_2(4\text{-Hcptpy})_2Cl_4]_n \cdot 2nC_2H_5OH \cdot nH_2O$ (**5**)



$[Co_4(3\text{-cptpy})_4(HCOO)_4(H_2O)_2]_n$ (**6**) $[Mn(3\text{-cptpy})_2]_n$ (**7**)

Fig. S1. The measured and simulated powder X-ray diffraction patterns of **1**, **2**, and **4**−**7**

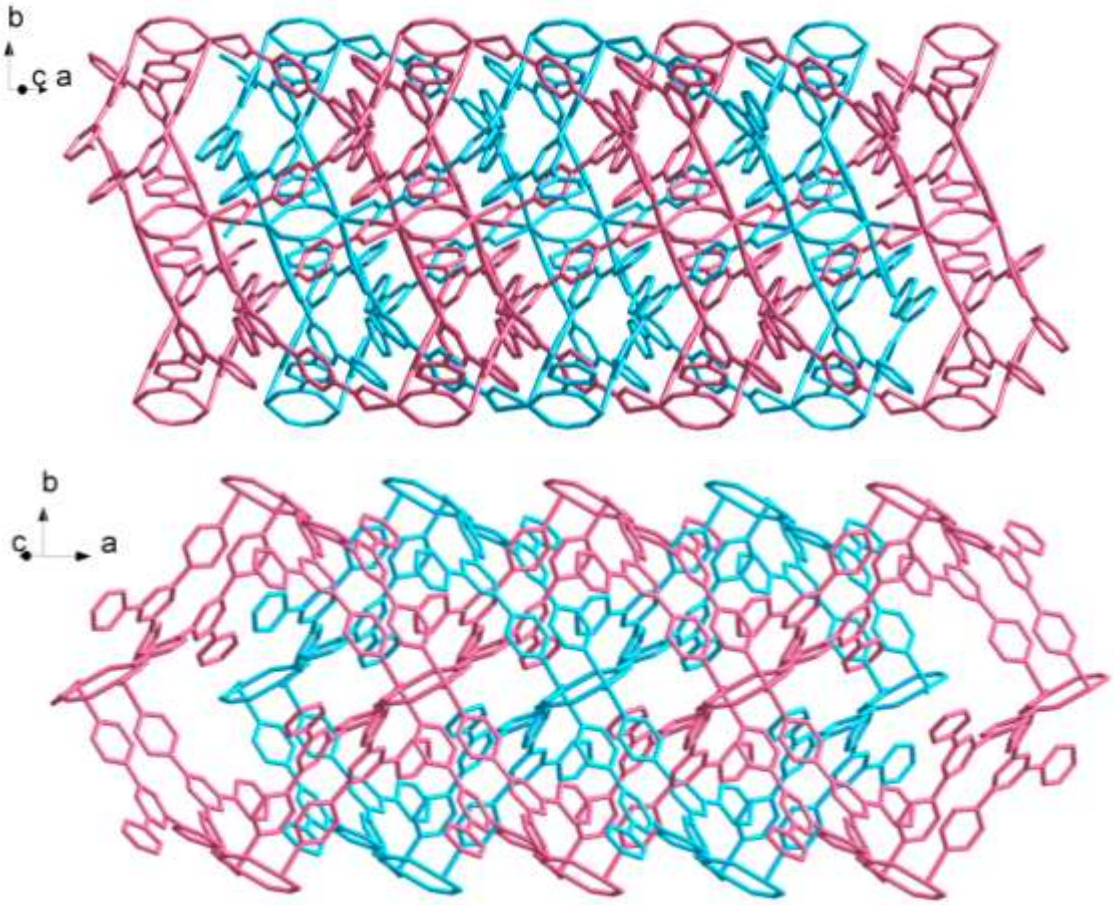


Fig. S2 The 2-fold interpenetrating framework of **1** along different directions

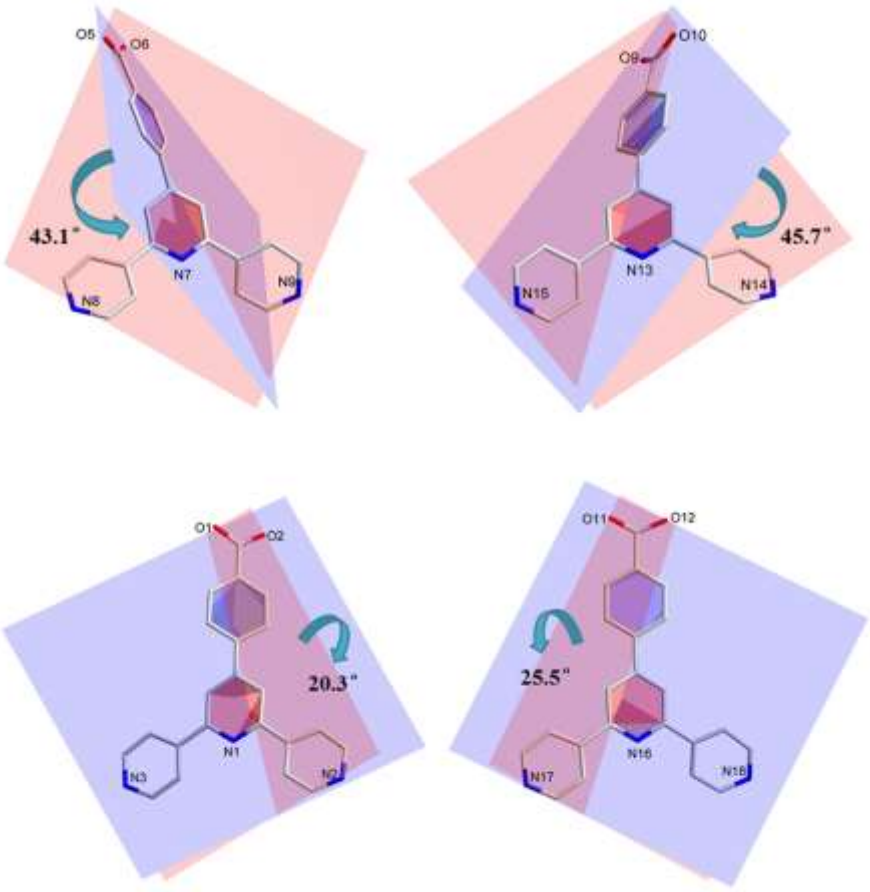


Fig. S3 Different dihedral angles between the phenyl ring and the central pyridyl group of 4-cptpy^{-} ligands in **3**

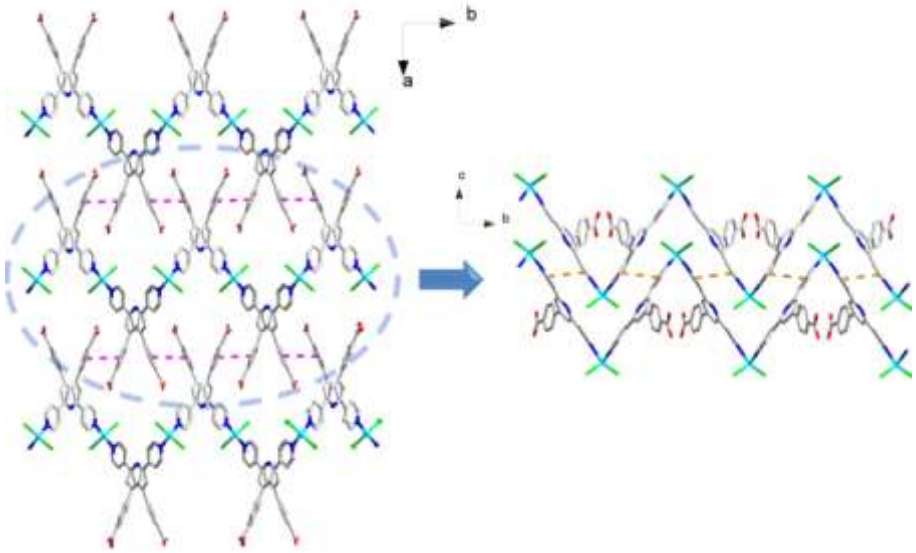
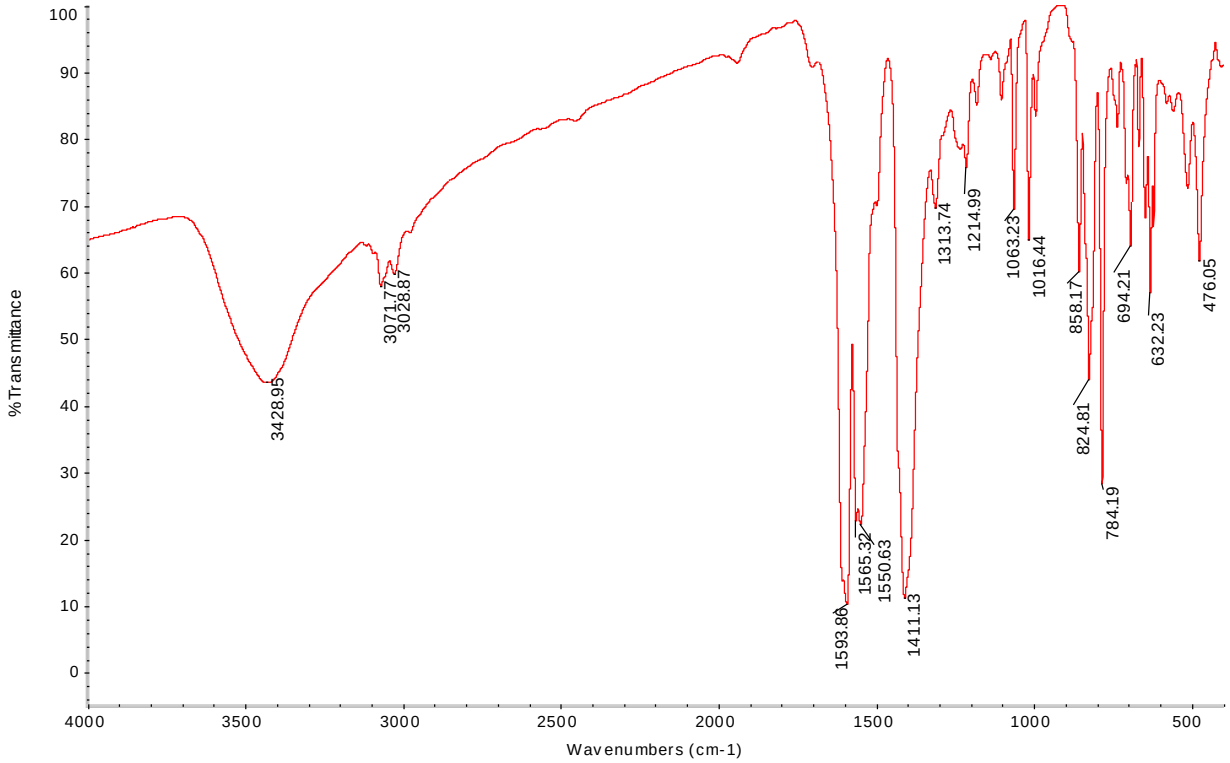
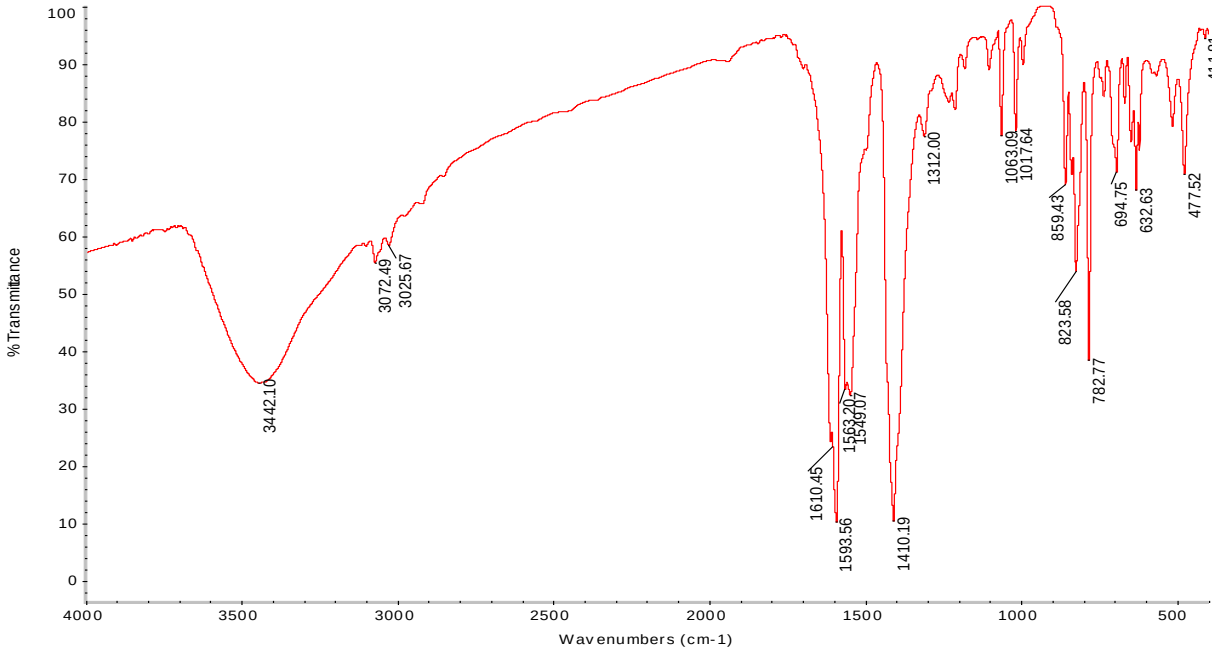


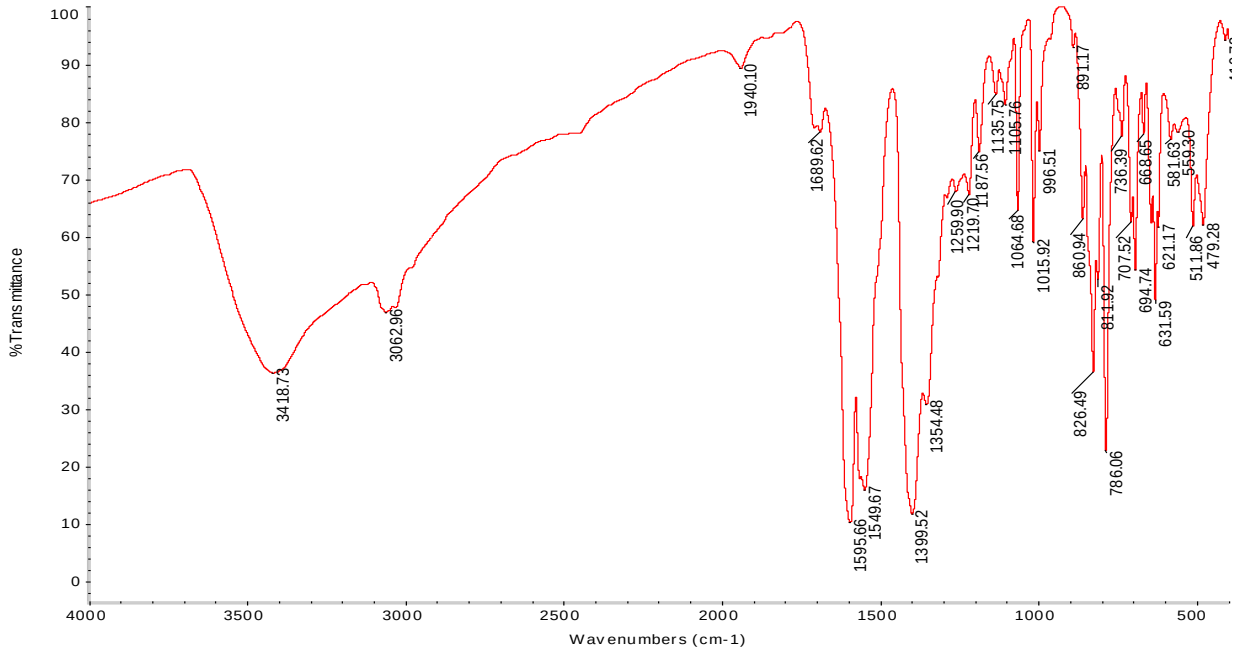
Fig. S4 The 3D supramolecular framework of **5** assembled via π−π interactions of phenyl rings (left) and pyridyl rings (right) along different directions.



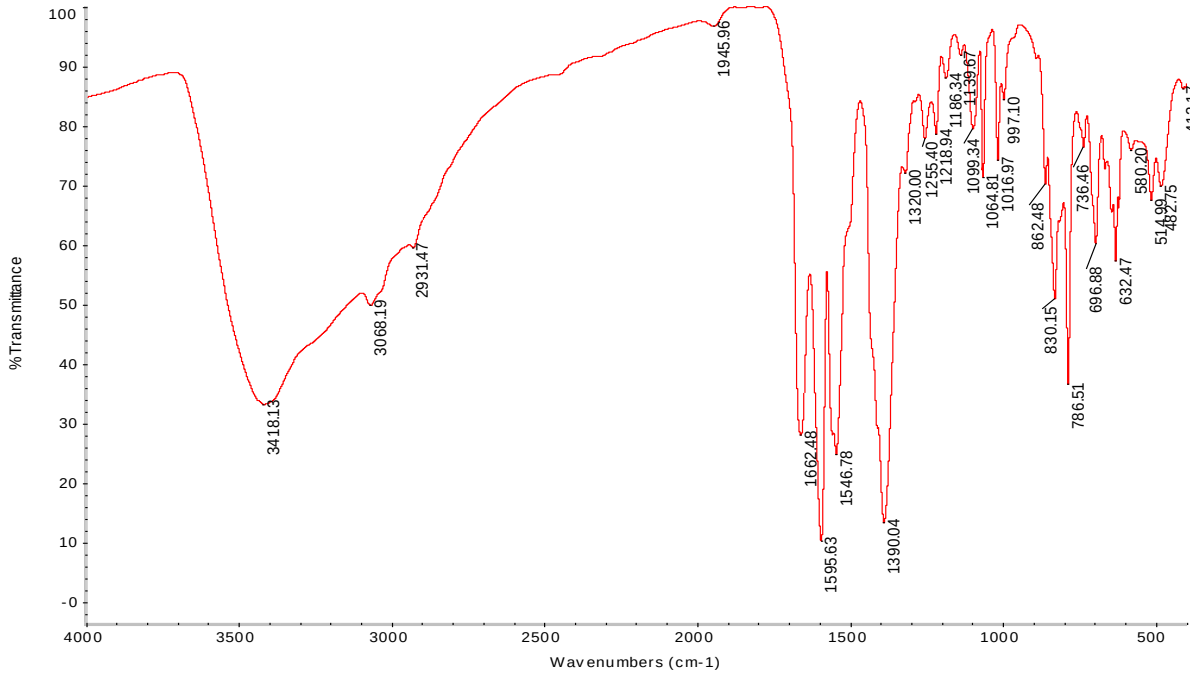
IR spectrum of $[Mn(4\text{-cptpy})_2]_n$ (**1**)



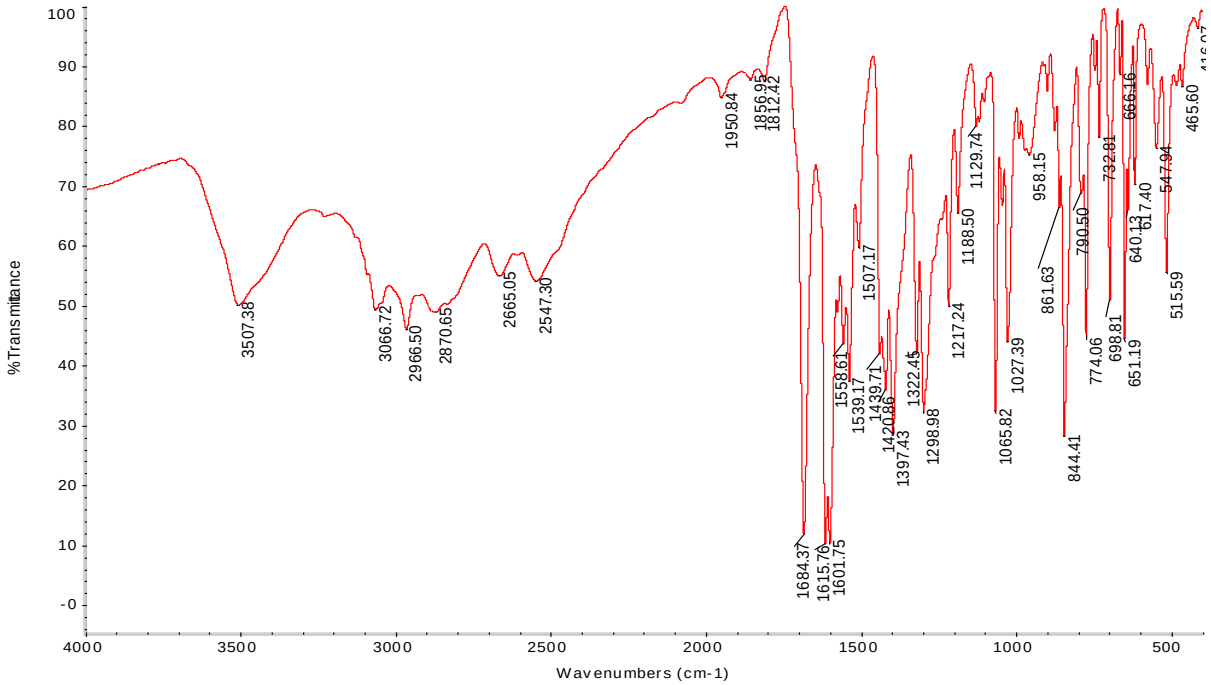
IR spectrum of $[Co(4\text{-cptpy})_2]_n$ (**2**)



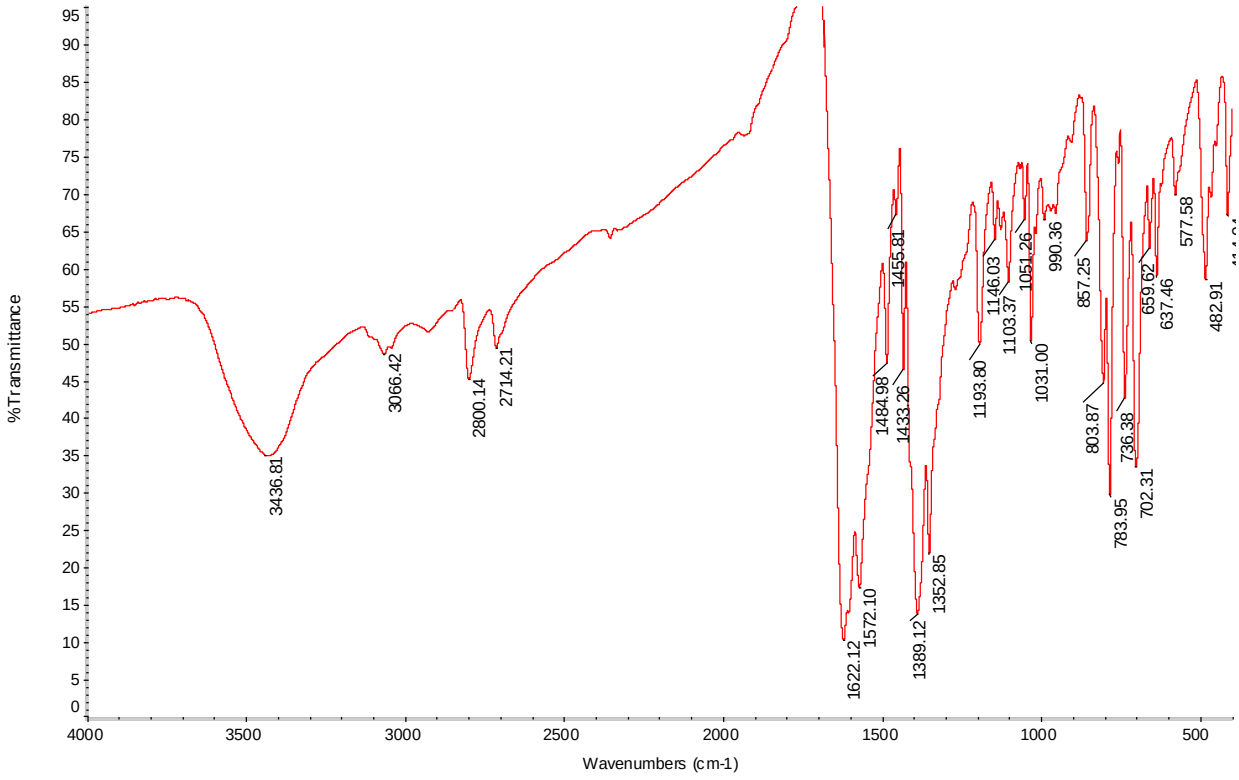
IR spectrum of $[Mn_3(4\text{-cptpy})_6(H_2O)]_n \cdot 2nH_2O$ (**3**)



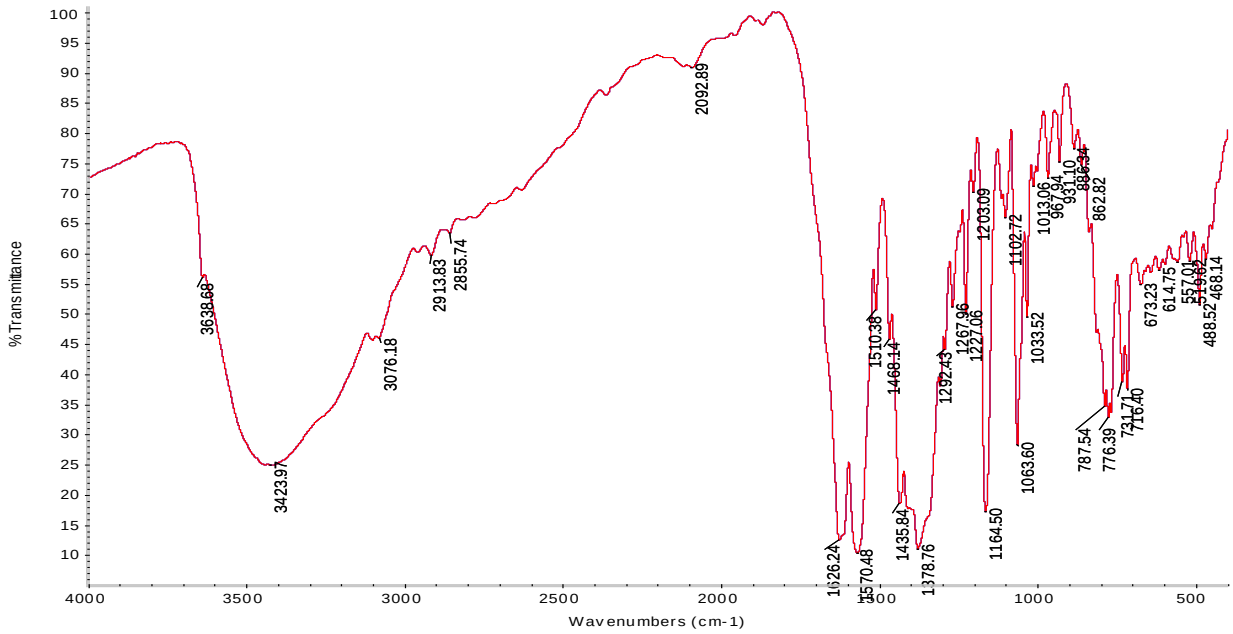
IR spectrum of $[Co(4\text{-cptpy})(HCOO)(H_2O)]_n \cdot n$DMF (**4**)



IR spectrum of $[Zn_2(4\text{-Hcptpy})_2Cl_4]_n \cdot 2nC_2H_5OH \cdot nH_2O$ (**5**)

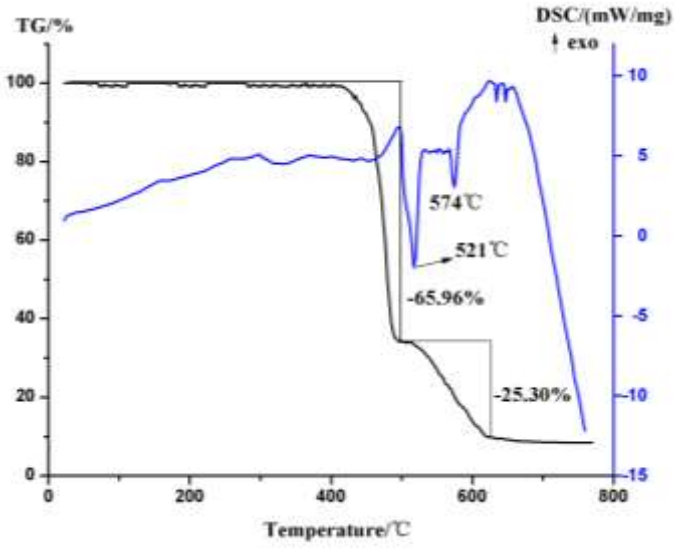


IR spectrum of $[Co_4(3\text{-cptpy})_4(HCOO)_4(H_2O)_2]_n$ (**6**)

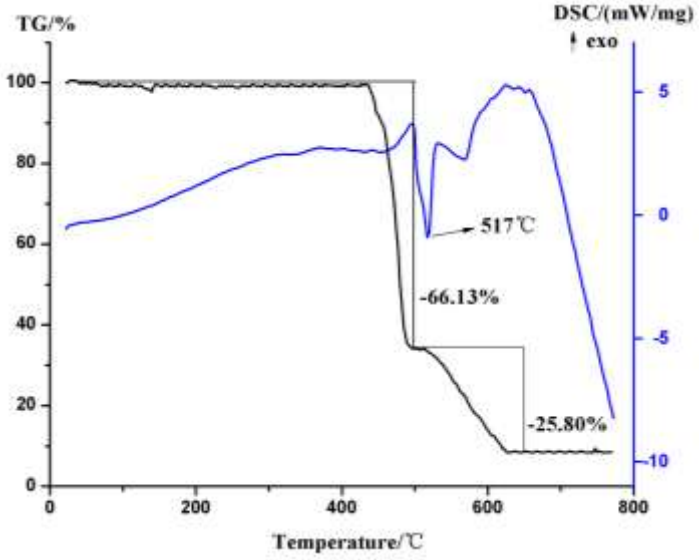


IR spectrum of $[Mn(3\text{-cptpy})_2]_n$ (**7**)

Fig. S5 The FT-IR spectra of complexes **1**−**7**.



TG-DSC of $[Mn(4\text{-cptpy})_2]_n$ (**1**)



TG-DSC of $[Co(4\text{-cptpy})_2]_n$ (**2**)

Fig. S6 Thermal analysis curves of **1** and **2**.