Supplementary Information

Table S1 Selected bond distances (Å) and angles (°) for complexes 1–6[a]

		1			
Co(1)-O(4)#1	2.009(4)	Co(1)-O(1)	2.038(3)	Co(1)-N(1)#2	2.041(4)
Co(1)-N(4)	2.041(4)	Co(1)-O(2)	2.348(4)		
O(4)#1-Co(1)-O(1)	107.19(15)	O(4)#1-Co(1)-N(1)#2	106.06(17)	O(1)-Co(1)-N(1)#2	130.87(17)
O(4)#1-Co(1)-N(4)	94.54(16)	O(1)-Co(1)-N(4)	104.93(15)	N(1)#2-Co(1)-N(4)	107.36(17)
N(4)-Co(1)-O(2)	86.64(15)	O(4)#1-Co(1)-O(2)	166.03(14)	O(1)-Co(1)-O(2)	59.22(13)
N(1)#2-Co(1)-O(2)	86.77(16)				
		2			
Ni(1)-N(1)	2.023(3)	Ni(1)-N(3)	2.027(3)	Ni(1)-O(1)	2.174(2)
Ni(1)-O(2)	2.103(2)	Ni(1)-O(3)#3	2.082(2)	Ni(1)-O(4)#3	2.189(2)
N(1)-Ni(1)-N(3)	98.63(12)	N(1)-Ni(1)-O(3)#3	100.39(10)	N(3)-Ni(1)-O(3)#3	96.35(11)
N(1)-Ni(1)-O(2)	98.55(10)	N(3)-Ni(1)-O(2)	95.05(11)	O(3)#3-Ni(1)-O(2)	156.12(9)
N(1)-Ni(1)-O(1)	159.96(10)	N(3)-Ni(1)-O(1)	86.18(11)	O(3)#3-Ni(1)-O(1)	98.37(9)
O(2)-Ni(1)-O(1)	61.54(8)	N(1)-Ni(1)-O(4)#3	92.96(11)	N(3)-Ni(1)-O(4)#3	156.71(11)
O(3)#3-Ni(1)-O(4)#3	61.54(9)	O(2)-Ni(1)-O(4)#3	103.16(9)	O(1)-Ni(1)-O(4)#3	89.81(9)
		3			
Ni(1)-N(1)	2.032(4)	Ni(1)-N(3)	2.029(3)	Ni(1)-O(1)	2.073(3)
Ni(1)-O(2)	2.173(3)	Ni(1)-O(3)#4	2.055(2)	Ni(1)-O(4)#4	2.215(3)
N(3)-Ni(1)-N(1)	95.89(14)	N(3)-Ni(1)-O(3)#4	99.16(12)	N(1)-Ni(1)-O(3)#4	96.16(12)
N(3)-Ni(1)-O(1)	99.84(11)	N(1)-Ni(1)-O(1)	94.64(13)	O(3)#4-Ni(1)-O(1)	157.01(11)
N(3)-Ni(1)-O(2)	161.88(11)	N(1)-Ni(1)-O(2)	88.90(12)	O(3)#4-Ni(1)-O(2)	97.68(10)
O(1)-Ni(1)-O(2)	62.27(10)	N(3)-Ni(1)-O(4)#4	92.55(13)	N(1)-Ni(1)-O(4)#4	157.21(12)
O(3)#4-Ni(1)-O(4)#4	61.54(10)	O(1)-Ni(1)-O(4)#4	104.73(11)	O(2)-Ni(1)-O(4)#4	89.60(11)
		4			
Ni(1)-N(1)#5	2.065(3)	N(3)-Ni(1)	2.053(3)	Ni(1)-O(2)	2.045(2)
Ni(1)-O(6)	2.095(2)	Ni(1)-O(8)	2.118(2)	Ni(1)-O(7)	2.132(2)
O(2)-Ni(1)-N(3)	171.86(11)	O(2)-Ni(1)-N(1)#5	91.07(10)	N(3)-Ni(1)-N(1)#5	94.62(11)
O(2)-Ni(1)-O(6)	83.76(9)	N(3)-Ni(1)-O(6)	90.47(11)	N(1)#5-Ni(1)-O(6)	89.57(11)

O(2)-Ni(1)-O(8)	90.40(8)	N(3)-Ni(1)-O(8)	95.61(10)	N(1)#5-Ni(1)-O(8)	87.80(10)
O(6)-Ni(1)-O(8)	173.55(8)	O(2)-Ni(1)-O(7)	86.23(9)	N(3)-Ni(1)-O(7)	88.32(10)
N(1)#5-Ni(1)-O(7)	176.29(10)	O(6)-Ni(1)-O(7)	92.67(10)	O(8)-Ni(1)-O(7)	89.66(9)
			5		
N(1)-Zn(1)	2.026(3)	N(4)-Zn(1)#6	2.008(3)	O(1)-Zn(1)	1.951(3)
O(3)-Zn(1)#7	1.979(3)				
O(1)-Zn(1)-O(3)#6	112.35(13)	O(1)-Zn(1)-N(4)#6	113.84(14)	O(3)#7-Zn(1)-N(4)#6	101.71(14)
O(1)-Zn(1)-N(1)	94.24(13)	O(3)#7-Zn(1)-N(1)	117.48(14)	N(4)#6-Zn(1)-N(1)	117.84(14)
			6		
Cd(1)-N(1)#8	2.271(3)	Cd(1)-N(3)	2.276(3)	Cd(1)-O(2)	2.384(3)
Cd(1)-O(6)	2.398(3)	Cd(1)-O(4)#9	2.404(3)		
N(1)#8-Cd(1)-N(3)	94.59(12)	N(1)#8-Cd(1)-O(2)	95.13(11)	N(3)-Cd(1)-O(2)	135.63(10)
N(1)#8-Cd(1)-O(6)	174.64(10)	N(3)-Cd(1)-O(6)	90.70(11)	O(2)-Cd(1)-O(6)	80.46(9)
N(1)#8-Cd(1)-O(4)#9	102.42(12)	N(3)-Cd(1)-O(4)#9	83.20(11)	O(2)-Cd(1)-O(4)#9	135.92(10)
O(6)-Cd(1)-O(4)#9	79.01(11)				

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y+1/2,-z+1/2, #2 -x+1,-y,-z for **1**; #3 -x+1/2,y-1/2,-z+3/2 for **2**; #4 -x+3/2,y+1/2,-z+3/2 for **3**; #5 -x+1,-y+2,-z+2 for **4**, #6 -x+2,-y,-z, #7 -x+2,-y,-z+1for **5**; #8 x+1,y,z, #9 -x+2,-y+2,-z+1 for **6**.

Table S2 Hydrogen Bonds Data for Complexes 2, 4 and 6[a]

D-H···A	d(D-H)/ Å	d(H···A) /Å	<DHA/deg	d(D···A) /Å
		2		
O6-H6A···O5#1	0.852	2.096	161.03	2.915
O6-H6B···O2#1	0.851	2.028	170.98	2.872
		4		
O6-H6C···O5	0.843	2.034	154.46	2.818
O6-H6D···O9#2	0.845	1.922	165.53	2.748
O7-H7C···O4#2	0.849	1.886	160.31	2.701
O7-H7D···O5#3	0.847	1.904	174.10	2.748
O8-H8A···O5#3	0.850	1.900	163.05	2.724
O8-H8B···O3	0.849	1.895	157.52	2.699
O9-H9A···O4	0.855	2.020	152.30	2.805

O9-H9B···O7	0.850	2.144	162.93	2.967
		6		
O6-H6B···O2#4	0.854	1.941	161.64	2.765

Symmetry transformations used to generate equivalent atoms: #1 x, -y+1, z-1/2 for **2**; #2 -x+1, -y+1, -z+2, #3 x+1, y, z for **4;** #4-x+2, -y+2, -z+1 for **6**.

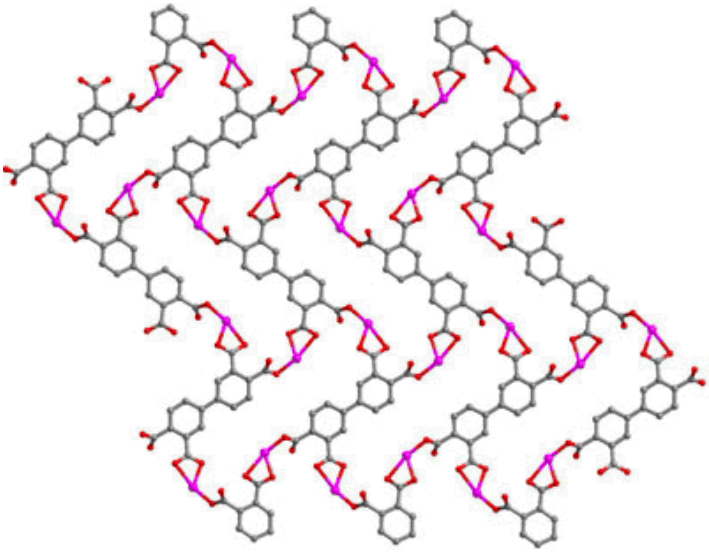


Figure S1 2D [Co_2(bptc)] layer of compound **1**.

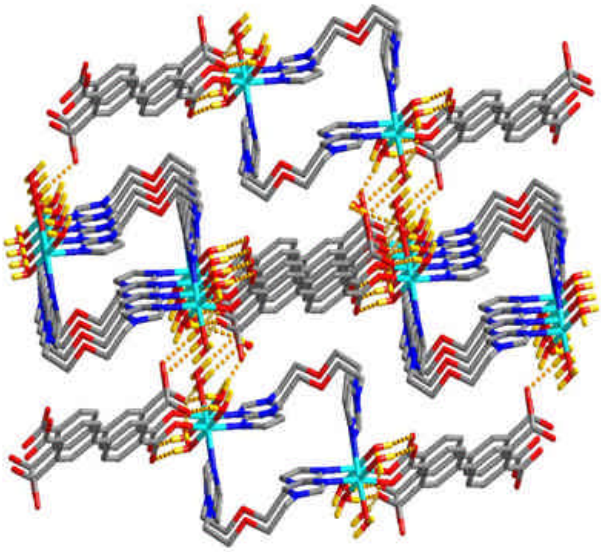


Figure S2 3D supramolecular framework of compound **4** (the dotted golden line represents the O-H···O H-bonds).

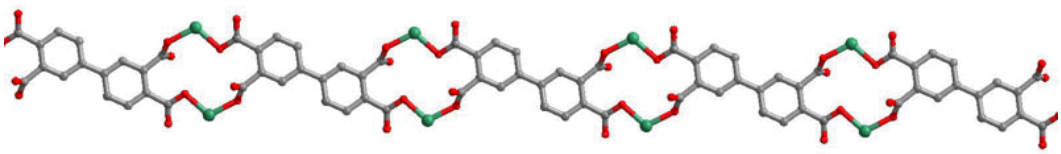
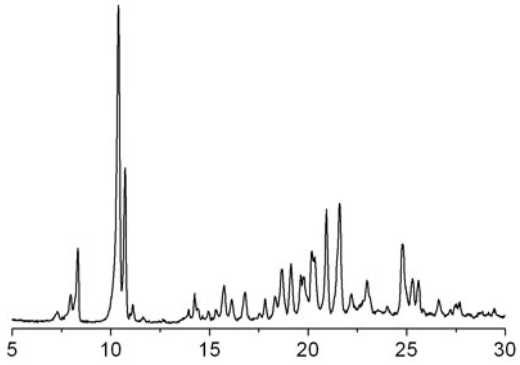
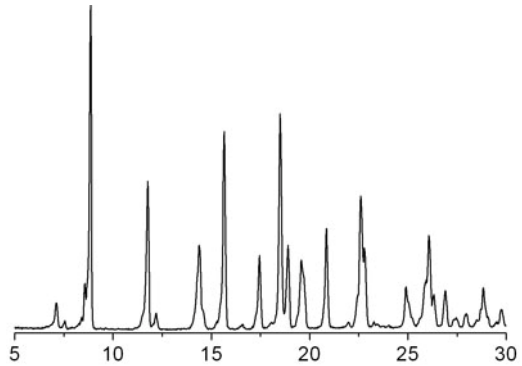


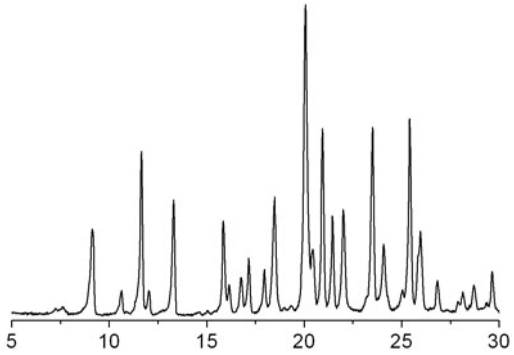
Figure S3 1D [$Zn(bptc)_{0.5}$] polymeric chain of compound **5**.



The powder X-ray diffraction (PXRD) pattern of compound **3**



The powder X-ray diffraction (PXRD) pattern of compound **4**



The powder X-ray diffraction (PXRD) pattern of compound **5**

Figure S4. The measured powder X-ray diffraction (PXRD) patterns (a) for **3**; (b) for **4**; (c) for **5**.