Support materials

Coordination Polymers of Biphenyl-2,4,2',4'-Tetracarboxylic Acid—Synthesis, Structures and Adsorption Properties

.

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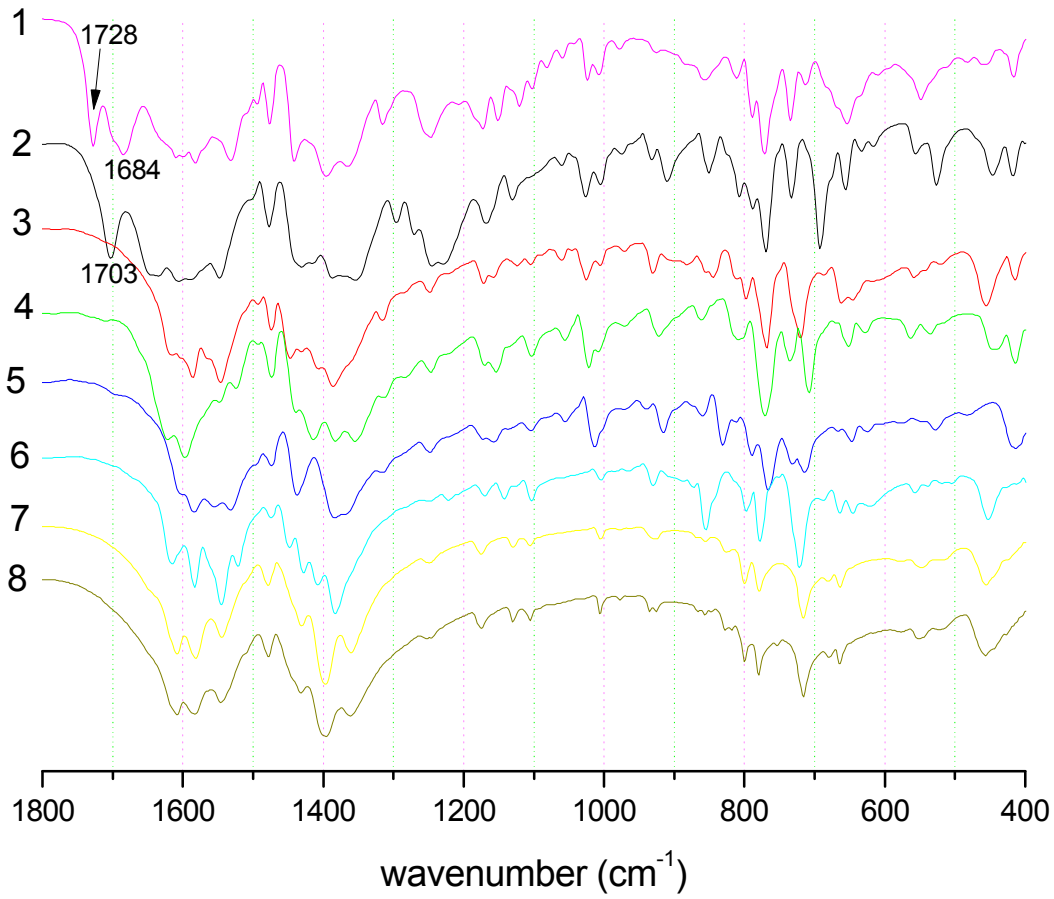


Fig. s1. IR spectra of complex **1**~**8**

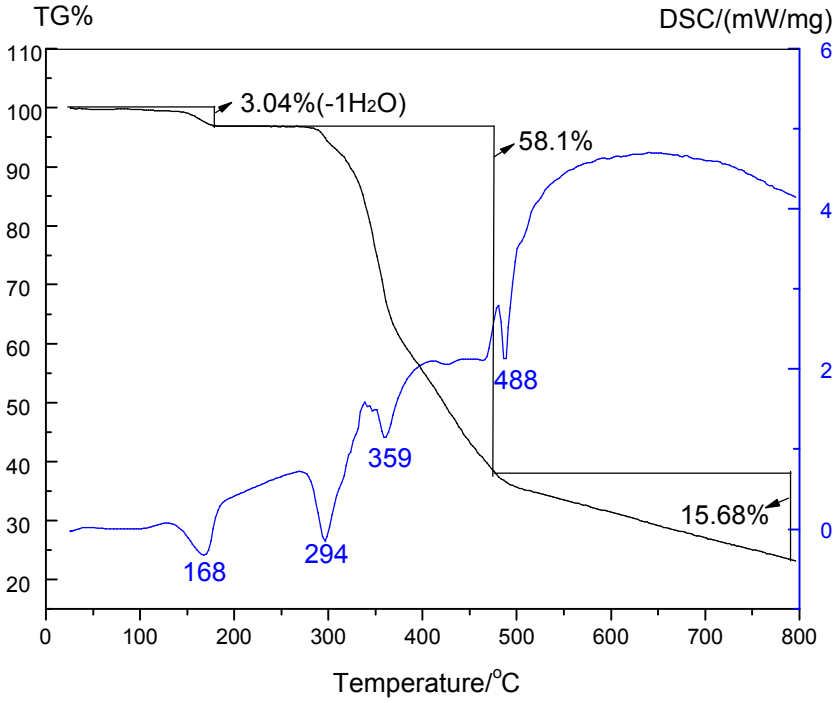


Fig. s2. TG of $[Zn(2,4\text{-}H_2bptc)(2,2'\text{-}bipy)\cdot H_2O]_n$[1] (**1**)

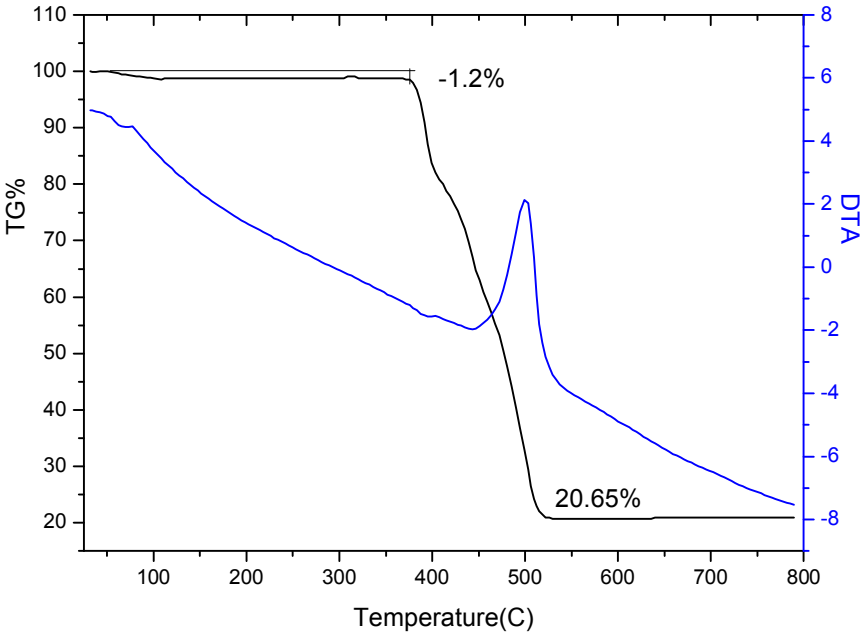


Fig. s3. TG of $\{[Zn_3(2,4\text{-Hbptc})_2(2,2'\text{-bpy})_2\cdot]\cdot 2H_2O\}_n$[1] **(2)**

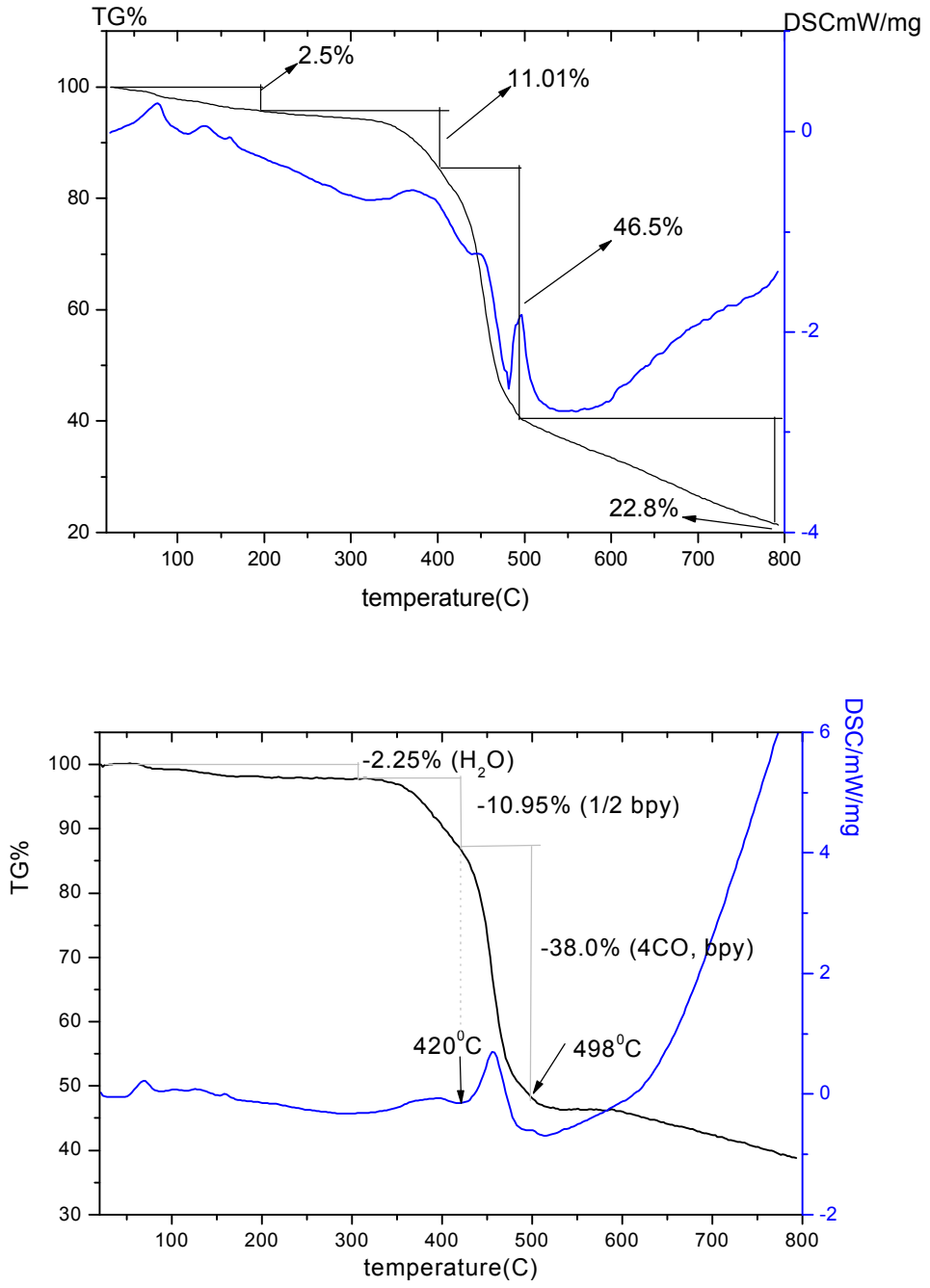


Fig. s4. TG of $\{[Zn_2(2,4\text{-bptc})(2,2'\text{-bpy})]\cdot(2,2'\text{-bpy})_{0.5}\cdot(H_2O)\}_n$ [3] **(3)** in air (top) and nitrogen (bottom)

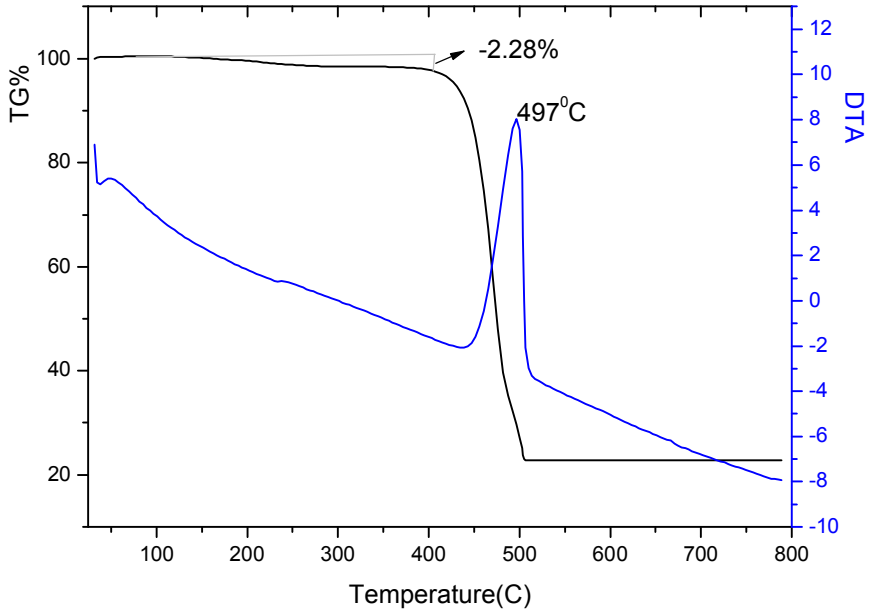


Fig. s5. TG curve of Complex $\{[Zn_2(2,4\text{-bptc})(2,2'\text{-bpy})_2](H_2O)\}_n$[3] **(4)**

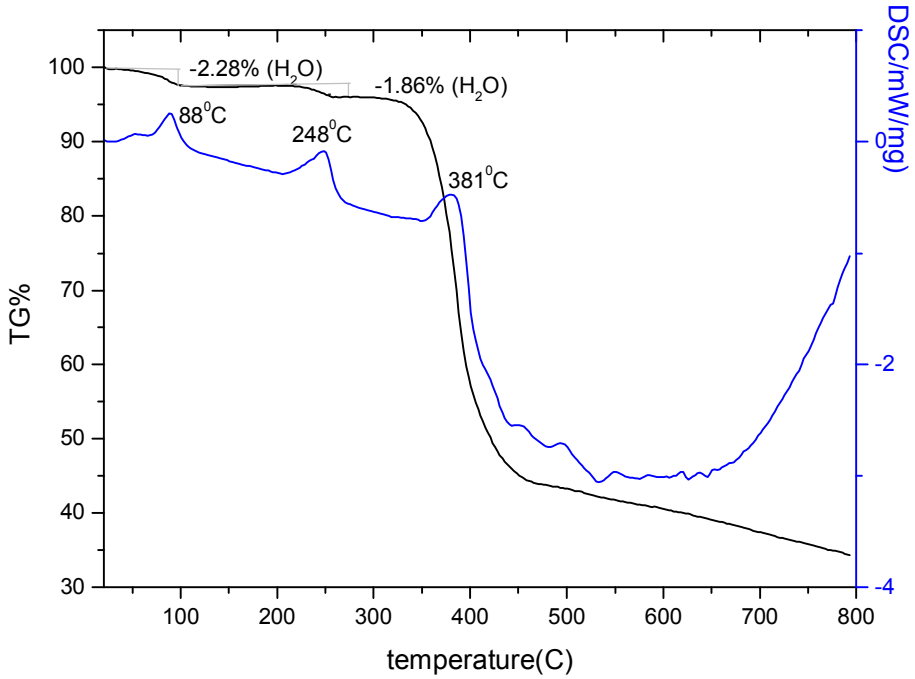


Fig. S6. TG curve of $\{[Cd_2\cdot(2,4\text{-bptc})\cdot(2,2\text{-bpy})_2\cdot H_2O]\cdot H_2O\}_n$ **(5)**

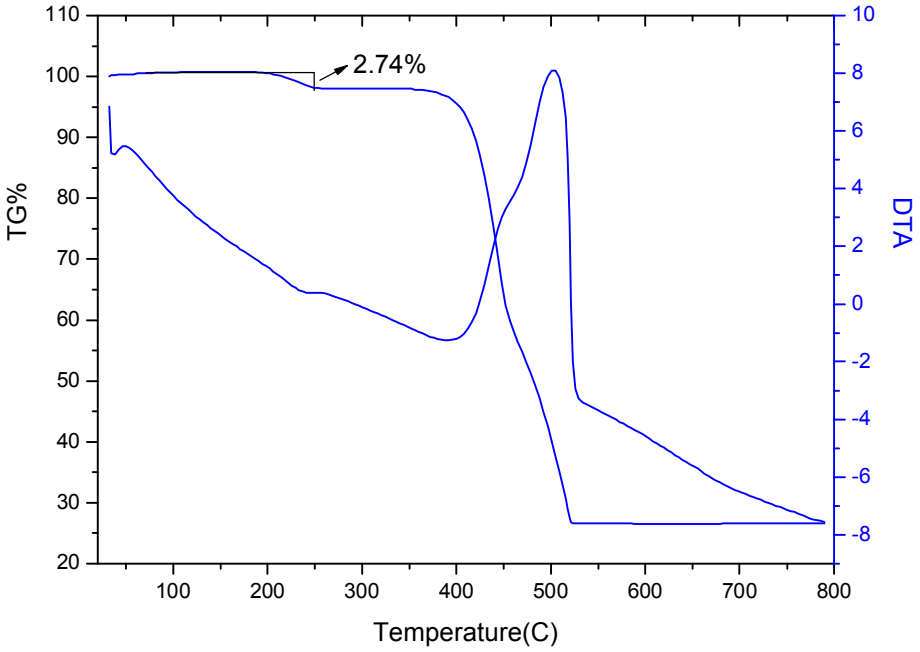


Fig. s7. TG curve of {[Zn_2·(2,4-bptc)·(phen)·H_2O]$_n$}[3] **(6)**

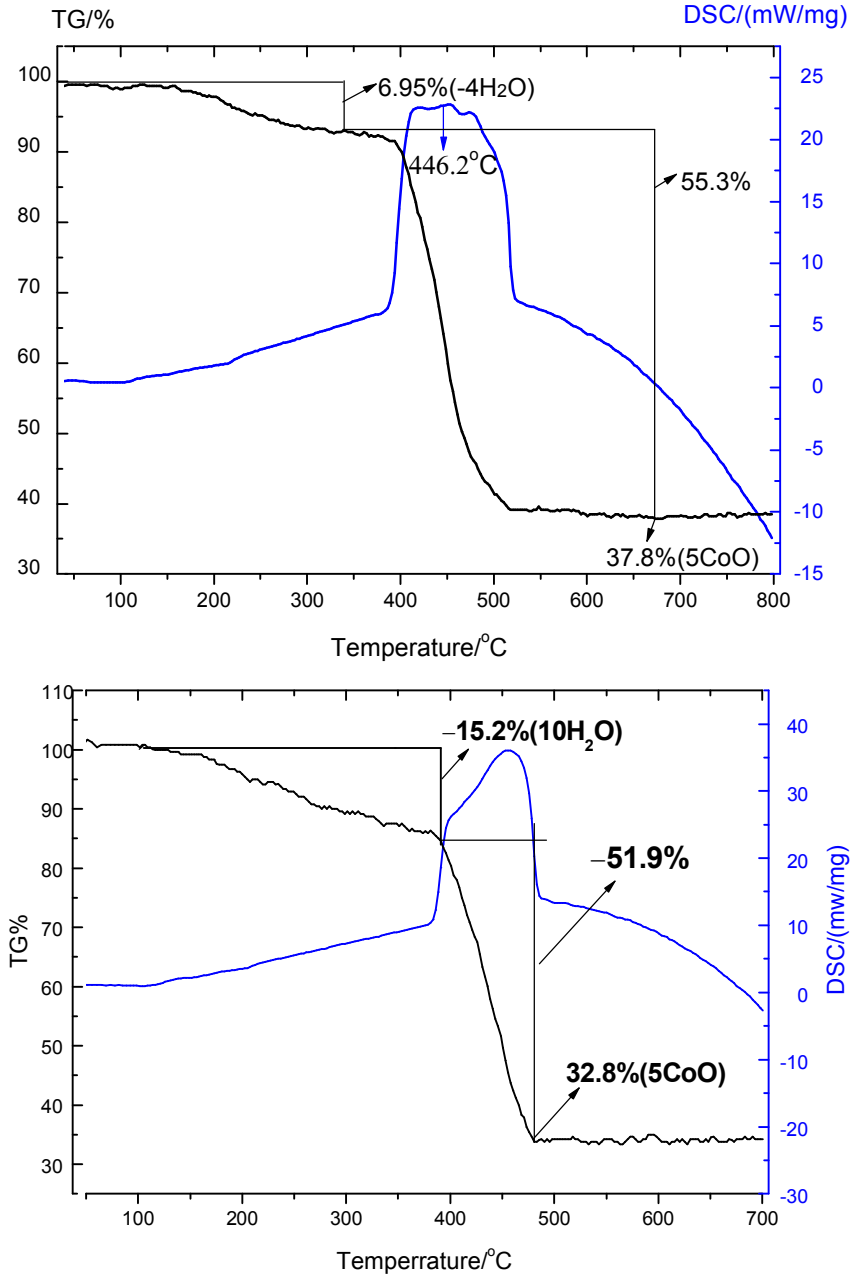


Fig. s8. TG of $\{[Co_5(2,4\text{-bptc})_2(\mu_3\text{-}OH)_2(\mu_2\text{-}H_2O)_2(\mu_1\text{-}H_2O)_2]\cdot 2H_2O\}_n$ **(7)** and $\{[Co_5(2,4\text{-bptc})_2(\mu_3\text{-}OH)(\mu_2\text{-}H_2O)_2(\mu_1\text{-}H_2O)_2]\cdot 6H_2O\}_n$ **(8)**.

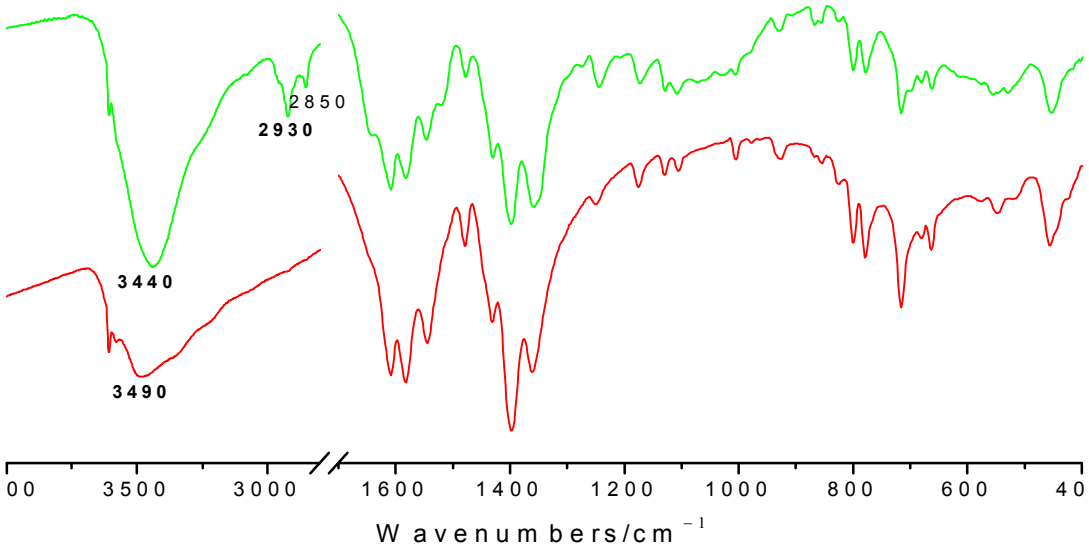
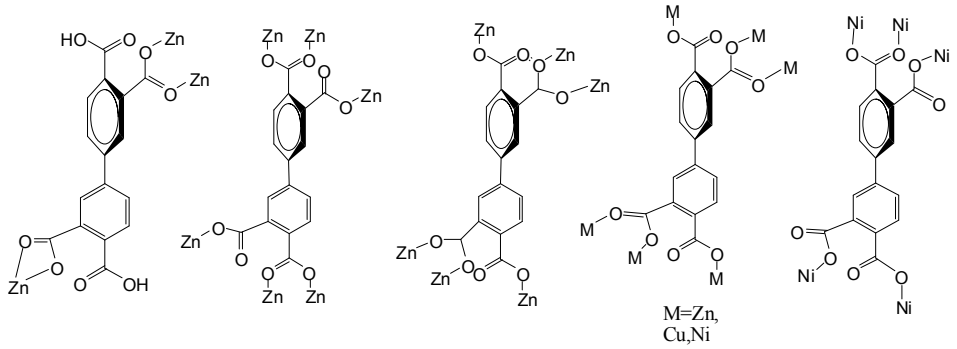
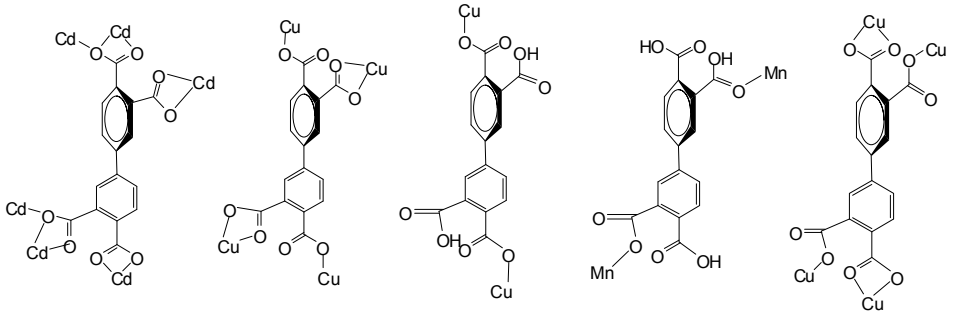


Fig. s9. IR of $\{[Co_5(2,4\text{-bptc})_2(\mu_3\text{-OH})(\mu_2\text{-}H_2O)_2(\mu_1\text{-}H_2O)_2]\cdot 6H_2O\}_n$ (**8**) (red) and ethanol adsorbed dehydrated sample of **8** (blue)



ref 1 ref 1 ref 1 ref 2 ref 2

M=Zn, Cu,Ni



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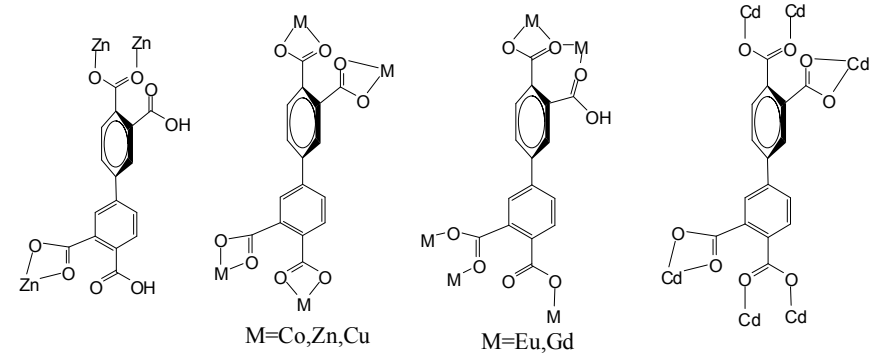
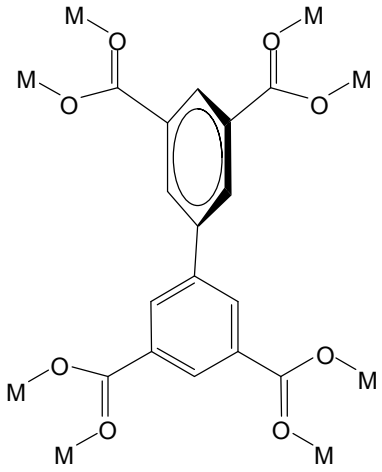


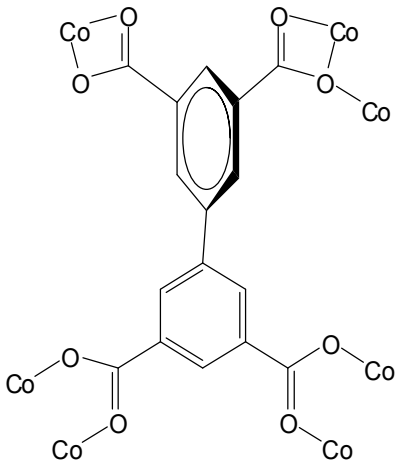
ref 4 ref 1,3,5 ref 6 ref 7

M=Co,Zn,Cu M=Eu,Gd

Scheme s1. Coordination mode of 3,4-bptc^{4-} complexes

1.Ji-Jiang Wang, Lei Gou, et al, *Crystal Growth & Design,* 2007, **7**, 1514-1521.
2. Shourong Zhu, Hui Zhang et al, *Transition Met Chem* 2008, **33**,669–680.
3. Guo-Ping Yang, Yao-Yu Wang et al, *Eur. J. Inorg. Chem.* 2007, 3892–3898.
4. Xin-Long Wang, Chao Qin, et al, *Eur. J. Inorg. Chem.* 2005, 3418–3421.
5. Li-Xin Sun, Yan Qi, et al, *Crystal Growth & Design,* 2009, **9**, 2995-2998.
6. Danfeng Weng, Xiangjun Zheng, et al, *Dalton Trans.,* 2007, 4822–4828.
7 .Ji-Jiang Wang, Meng-Lin Yang et al, *Z. Anorg. Allg. Chem*. 2007, 341-345





Scheme s2 Coordination mode of 3,5-bptc^{4-} complexes

1. Banglin Chen, Nathan W. Ockwig, et al, *Inorg. Chem.*, 2005, **44**, 181-183.

2.Banglin Chen, Nathan W. Ockwig,et al, *Angew. Chem. Int. Ed.* 2005, **44**, 4745 –4749

3.Xiang Lin, Irvin Telepeni et al, *J. Am. Chem. Soc.* 2009, **131**, 2159–2171

Table s1. Selected bond length [Å] and angle [°] of complex **1**

Zn(1)-O(1)	1.978(2)	Zn(1)-O(4)#1	2.015(3)
Zn(1)-N(1)	2.103(3)	Zn(1)-O(1W)	2.104(3)
Zn(1)-N(2)	2.129(3)		
O(1)-Zn(1)-O(4)#1	108.32(11)	O(1)-Zn(1)-N(1)	111.83(12)
O(4)#1-Zn(1)-N(1)	138.66(12)	O(1)-Zn(1)-O(1W)	91.69(11)
O(4)#1-Zn(1)-O(1W)	95.37(12)	N(1)-Zn(1)-O(1W)	92.90(13)
O(1)-Zn(1)-N(2)	96.22(11)	O(4)#1-Zn(1)-N(2)	89.18(12)
N(1)-Zn(1)-N(2)	77.29(13)	O(1W)-Zn(1)-N(2)	169.16(12)

Symmetry transformations used to generate equivalent atoms:
#1 x-1/2,-y+1/2,z+1/2 #2 x+1/2,-y+1/2,z-1/2

Table S2. Hydrogen bonds for **1** [Å and °].

D-H . . . A	d (D-H)	d(H...A)	d(D...A)	<(DHA)
O(6)-H(6A)...O(3)#3	0.82	1.77	2.566(4)	163.6
O(7)-H(7)...O(5)#4	0.82	2.23	2.856(5)	134.0
O(7)-H(7)...O(1)#4	0.82	2.67	3.268(6)	131.1
O(1W)-H(1WA)...O(2)	0.82	1.87	2.590(4)	146.3
O(1W)-H(1WB)...O(5)#5	0.89(5)	1.98(5)	2.830(4)	159(4)

Symmetry transformations used to generate equivalent atoms:
#1 x-1/2,-y+1/2,z+1/2 #2 x+1/2,-y+1/2,z-1/2
#3 x+1/2,-y+1/2,z+1/2 #4 -x+1/2,y-1/2,-z+3/2
#5 x-1,y,z

Table s3. Selected bond length [Å] and angle [°] of complex **2**.

Zn(1)-O(3)#1	2.004(3)	Zn(1)-O(5)#2	2.008(3)
Zn(1)-N(2)	2.046(4)	Zn(1)-O(1)	2.055(3)
Zn(1)-N(1)	2.125(4)	Zn(2)-O(4)#3	2.019(3)
Zn(2)-O(4)#1	2.019(3)	Zn(2)-O(5)#2	2.171(3)
Zn(2)-O(5)	2.171(3)	Zn(2)-O(1)#2	2.196(3)
Zn(2)-O(1)	2.196(3)	Zn(2)-Zn(1)#2	3.1226(7)
O(3)#1-Zn(1)-O(5)#2	90.35(13)	O(3)#1-Zn(1)-N(2)	95.23(15)
O(5)#2-Zn(1)-N(2)	141.06(15)	O(3)#1-Zn(1)-O(1)	93.81(13)
O(5)#2-Zn(1)-O(1)	84.54(13)	N(2)-Zn(1)-O(1)	133.20(15)
O(3)#1-Zn(1)-N(1)	173.09(15)	O(5)#2-Zn(1)-N(1)	95.61(15)
N(2)-Zn(1)-N(1)	77.93(16)	O(1)-Zn(1)-N(1)	90.23(14)
O(4)#3-Zn(2)-O(4)#1	180	O(4)#3-Zn(2)-O(5)#2	89.92(12)
O(4)#1-Zn(2)-O(5)#2	90.08(12)	O(4)#3-Zn(2)-O(5)	90.08(12)
O(4)#1-Zn(2)-O(5)	89.92(12)	O(5)#2-Zn(2)-O(5)	180
O(4)#3-Zn(2)-O(1)#2	87.24(12)	O(4)#1-Zn(2)-O(1)#2	92.76(12)
O(5)#2-Zn(2)-O(1)#2	102.49(12)	O(5)-Zn(2)-O(1)#2	77.51(12)
O(4)#3-Zn(2)-O(1)	92.76(12)	O(4)#1-Zn(2)-O(1)	87.23(12)
O(5)#2-Zn(2)-O(1)	77.51(12)	O(5)-Zn(2)-O(1)	102.49(12)
O(1)#2-Zn(2)-O(1)	180	O(4)#3-Zn(2)-Zn(1)#2	76.05(9)
O(4)#1-Zn(2)-Zn(1)#2	103.95(9)	O(5)#2-Zn(2)-Zn(1)#2	140.30(8)
O(5)-Zn(2)-Zn(1)#2	39.70(8)	O(1)#2-Zn(2)-Zn(1)#2	41.01(8)
O(1)-Zn(2)-Zn(1)#2	138.99(8)		

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z #2 -x+1,-y+1,-z+1 #3 -x+2,-y+1,-z+1

#4 x+1,y,z

Table s4. Selected bond length [Å] and angle [°] of complex **3**.

Zn(1)-O(2)#1	1.936(2)	Zn(1)-O(3)#2	1.940(2)
Zn(1)-O(7)	1.979(2)	Zn(1)-O(6)#3	2.031(2)
Zn(1)-O(8)	2.412(3)	Zn(2)-O(5)#4	1.993(3)
Zn(2)-O(1)	2.033(2)	Zn(2)-O(4)#5	2.042(3)
Zn(2)-N(2)	2.098(3)	Zn(2)-N(1)	2.146(3)
O(2)#1-Zn(1)-O(3)#2	116.28(11)	O(2)#1-Zn(1)-O(7)	113.02(12)
O(3)#2-Zn(1)-O(7)	123.76(11)	O(2)#1-Zn(1)-O(6)#3	105.49(11)
O(3)#2-Zn(1)-O(6)#3	97.29(11)	O(7)-Zn(1)-O(6)#3	94.15(11)
O(2)#1-Zn(1)-O(8)	93.57(12)	O(3)#2-Zn(1)-O(8)	92.68(11)
O(7)-Zn(1)-O(8)	58.58(10)	O(6)#3-Zn(1)-O(8)	151.61(10)
O(5)#4-Zn(2)-O(1)	96.14(11)	O(5)#4-Zn(2)-O(4)#5	125.96(10)
O(1)-Zn(2)-O(4)#5	95.25(11)	O(5)#4-Zn(2)-N(2)	107.33(12)
O(1)-Zn(2)-N(2)	90.61(12)	O(4)#5-Zn(2)-N(2)	125.17(12)
O(5)#4-Zn(2)-N(1)	95.49(12)	O(1)-Zn(2)-N(1)	164.95(12)
O(4)#5-Zn(2)-N(1)	85.58(12)	N(2)-Zn(2)-N(1)	76.80(14)

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,-y+1/2,z-1/2 #2 -x+2,-y,-z
#3 -x+1,-y,-z #4 -x+3/2,y+1/2,-z+1/2
#5 -x+5/2,y+1/2,-z+1/2 #6 -x,-y,-z+1
#7 x+1/2,-y+1/2,z+1/2 #8 -x+5/2,y-1/2,-z+1/2
#9 -x+3/2,y-1/2,-z+1/2

Table s5. Selected bond length [Å] and angle [°] of complex **4**

Zn(1)-O(3)#1	1.959(2)	Zn(1)-O(5)	1.998(2)
Zn(1)-O(1)#2	2.086(2)	Zn(1)-N(2)	2.120(3)
Zn(1)-N(1)	2.126(2)	Zn(2)-O(8)#3	1.967(2)
Zn(2)-O(2)#2	2.014(2)	Zn(2)-O(6)	2.088(2)
Zn(2)-N(3)	2.099(3)	Zn(2)-N(4)	2.131(3)
O(3)#1-Zn(1)-O(5)	110.41(9)	O(3)#1-Zn(1)-O(1)#2	95.59(8)
O(5)-Zn(1)-O(1)#2	90.08(9)	O(3)#1-Zn(1)-N(2)	101.54(9)
O(5)-Zn(1)-N(2)	148.03(9)	O(1)#2-Zn(1)-N(2)	87.72(9)
O(3)#1-Zn(1)-N(1)	111.97(9)	O(5)-Zn(1)-N(1)	90.84(10)
O(1)#2-Zn(1)-N(1)	150.12(9)	N(2)-Zn(1)-N(1)	76.01(10)
O(8)#3-Zn(2)-O(2)#2	96.82(9)	O(8)#3-Zn(2)-O(6)	104.76(9)
O(2)#2-Zn(2)-O(6)	86.55(9)	O(8)#3-Zn(2)-N(3)	108.19(9)
O(2)#2-Zn(2)-N(3)	154.99(9)	O(6)-Zn(2)-N(3)	87.33(10)
O(8)#3-Zn(2)-N(4)	102.41(10)	O(2)#2-Zn(2)-N(4)	98.03(10)
O(6)-Zn(2)-N(4)	151.70(9)	N(3)-Zn(2)-N(4)	76.73(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y+1/2,-z+1/2 #2 x,-y+1/2,z-1/2

#3 -x+1,-y+1,-z+1 #4 x,-y+1/2,z+1/2

#5 -x,y-1/2,-z+1/2

Table s6. Selected bond length [Å] and angle [°] of complex **5**

Cd(1)-O(8)#1	2.274(3)	Cd(1)-O(1)	2.328(3)
Cd(1)-N(2)	2.332(4)	Cd(1)-N(1)	2.363(3)
Cd(1)-O(6)#2	2.361(4)	Cd(1)-O(5)#2	2.516(3)
Cd(1)-O(7)#1	2.577(3)	Cd(2)-O(2)	2.216(3)
Cd(2)-O(1W)	2.229(3)	Cd(2)-O(3)#3	2.285(3)
Cd(2)-N(3)	2.314(4)	Cd(2)-N(4)	2.352(4)
Cd(2)-O(4)#3	2.455(3)		
O(8)#1-Cd(1)-O(1)	90.43(13)	O(8)#1-Cd(1)-N(2)	132.76(13)
O(1)-Cd(1)-N(2)	127.93(13)	O(8)#1-Cd(1)-N(1)	96.51(14)
O(1)-Cd(1)-N(1)	79.60(13)	N(2)-Cd(1)-N(1)	69.51(13)
O(8)#1-Cd(1)-O(6)#2	91.60(13)	O(1)-Cd(1)-O(6)#2	111.07(14)
N(2)-Cd(1)-O(6)#2	97.18(14)	N(1)-Cd(1)-O(6)#2	166.61(14)
O(8)#1-Cd(1)-O(5)#2	133.33(12)	O(1)-Cd(1)-O(5)#2	78.24(13)
N(2)-Cd(1)-O(5)#2	86.14(13)	N(1)-Cd(1)-O(5)#2	124.78(13)
O(6)#2-Cd(1)-O(5)#2	53.11(12)	O(8)#1-Cd(1)-O(7)#1	53.30(12)
O(1)-Cd(1)-O(7)#1	139.98(13)	N(2)-Cd(1)-O(7)#1	80.50(12)
N(1)-Cd(1)-O(7)#1	87.64(13)	O(6)#2-Cd(1)-O(7)#1	88.70(13)
O(5)#2-Cd(1)-O(7)#1	137.50(12)	O(2)-Cd(2)-O(1W)	86.15(13)
O(2)-Cd(2)-O(3)#3	139.02(12)	O(1W)-Cd(2)-O(3)#3	93.59(13)
O(2)-Cd(2)-N(3)	87.50(14)	O(1W)-Cd(2)-N(3)	152.32(16)
O(3)#3-Cd(2)-N(3)	108.62(13)	O(2)-Cd(2)-N(4)	129.53(14)
O(1W)-Cd(2)-N(4)	93.26(16)	O(3)#3-Cd(2)-N(4)	91.42(14)
N(3)-Cd(2)-N(4)	70.49(16)	O(2)-Cd(2)-O(4)#3	89.65(12)
O(1W)-Cd(2)-O(4)#3	118.78(14)	O(3)#3-Cd(2)-O(4)#3	54.89(10)
N(3)-Cd(2)-O(4)#3	88.07(14)	N(4)-Cd(2)-O(4)#3	132.25(14)

Symmetry transformations used to generate equivalent atoms:
#1 -x+3/2,y+1/2,-z+3/2 #2 x-1,y,z
#3 -x+1,-y+1,-z+1 #4 -x+3/2,y-1/2,-z+3/2
#5 x+1,y,z

Table s7. Hydrogen bonds for complex **5**

D-H . . . A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(1WB)...O(3)#2	0.85	1.84	2.667(5)	163.1
O(1W)-H(1WA)...O(5)#2	0.85	1.97	2.682(5)	140.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+3/2,y+1/2,-z+3/2 #2 x-1,y,z #3 -x+1,-y+1,-z+1
#4 -x+3/2,y-1/2,-z+3/2 #5 x+1,y,z

Table s8. Selected bond length [Å] and angle [°] of complex **6**

Zn(1)-O(1)	1.9808(18)	Zn(1)-N(1)	2.045(2)
Zn(1)-O(4)#1	2.063(2)	Zn(1)-N(2)	2.084(2)
Zn(1)-O(3)#1	2.1861(18)	Zn(1)-C(20)#1	2.448(3)
Zn(2)-O(7)#2	2.0102(17)	Zn(2)-O(8)#3	2.0349(16)
Zn(2)-O(2)	2.0514(18)	Zn(2)-O(1W)	2.100(2)
Zn(2)-O(5)	2.1110(18)	Zn(2)-Zn(2)#4	3.1462(7)
O(1)-Zn(1)-N(1)	106.37(8)	O(1)-Zn(1)-O(4)#1	111.86(8)
N(1)-Zn(1)-O(4)#1	140.85(9)	O(1)-Zn(1)-N(2)	96.92(8)
N(1)-Zn(1)-N(2)	81.16(9)	O(4)#1-Zn(1)-N(2)	101.88(8)
O(1)-Zn(1)-O(3)#1	109.07(7)	N(1)-Zn(1)-O(3)#1	98.21(8)
O(4)#1-Zn(1)-O(3)#1	61.79(7)	N(2)-Zn(1)-O(3)#1	152.90(8)
O(1)-Zn(1)-C(20)#1	112.65(8)	N(1)-Zn(1)-C(20)#1	123.19(9)
O(7)#2-Zn(2)-O(8)#3	153.59(7)	O(7)#2-Zn(2)-O(2)	106.37(7)
O(8)#3-Zn(2)-O(2)	99.87(7)	O(7)#2-Zn(2)-O(1W)	92.27(8)
O(8)#3-Zn(2)-O(1W)	94.16(7)	O(2)-Zn(2)-O(1W)	82.33(8)
O(7)#2-Zn(2)-O(5)	86.02(7)	O(8)#3-Zn(2)-O(5)	84.69(7)
O(2)-Zn(2)-O(5)	104.22(7)	O(1W)-Zn(2)-O(5)	173.44(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x-1/2,y-1/2,-z+1/2 #2 -x+1,-y,-z+1
#3 x-1,y,z #4 -x,-y,-z+1 #5 -x-1/2,y+1/2,-z+1/2
#6 x+1,y,z

Table s9. Hydrogen bonds for complex **6** [Å and deg.].

D-H . . . A	d (D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(1WA)...O(3)#1	0 . 8 6(4)	2.01(4)	2.851(3)	167(3)
O(1W)-H(1WB)...O(5)#4	0.82	2.52	2.935(3)	112.6
O(1W)-H(1WB)...O(6)#4	0.82	1.86	2.667(3)	169.1

Symmetry transformations used to generate equivalent atoms:

#1 -x-1/2,y-1/2,-z+1/2 #2 -x+1,-y,-z+1 #3 x-1,y,z
#4 -x,-y,-z+1 #5 -x-1/2,y+1/2,-z+1/2 #6 x+1,y,z

Table s10. Selected bond length [Å] and angle [°] of complex **7**

Co(1)-O(4)#1	2.073(4)	Co(1)-O(4)#2	2.073(4)
Co(1)-O(5)#3	2.142(4)	Co(1)-O(5)	2.142(4)
Co(1)-O(1)	2.292(4)	Co(1)-O(1)#3	2.292(4)
Co(2)-O(3)#2	2.028(4)	Co(2)-O(7)#4	2.042(5)
Co(2)-O(1W)	2.045(4)	Co(2)-O(5)#3	2.104(4)
Co(2)-O(1)	2.121(4)	Co(2)-O(2W)#5	2.322(4)
Co(3)-O(2)#5	2.049(5)	Co(3)-O(1W)#5	2.086(4)
Co(3)-O(3W)	2.086(4)	Co(3)-O(8)#4	2.104(4)
Co(3)-O(1W)	2.108(4)	Co(3)-O(2W)	2.197(4)
O(4)#1-Co(1)-O(4)#2	180.0	O(4)#1-Co(1)-O(5)	92.27(16)
O(4)#2-Co(1)-O(5)	87.73(16)	O(4)#1-Co(1)-O(5)#3	87.73(16)
O(4)#2-Co(1)-O(5)#3	92.27(16)	O(5)-Co(1)-O(5)#3	180.0
O(4)#1-Co(1)-O(1)#3	94.98(15)	O(4)#2-Co(1)-O(1)#3	85.02(15)
O(5)-Co(1)-O(1)#3	73.31(15)	O(5)#3-Co(1)-O(1)#3	106.69(15)
O(4)#1-Co(1)-O(1)	85.02(15)	O(4)#2-Co(1)-O(1)	94.98(15)
O(5)-Co(1)-O(1)	106.69(15)	O(5)#3-Co(1)-O(1)	73.31(15)
O(1)#3-Co(1)-O(1)	180.0	O(3)#2-Co(2)-O(7)#4	87.89(19)
O(3)#2-Co(2)-O(1W)	95.78(17)	O(7)#4-Co(2)-O(1W)	97.98(17)
O(3)#2-Co(2)-O(5)#3	92.57(16)	O(7)#4-Co(2)-O(5)#3	88.79(17)
O(1W)-Co(2)-O(5)#3	169.41(16)	O(3)#2-Co(2)-O(1)	87.07(17)
O(7)#4-Co(2)-O(1)	165.32(17)	O(1W)-Co(2)-O(1)	96.23(16)
O(5)#3-Co(2)-O(1)	77.68(16)	O(3)#2-Co(2)-O(2W)#5	170.74(17)
O(7)#4-Co(2)-O(2W)#5	88.78(17)	O(1W)-Co(2)-O(2W)#5	76.13(15)
O(5)#3-Co(2)-O(2W)#5	96.00(15)	O(1)-Co(2)-O(2W)#5	98.18(16)
O(2)#5-Co(3)-O(3W)	86.00(19)	O(2)#5-Co(3)-O(1W)#5	97.91(17)
O(3W)-Co(3)-O(1W)#5	170.48(18)	O(2)#5-Co(3)-O(8)#4	91.27(19)
O(3W)-Co(3)-O(8)#4	99.79(19)	O(1W)#5-Co(3)-O(8)#4	88.83(17)
O(2)#5-Co(3)-O(1W)	177.42(18)	O(3W)-Co(3)-O(1W)	91.63(17)
O(1W)#5-Co(3)-O(1W)	84.26(16)	O(8)#4-Co(3)-O(1W)	90.16(17)
O(2)#5-Co(3)-O(2W)	91.76(18)	O(3W)-Co(3)-O(2W)	93.11(18)
O(1W)#5-Co(3)-O(2W)	78.16(16)	O(8)#4-Co(3)-O(2W)	166.92(18)
O(1W)-Co(3)-O(2W)	87.32(16)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+2 #2 x+1,y,z #3 -x+2,-y,-z+2
#4 -x+5/2,y-1/2,-z+3/2 #5 -x+2,-y,-z+1
#6 x-1,y,z #7 -x+5/2,y+1/2,-z+3/2

Table s11. Selected bond length [Å] and angle [°] of complex **8**

Co(1)-O(7)#1	2.012(3)	Co(1)-O(2W)#2	2.060(3)
Co(1)-O(1)	2.065(3)	Co(1)-O(4)#3	2.107(3)
Co(1)-O(5)#4	2.121(3)	Co(1)-O(1W)	2.300(3)
Co(2)-O(8)#5	2.013(3)	Co(2)-O(8)#6	2.013(3)
Co(2)-O(5)	2.168(3)	Co(2)-O(5)#7	2.168(3)
Co(2)-O(4)	2.194(3)	Co(2)-O(4)#7	2.194(3)
Co(3)-O(2)	2.038(3)	Co(3)-O(2W)	2.056(3)
Co(3)-O(6)#8	2.104(3)	Co(3)-O(2W)#2	2.116(3)
Co(3)-O(3W)	2.140(4)	Co(3)-O(1W)	2.176(3)
O(7)#1-Co(1)-O(2W)#2	98.95(12)	O(7)#1-Co(1)-O(1)	86.99(13)
O(2W)#2-Co(1)-O(1)	91.22(12)	O(7)#1-Co(1)-O(4)#3	91.13(12)
O(2W)#2-Co(1)-O(4)#3	169.91(12)	O(1)-Co(1)-O(4)#3	88.95(12)
O(7)#1-Co(1)-O(5)#4	88.85(12)	O(2W)#2-Co(1)-O(5)#4	101.96(11)
O(1)-Co(1)-O(5)#4	166.65(12)	O(4)#3-Co(1)-O(5)#4	78.45(11)
O(7)#1-Co(1)-O(1W)	176.73(13)	O(2W)#2-Co(1)-O(1W)	77.83(11)
O(1)-Co(1)-O(1W)	93.59(12)	O(4)#3-Co(1)-O(1W)	92.09(11)
O(5)#4-Co(1)-O(1W)	91.29(11)	O(8)#5-Co(2)-O(8)#6	180.0
O(8)#5-Co(2)-O(5)	87.02(12)	O(8)#6-Co(2)-O(5)	92.98(12)
O(8)#5-Co(2)-O(5)#7	92.98(12)	O(8)#6-Co(2)-O(5)#7	87.01(12)
O(5)-Co(2)-O(5)#7	180.00(5)	O(8)#5-Co(2)-O(4)	83.93(11)
O(8)#6-Co(2)-O(4)	96.07(11)	O(5)-Co(2)-O(4)	104.40(11)
O(5)#7-Co(2)-O(4)	75.60(11)	O(8)#5-Co(2)-O(4)#7	96.07(11)
O(8)#6-Co(2)-O(4)#7	83.93(11)	O(5)-Co(2)-O(4)#7	75.60(11)
O(5)#7-Co(2)-O(4)#7	104.40(11)	O(4)-Co(2)-O(4)#7	179.998(1)
O(2)-Co(3)-O(2W)	177.74(14)	O(2)-Co(3)-O(6)#8	85.21(13)
O(2W)-Co(3)-O(6)#8	96.41(12)	O(2)-Co(3)-O(2W)#2	98.59(12)
O(2W)-Co(3)-O(2W)#2	82.83(12)	O(6)#8-Co(3)-O(2W)#2	96.08(12)
O(2)-Co(3)-O(3W)	85.07(15)	O(2W)-Co(3)-O(3W)	93.34(14)
O(6)#8-Co(3)-O(3W)	89.97(15)	O(2W)#2-Co(3)-O(3W)	173.15(14)
O(2)-Co(3)-O(1W)	87.10(12)	O(2W)-Co(3)-O(1W)	91.45(12)
O(6)#8-Co(3)-O(1W)	170.46(13)	O(2W)#2-Co(3)-O(1W)	79.50(11)
O(3W)-Co(3)-O(1W)	94.98(14)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+5/2,y-1/2,-z+3/2 #2 -x+1,-y+1,-z+1
#3 x-1/2,-y+3/2,z+1/2 #4 -x+3/2,y-1/2,-z+3/2
#5 x-1,y,z #6 -x+3,-y+2,-z+1 #7 -x+2,-y+2,-z+1
#8 x-1/2,-y+3/2,z-1/2 #9 x+1/2,-y+3/2,z-1/2
#10 -x+3/2,y+1/2,-z+3/2 #11 x+1/2,-y+3/2,z+1/2
#12 -x+5/2,y+1/2,-z+3/2 #13 x+1,y,z