Supplementary Material (ESI) for Dalton Transactions

Supplementary materials

Isomorphic coordination polymers of Cobalt(II), Zinc(II) with a flexible ligand of cis, cis, cis-1, 2, 3, 4-cyclopentanetetracarboxylic acid and their molecular alloy: crystal structures, thermal decomposition mechanisms and magnetic properties

Liang-Fang Huang, Chang-Chun Ji, Zhen-Zhong Lu, Xiao-Qiang Yao, Jin-Song Hu and He-Gen Zheng*

State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing National Laboratory of Microstructures, Nanjing University, Nanjing 210093, P. R. China

E-mail: zhenghg@nju.edu.cn

Fig. S1 Neighboring three-nuclear unit to form a chain by carboxylate along the *b*-axis direction and packing diagram of 3D supramolecular framework in **2** (dotted lines show hydrogen bonds).

Fig. S2 Neighboring three-nuclear unit to form a chain by carboxylate along the *b*-axis direction and packing diagram of 3D supramolecular framework in **3** (dotted lines show hydrogen bonds).

Fig. S3 XPS spectra of Zn 2p and Co 2p for complex **3**.

Fig. S4 (a) EDS spectra for complex **3** (b) Typical SEM image from complex **3**.

Fig. S5 Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of complex **1** at 293K.

Fig. S6 Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of complex **2** at 293K.

Fig. S7 Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of complex **3** at 293K.

Fig. S8 Temperature dependence of $\chi_M T$ for **1** (inset: plot of χ_M^{-1} versus T, open circles and red line represent experimental data and fits).

Fig. S9 Temperature dependence of $\chi_M T$ for **3** (open circles represent experimental data).

Table S1 Selected bond lengths (Å) and bond angles (°) for **1**, **2** and **3**.

Table S2 XPS peak table of complex **3**.

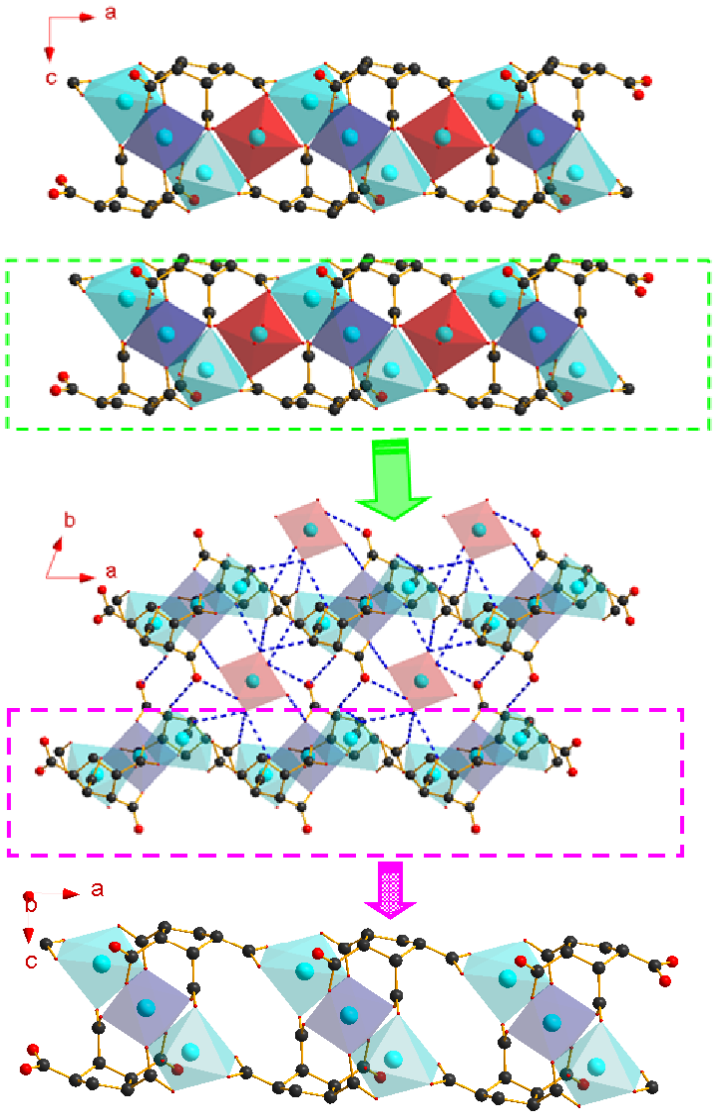


Fig. S1 Neighboring three-nuclear unit to form a chain by carboxylate along the *b*-axis direction and packing diagram of 3D supramolecular framework in **2** (dotted lines show hydrogen bonds).

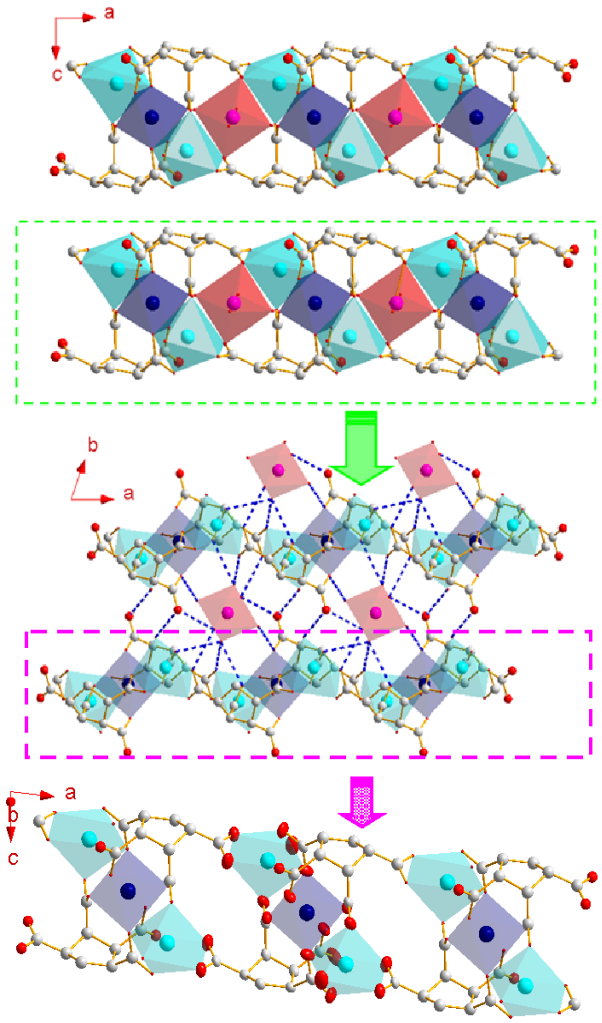


Fig. S2 Neighboring three-nuclear unit to form a chain by carboxylate along the *b*-axis direction and packing diagram of 3D supramolecular framework in **3** (dotted lines show hydrogen bonds).

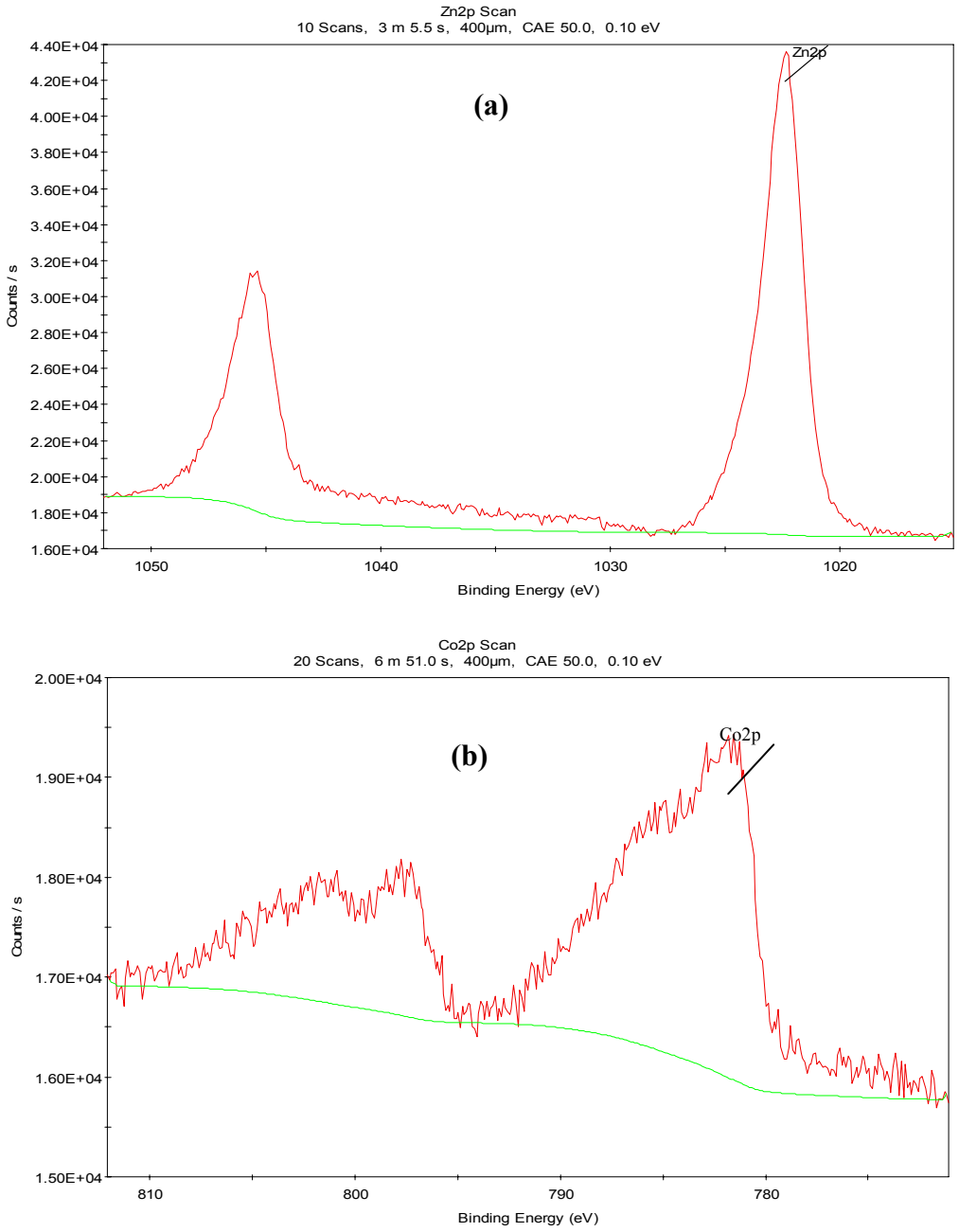
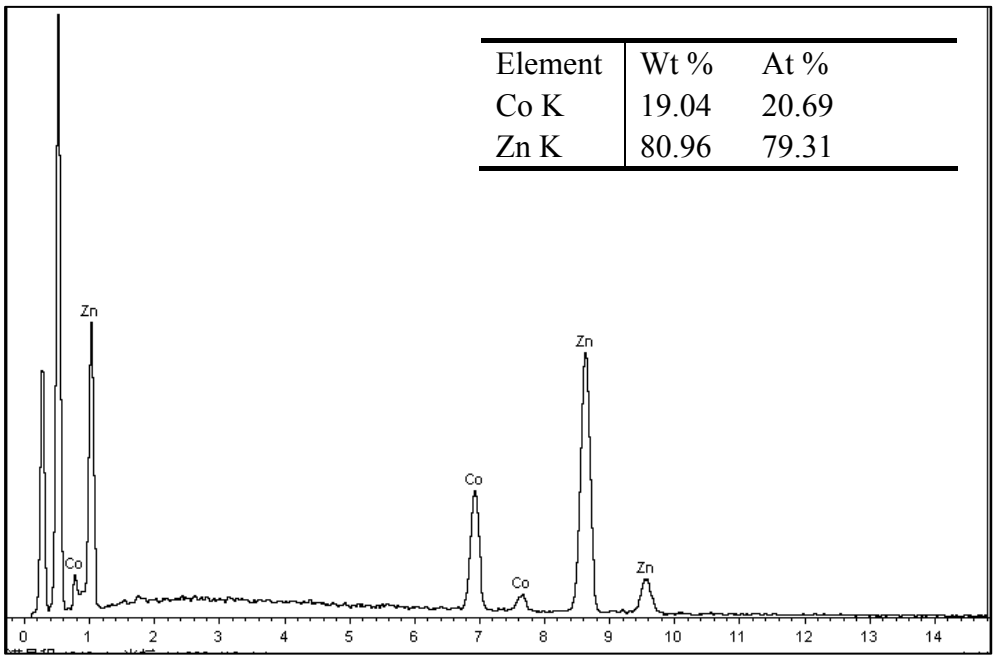
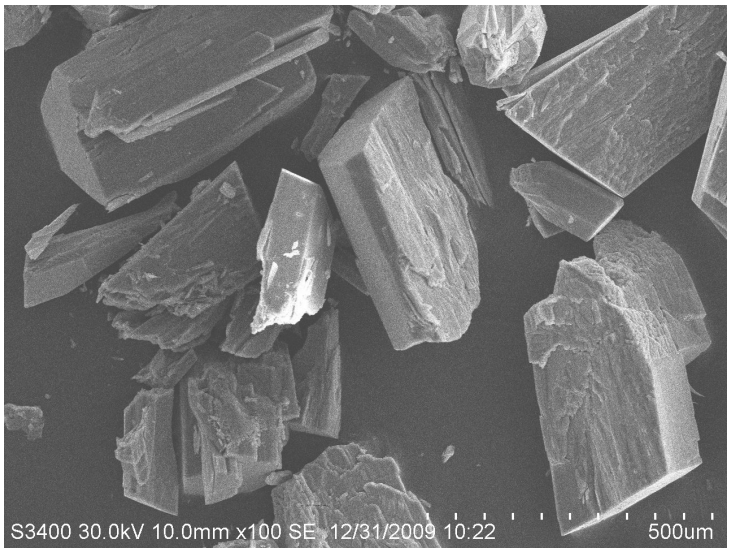


Fig. S3 XPS spectra of Zn 2p and Co 2p for complex **3**.



(a)



(b)

Fig. S4 (a) EDS spectra for complex **3** (b) Typical SEM image from complex **3**.

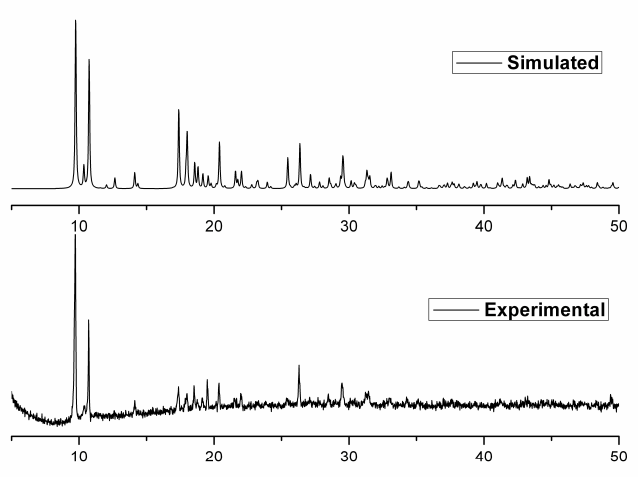


Fig. S5 Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of complex **1** at 293K.

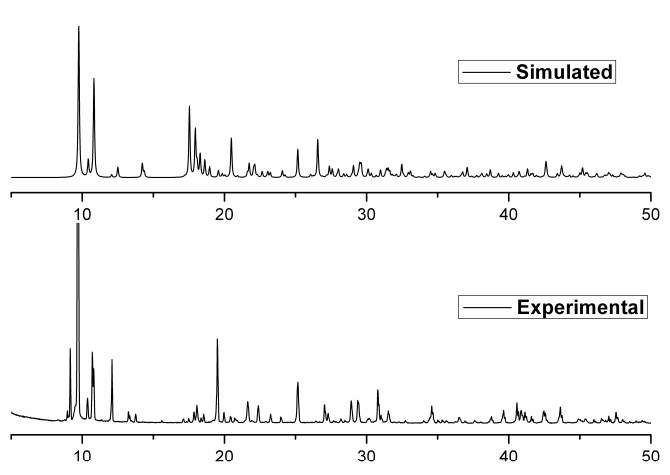


Fig. S6 Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of complex **2** at 293K.

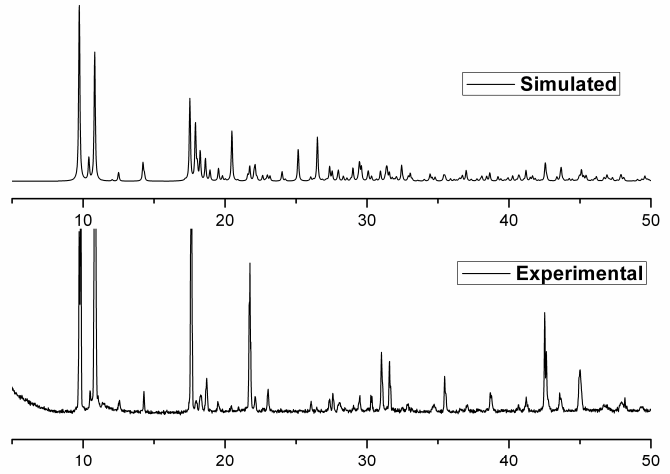


Fig. S7 Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of complex **3** at 293K

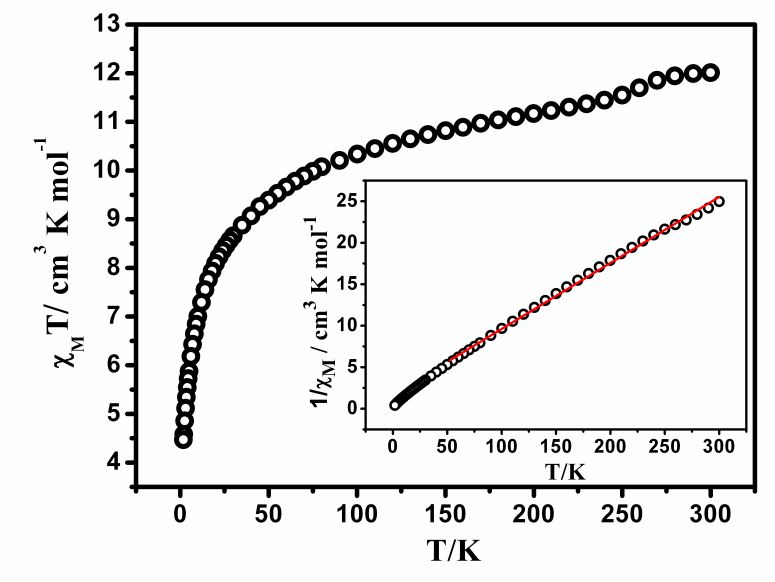


Fig. S8 Temperature dependence of $\chi_M T$ for **1** (inset: plot of χ_M^{-1} versus T, open circles and red line represent experimental data and fits).

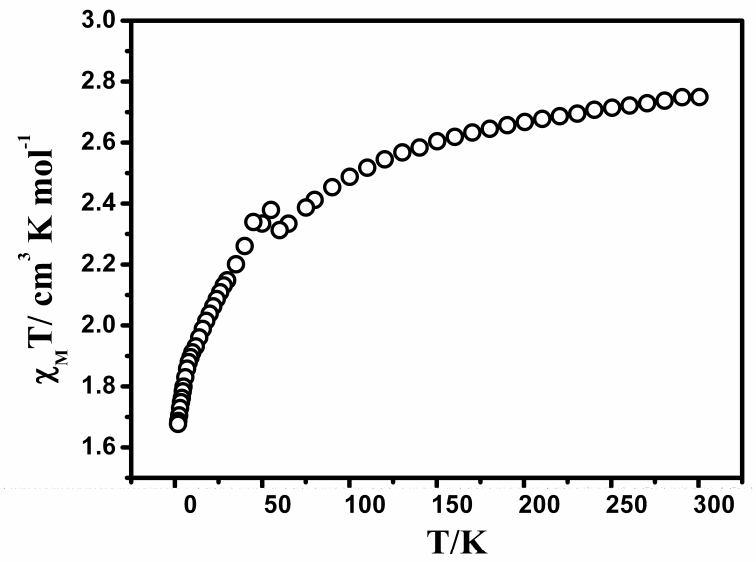


Fig. S9 Temperature dependence of $\chi_M T$ for **3** (open circles represent experiemental data).

Table S1 Selected bond lengths (Å) and angles (◦) for complexes **1**, **2** and **3**

		Complex **1**	
Co1-O7	2.056(3)	Co2-O9	2.067(3)
Co1-O8	2.061(3)	Co2-O3	2.070(3)
Co1-O6	2.113(3)	Co3-O12	2.071(3)
Co1-O4	2.161(3)	Co3-O10	2.074(3)
Co1-O3	2.197(3)	Co3-O11	2.079(3)
Co1-O5	2.197(3)	O2-Co2-O9	89.93(11)
O7-Co1-O8	93.38(14)	O2-Co2-O9#1	90.07(11)
O7-Co1-O6	100.61(12)	O9-Co2-O9#1	180.0 2_766
O8-Co1-O6	92.17(12)	O2-Co2-O3	90.65(11)
O7-Co1-O4	156.46(12)	O2-Co2-O3#1	89.35(11)
O8-Co1-O4	95.81(13)	O9-Co2-O3	85.28(11)
O6-Co1-O4	100.65(12)	O9-Co2-O3#1	94.72(11)
O7-Co1-O3	100.01(11)	O3-Co2-O3#1	180.000(1)
O8-Co1-O3	85.74(12)	O12-Co3-O12#3	180.0 2_656
O6-Co1-O3	159.36(11)	O12-Co3-O10	89.13(14)
O4-Co1-O3	59.27(10)	O12-Co3-O10#3	90.87(14)
O7-Co1-O5	96.68(13)	O10-Co3- O10#3	180.0
O8-Co1-O5	151.86(12)	O10-Co3- O11	92.72(13)
O6-Co1-O5	60.19(11)	O10-Co3- O11#3	87.28(13)
O4-Co1-O5	85.23(12)	O12-Co3- O11	90.67(14)
O3-Co1-O5	118.01(11)	O12-Co3- O11#3	89.33(14)
O2-Co2-O2#1	180.00(16)	O11-Co3- O11#3	180.0
Co2-O2	2.060(3)		
		Complex **2**	
Zn1-O7	2.017(3)	Zn2-O2	2.035(3)
Zn1-O8	2.067(3)	Zn2-O9	2.0813)
Zn1-O6	2.094(3)	Zn2-O3	2.097(3)
Zn1-O4	2.211(3)	Zn3-O12	2.065(3)
Zn1-O3	2.217(3)	Zn3-O10	2.096(3)
Zn1-O5	2.247(3)	Zn3-O11	2.091(3)
O7-Zn1-O8	93.38(13)	O2-Zn2-O9#1	88.93(10)
O7-Zn1-O6	108.59(11)	O9-Zn2-O9#1	180.00(14)
O8-Zn1-O6	91.64(12)	O2-Zn2-O3	88.73(11)
O7-Zn1-O4	152.32(11)	O2-Zn2-O3#1	91.27(11)
O8-Zn1-O4	98.07(13)	O9-Zn2-O3	86.05(10)
O6-Zn1-O4	96.18(11)	O9-Zn2-O3#1	93.95(10)
O7-Zn1-O3	96.94(10)	O3-Zn2-O3#1	180.000(1)
O8-Zn1-O3	89.18(11)	O12-Zn3-O12#3	180.000(1)
O6-Zn1-O3	154.35(10)	O12-Zn3-O10	88.57(12)
O4-Zn1-O3	58.37(10)	O12-Zn3-O10#3	91.43(12)
O7-Zn1-O5	96.44(11)	O10-Zn3- O10#3	180.0
O8-Zn1-O5	151.39(12)	O10-Zn3- O11	87.56(12)

O6-Zn1-O5	59.76(10)	O11-Zn3- O10#3	92.44(12)
O4-Zn1-O5	85.29(11)	O11-Zn3- O11#3	180.0
O3-Zn1-O5	116.02(11)	O12-Zn3- O11	91.07(12)
O2-Zn2-O2#1	180.00(16)	O12-Zn3- O11#3	88.93(12)
O2-Zn2-O9	91.07(10)		
	Complex **3**		
Zn1-O7	2.016(4)	Co2-O2	2.042(4)
Zn1-O8	2.059(4)	Co2-O9	2.078(4)
Zn1-O6	2.109(4)	Co2-O3	2.081(4)
Zn1-O4	2.203(5)	Co3-O12	2.068(4)
Zn1-O3	2.216(4)	Co3-O10	2.102(4)
Zn1-O5	2.248(5)	Co3-O11	2.088(4)
O7-Zn1-O8	93.7(2)	O2-Co2-O9#1	89.07(15)
O7-Zn1-O6	108.36(16)	O9-Co2-O9#1	180.00(5)
O8-Zn1-O6	91.18(17)	O2-Co2-O3	88.79(16)
O7-Zn1-O4	152.64(16)	O2-Co2-O3#1	91.21(16)
O8-Zn1-O4	97.9(2)	O9-Co2-O3	85.89(15)
O6-Zn1-O4	96.15(16)	O9-Co2-O3#1	94.11(15)
O7-Zn1-O3	97.01(15)	O3-Co2-O3#1	180.0
O8-Zn1-O3	89.88(17)	O12-Co3-O12#3	180.0
O6-Zn1-O3	154.48(16)	O12-Co3-O10	91.13(17)
O4-Zn1-O3	58.47(15)	O12-Co3-O10#3	88.87(17)
O7-Zn1-O5	96.31(17)	O10-Co3- O10#3	180.0
O8-Zn1-O5	151.07(17)	O10-Co3- O11	92.76(17)
O6-Zn1-O5	59.90(15)	O10-Co3- O11#3	87.24(17)
O4-Zn1-O5	85.41(18)	O11-Co3- O11#3	180.0
O3-Zn1-O5	115.62(17)	O12-Co3- O11#3	91.48(18)
O2-Co2-O2#1	180. 0	O12-Co3- O11	88.52(18)
O2-Co2-O9	90.93(15)		

Symmetry codes : #1 = 2-x, 1-y, 1-z; #2 = -1+x, y, z; #3 = 1-x, -y, 1-z; #4 = 1+x, y, z.

Table S2 XPS Peak table of complex **3**

Name	Start BE	Peak BE	End BE	PP Hgt (N)	PP At. %
C1s	297.98	285.13	279.18	33.56	46.49
O1s	544.98	532.05	525.18	22.95	31.78
Co2p	811.98	781.62	771.18	3.82	5.29
Zn2p	1051.98	1022.41	1015.18	11.87	16.44