

Impact of N-donor auxiliary ligands on three new Co(II)-based coordination polymers with symmetrical tetracarboxylate ligands: magnetism study

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Contents

Figure S1. The coordination modes of **L** in **1-3**.

Figure S2. Simulated and observed PXRD patterns of CPs **1-3**.

Figure S3. Infrared spectra of CPs **1-3**.

Figure S4. The TG curves of CPs **1-3**.

Table S1. Crystal data and structure refinement for CPs **1-3**.

Table S2. Selected Bond Lengths (Å) and angles (°) for CPs **1-3**.

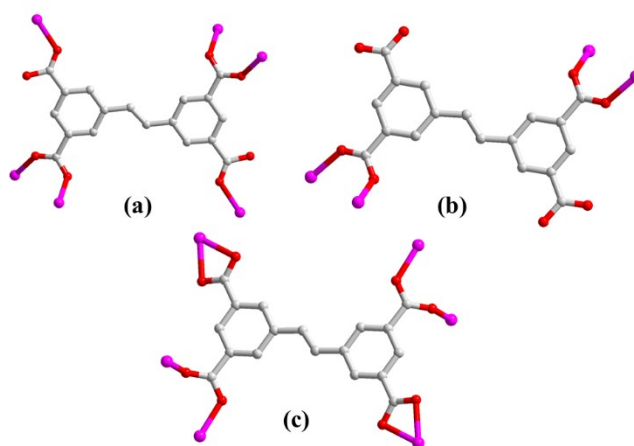


Figure S1. The coordination modes of **L** in **1-3**.

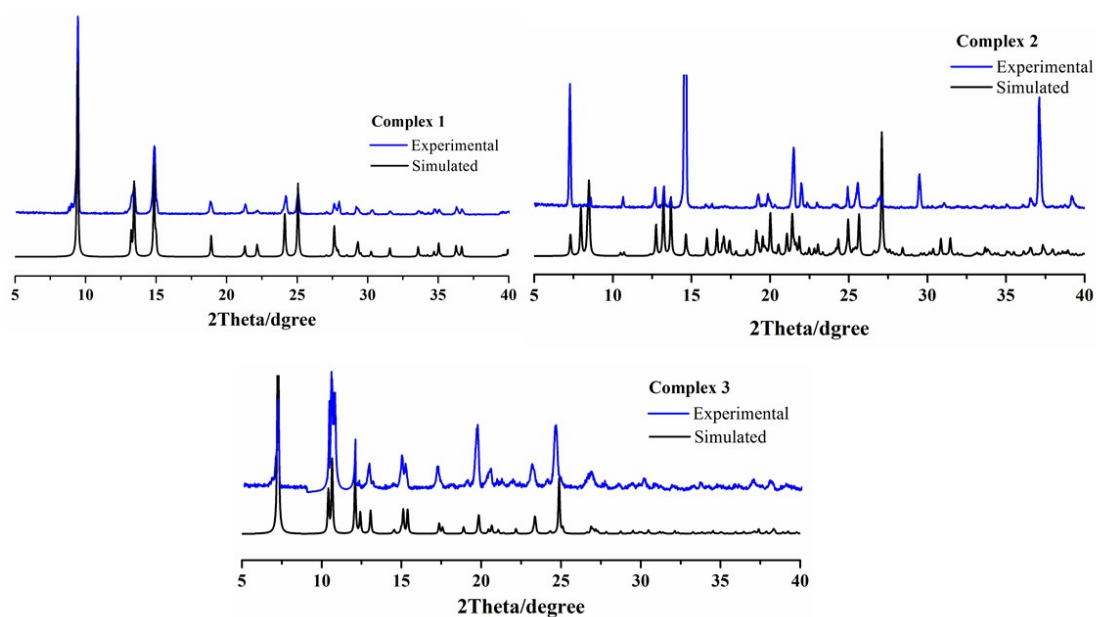


Figure S2. Simulated and observed PXRD patterns of CPs **1-3**.

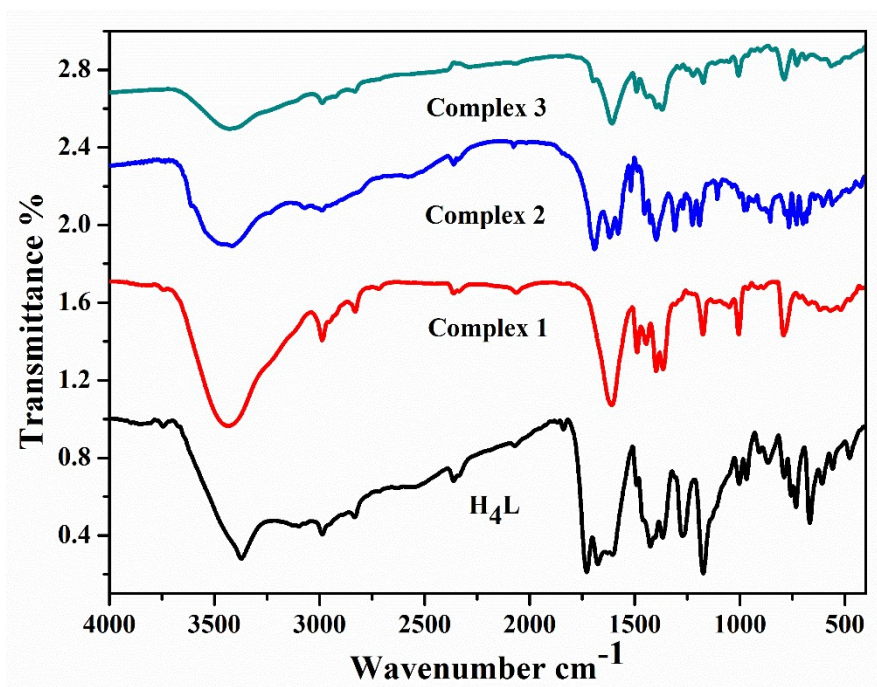


Figure S3. Infrared spectra of CPs 1-3.

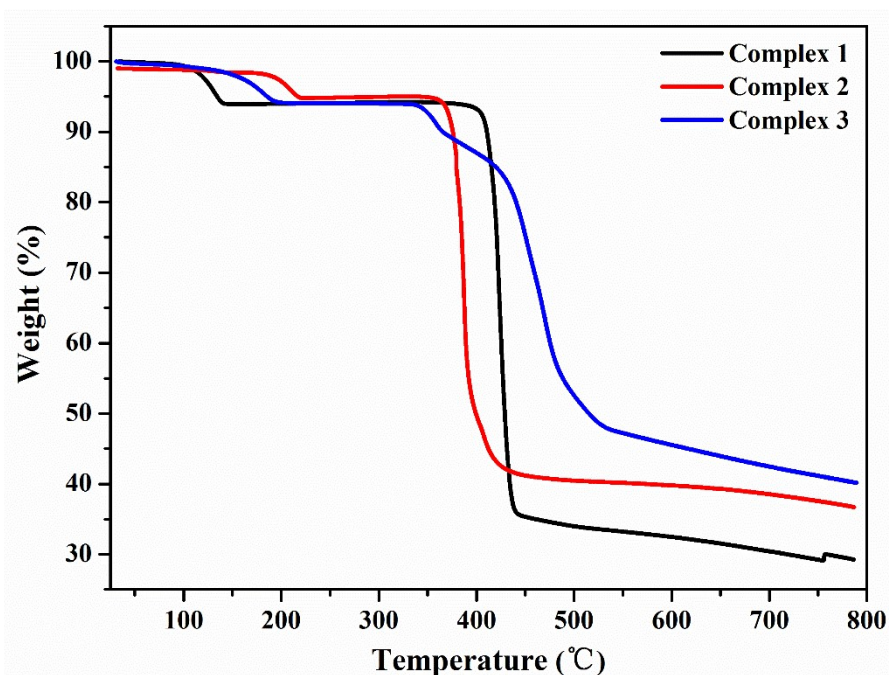


Figure S4. The TG curves of CPs 1-3.

Table S1. Crystal data and structure refinement for CPs 1-3.

Complex	1	2	3
Empirical formula	$C_{18}H_{10}CoO_8$	$C_{39}H_{28}CoN_2O_{14}$	$C_{37}H_{26}Co_2N_4O_{14}$
Formula weight	413.19	807.56	868.48
Temperature (K)	298	293	296

Wavelength (Å)	1.54184	1.54184	0.710730
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	$P2_1/c$	$P\bar{1}$	$P\bar{1}$
Unit cell dimension			
a (Å)	4.4234(2)	11.6020(7)	8.0125(7)
b (Å)	13.3689(5)	12.0259(8)	9.6714(8)
c (Å)	13.1637(5)	14.2958(9)	13.1079(11)
α (°)	90	68.618(6)	109.886(2)
β (°)	90.391(3)	66.501(6)	90.701(3)
γ (°)	90	88.714(5)	112.409(3)
V (Å ³)	778.43(5)	1685.6(2)	871.22(13)
Z	2	2	1
D_{calc} (Mg m ⁻³)	1.763	1.591	1.655
μ (mm ⁻¹)	9.11	4.69	1.03
$F(000)$	418	830	442
Crystal size (mm)	0.07 × 0.05 × 0.04	0.12 × 0.12 × 0.11	0.08 × 0.06 × 0.03
θ range (°)	4.7 to 75.1	3.7 to 71.1	2.4 to 27.5
Index ranges	-3 ≤ h ≤ 5, -15 ≤ k ≤ 15, -15 ≤ l ≤ 15	-12 ≤ h ≤ 13, -13 ≤ k ≤ 14, -17 ≤ l ≤ 17	-8 ≤ h ≤ 10, -12 ≤ k ≤ 11, -16 ≤ l ≤ 17
Reflections collected	4196	10881	7684
Independent reflection	1369 [$R_{\text{int}} = 0.043$]	6027 [$R_{\text{int}} = 0.037$]	3949 [$R_{\text{int}} = 0.026$]
Data/restraints/parameters	1369/0/125	6027/156/509	3949/140/309
Final R_1 , wR_2 indices	0.037, 0.096	0.058, 0.147	0.041, 0.104
$[I > 2\sigma(I)]$			
R_1 , wR_2 indices (all data)	0.049, 0.101	0.029, 0.157	0.049, 0.111
GOF	1.05	1.10	1.02
$\Delta\rho_{\text{max,min}}$ (e Å ⁻³)	0.42/-0.60	1.01/-0.60	0.78/-0.75

Table S2. Selected Bond Lengths (Å) and angles (°) for CPs 1-3.

Complex 1					
Co1—O1#1	2.1464 (17)	Co1—O2#3	2.0433 (18)	Co1—O3#4	2.0974 (18)
Co1—O1#2	2.1464 (18)	Co1—O2	2.0432 (18)	Co1—O3#5	2.0974 (18)
O1#2—Co1—O1#1	180.0	O2—Co1—O3#4	94.57 (8)		
O2#3—Co1—O1#1	92.93 (7)	O2#3—Co1—O3#4	85.43 (8)		
O2—Co1—O1#2	92.93 (7)	O3#4—Co1—O1#1	88.18 (7)		

O2—Co1—O1#1	87.07 (7)	O3#5—Co1—O1#2	88.18 (7)
O2#3—Co1—O1#2	87.07 (7)	O3#5—Co1—O1#1	91.82 (7)
O2—Co1—O2#3	180.0	O3#4—Co1—O1#2	91.82 (7)
O2#3—Co1—O3#5	94.57 (8)	O3#4—Co1—O3#5	180.0
O2—Co1—O3#5	85.43 (8)		

Symmetry codes for #1 $-x, y+1/2, -z+1/2$; #2 $x, -y+3/2, z+1/2$; #3 $-x, -y+2, -z+1$; #4 $-x+1, -y+2, -z+1$; #5 $x-1, y, z$; #6 $-x, y-1/2, -z+1/2$; #7 $x+1, y, z$; #8 $-x+2, -y+1, -z+1$.

Complex 2

Co1—O14	2.048 (3)	Co1—O1#1	2.097 (3)	Co1—N1	2.144 (3)
Co1—O2	2.051 (3)	Co1—N2	2.100 (3)	Co1—O13	2.288 (3)
O14—Co1—O2	95.62 (11)	O1#1—Co1—N1	86.40 (12)		
O14—Co1—O1#1	94.18 (12)	N2—Co1—N1	78.45 (11)		
O2—Co1—O1#1	106.62 (12)	O14—Co1—O13	82.99 (12)		
O14—Co1—N2	173.26 (11)	O2—Co1—O13	77.53 (12)		
O2—Co1—N2	91.02 (11)	O1#1—Co1—O13	175.24 (11)		
O1#1—Co1—N2	85.03 (11)	N2—Co1—O13	97.33 (12)		
O14—Co1—N1	94.82 (11)	N1—Co1—O13	90.02 (12)		
O2—Co1—N1	162.62 (11)				

Symmetry codes for #1 $-x+2, -y, -z+2$; #2 $-x+3, -y, -z+1$.

Complex 3

Co1—O1	2.0358(16)	Co1—O1W	2.095(2)	Co1—O3#2	2.1242(16)
Co1—O2#1	2.0641(18)	Co1—N1	2.115(9)	Co1—O4#2	2.2736(18)
O1—Co1—O2#1	94.63(7)	O1W—Co1—O3#2	88.10(8)		
O1—Co1—O1W	81.12(8)	N1—Co1—O3#2	93.0(3)		
O2#1—Co1—O1W	173.13(8)	O1—Co1—O4#2	88.11(6)		
O1—Co1—N1	119.1(3)	O2#1—Co1—O4#2	90.86(7)		
O2#1—Co1—N1	91.60(19)	O1W—Co1—O4#2	94.37(9)		

O1W—Co1—N1	85.8(2)	N1—Co1—O4#2	152.3(3)
O1—Co1—O3#2	144.88(7)	O3#2—Co1—O4#2	59.34(6)
O2#1—Co1—O3#2	98.41(7)		

Symmetry codes for #1 $-x+1, -y+1, -z+1$; #2 $x-1, y-1, z$; #3 $-x+2, -y+2, -z+2$; #4 $x+1, y+1, z$.
