<Electronic Supplementary Information>

Auxiliary ligand-induced structural diversities of octacyanometalates-based coordination polymers towards diverse magnetic properties

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Table S1. Selected Bond Lengths (Å) and Angles (°) of CPs 1, 2, and 3.

CP-1		CP-2		CP-3	
W(1)–C(1)#1	2.164(4)	Mo(1)–C(1)#1	2.146(5)	W(1)–C(1)	2.037(7)
W(1)–C(2)#3	2.153(4)	Mo(1)–C(2)#2	2.157(5)	W(1)–C(1)#1	2.037(7)
Co(1)-O(2)#4	2.126(3)	Co(1)-O(1)#4	2.126(3)	W(1)–C(2)#2	2.099(7)
Co(1)–O(3)#4	2.072(3)	Co(1)–O(2)#4	2.073(3)	W(1)–C(2)#3	2.099(7)
Co(1)–N(2)	2.074(4)	Co(1)–N(1)	2.068(4)	Co(1)–N(1)#4	2.116(8)
Cl(1)–O(1)#5	1.411(6)	Cl(1)–O(3)#5	1.436(6)	Co(1)–N(3)	1.905(6)
Cl(1)–O(1)#6	1.411(6)	Cl(1)–O(3)#6	1.436(6)	Co(1)–N(3)#5	1.905(6)
Cl(1)–O(1)#7	1.411(6)	Cl(1)–O(3)#7	1.436(6)	N(4)–N(4)#6	1.252(6)
N(1)-C(1)-W(1)	178.7(4)	N(1)-C(1)-Mo(1)	176.4(4)	C(1)–W(1)–C(1)#2	97.07(1)
N(2)-C(2)-W(1)	176.9(4)	N(2)-C(2)-Mo(1)	178.6(4)	C(1)–W(1)–C(2)	74.02(2)
C(2)-N(2)-Co(1)	160.5(4)	C(1)-N(1)-Co(1)	160.6(4)	C(1)#2–W(1)–C(2)	148.9(3)
C(1)#2–W(1)–C(2)#1	75.8(2)	C(1)–Mo(1)–C(2)#3	142.2(2)	C(1)#3–W(1)–C(2)	72.2(3)
C(1)#1–W(1)–C(2)	142.3(2)	C(1)#1–Mo(1)–C(2)	75.5(2)	C(2)–W(1)–C(2)#2	128.0(2)
C(1)#2–W(1)–C(2)	71.7(2)	C(1)#1–Mo(1)–C(2)#3	71.5(2)	C(2)#2–W(1)–C(2)#3	76.6(4)
C(2)#1–W(1)–C(2)	131.8(1)	C(2)#3–Mo(1)–C(2)	94.8(7)	N(3)–Co(1)–N(3)#5	83.8(4)
C(2)–W(1)–C(2)#3	70.6(2)	C(2)–Mo(1)–C(2)#1	146.3(2)	N(3)–Co(1)–N(1)#4	94.3(2)
O(3)#4–Co(1)–N(2)	90.5(1)	O(2)#4–Co(1)–N(1)	90.3(2)	N(1)#4–Co(1)–N(1)	160.92(1)
O(3)–Co(1)–N(2)	89.5(1)	O(2)–Co(1)–O(1)#4	87.8(1)	N(3)#5-Co(1)-N(1)#4	99.9(2)

Symmetry transformations used to generate equivalent atoms of CP-1:
#1 –y–3/4, x+1/4, –z+1/4 #2 y–1/4, –x–3/4, –z+1/4 #3 –x–1, –y–1/2, z+0 #4 –x–1, –y–1, –z #5 y–1/4, –x–7/4, –z+1/4 #6 –x–2, –y–3/2, z+0 #7 –y–7/4, x+1/4, –z+1/4

Symmetry transformations used to generate equivalent atoms of CP-2:
#1 –x–1, –y–1/2, z+0 #2 –y–3/4, x+1/4, –z+1/4 #3 y–1/4, –x–3/4, –z+1/4 #4 –x–3/2, –y–1/2, –z+1/2 #5 y–1/4, –x–7/4, –z+1/4 #6 –y–7/4, x+1/4, –z+1/4 #7 –x–2, –y–3/2, z+0

Symmetry transformations used to generate equivalent atoms of CP-3:
#1 –x+0, –y+1/2, z+0 #2 y–1/4, –x+1/4, –z+3/4 #3 –y+1/4, x+1/4, –z+3/4 #4 –x, –y, –z+1 #5 x, –y, –z+1 #6 –y+1/4, –x+1/4, –z+7/4

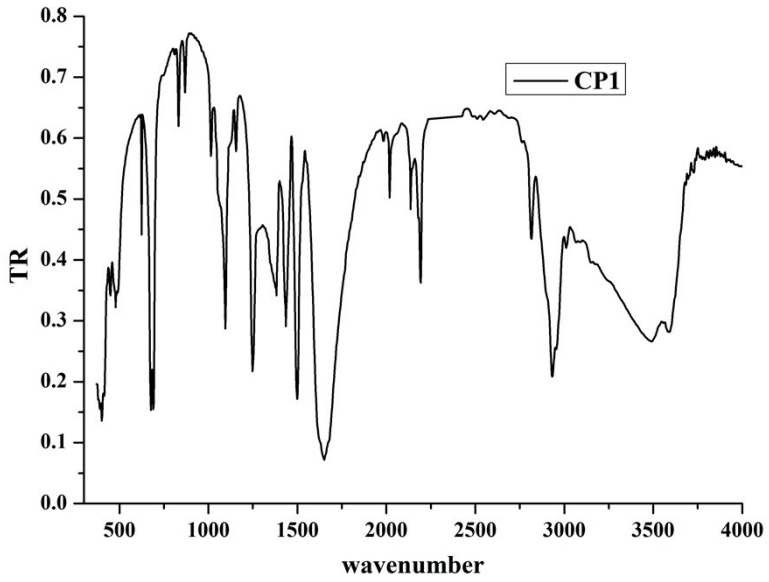

Fig. S1 IR spectrum of CP-1.

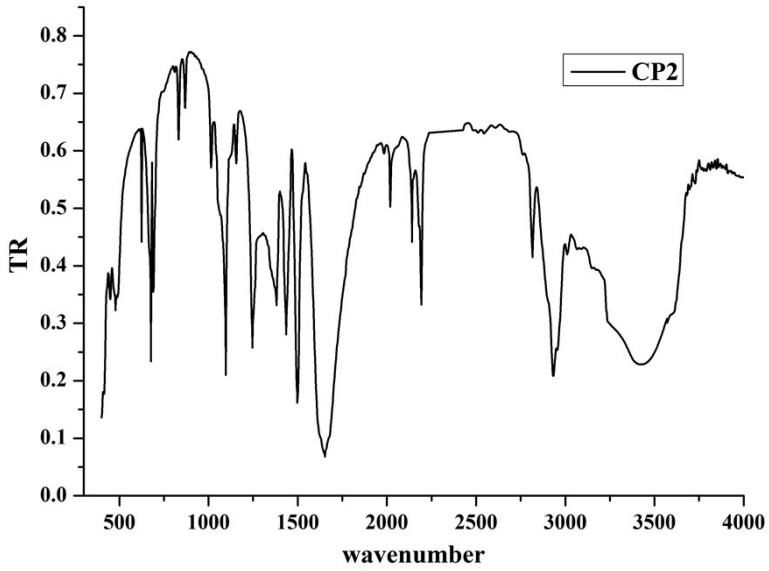

Fig. S2 IR spectrum of CP-2.

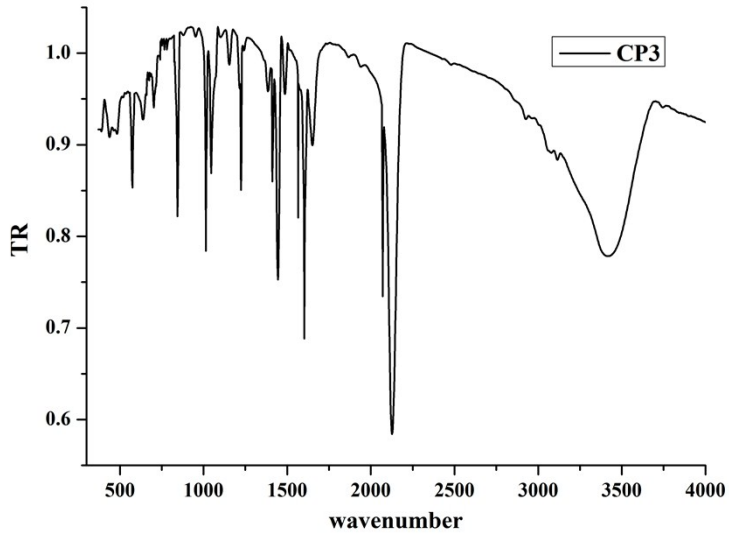

Fig. S3 IR spectrum of CP-3.

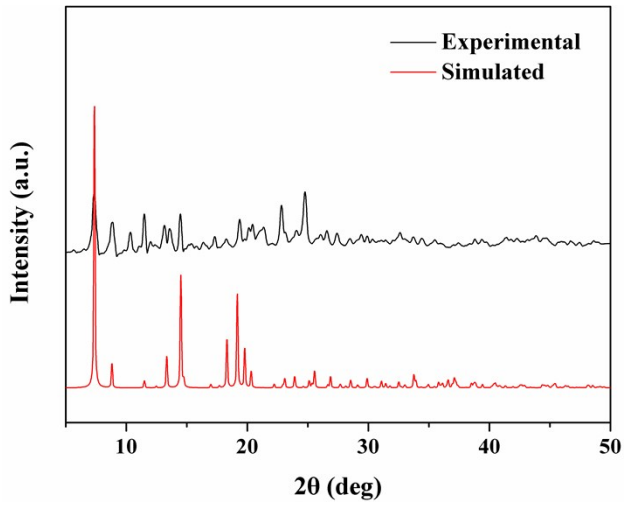

Fig. S4 The experimental powder X-ray diffraction pattern (wavelength λ = 1.5406 Å) of CP-3. The simulated diffraction pattern generated from the single-crystal X-ray diffraction data is given for comparison.

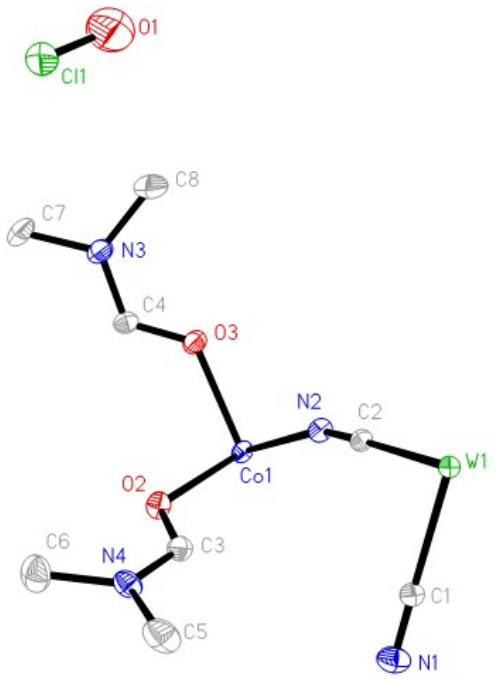

Fig. S5 *ORTEP* diagram of CP-1 with displacement ellipsoids of 30% probability level. Hydrogen atoms were omitted for clarity.

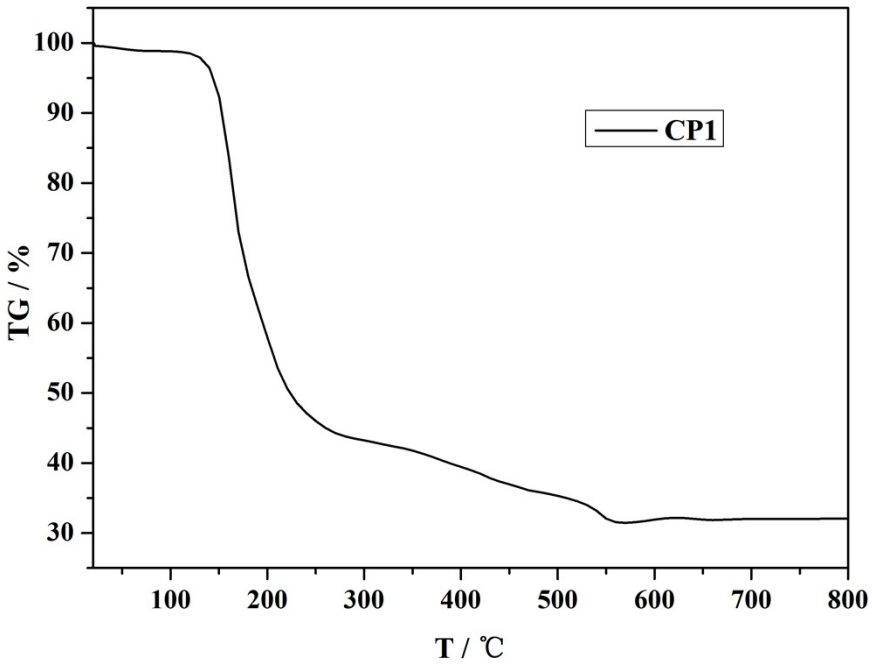

Fig. S6 TGA curve of CP-1.

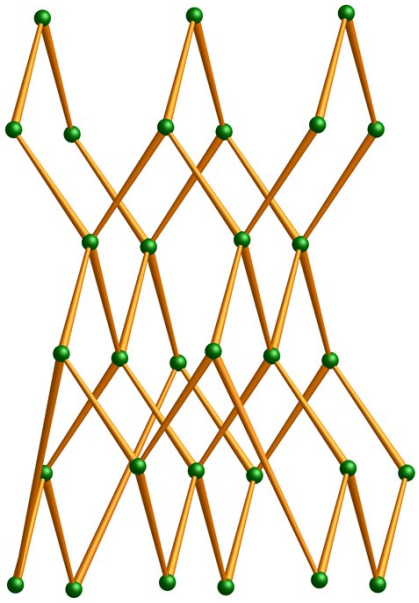

Fig. S7 The topological structure of CP-1.

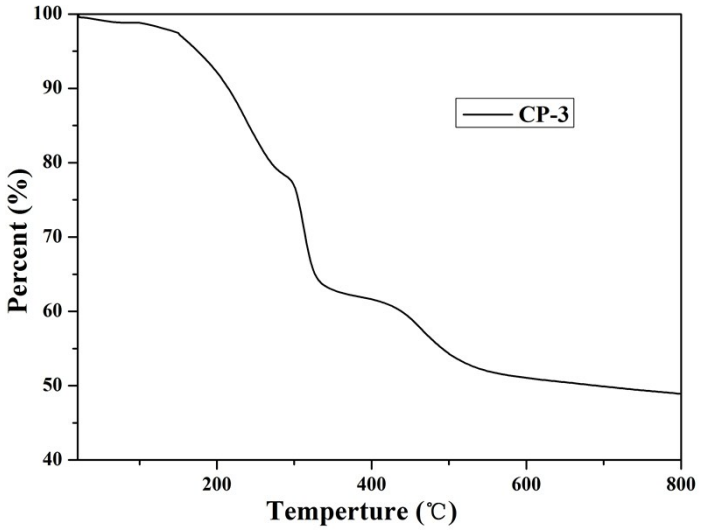

Fig. S8 TGA curve of CP-3.

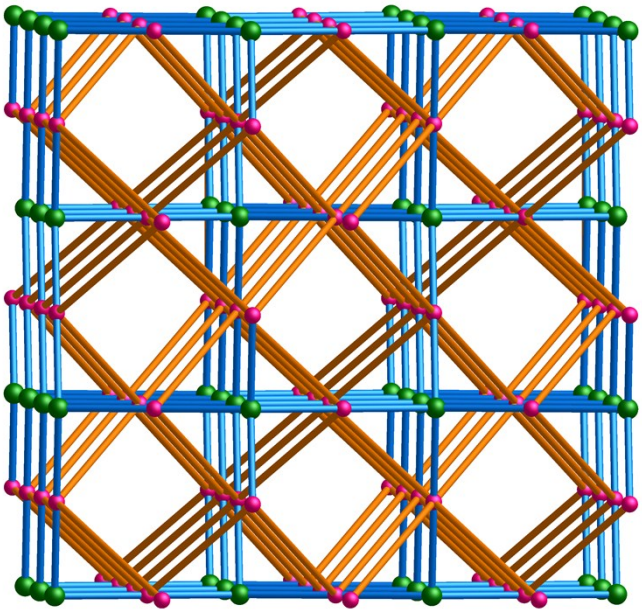

Fig. S9 Topological structure of CP-3.

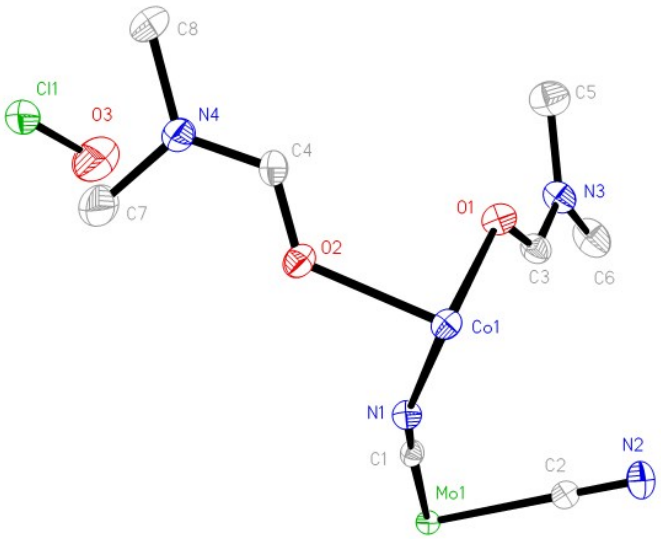

Fig. S10 *ORTEP* diagram of CP-2 with displacement ellipsoids of 30% probability level. Hydrogen atoms were omitted for clarit.