

Supporting Information

Solvent controlled metal coordination polymers of Co(II) with different topological structures and properties

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Physical Measurements

The contents of C, H, and N were determined by a Perkin-Elmer elemental analyzer. Infrared spectra were taken on a Bruker TENOR 27 spectrometer in the region of 4000–400 cm^{-1} . Powder X-ray diffraction patterns (PXRD) were carried out at room temperature on a D/Max-2500 X-ray diffractometer with Cu-K α radiation ($\lambda = 1.5406 \text{ \AA}$). Thermogravimetric test (TG) was measured in the temperature range of 25–800 $^{\circ}\text{C}$ on a NETZSCH TG 209 instrument under N_2 atmosphere. N_2 sorption isotherms were performed from 0 to 1 bar at 77 K with liquid nitrogen by a volumetric method on a Micromeritics ASAP 2020HD88 surface area and pore analyzer. The low pressure gas sorption data of CO_2 at 298 K was carried out on the same instruments.

Crystallographic Data and Diagrams

X-Ray crystallography. Crystallographic data for **Co-(1-3)** were all collected on an Agilent SuperNova (Dual, Cu at zero, AtlasS2, CCD) diffractometer equipped with graphite-monochromated Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$), using the φ - ω scan technique. Semiempirical multiscan absorption corrections were applied by SCALE3

ABSPACK, and the programs CrysAlisPro were used for integration of the diffraction profiles. The structures were solved by direct methods with the ShelXT-2015 structure solution program and refined using least squares minimization by with the ShelXL-2015 refinement package. Some restraints are employed, such as ISOR (anisotropic parameter), DFIX (restricting the distance between two atoms) to solve the disorder of the O atoms. All non-hydrogen atoms were refined anisotropically, and hydrogen atoms were located geometrically and refined isotropically.

Table S1. Selected bond lengths (Å) and bond angles (°) for complex **Co-1**.

Co(1)-O(1)#1	2.058(4)	O(1)-Co(1)-O(3)#1	88.78(16)
Co(1)-O(1)	2.058(4)	O(1)-Co(1)-N(1)#3	88.54(19)
Co(1)-O(3)#1	2.133(4)	O(1)#1-Co(1)-O(1)	180.0
Co(1)-O(3)	2.133(4)	O(1)-Co(1)-O(3)	91.22(16)
Co(1)-N(1)#2	2.142(5)	O(1)-Co(1)-N(1)#2	91.46(19)
Co(1)-N(1)#3	2.142(5)	O(3)#1-Co(1)-N(1)#2	90.58(19)
N(1)-Co(1)#4	2.142(5)	O(3)-Co(1)-N(1)#2	89.42(19)

#1: -x+2, -y+1, -z+1; #2: -x+2, -y, -z+1; #3: x, y+1, z; #4: x, y-1, z; #5: -x+1, -y+1, -z

Table S2. Selected bond lengths (Å) and bond angles (°) for complex **Co-2**.

Co(1)-O(1)	2.028(4)	O(1)-Co(1)-O(2)	58.71(13)
Co(1)-O(2)	2.373(4)	O(1)-Co(1)-O(3)#1	102.60(15)
Co(1)-O(3)#1	2.104(3)	O(1)-Co(1)-O(7)	82.56(17)
Co(1)-O(5)	1.992(4)	O(1)-Co(1)-N(6)#2	143.47(16)
Co(1)-O(7)	2.254(4)	O(3)#1-Co(1)-O(2)	90.78(13)
Co(1)-N(6)#2	2.061(4)	O(3)#1-Co(1)-O(7)	172.28(16)
Co(2)-O(4)#2	2.139(3)	O(5)-Co(1)-O(1)	95.71(19)
Co(2)-N(3)	2.142(3)	O(5)-Co(1)-O(2)	153.98(18)
Co(2)-N(9)#5	2.130(3)	O(5)-Co(1)-O(3)#1	90.50(16)
N(6)#2-Co(1)-O(7)	85.98(16)	O(5)-Co(1)-O(7)	83.21(18)
N(6)#2-Co(1)-O(3)#1	92.97(14)	O(5)-Co(1)-N(6)#2	117.24(19)
N(6)#2-Co(1)-O(7)	85.98(16)	O(7)-Co(1)-O(2)	96.84(16)
O(4)#2-Co(2)-N(3)	95.99(13)	N(6)#2-Co(1)-O(2)	88.64(14)
O(4)#3-Co(2)-N(3)	84.01(13)	O(4)#2-Co(2)-N(3)#4	84.01(13)
O(4)#2-Co(2)-N(9)#6	94.4(3)	N(3)-Co(2)-N(9)#6	89.0(4)
N(3)-Co(2)-N(3)#4	180.0	N(9)#5-Co(2)-N(3)	87.9(18)
N(9)#6-Co(2)-N(3)	92.1(18)	N(9)#6-Co(2)-O(4)#3	92.7(11)
N(9)#5-Co(2)-O(4)#3	87.3(11)	N(9)#5-Co(2)-N(9)#A6	172.5(16)

#1: 1-x, 1-y, 1-z; #2: x, 1+y, z; #3: -x, 1-y, 1-z; #4: -x, 2-y, 1-z; #5: 1-x, 2-y, 1-z; #6: -1+ x, y, z.

Table S3. Selected bond lengths (Å) and bond angles (°) for complex **Co-3**.

Co(1)-O(1)#1	2.1088(13)	O(1)#1-Co(1)-O(1)	180.0
Co(1)-O(1)	2.1088(13)	O(1)-Co(1)-N(1)#1	95.27(6)
Co(1)-N(1)	2.1489(16)	N(1)#1-Co(1)-N(1)	180.00(10)
Co(1)-N(1)#1	2.1489(16)	O(1)-Co(1)-N(1)	84.73(6)
Co(1)-N(6)#2	2.1431(18)	O(1)#1-Co(1)-N(1)	95.27(6)
Co(1)-N(6)#3	2.1431(18)	O(1)#1-Co(1)-N(6)#2	93.46(6)
N(6)#2-Co(1)-N(1)#1	88.16(7)	N(6)#2-Co(1)-N(1)	91.84(7)
O(1)-Co(1)-N(6)#3	93.46(6)	N(6)#2-Co(1)-N(6)#3	180.0
O(1)-Co(1)-N(6)#2	86.54(6)	N(6)#3-Co(1)-N(1)	88.16(7)

#1: 1-x, 2-y, -z; #2: 2-x, 2-y, -z; #3: -1+x, y, z.

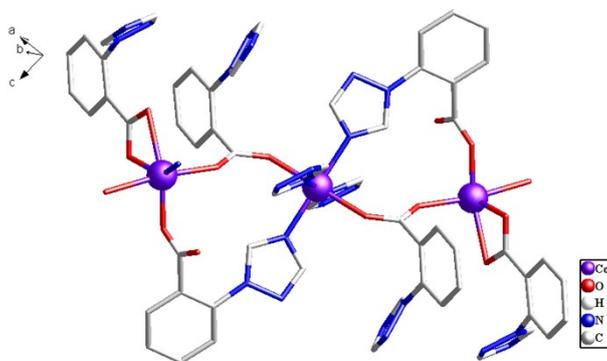


Figure S1. Trinuclear cobalt cluster $[\text{Co}_3(\text{COO})_2(\text{H}_2\text{O})_2]$ in **Co-2**.

Powder X-ray Diffraction

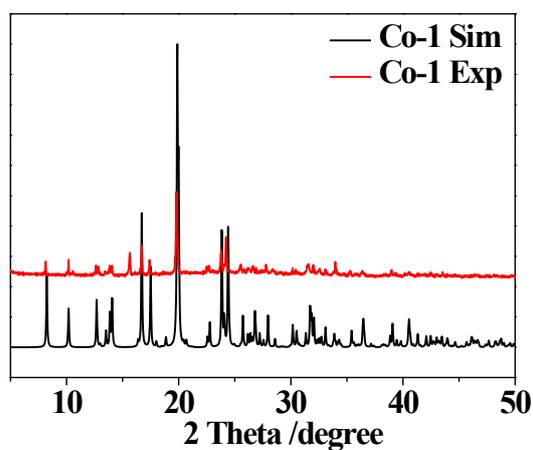


Figure S2. Powder X-ray diffractions of **Co-1**.

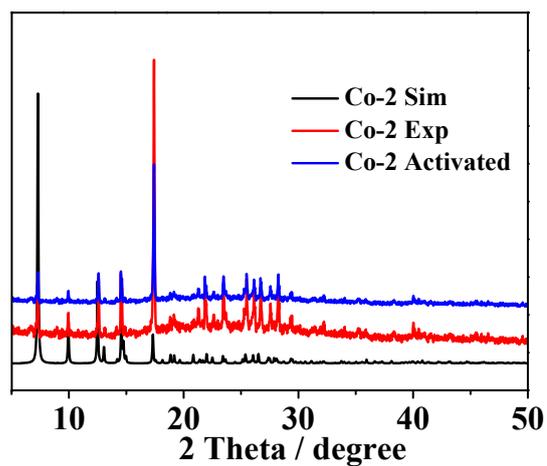


Figure S3. Powder X-ray diffractions of Co-2.

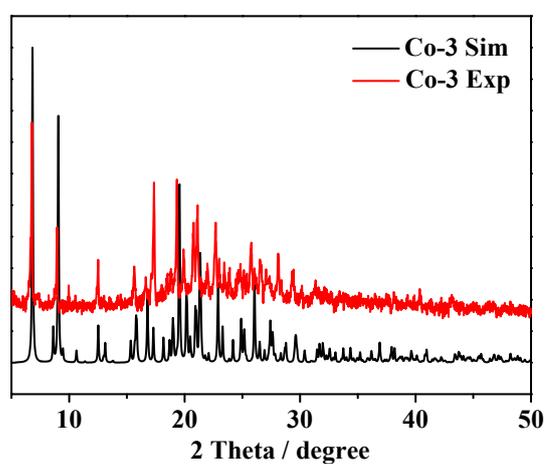


Figure S4. Powder X-ray diffractions of Co-3.

Thermal Gravimetric Analysis Curves

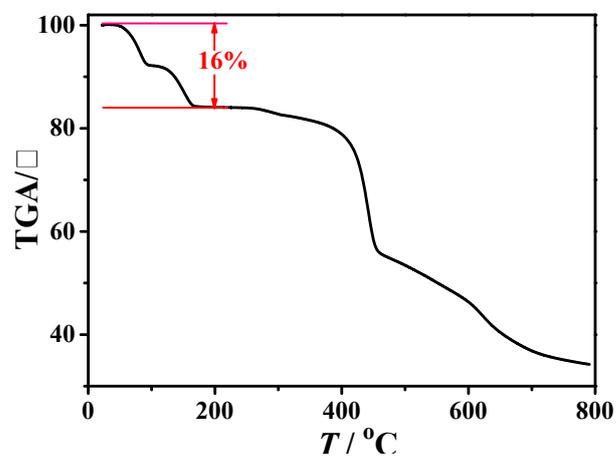


Figure S5. Weight loss curve for Co-1.

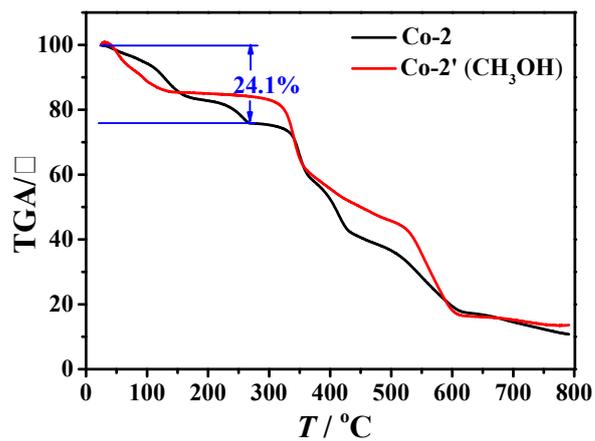


Figure S6. Weight loss curves for Co-2 and Co-2' after methanol exchange

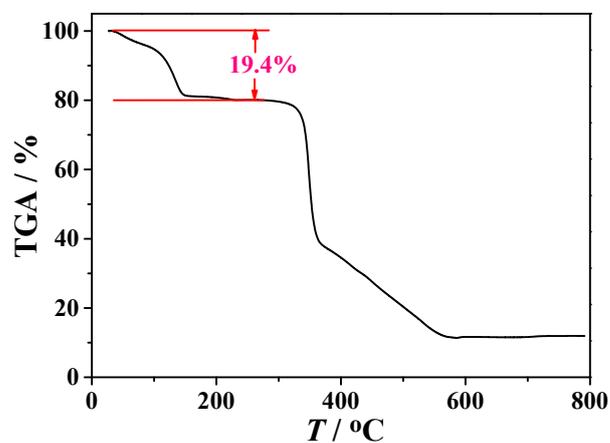


Figure S7. Weight loss curve for Co-3.

Dynamic Magnetic Measurement Results

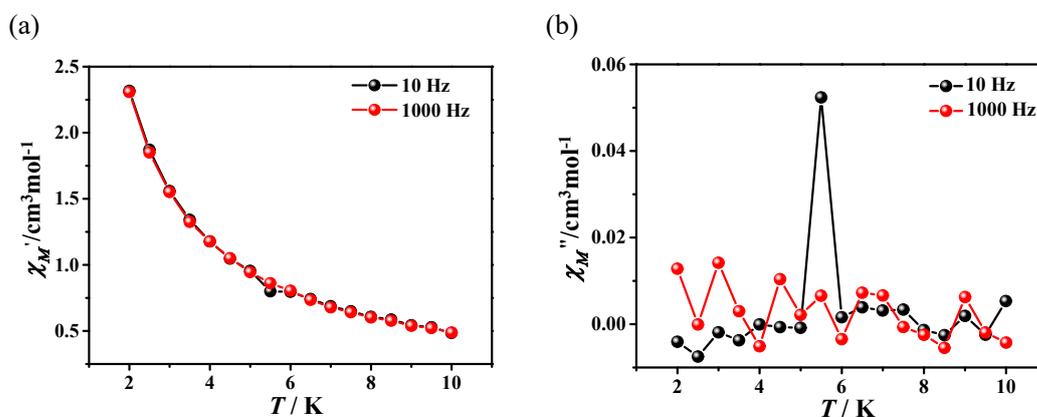


Figure S8. In-phase (χ') (a) and out-of-phase signals (χ'') (b) components of the ac magnetic susceptibility for Co-2 under zero dc field with an oscillation of 3 Oe.

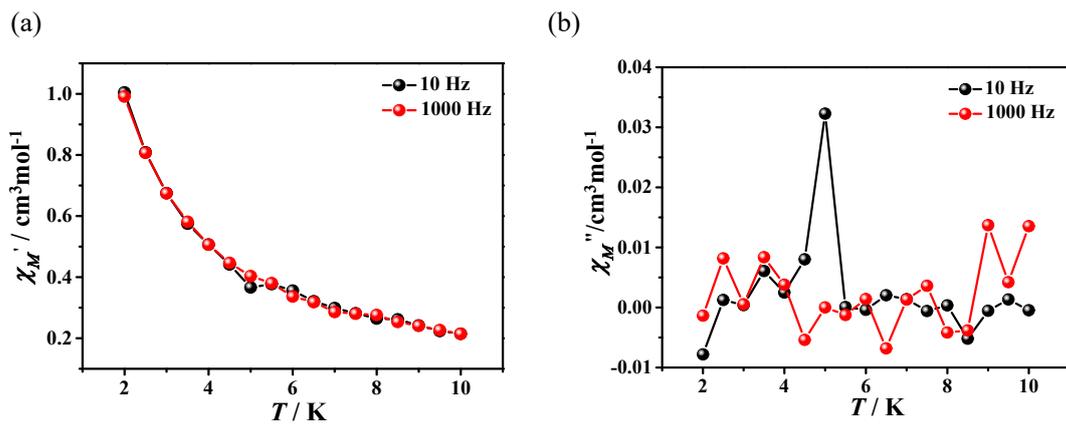


Figure S9. In-phase (χ') (a) and out-of-phase signals (χ'') (b) components of the ac magnetic susceptibility for Co-3 under zero dc field with an oscillation of 3 Oe.