

Supporting Information

Highly-connected, porous coordination polymers based on $[M_4(\mu_3\text{-OH})_2]$ ($M = \text{Co}^{\text{II}}$ and Ni^{II}) clusters: different networks, adsorption and magnetic properties

5 Qing Chen,^a Wei Xue,^a Jian-bin Lin,^a Rui-biao Lin,^a Ming-Hua Zeng,^{*b} and Xiao-Ming Chen^{*a}

^a MOE Key Laboratory of Bioinorganic and Synthetic Chemistry, State Key Laboratory of Optoelectronic Materials and Technologies, School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, P. R. China.

^b Key Laboratory for the Chemistry and Molecular Engineering of Medicinal Resources (Ministry of Education of China), School of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin 541004, P. R. China

Corresponding authors: cxm@mail.sysu.edu.cn (X.-M. Chen) and zmh@mailbox.gxnu.edu.cn (M.-H. Zeng).

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

1					
Co1-O7	2.046(3)	Co1-O2	2.057(3)	Co1-O9a	2.064(3)
Co1-O1	2.104(3)	Co1-N1b	2.143(4)	Co1-O5	2.147(3)
Co2-O1	2.055(3)	Co2-O10a	2.096(3)	Co2-N3c	2.113(3)
Co2-O2	2.120(3)	Co2-O3	2.204(3)	Co3-O1	2.026(3)
Co3-O8	2.051(3)	Co3-O4	2.074(3)	Co3-N5	2.118(4)
Co3-O14	2.117(3)-	Co3-O5	2.220(3)	Co4-O2	2.045(3)
Co4-O13	2.095(3)	Co4-O6	2.112(3)	Co4-N4d	2.166(4)
Co4-O3	2.214(3)	O7-Co1-O2	175.75(1)	O7-Co1-O9a	89.09(1)
O2-Co1-O9a	94.20(1)	O7-Co1-O1	91.77(1)	O2-Co1-O1	85.51(1)
O9a-Co1-O1	90.44(1)	O7-Co1-N1b	86.50(1)	O2-Co1-N1b	96.40(1)

O9a-Co1-N1b	86.17(1)	O1-Co1-N1b	176.22(1)	O7-Co1-O5	88.54(1)
O2-Co1-O5	87.81(1)	O9a-Co1-O5	171.16(1)	O1-Co1-O5	81.13(1)
N1b-Co1-O5	102.18(1)	O11-Co2-O1	177.44(1)	O11-Co2-O10a	86.90(1)
O1-Co2-O10a	91.89(1)	O11-Co2-N3c	89.32(1)	O1-Co2-N3c	92.96(1)
O11-Co2-O2	92.73(1)	O1-Co2-O2	85.14(1)	O10a-Co2-O2	95.43(1)
N3c-Co2-O2	173.24(1)	O11-Co2-O3	88.39(1)	O1-Co2-O3	92.70(1)
O10a-Co2-O3	174.51(1)	N3c-Co2-O3	91.68(1)	O2-Co2-O3	81.95(1)
O1-Co3-O8	94.21(1)	O1-Co3-O4	92.60(1)	O8-Co3-O4	171.93(1)
O1-Co3-N5	171.83(1)	O8-Co3-N5	87.24(1)	O4-Co3-N5	86.62(1)
O1-Co3-O14	96.09(1)	O8-Co3-O14	86.59(1)	O4-Co3-O14	88.40(1)
N5-Co3-O14	92.02(1)	O1-Co3-O5	81.11(1)	O8-Co3-O5	88.59(1)
O4-Co3-O5	96.73(1)	N5-Co3-O5	90.90(1)	O2-Co4-O13	94.23(1)
O2-Co4-O12	89.51(1)	O13-Co4-O12	87.57(1)	O2-Co4-O6	94.92(1)
O13-Co4-O6	86.67(1)	O12-Co4-O6	172.98(1)	O2-Co4-N4d	171.39(1)
O13-Co4-N4d	94.24(1)	O12-Co4-N4d	89.32(1)	O6-Co4-N4d	87.11(1)
O2-Co4-O3	83.39(1)	O13-Co4-O3	174.36(1)	O12-Co4-O3	87.30(1)
O6-Co4-O3	98.61(1)	N4d-Co4-O3	88.04(1)		

Symmetry codes: *a*) $x+1/2, -y+1/2, z+1/2$; *b*) $-x+5/2, y-1/2, -z+1/2$; *c*) $-x+3/2, y+1/2, -z+1/2$; *d*) $-x+2, -y+1, -z$.

2

Ni1-O2	2.039(3)	Ni1-O7a	2.042(2)	Ni1-O1	2.046(3)
Ni1-O9b	2.057(2)	Ni1-N2	2.099(3)	Ni1-O5	2.114(2)
Ni2-O1	2.047(3)	Ni2-O2	2.050(3)	Ni2-N1	2.076(3)
Ni2-O8a	2.081(2)	Ni2-O12c	2.086(3)	Ni2-O3	2.145(2)
Ni3-O10b	2.033(2)	Ni3-O1	2.036(3)	Ni3-O4	2.057(3)
Ni3-N5	2.08(2)	Ni3-N4	2.120(3)	Ni3-O5	2.155(3)
Ni4-O14d	2.006(9)	Ni4-O11c	2.015(3)	Ni4-O2	2.022(3)
Ni4-O6	2.025(3)	Ni4-N3e	2.128(3)	Ni4-O3	2.240(3)
O10b-Ni3-O1	95.91(1)	O10b-Ni3-O4	171.52(1)	O1-Ni3-O4	91.36(1)
O10b-Ni3-N5	83.0(7)	O1-Ni3-N5	94.8(6)	O4-Ni3-N5	92.0(6)
O10b-Ni3-N4	86.93(1)	O1-Ni3-N4	172.53(1)	O4-Ni3-N4	86.39(1)
N5-Ni3-N4	92.4(6)	O10b-Ni3-O5	86.25(1)	O1-Ni3-O5	81.00(1)
O4-Ni3-O5	99.24(1)	N5-Ni3-O5	168.0(5)	N4-Ni3-O5	92.31(1)
O14d-Ni4-O11c	90.6(2)	O14d-Ni4-O2	99.4(3)	O11c-Ni4-O2	92.56(1)
O14d-Ni4-O6	87.8(2)	O11c-Ni4-O6	172.36(1)	O2-Ni4-O6	95.07(1)
O14d-Ni4-N3e	86.7(3)	O11c-Ni4-N3e	86.49(1)	O2-Ni4-N3e	173.89(1)
O6-Ni4-N3e	85.97(1)	O14d-Ni4-O3	172.9(2)	O11c-Ni4-O3	82.39(1)

O2-Ni4-O3	79.86(1)	O6-Ni4-O3	99.36(1)	N3e-Ni4-O3	94.04(1)
O2-Ni1-O7a	90.18(1)	O2-Ni1-O1	85.04(1)	O7a-Ni1-O1	93.89(1)
O2-Ni1-O9b	175.68(1)	O7a-Ni1-O9	87.66(1)	O1-Ni1-O9b	91.37(1)
O2-Ni1-N2	96.00(1)	O7a-Ni1-N2	85.92(1)	O1-Ni1-N2	178.94(1)
O9b-Ni1-N2	87.58(1)	O2-Ni1-O5	90.32(1)	O7a-Ni1-O5	175.58(1)
O1-Ni1-O5	81.78(1)	O9b-Ni1-O5	91.55(1)	N2-Ni1-O5	98.40(1)
O1-Ni2-O2-	84.74(1)	O1-Ni2-N1	95.27(1)	O2-Ni2-N1	177.74(1)
O1-Ni2-O8a	94.54(1)	O2-Ni2-O8a	92.67(1)	O2-Ni2-O3	81.55(1)
O1-Ni2-O12c	177.90(1)	O2-Ni2-O12c	93.41(1)	O12c-Ni2-O3	88.08(1)
O8a-Ni2-O12c	86.55(1)	O1-Ni2-O3	90.65(1)	O8a-Ni2-O3	171.86(1)
N1-Ni2-O3	96.19(1)				

Symmetry codes: *a*) $x+1/2, -y+1/2, z+1/2$; *b*) $-x+1/2, y+1/2, -z+1/2$; *c*) $-x+3/2, y-1/2, -z+1/2$; *d*) $x+1, y, z$; *e*) $-x+1, -y, -z$.

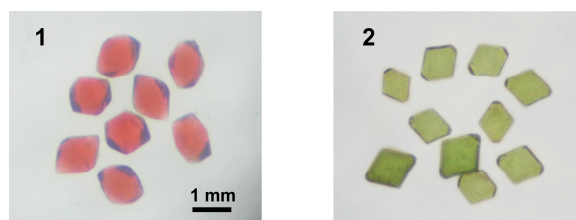


Fig. S1. Photos of chosen single crystals of **1** and **2**.

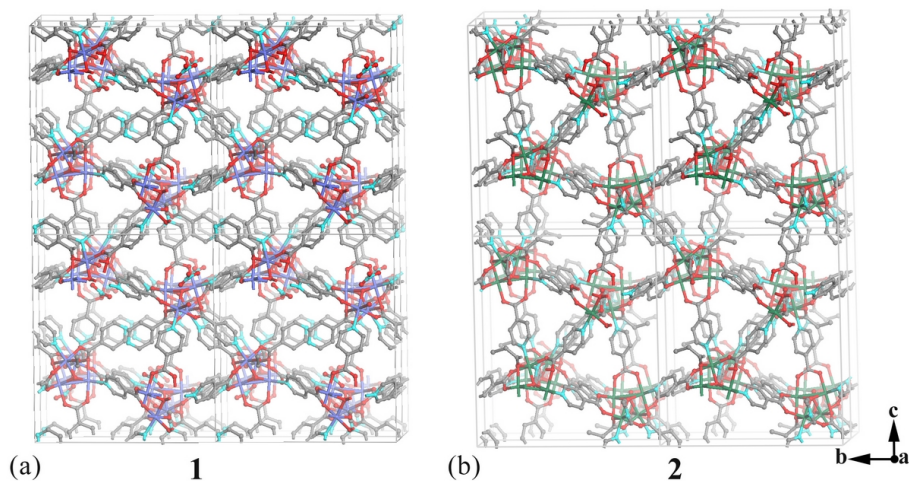


Fig. S2. Views of the 3D molecular packing patterns of **1** (a) and **2** (b).

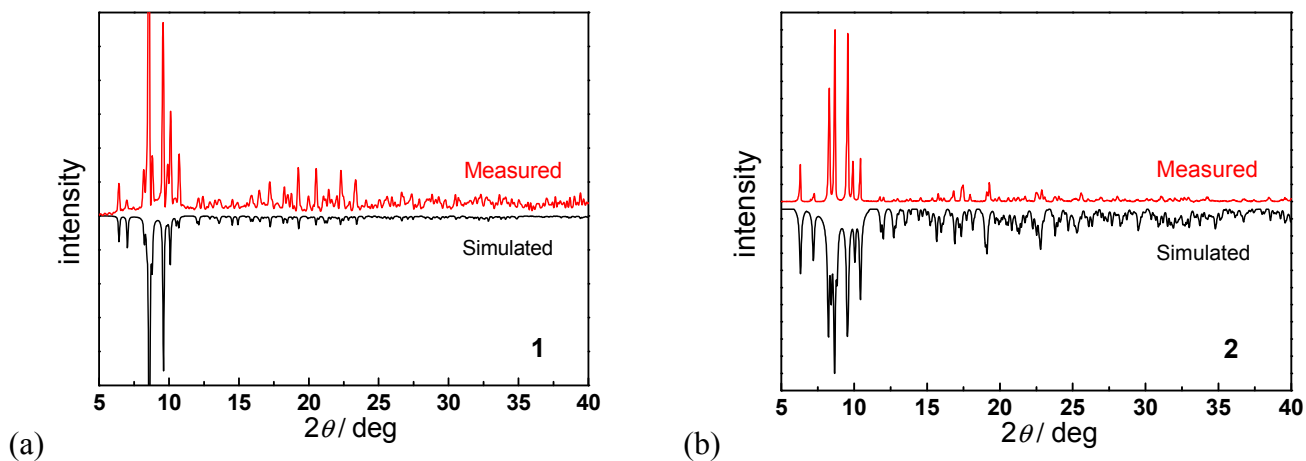


Fig. S3. Measured and simulated PXRD patterns of **1** and **2**.

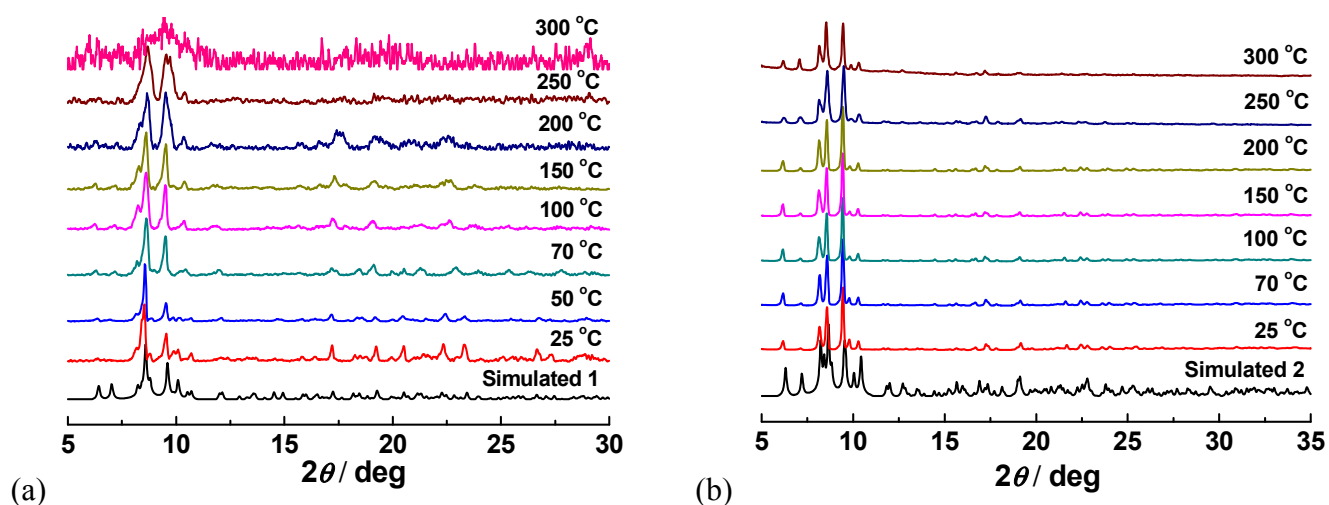


Fig. S4. The variable-temperature PXRD patterns of **1** (a) and **2** (b).

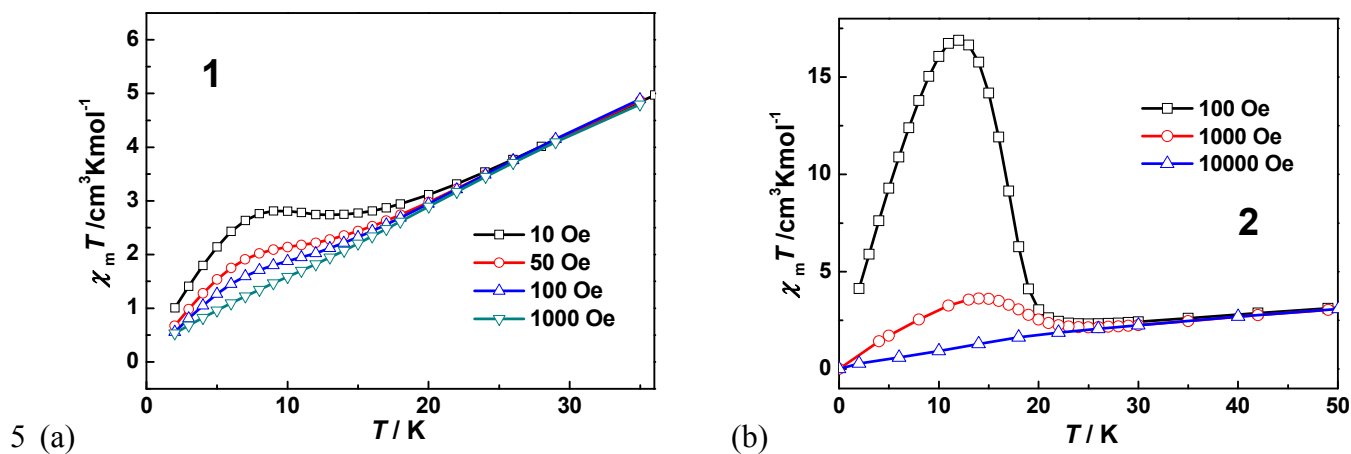


Fig. S5. The temperature dependence of the magnetic susceptibility under different static fields in the low temperature range for **1** (a) and **2** (b).

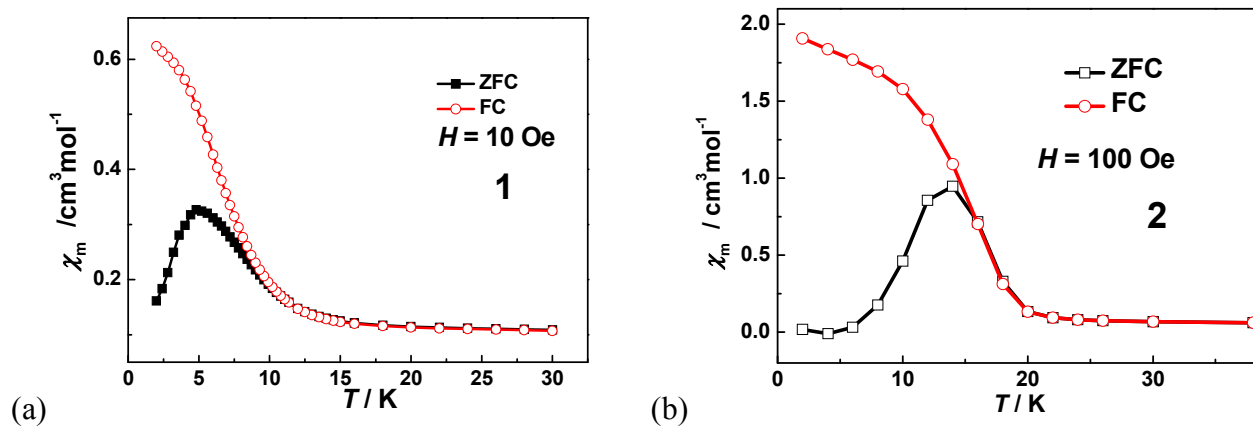


Fig. S6. ZFCM-FCM curves of **1** (a) and **2** (b).

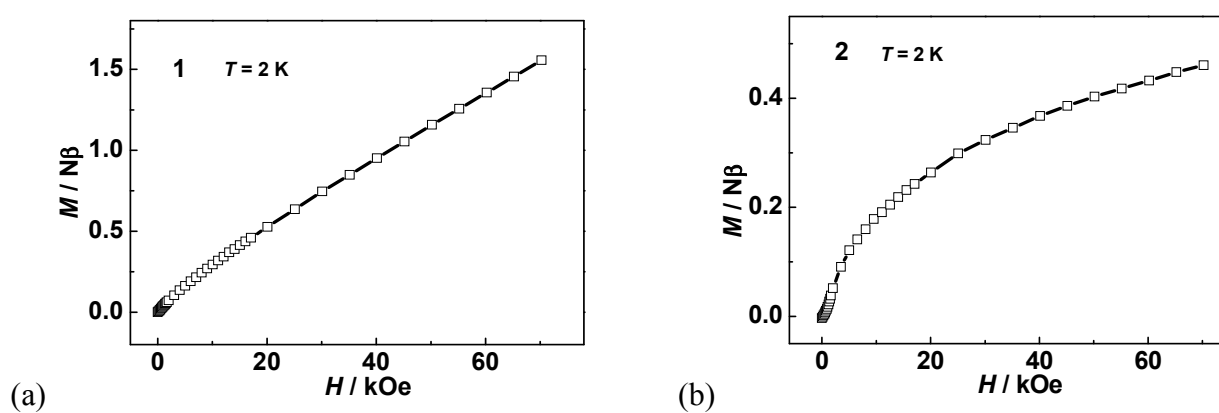


Fig. S7. The isothermal magnetization and hysteresis loops (inset) of **1** (a) and **2** (b) at 2 K .