

Supporting Information for

Crystal Engineering to Control the Magnetic Interaction between Weak Ferromagnetic Single-Chain Magnets Assembled in 3D Framework

Lei Su,^a Wei-Chao Song,^b Jiong-Peng Zhao,^{*a} Fu-Chen Liu^{*a}

^a School of Chemistry and Chemical Engineering, Tianjin University of Technology, Tianjin 300384, P.R. China.

^b Tianjin Key Laboratory of Structure and Performance for Functional Molecules, College of Chemistry, Tianjin Normal University, Tianjin 300387, P. R. China

* Corresponding author. E-mail: horryzhao@yahoo.com, fuchenliutj@yahoo.com

Table S1. Selected bond lengths [Å] for **1** and **2**.

	1	2
Co1—O6	1.968 (4)	1.9584 (19)
Co1—O1	2.094 (5)	2.074 (2)
Co1—O3	2.094 (5)	2.076 (2)
Co1—O4	2.162 (5)	2.113 (2)
Co1—N1 ⁱ	2.178 (6)	2.151 (3)
Co1—O5	2.271 (5)	2.251 (2)
Co2—O2	2.053 (5)	2.048 (2)
Co2—O7 ⁱⁱ	2.086 (5)	2.069 (2)
Co2—O7 ⁱⁱⁱ	2.094 (5)	2.092 (2)
Co2—O7	2.126 (5)	2.130 (2)
Co2—O4	2.153 (5)	2.128 (2)
Co2—O5	2.154 (5)	2.176 (2)
Co1 ^{iv} —O6—Co1	118.4 (3)	116.43 (17)
Co2—O4—Co1	101.9 (2)	103.28 (10)
Co2—O5—Co1	98.4 (2)	97.34 (9)
Co2—O7—Co2 ⁱⁱⁱ	90.56 (19)	90.58 (8)
Co2 ⁱⁱ —O7—Co2 ⁱⁱⁱ	102.9 (2)	102.46 (10)
Co2 ⁱⁱ —O7—Co2	96.1 (2)	97.83 (9)

Symmetry Code: ⁱ $y-1, -x+1, -z+3/2$; ⁱⁱ $-y+3/2, -x+3/2, -z+3/2$; ⁱⁱⁱ $y-1/2, x+1/2, -z+3/2$; ^{iv} $x, y, -z+2$

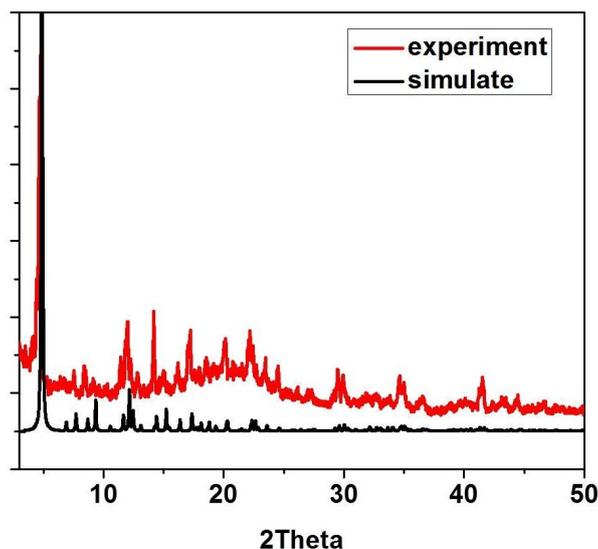


Fig.S1 Powder X-ray diffraction pattern of **2**

Experimental Section

X-ray Crystallography. The single-crystal X-ray diffraction data of **2** were collected on a Rigaku 007HF XtaLAB P200 diffractometer at 113 (2) K. The program *CrystalClear*^{S1} was used for the integration of the diffraction profiles. The structure was solved by direct method using the SHELXS program of the SHELXTL package and refined by full-matrix least-squares methods with SHELXL (semi-empirical absorption corrections were applied by using the SADABS program).^{S2} The non-hydrogen atoms were located in successive difference Fourier syntheses and refined with anisotropic thermal parameters on F^2 . All hydrogen atoms were generated theoretically at the specific atoms and refined isotropically with fixed thermal factors. The selected bond lengths and angles are given in Tables S1.

Magnetic measurements. The magnetic measurements were performed by an MPMS XL-7T SQUID magnetometer with polycrystals of **2**. Diamagnetic corrections were estimated by using Pascal constants and background corrections by experimental measurement on sample holders.

References

- S1. G. M. Sheldrick, *SHELXL97, Program for Crystal Structure Refinement*; University of Göttingen: Göttingen, Germany, 1997.
- S2. *CrystalClear and CrystalStructure*; Rigaku/MSK: The Woodlands, TX, 2005.

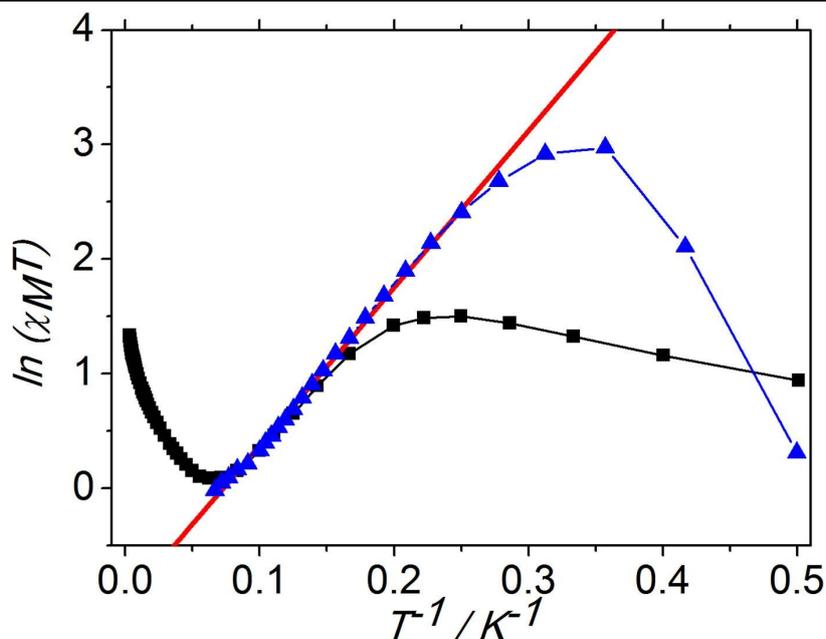


Fig. S2 Logarithm of $\chi_m T$ vs $1/T$ plots (assuming one Co^{II} ions per formula unit) of **2**. The dc susceptibility (■) was collected at 0.1 T and ac susceptibility (▲) was obtained at a frequency of 100 Hz under oscillating field of 3.5 Oe. The red line is the result of fitting by $\chi_m T = C_{\text{eff}} \exp(\Delta/k_B T)$ between 15 K and 5 K with the energy gap of $\Delta/k_B = 13.72$ K and $C_{\text{eff}} = 0.38 \text{ cm}^3 \text{ mol}^{-1} \text{ K}$.

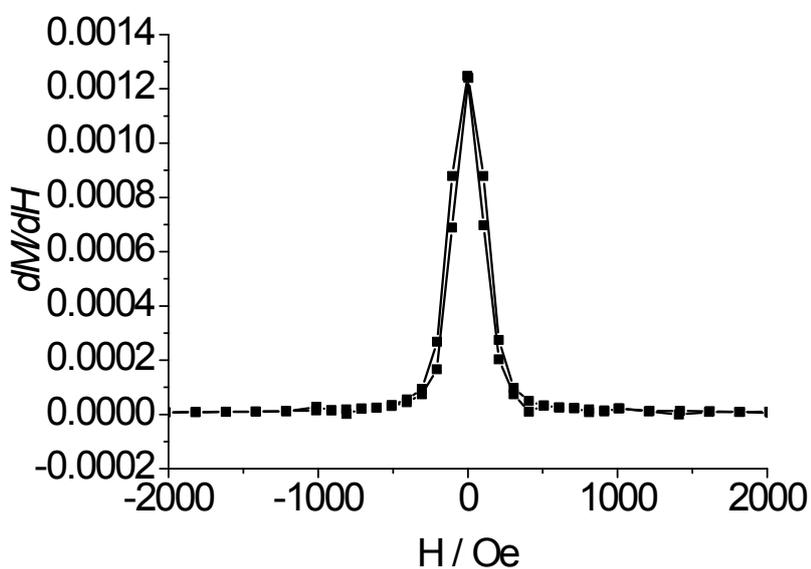


Fig. S3 Plot of the magnetic data as dM/dH vs H for **2**.