Supporting Information

Combination of cobalt-water chain into 2D network with *cis*-1,4-cyclohexanedicarboxylate bridge exhibiting spin-canted antiferromagnetism

Zhong-Yi Li,* Yuan-Qing Cao, Xiang-Ming Zhang, Ya-Lan Xu, Guang-Xiu Cao, Fu-Li Zhang, Su-Zhi Li, Fu-Qiang Zhang and Bin Zhai*

Materials and Physical measurements. All chemicals were obtained from commercial sources and used without further purification. Elemental analyses were determined by a Vario EL III elemental analyzer. FT-IR spectra were recorded in the range of 4000-400 cm^{-1} on a JASCO FT/IR-430 spectrometer with KBr pellets. Powder X-ray diffraction (PXPD) measurements were carried out on a Bruker D8 ADVANCE X-ray Diffractometer using Cu Kα (λ = 1.5418 Å) at room temperature. Thermogravimetric analyses were performed under a flow of nitrogen (40 mL/min) at a ramp rate of 10 °C/min, using a NETZSCH STA 449F3 instrument. Magnetic measurements were performed on a Quantum Design SQUID magnetometer MPMS XL-7. The data was corrected for the sample holder and the diamagnetic contributions.

X-ray Crystallography. Crystallographic data of complex **1** were collected on a Bruker D8 Quest CMOS area detector system with graphite-monochromated Mo-Kα (λ = 0.71073 Å) radiation. Data reduction and unit cell refinement were performed with Smart-CCD software[1]. The structure solution was performed using SHELXS-2016 while the refinement was performed using SHELXL based on F^2 through the full-matrix least-squares routine.[2] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms on organic ligands were placed in idealised positions and refined using a riding model. Hydrogen atoms on the terminal and bridged water molecules were initially found on Fourier difference maps and then restrained by using the DFIX instruction. Exceptionally, no attempts were made to locate the hydrogen atoms on the free water molecule. A summary of the important crystal and structure refinement data of **1** was given in Table S1. Selected bond lengths and angles were listed in Table S2.

Reference:

1 *XSCANS* (Version 2.1), Siemens Analytical X-Ray Instruments Inc., Madison, WI, 1994.

2 (a) G. M. Sheldrick, *Acta Crystallogr.*, Sect. A: Fundam. Crystallogr., 2008, 112; (b) O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339.

Thermogravimetric Analyses. To investigate the thermostability of compound **1**, thermogravimetric analysis was carried out under a N_2 atmosphere in the range of 30–600 ℃. As shown in Fig. S4, the TG curve of **1** has two mass steps. In the first step, the 28.6% weight loss from 30 to 400 ℃ corresponds to the departure of two free and three coordinated water molecules for each formula unit (calculated 28.2% for **1**). After 400 °C, the curve shows a striking weight loss, indicating complete decomposition of the fromwork.

Table S1. Crystal data and structure refinement of **1**.

	1
Formula	$C_8H_{16}CoO_7$, 2.5(H_2O)
Mr.	283.14
T (K)	296(2)
Cryst. system	Monoclinic
Space group	*P2(1)/c*
a /Å	9.8852(5)
b /Å	16.8825(9)
c /Å	8.1720(4)
α/°	90
β/°	93.423(2)
γ/°	90
V (Å^3)	1361.37(12)
Z	4
$d_{calcd.}$, g/cm^3	1.381
μ(mm^{-1})	1.275
F(000)	588
Reflections collected/ unique	23547 / 9988
R(int)	0.0523
GOF on F^2	1.118
$R1^a(I > 2\sigma(I))$	0.0594
$wR2^b$(all data)	0.1589

$^aR1 = \sum(||F_o|-|F_c||) / \sum |F_o|$, $^bwR2 = \{\sum w [(F^2_o - F^2_c)] / \sum w [(F^2_o)^2]\}^{0.5}$

Table S2. Selected bond lengths (Å) and angles (°) for **1**.

Co(1)-O(5)	2.036(5)
Co(1)-O(1)	2.051(4)
Co(1)-O(3)#1	2.054(4)
Co(1)-O(7)	2.079(5)
Co(1)-O(6)	2.183(4)
Co(1)-O(6)#2	2.264(4)
O(5)-Co(1)-O(1)	91.1(2)
O(5)-Co(1)-O(3)#1	176.4(2)
O(1)-Co(1)-O(3)#1	92.4(2)
O(5)-Co(1)-O(7)	87.4(3)
O(1)-Co(1)-O(7)	178.4(2)
O(3)#1-Co(1)-O(7)	89.0(2)
O(5)-Co(1)-O(6)	94.75(18)
O(1)-Co(1)-O(6)	86.44(17)
O(3)#1-Co(1)-O(6)	86.24(17)
O(7)-Co(1)-O(6)	94.38(18)
O(5)-Co(1)-O(6)#2	84.82(18)
O(1)-Co(1)-O(6)#2	92.53(17)
O(3)#1-Co(1)-O(6)#2	94.25(16)
O(7)-Co(1)-O(6)#2	86.65(18)

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

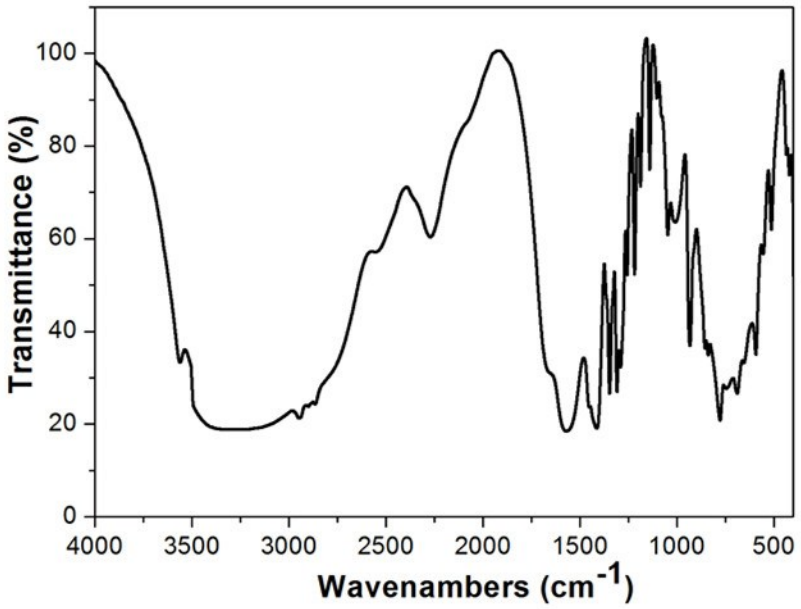
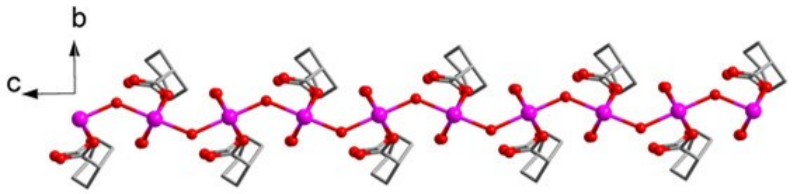
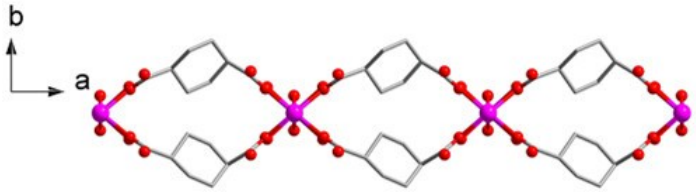


Fig. S1 The IR spectrum of **1**.



(a)



(b)

Fig. S2 (a) View of the 2D layer structure of **1** viewed along a axis. (b) View of the 2D layer structure of **1** viewed along c axis. The hydrogen atoms have been omitted for clarity.

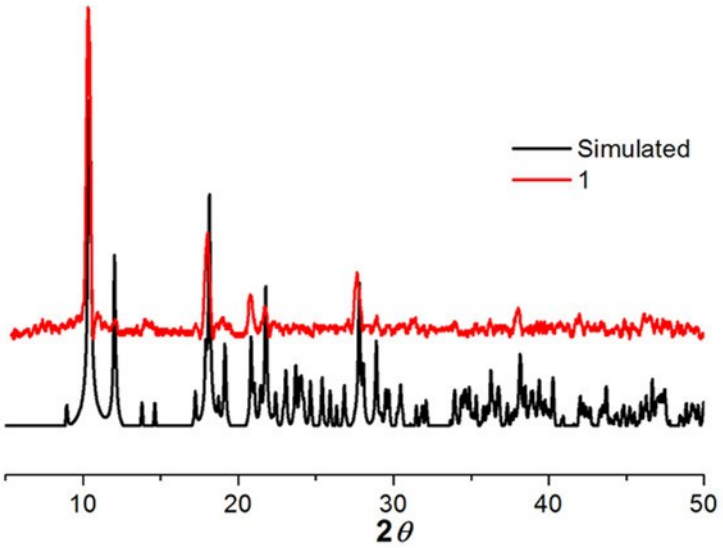


Fig. S3 Powder X-ray diffraction (PXRD) patterns of **1**.

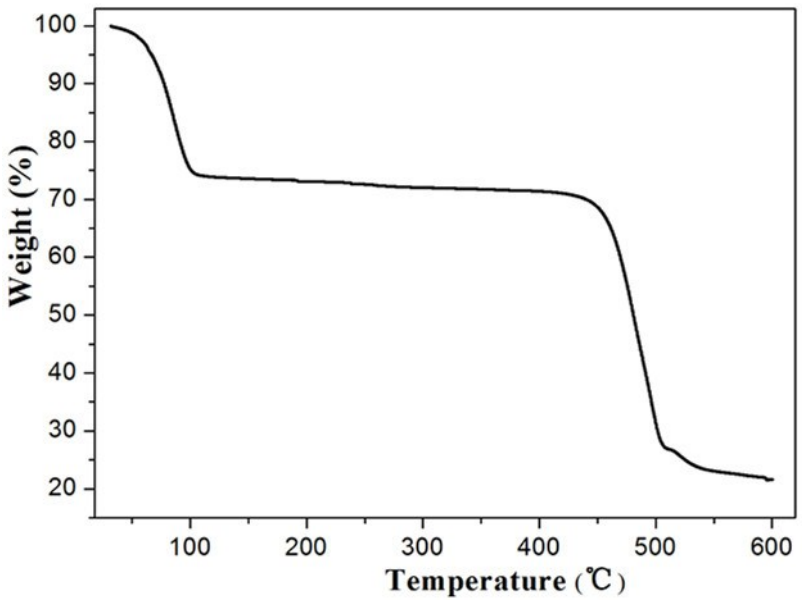


Fig. S4 TG curve for **1**in a nitrogen atmosphere (10 °C/min).

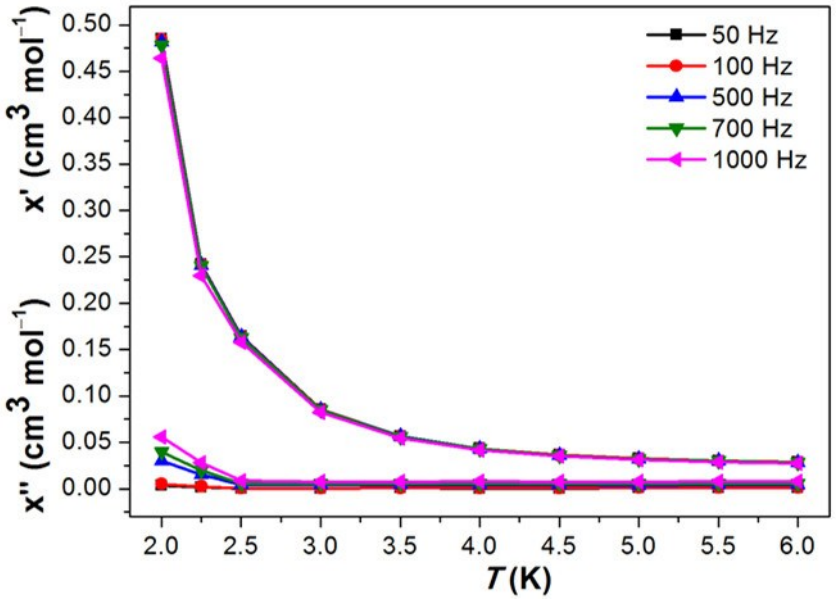


Fig. S5 Temperature dependence of the ac susceptibility for 1 at various frequencies and in a zero dc and 2 Oe ac applied field.

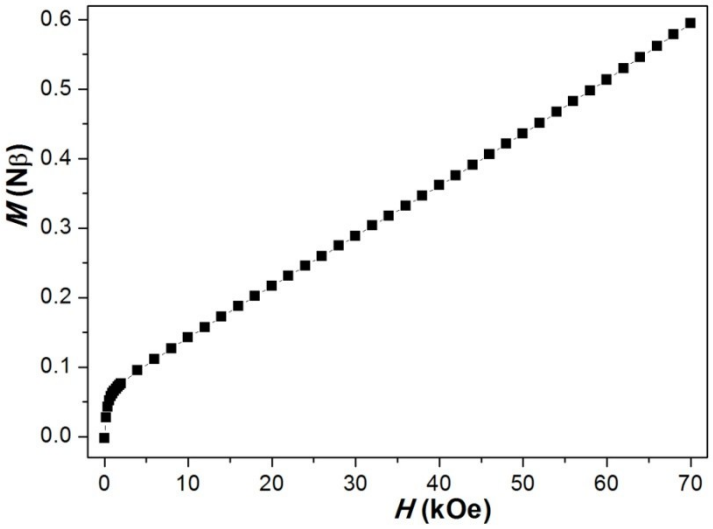


Fig. S6 Field dependence of the magnetization of **1** at 2.0 K.