Supporting Information

One-dimensional cobalt(II) coordination polymer featuring single-ion-magnet-type field-induced slow magnetic relaxation

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Table S1. Crystal data and structure refinement summary for compound **1**.

compound	**1**
Empirical formula	$C_{32}H_{36}CoN_8O_8$
Formula weight	719.62
Crystal system	triclinic
Space group	*P* -1
a / (Å)	8.6876(6)
b / (Å)	8.8285(6)
c / (Å)	11.1967(5)
α / (°)	74.149(5)
β / (°)	89.728(5)
γ / (°)	78.065(6)
V (Å^3)	807.04(9)
Z	1
Calculated density D_e / mg · m^{-3}	1.481
Absorption coeff.(μ)mm^{-1}	0.597
F(000)	375
R(int)	0.0262
Θ range / (°)	2.97 to 29.14
Reflections collected / unique	10791 / 3768
Parameters refined	231
Final *R* indices [I>2σ(I)]	R_1 = 0.0348, wR_2 = 0.0814
R indices (all data)	R_1 = 0.0421, wR_2 = 0.0862
Temp.(K)	293(2)

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

			1		
Co(1)-O(4)	2.0901(13)	N(6)-C(5)	1.337(2)	O(4A)-Co(1)-N(6)	91.91(5)
Co(1)-O(2)	2.0981(11)	C(2)-C(3)	1.466(2)	C(6)-N(6)-Co(1)	122.88(11)
Co(1)-N(6)	2.1488(14)	O(7)-C(3)	1.361(2)	O(2)-C(1)-O(3)	124.49(14)
O(2)-C(1)	1.2463(19)	O(2)-Co(1)-N(6)	92.68(5)	O(2A) -Co(1)-O(2)	180.0
O(3)-C(1)	1.266(2)	C(1)-O(2)-Co(1)	131.20(10)	O(4A) -Co(1)-O(4)	180.00(2)
C(1)-C(8)	1.520(2)	O(4A)-Co(1)-O(2A)	86.15(5)	N(6)-Co(1)-N(6A)	180.0

Table S3. Relaxation fitting parameters from least-squares fitting of $\chi(f)$ data under 1200 Oe dc field of **1**.

T(K)	χ_T	χ_S	α_1	α_2
2	2.221	0.186	0.0008	0.280
2.2	1.861	0.128	0.0014	0.264
2.5	1.820	0.124	0.0032	0.241
2.8	1.776	0.121	0.0065	0.195
3	1.668	0.111	0.0087	0.184
3.2	1.572	0.102	0.011	0.179
3.5	1.515	0.595	0.019	0.153
3.8	1.462	0.089	0.021	0.128
4	0.230	0.064		0.111
4.2	0.219	0.060		0.090
4.5	0.205	0.059		0.044
4.8	0.193	0.053		0.028
5	0.185	0.043		0.032
5.5	0.169	0.031		0.006

Table S4. ZFS parameters and relaxation parameters with easy-axis anisotropy of octahedral Co(II) ion.

Compounds	Chromophere	Calculated value by SHAPE analysis	D/cm^{-1}	DC field/Oe	U_{eff}/K	τ_0/s
$[Co(H_2L_1)_2]\cdot 2THF$[35a]	CoN_4O_2	5.54	-30.4	1000	7.3	8.4×10^{-6}
$[Co(HL_2)_2]$[35a]	CoN_4O_2	5.91	-18.4	1000	10.2	6.1×10^{-6}
$[Co(H_2L_3)_2]\cdot CH_2Cl_2$[35a]	CoN_4O_2	4.99	-27.4	1000	14.1	1.2×10^{-5}
$[Co^{III}Co^{II}(LH_2)_2(Cl)(H_2O)]\cdot 4(H_2O)$[35b]	CoN_2O_4	0.856	-7.4	1000	11.4	6.1×10^{-6}
$[Co^{III}Co^{II}(LH_2)_2(Br)(H_2O)]\cdot 4(H_2O)$ [35b]	CoN_2O_4	0.742	-9.7	1000	20.8	1.0×10^{-6}
$[Co(dca)_2(bim)_4]$[35c]	CoN_6	0.031	-69.6	2500	11.1	0.87×10^{-6}
$[Co(dca)_2(bim)_2]$[35c]	CoN_6	0.039	-74.3	2500	13.2	1.54×10^{-6}
$[Co(dca)_2(bmim)_2]$[35c]	CoN_6	0.048	-75.8	2500	22.1	0.63×10^{-6}
$\{[(Tpm)Co(DMF)W(CN)_8]_2[Co(DMF)_4]\cdot 2DMF\}$[35d]	CoN_5O	--	--	500	55.1	3.8×10^{-10}
$[Co(3\text{-}Hppt)_2(adip)(2H_2O)]\cdot 2H_2O$ this work	CoN_2O_4	0.148	-33.9	1200	38.8	6.68×10^{-8}

Table S5. Calculated energy levels (cm^{-1}), ***g*** (g_x, g_y, g_z) tensors of the ground doublets of the Co^{II} by CASSCF (***a***) and CASPT2 (***b***).

a			***b***		
E/cm^{-1}	***g***		E/cm^{-1}	***g***	
0.0	g_x	1.951	0.0	g_x	1.937
	g_y	2.899		g_y	3.078
	g_z	7.478		g_z	7.267
222.9	g_x	1.600	223.1	g_x	1.581
	g_y	2.333		g_y	2.076
	g_z	4.722		g_z	5.013

Table S6. Calculated spin-free energies (cm^{-1}) of the lowest ten terms (S = 3/2) of the Co^{II} by CASSCF (***a***) and CASPT2 (***b***).

spin-free states	***a***	***b***
	E/cm^{-1}	E/cm^{-1}
1	0.0	0.0
2	331.0	418.7
3	1008.6	1078.8
4	7618.1	8513.9
5	7886.6	8766.9
6	8189.8	9129.9
7	16543.8	18412.1
8	22509.3	20394.6
9	23328.9	20957.6
10	24705.7	22739.8

Table S7. Calculated weights of the five most important spin-orbit-free states for the lowest two spin-orbit states of the Co^{II} by CASSCF (***a***) and CASPT2 (***b***).

methods	Spin-orbit states	Energy(cm^{-1})	Spin-free states, Spin, Weights				
CASSCF	1	0.0	1,1.5,0.6576	2,1.5,0.2748	3,1.5,0.0645	6,1.5,0.0011	21,0.5,0.0006
	2	222.9	1,1.5,0.8412	2,1.5,0.1124	3,1.5,0.0415	5,1.5,0.0019	6,1.5,0.0010
CASPT2	1	0.0	1,1.5,0.6994	2,1.5,0.2357	3,1.5,0.0618	6,1.5,0.0009	22,0.5,0.0006
	2	223.1	1,1.5,0.8711	2,1.5,0.0867	3,1.5,0.0376	5,1.5,0.0015	6,1.5,0.0010

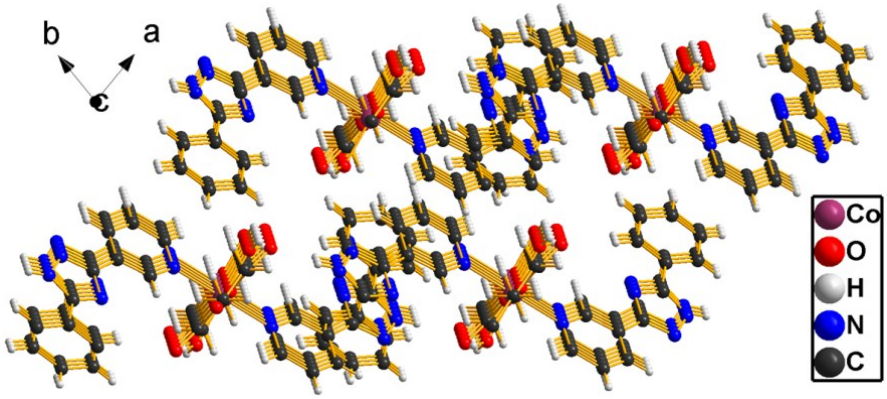

Figure S1. 3D supramolecular structure of **1**.

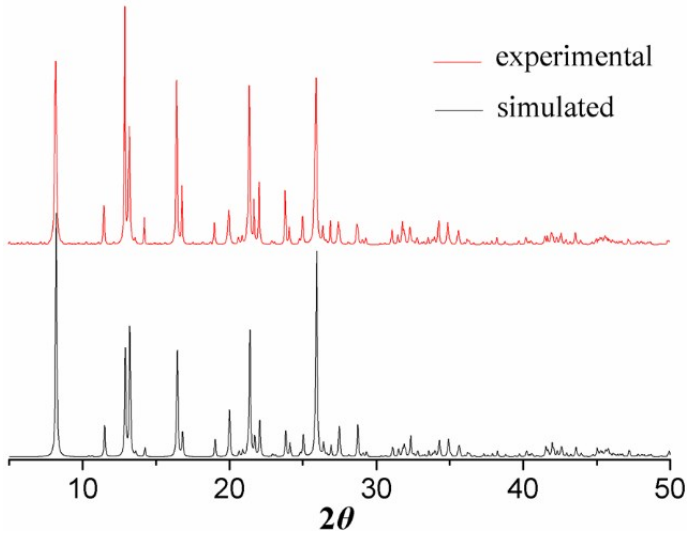

Figure S2. PXRD patterns for compound **1.**

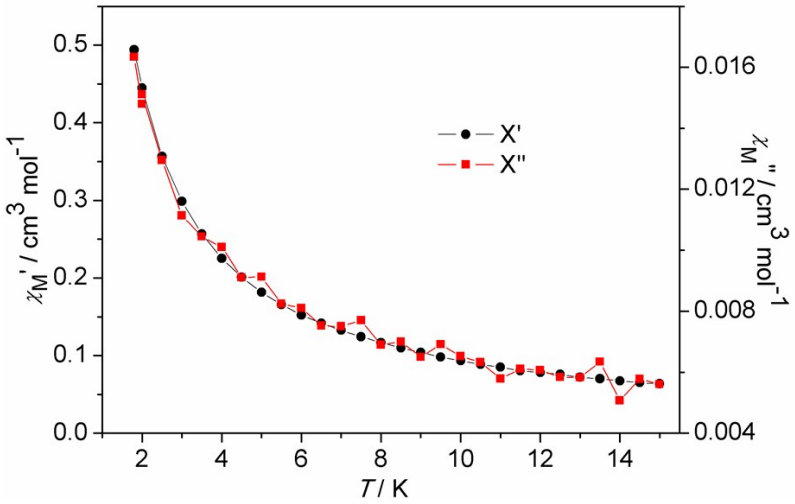

Figure S3. The ac magnetic susceptibility measurements for **1** in 0 Oe static field.

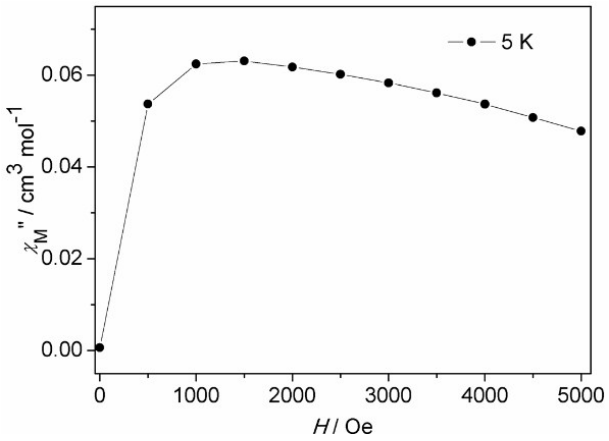

Figure S4. Plot of χ''_M vs H for compound **1** at 5 K.

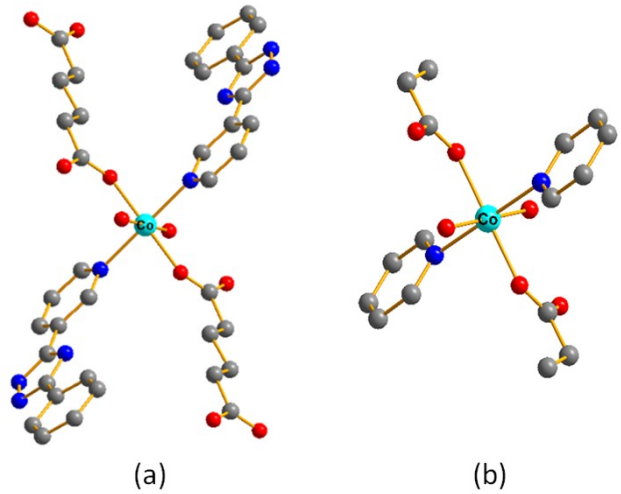

Figure S5. Calculated complete structure (***a***) extracted from complex **1** for CASSCF calculation, and the simplified model structure (***b***) for CASPT2 calculation; H atoms are omitted.