Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary materials for

Fine-tuning effect of auxiliary ligand on two trigonal-bipyramid cobalt(II) complexes exhibiting field-Induced slow magnetic relaxation

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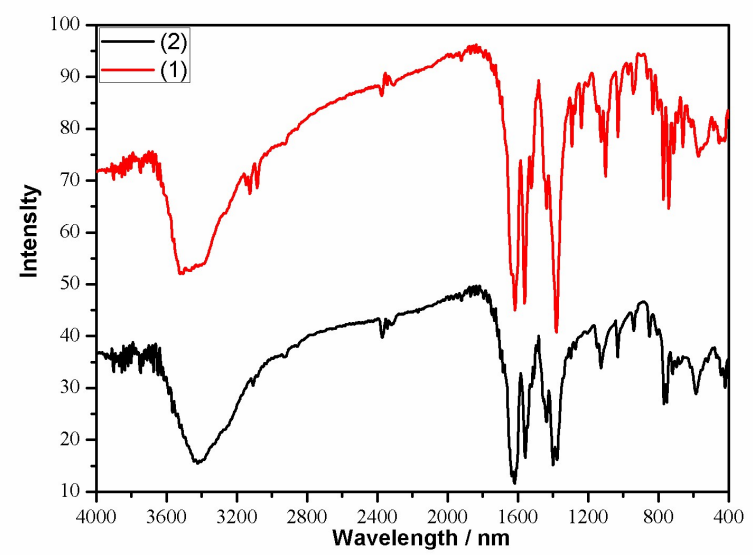
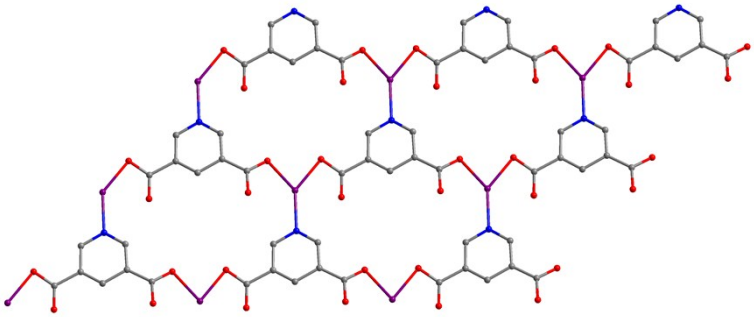
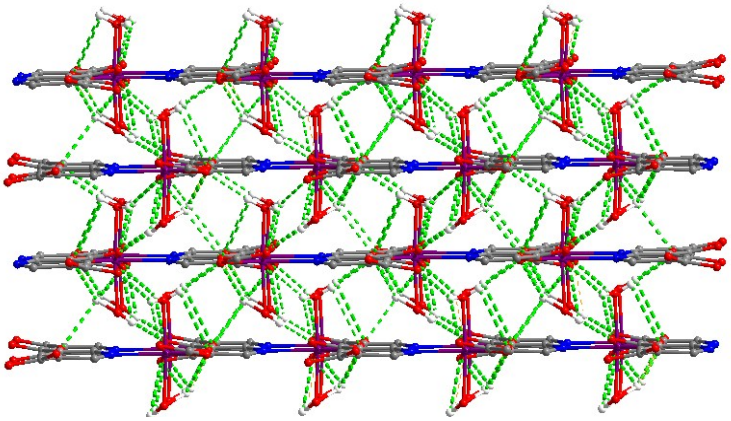


Fig. S1. The IR spectra of **1** and **2**

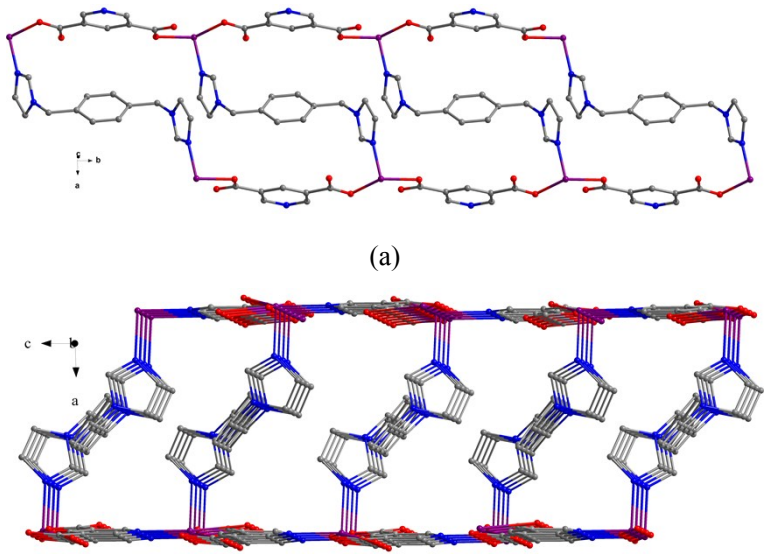


(a)



(b)

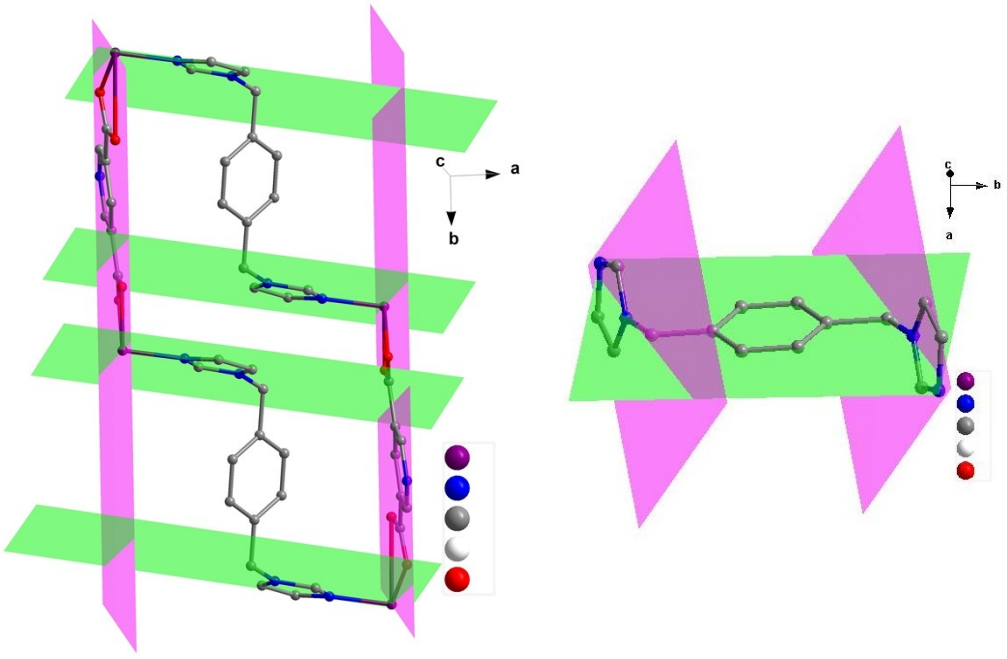
Fig. S2 (a) 2D network of complex **1** in ab-plane; (b) 3D network of **1**



(a)

(b)

Fig. S3 (a) The 1D ladder chain structure of **2**; (b) the 1D double layer structure with (4,4) rhombic grid in the *ac* plane of **2**



(a) (b)

Fig.S4 The different types of planes for (4,4) rhombic grid (a) and 1,2-BIYB ligands (b)

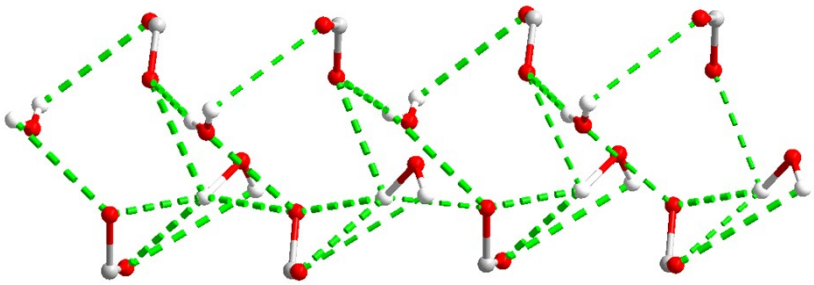


Fig.S5 The hydrogen bonding interactions in **2**

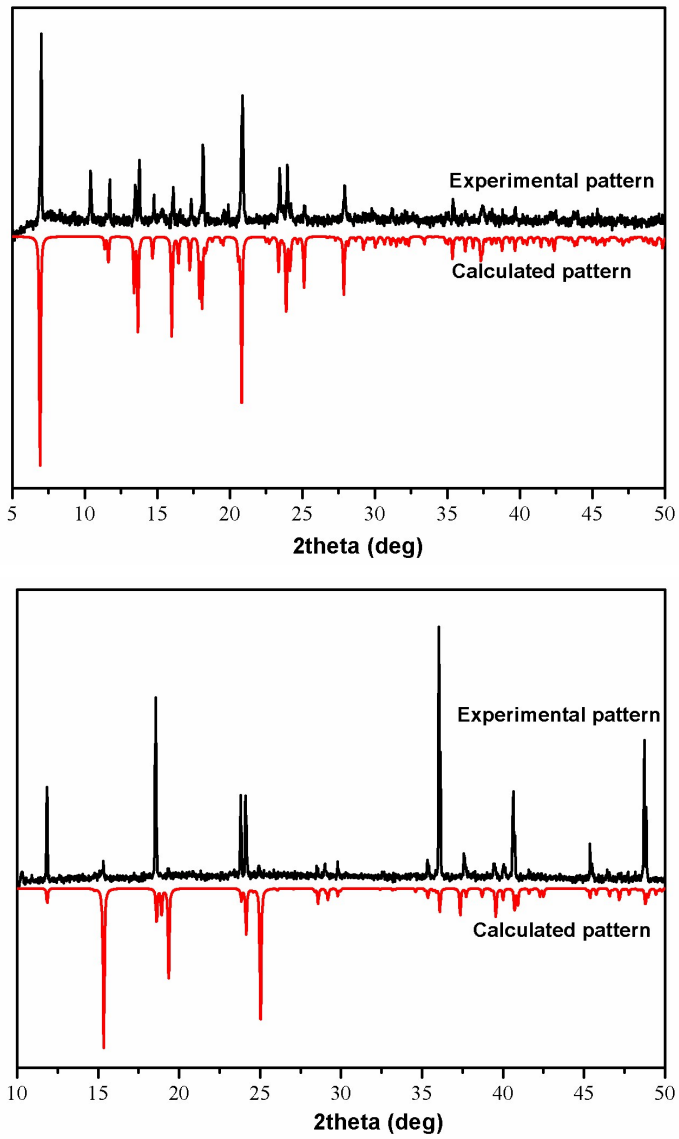


Fig. S6. PXRD patterns for compound **1** and **2**

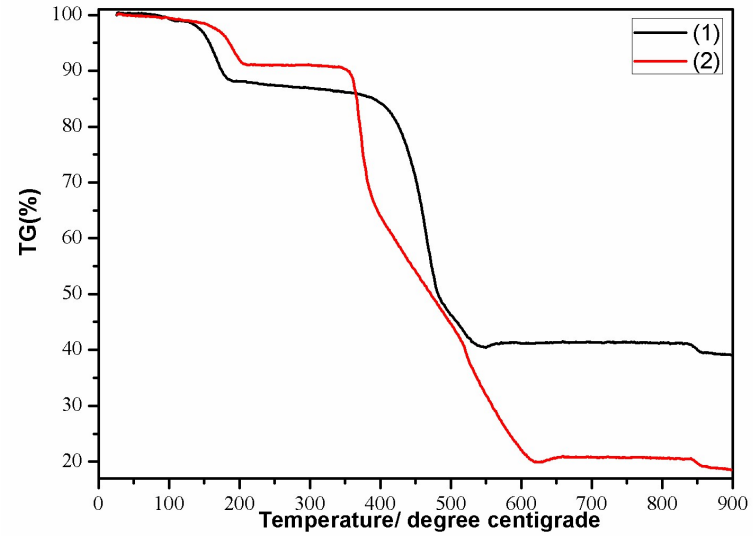


Fig.S7. The thermal stabilities of **1** and **2**

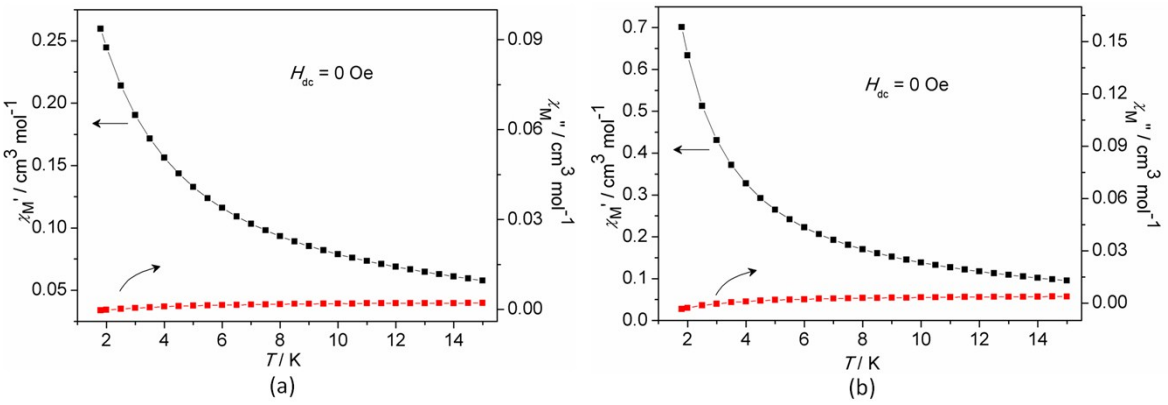


Fig. S8. Temperature dependence of the in-phase (χ′) and out-ofphase (χ″) of the ac susceptibilities for **1** (a) and 2 (b) under zero dc field.

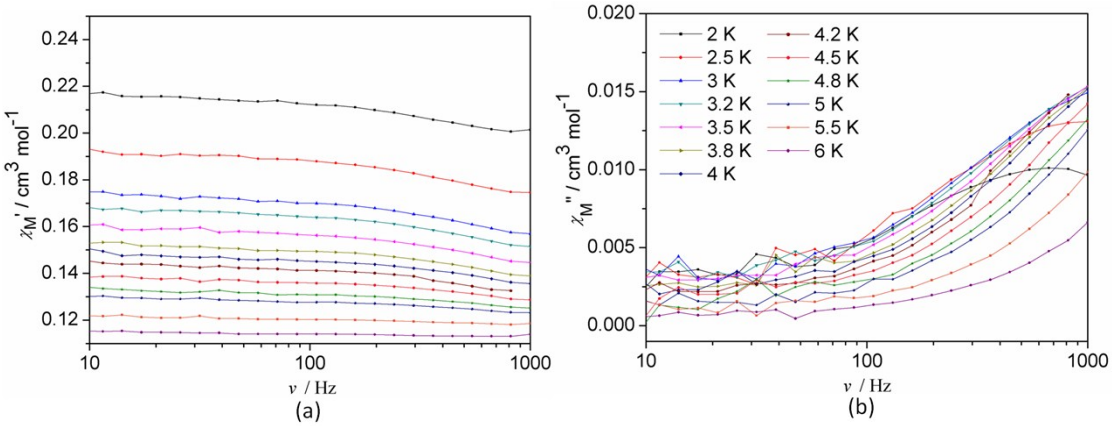


Fig. S9 Frequency dependence of χ′ and χ″ susceptibilities for **1** at applied DC fields of 3000 Oe.

Table S1 Crystal data and structure refinement summary for **2**

Compound	2		
T/K	293(2)	*Γ* (°)	90.00
Empirical formula	$C_{14}H_{14}N_3O_6Co$	*V* / Å^{-3}	1514.7(5)
Formula weight	379.21	D_c/ Mg•m^{-3}	1.663
Crystal system	monoclinic	*F*(000)	776
Space group	P2(1)/c	Reflections collected	8955
a/ Å	12.804(2)	Data/restraints/parameters	3638/229/4
b/ Å	9.8015(17)	*Z*	4
c/ Å	12.078(2)	final *R*	0.0372
α (°)	90.00	w_R indices(all data)	0.0768
β(°)	92.057(3)	GOF on F^2	1.03

Table S2 Selected bond lengths (Å) and angles (°) for **2**

Compound	2				
Co1-O1#1	2.0464(17)	Co1-O3#2	2.0630(18)	Co1-N1	2.077(2)
Co1-O5	2.102(2)	Co1- N2	2.1349(19)	O1#1-Co1- N1	90.72(8)
O3#2-Co1-N1	98.19(9)	O1#1-Co1-O3	130.71(7)	O1#1-Co1-O5	84.78(8)
O3#2-Co1-O5	87.58(9)	N1-Co1-O5	174.16(9)	O1#1-Co1-N2	135.84(7)
O3#2-Co1-N2	91.91(7)	N1-Co1-N2	94.24(8)	O5-Co1-N2	86.46(8)

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

Table S3 The geometrical parameters of all hydrogen bonds for **2**

D-H···A	d (D-H)/Å	d (H···A)/ Å	d (D-H···A)/Å	∠DHA/°
O(5)-H(5)A···O(1)#1	0.85(2)	2.01(2)	2.824(3)	160(2)
O(5)-H(5)B···O(3)#2	0.86(3)	1.92(3)	2.762(3)	168(3)
O(6) -H(6)A···O(3)#3	0.87(4)	2.06(4)	2.858(3)	153(4)
O(6)-H(6)A···O(1)	0.86(4)	2.07(4)	2.923(4)	168(4)

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

Table S4. Selected magneto-structural data for some 2D Co^{2+} compounds

L.p	Compound	Intralayer Co… Co distances/ Å	Magnetic properties	Ref
1	$[Co(dmpzm)(\mu_{1,5}\text{-dca})_2]_n$	7.4900 8.7527	isolated cations ma	1
2	$[Co_2(\mu_{1,5}\text{-dca})_4(4\text{-cypy})_4]_n$	7.745 8.037 8.349 8.404	AF (J = -0.80 cm^{-1})	2
3	$[Co(\mu_{1,5}\text{-dca})_2(3\text{-cypy})_2]_n$	8.194	AF (J = -1.18 cm^{-1})	2
4	$[Co(btrm)_2(\mu_{1.5}\text{-dca})]ClO_4$	8.539	AF(J not given)	3
5	$[Co(\mu_{1.5}\text{-dca})_2(dmdpy)]_n$	8.102	AF (J = -0.08 cm^{-1})	4
6	$[Co(azbbpy)(4,4'\text{-bipy})_{0.5}(DMF)(NCS)_2]\cdot MeOH$	13.92	magnetically isolated cations	5
7	$[Co(azbbpy)(bpe)_{0.5}(DMF)(NCS)_2]\cdot 0.25H_2O$	13.67	magnetically isolated cations	5
8	$[Co(atz)_2(dca)_2]_n$	8.041	magnetically isolated cations	6
9	$[Co(ppad)_2]n$	8.302	magnetically isolated cations	7
10	$[Co(tbta)N_3]ClO4\cdot 3CH_3CN$	8.186(1)	AF (J = -0.48 cm^{-1})	8
11	$[\{ArNdCMe\}_2(NPh)]Co(NCS)_2$	8.67		9
12	$[\{ArNdCMe\}_2(NPh)]Co(NCS)_2$	9.96		9

Table S5. The best results fitted for **2** under 1500 Oe dc field by a generalized Debye model

T(K)	χ_T	χ_S	α
2.0	0.54	0.19	0.32
2.2	0.50	0.17	0.31
2.5	0.46	0.17	0.28
2.8	0.42	0.15	0.27
3.0	0.40	0.15	0.24
3.2	0.38	0.15	0.21
3.5	0.35	0.14	0.18
3.8	0.33	0.12	0.19
4.0	0.31	0.12	0.15

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