Field-induced slow magnetic relaxation in two-dimensional and three-dimensional Co(II) coordination polymers

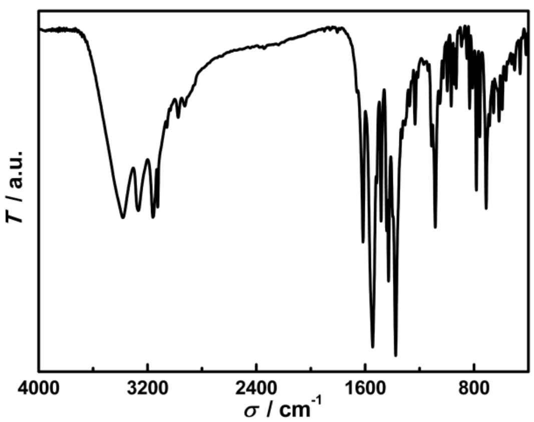
Deyun Ma,[b] Guo Peng,*[ac] Ying-Ying Zhang[c] and Bo Li*[d]

[a]College of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211816, P. R. China. Email: guopengnjtech@foxmail.com

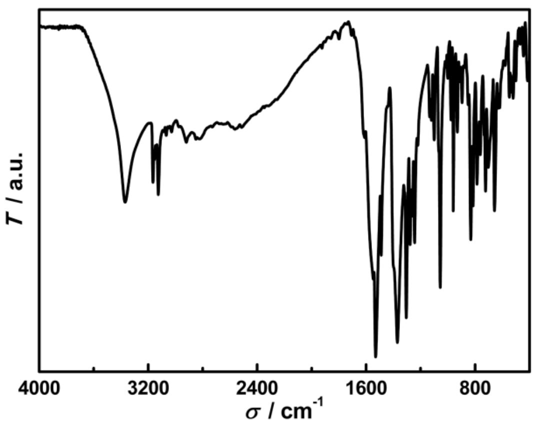
[b]School of Food and Pharmaceutical Engineering, Zhaoqing University, Zhaoqing 526061, P. R. China.

[c]Herbert Gleiter Institute of Nanoscience, School of Materials Science and Engineering, Nanjing University of Science and Technology, Nanjing 210094, P. R. China. Email: guopeng@njust.edu.cn

[d]College of Chemistry and Pharmaceutical Engineering, Nanyang Normal University, Nanyang 473061, P. R. China. Email: libozzu0107@163.com

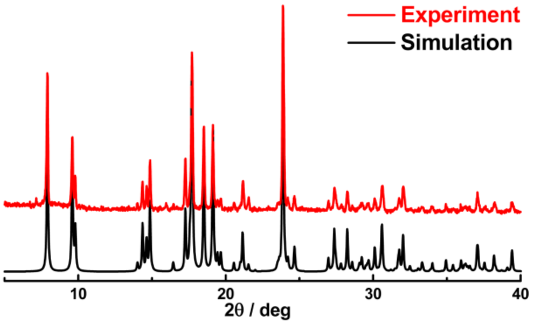


(a)

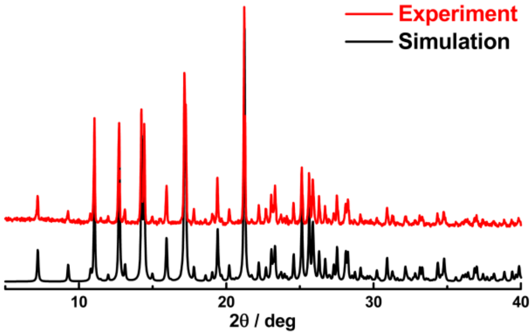


(b)

Fig. S1 IR spectra for complexes **1** (a) and **2** (b).



(a)



(b)

Fig. S2 Experimental and simulated PXRD patterns for complexes **1** (a) and **2** (b).

Table S1 Continuous shape measures (CShM) for complexes **1** and **2**

	1	2
HP-6 (D_{6h})	28.915	32.784
PPY-6 (C_{5V})	22.659	27.544
OC-6 (O_h)	**2.289**	**0.211**
TPR-6 (D_{3h})	14.539	14.727
JPPY-6 (C_{5v})	26.170	31.278

HP-6 = Hexagon, PPY-6 = Pentagonal pyramid, OC-6 = Octahedron, TPR-6 = Trigonal prism, JPPY-6 = Johnson pentagonal pyramid J2

Table S2 Hydrogen Bonds of **1** and **2**

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠(DHA)
		1		
O(5)–H(5A)···O(4)a	0.87	2.10	2.830(5)	142
C(5)–H(5B)···O(2)	0.89	1.94	2.712(5)	145
		2		
O(3)–H(3)···O(1)b	0.84	1.76	2.600(4)	173
O(6)–H(6A)···O(3)c	0.84	1.86	2.666(4)	162
O(6)–H(6B)···O(4)	0.84	1.86	2.596(4)	144

Symmetry codes: For **1**, a: 1+x, 1+y, z. For **2**, b: -1+x, y, z; c: 0.5+x, .05-y, 0.5+z.

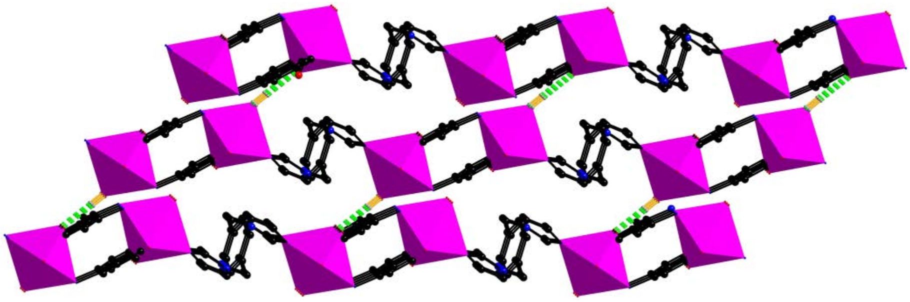


Fig. S3 The O-H···O hydrogen bonds (green dash lines) in the 3D supramolecular structure of **1**.

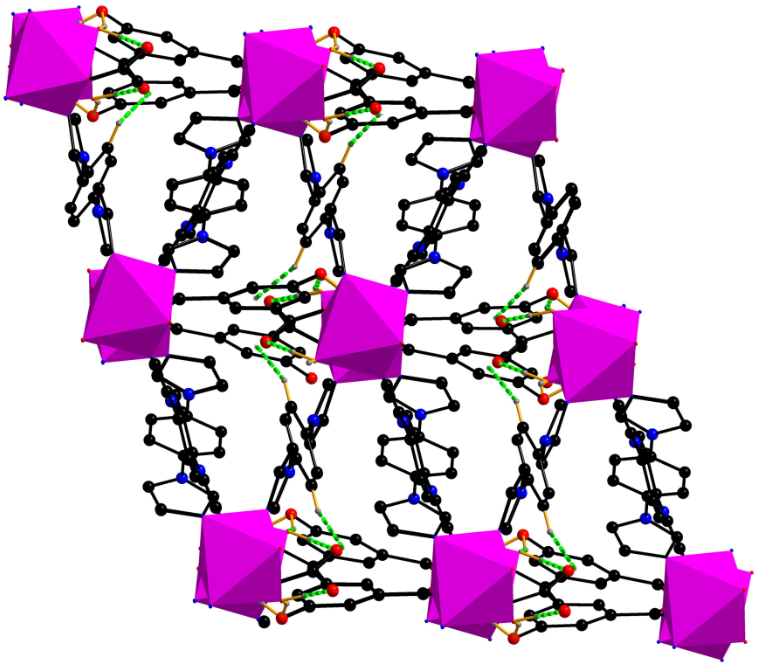
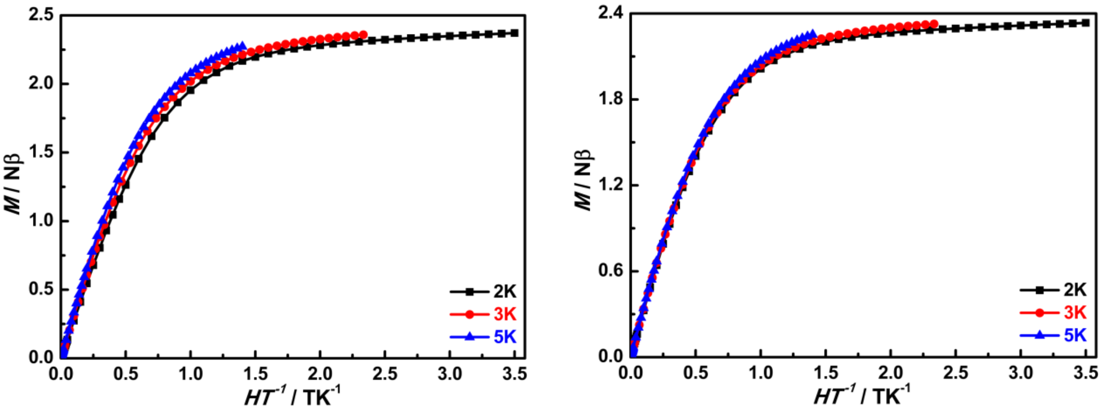
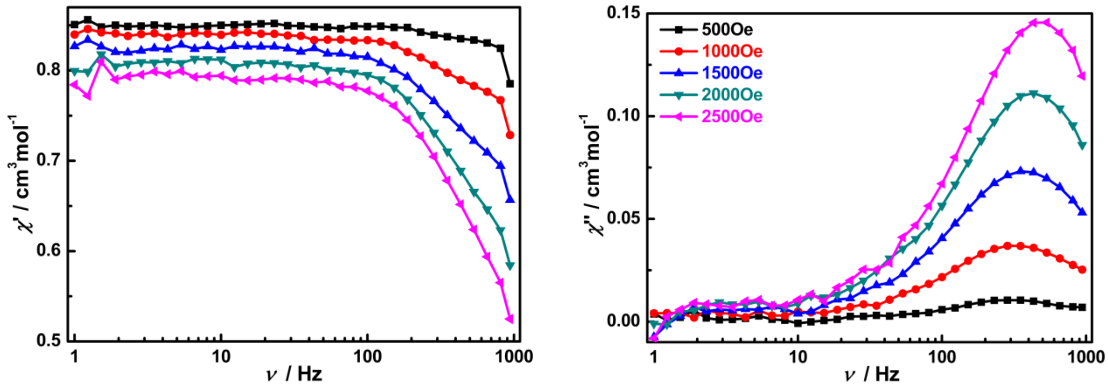


Fig. S4 The O-H···O hydrogen bonds and C-H···π stacking interactions (green dash lines) in the 3D framework of **2**.



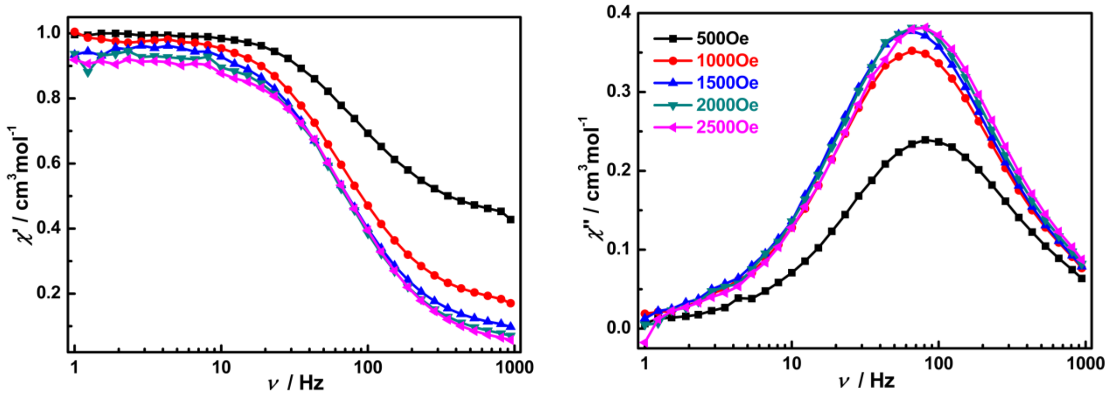
(a) (b)

Fig. S5 *M* vs. HT^{-1} plots for **1** (a) and **2** (b).



(a) (b)

Fig. S6 Frequency dependence of in-phase (a) and out-of-phase (b) ac susceptibility data under different dc fields at 2 K for **1**.



(a) (b)

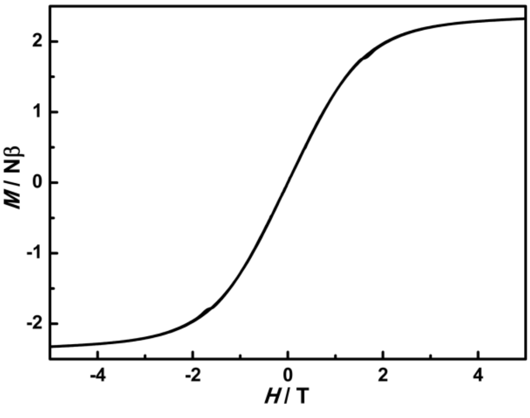
Fig. S7 Frequency dependence of in-phase (a) and out-of-phase (b) ac susceptibility data under different dc fields at 2 K for **2**.

Table S3 Cole-Cole parameters of **1** under 1000 Oe dc field

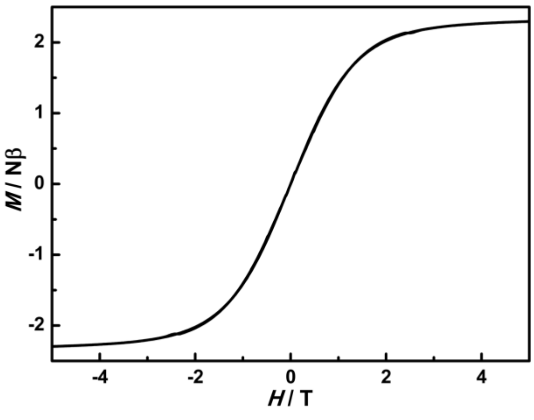
T / K	χ_S / cm^{-3}mol^{-1}	χ_T / cm^{-3}mol^{-1}	τ / s	α	R
2.0	7.56E-01	8.31E-01	5.50E-04	3.13E-02	4.01E-04
2.2	7.01E-01	7.74E-01	4.91E-04	2.94E-02	3.18E-04
2.4	6.52E-01	7.24E-01	4.35E-04	3.42E-02	2.23E-04
2.6	6.12E-01	6.82E-01	4.00E-04	2.91E-02	2.45E-04
2.8	5.75E-01	6.44E-01	3.64E-04	3.42E-02	1.84E-04
3.0	5.42E-01	6.11E-01	3.28E-04	4.83E-02	1.67E-04
3.2	5.16E-01	5.80E-01	2.97E-04	1.58E-02	2.87E-04
3.4	4.89E-01	5.53E-01	2.67E-04	4.32E-02	2.30E-04

Table S4 Cole-Cole parameters of **2** under 1000 Oe dc field

T / K	χ_S / cm^{-3}mol^{-1}	χ_T / cm^{-3}mol^{-1}	τ / s	α	R
2.0	1.62E-01	1.00E+00	2.30E-03	1.01E-01	1.72E-03
2.5	1.35E-01	8.04E-01	1.22E-03	9.52E-02	1.43E-03
3.0	1.23E-01	6.73E-01	6.53E-04	7.49E-02	9.43E-04
3.5	1.22E-01	5.80E-01	3.46E-04	4.23E-02	3.99E-04
4.0	1.37E-01	5.10E-01	1.90E-04	2.65E-15	4.16E-04
4.5	1.54E-01	4.59E-01	1.06E-04	6.03E-15	3.53E-04
5.0	2.05E-01	4.13E-01	7.32E-05	6.12E-15	3.45E-04



(a)



(b)

Fig. S8 Field dependence of the magnetization at 2 K for **1** (a) and **2** (b).

Table S5 Magnetic parameters of **1** and **2** compared with that of other high-dimensional Co(II) coordination polymers with SIM behavior

Compound	Dimension	SOC parameters	ZFS parameters	H_{dc} (Oe)	U_{eff} (K)	τ_0 (s)	Ref.
$[Co(1,4\text{-bimb})_{0.5}(5\text{-aip})(H_2O)]_n$	2D	α = 1.20, λ = -160 cm^{-1}, Δ = -119 cm^{-1}, g = 2.17, zJ = -0.085 cm^{-1}		1000	4.9	6.44×10^{-5}	This work
$[Co(1,4\text{-bib})_{1.5}(5\text{-hip})(H_2O)]_n$	3D	α = 1.26, λ = -160 cm^{-1}, Δ = -56.5 cm^{-1}, g = 2.12	D = -102 cm^{-1}, E = 0.36 cm^{-1}, g_{xy} = 1.92, g_z = 2.20	1000	18.4	1.83×10^{-6}	This work
$[Co(btm)_2(SCN)_2\cdot H_2O]_n$	1D		D = 56.6 cm^{-1}, E = 3.70 cm^{-1}, g = 2.49	1500	45.4	5.6×10^{-8}	1
$[Co(tdmmb)(bpe)][BF_4]_2\cdot 3CH_3CN$	1D		D = 21.7(7) cm^{-1}, E = −0.4(3) cm^{-1}, g = 2.121(1)	1000	19.0	7.5×10^{-6}	2
$[Co^{II}L_{N3O2})]_6[Co^{III}(CN)_6]_4\cdot 26H_2O$	1D		D = 21.4(6) cm^{-1}, E= −0.08(1) cm^{-1}, g_z = 2.121(1), g_{xy} = 2.328(5)	1500	9.1	1.9×10^{-6}	3
$[Co(bpg)_2(SCN)_2]\cdot 2DMF$	2D		D = 67.5(2) cm^{-1}, E = −2.32(3) cm^{-1}, g_{xy} = 2.48(1), g_z = 2.26(3)	1500	15.3	9.7×10^{-6}	4
$[Co(ppad)_2]_n$	2D	α = 1.48(1), λ =	D = 76 cm^{-1}, E =	2000	16.4	5.03×10^{-6}	5

		−147(1) cm^{-1}, Δ = −482(5) cm^{-1}	6.5cm^{-1}, g = 2.46				
$\{[Co(bmzbc)_2]\cdot 2DMF\}_n$	2D		D = 62.6 cm^{-1}, E = 13.4 cm^{-1}, g_x = 2.055, g_y = 2.362, g_z = 2.849	2000	11.8	1.3×10^{-5}	6
$[Co(azbbpy)(4,4'\text{-}bipy)_{0.5}(DMF)(NCS)_2]\cdot MeOH$	2D	α = 1.26(1), λ = −153(1) cm^{-1}, Δ = −350(2) cm^{-1}		1000	14	1.2×10^{-6}	7
$[Co(azbbpy)(bpe)_{0.5}(DMF)(NCS)_2]\cdot 0.25H_2O$	2D	α = 1.20(1), λ = −162(1) cm^{-1}, Δ = −630(5) cm^{-1}		1000	8.4	1.7×10^{-6}	7
$[Co(dca)_2(atz)_2]_n$	2D	α = 1.18(1), λ = −125(1) cm^{-1}, Δ = −509(10) cm^{-1}		1000	7.3	1.7×10^{-6}	8
$\{[Co(3,3'\text{-}Hbpt)_2(SCN)_2]\cdot 2H_2O\}_n$	2D		D = 70.1 cm^{-1}, E = 0.7 cm^{-1}, g_{xy} = 2.61, g_z = 2.64	1500	32.5	7.2×10^{-7}	9
$\{[(Co(NCS)_2)_3(TPT)_4]\cdot aH_2O\cdot bMeOH\}_n$	3D			600	7.0	8.68×10^{-6}	10
$[Co(bmzbc)_2(1,2\text{-}etdio)]_n$	3D			2000	16.8	1.2×10^{-7}	11
$[Co(NCS)_2(L)]\cdot 2H_2O\cdot CH_3OH$	3D		D = -86.91 cm^{-1}, E = 15.42 cm^{-1}, g_{xy} = 2.511, g_z = 2.181	800	7.05	1.09×10^{-5}	12

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