Supporting information

Chiral and kryptoracemic Dy(III) complexes with field-induced single molecule magnet behavior

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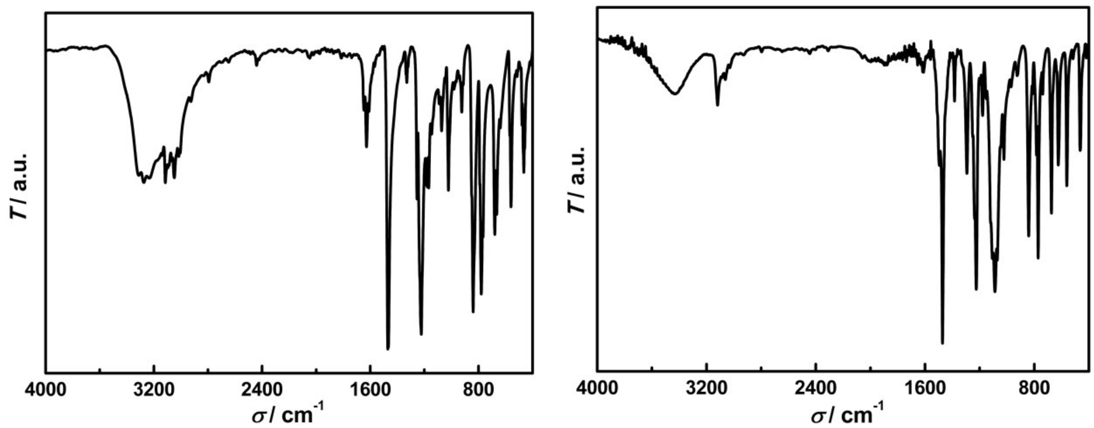


(a) (b)

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

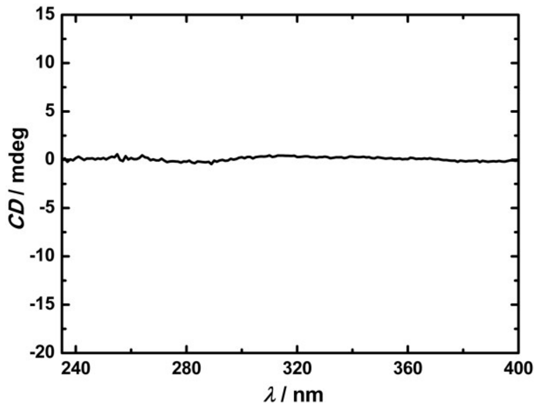
Table S1 Various experiments were carried out for crystalline products.

Lathanide salts	The ratio of PNO to Dy ions	Solvent	Products
$DyBr_3·6H_2O$	7:1	CH_3CN	1
$Dy(ClO_4)_3·6H_2O$	7:1 / 10:1 / 12:1/ 16:1	CH_3CN / CH_3OH / C_2H_5OH / CH_3CN+ C_2H_5OH	×
$Dy(NO_3)_3·6H_2O$	7:1	CH_3CN / C_2H_5OH / CH_3CN+C_2H_5OH / CH_3CN+CH_3OH	×
$Dy(OAc)_3·4H_2O$	7:1	CH_3CN / CH_3CN+C_2H_5OH / CH_3CN+CH_3OH	×
$Dy(OTf)_3$	7:1 / 8:1 / 10:1	CH_3CN / C_2H_5OH / CH_3OH	×
$Dy(NO_3)_3·6H_2O$+$DyCl_3·6H_2O$	7:1 (14:1:1)	CH_3CN	×
$Dy(NO_3)_3·6H_2O$+$Dy(ClO_4)_3·6H_2O$	7:1 (35:2:3 / 21:1:2)	C_2H_5OH	2
$Dy(NO_3)_3·6H_2O$+ $Dy(OTf)_3$	7:1 (35:1:4)	C_2H_5OH	×
$Dy(OTf)_3$+$Dy(acac)_3$	7:1 (35:4:1)	C_2H_5OH	×

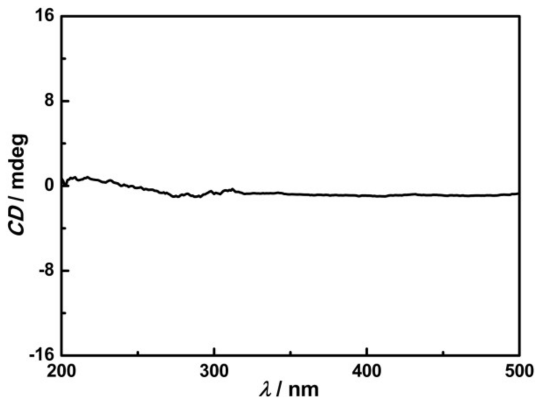
Table S2 Continuous shape measures (CShM) for complexes **1** and **2**.

Complexes	Ions	SAPR (D_{4d})	TDD (D_{2d})	JBTPR (C_{2v})	BTPR (C_{2v})
1	Dy1	1.928	**0.488**	2.328	1.534
2	Dy1	**1.271**	2.001	2.672	1.981
	Dy2	**1.689**	2.429	2.323	**1.687**

SAPR = Square antiprism, TDD = Triangular dodecahedron, JBTPR = Biaugmented trigonal prism J50, BTPR = Biaugmented trigonal prism.

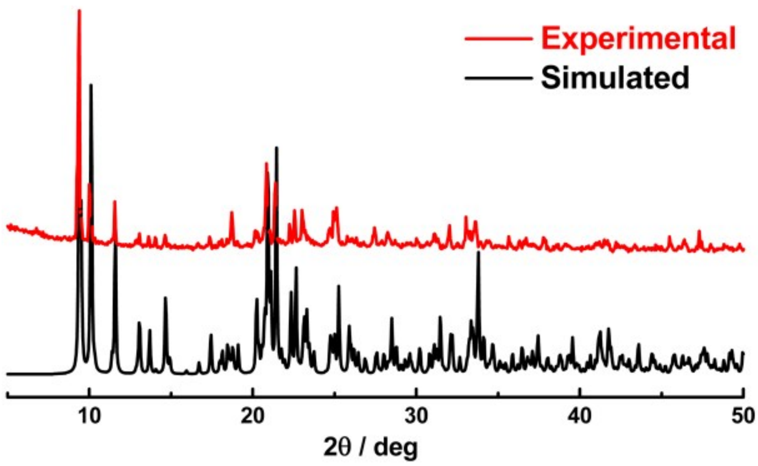


(a)

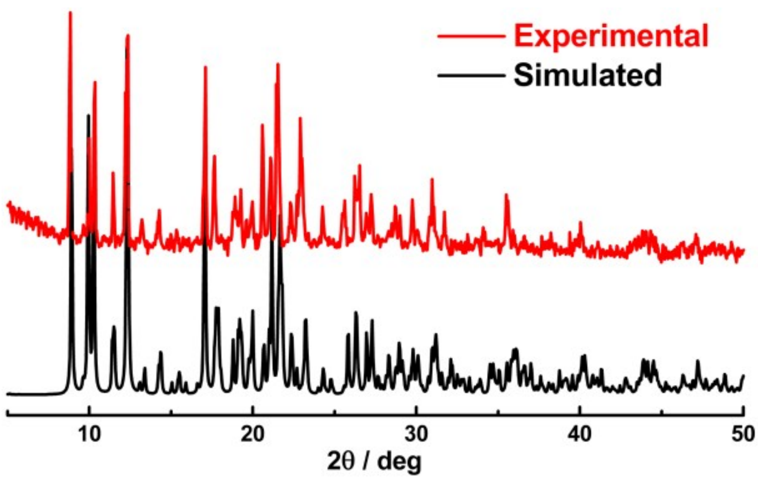


(b)

Fig. S2 Solid-state CD spectra of bulk samples for complexes **1** (a) and **2** (b).

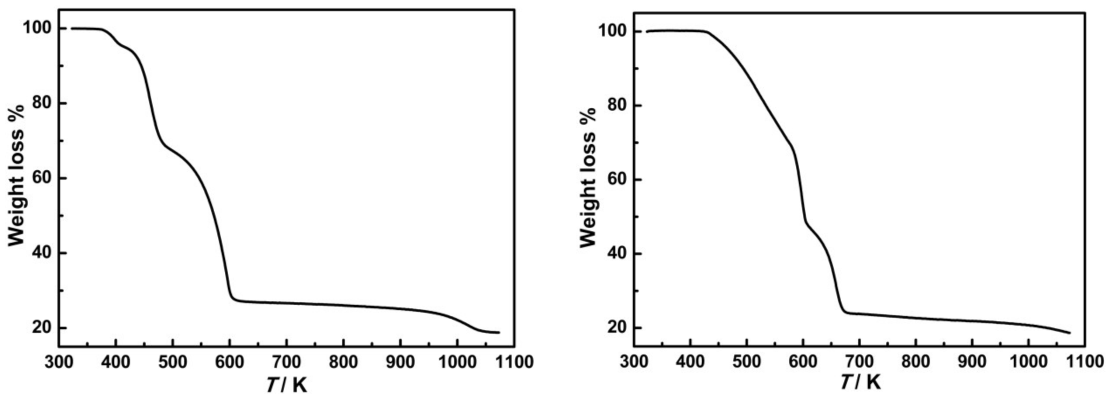


(a)



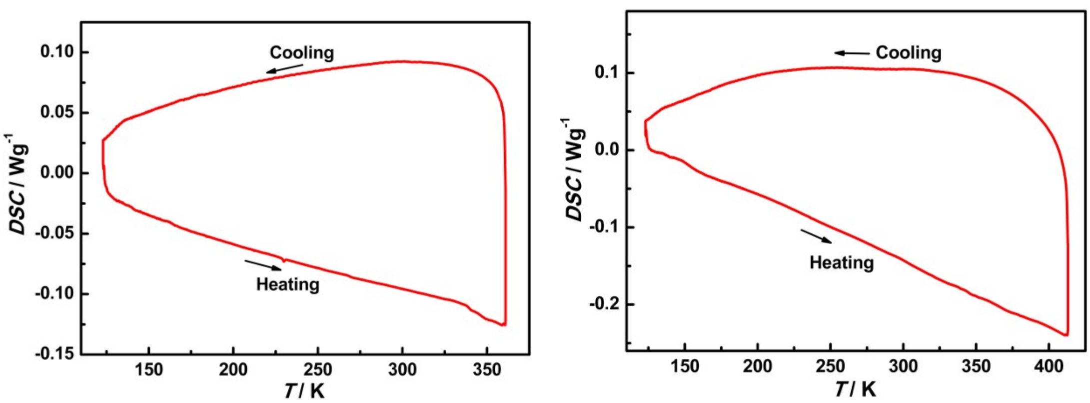
(b)

Fig. S3 Experimental and simulated PXRD patterns for complexes **1** (a) and **2** (b).



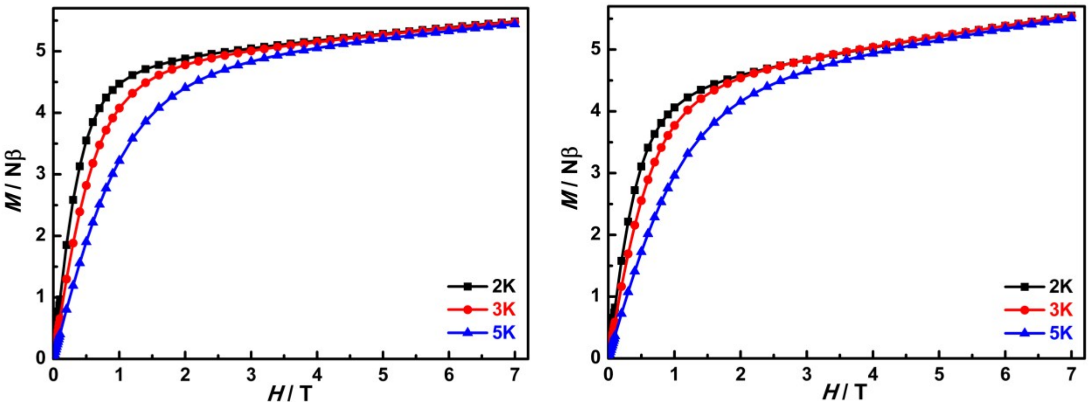
(a) (b)

Fig. S4 TGA curves for complexes **1** (a) and **2** (b).



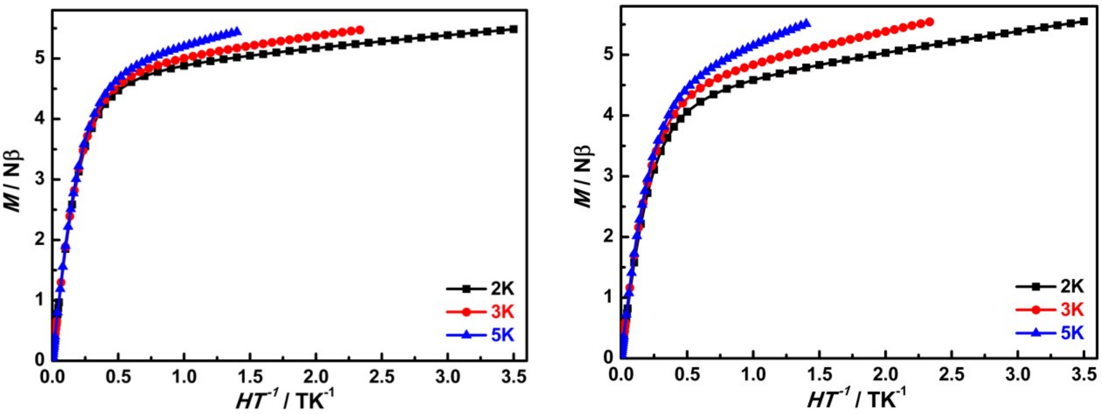
(a) (b)

Fig. S5 DSC curves for complexes **1** (a) and **2** (b).



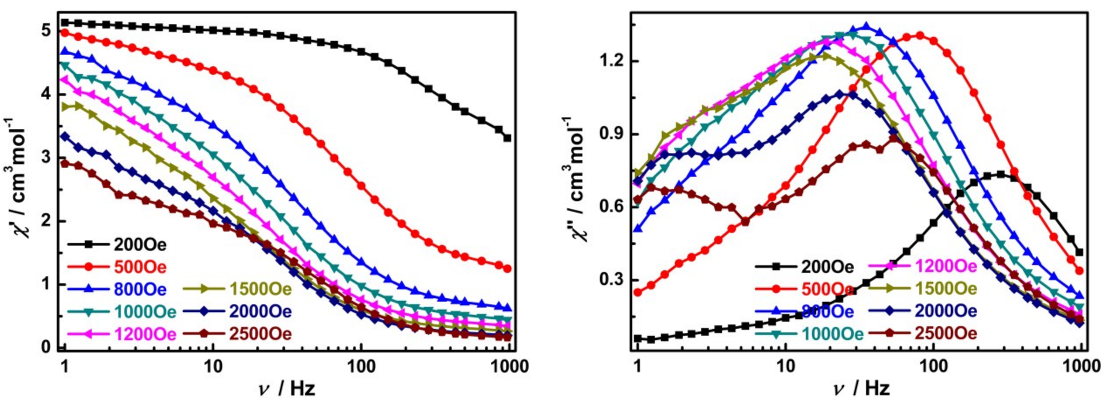
(a) (b)

Fig. S6 M vs. H plots for complexes **1** (a) and **2** (b).



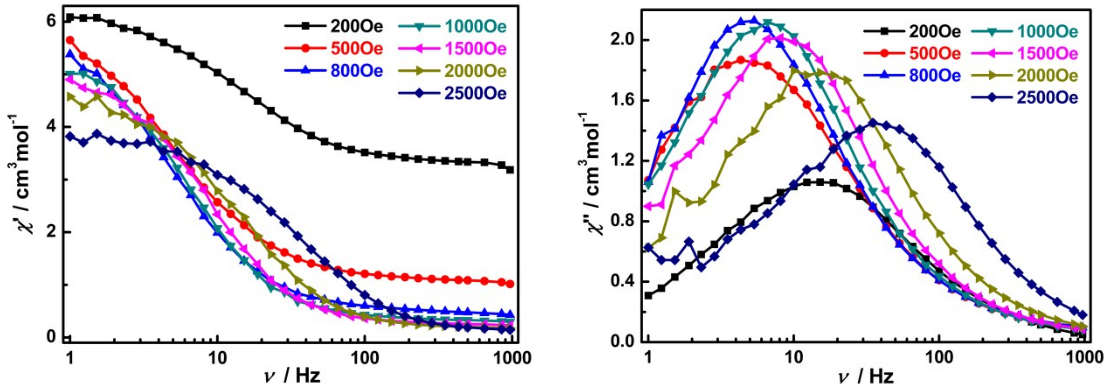
(a) (b)

Fig. S7 M vs. HT^{-1} plots for complexes **1** (a) and **2** (b).



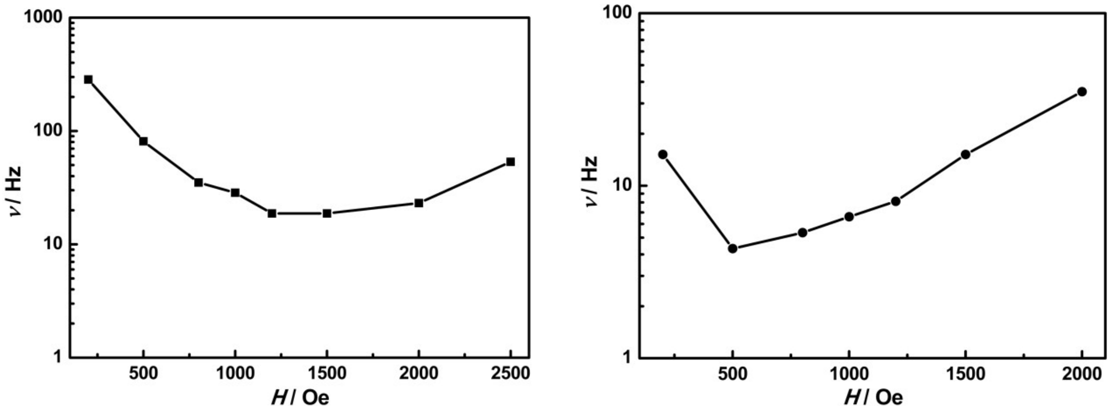
(a) (b)

Fig. S8 Frequency dependence of in-phase (a) and out-of-phase (b) ac susceptibility signals under different dc fields at 2K for **1**.



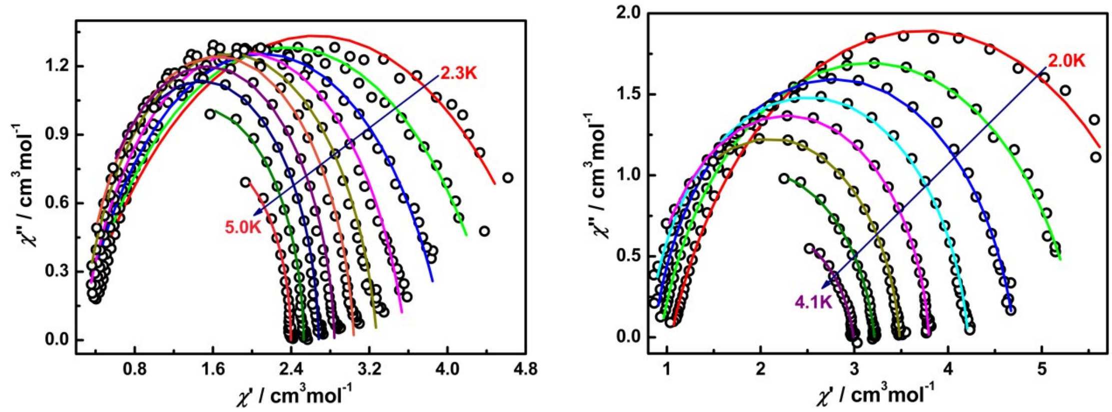
(a) (b)

Fig. S9 Frequency dependence of in-phase (a) and out-of-phase (b) ac susceptibility signals under different dc fields at 2K for **2**.



(a) (b)

Fig. S10 Field dependence of the characteristic frequency for complexes **1** (a) and **2** (b) at 2K.



(a) (b)

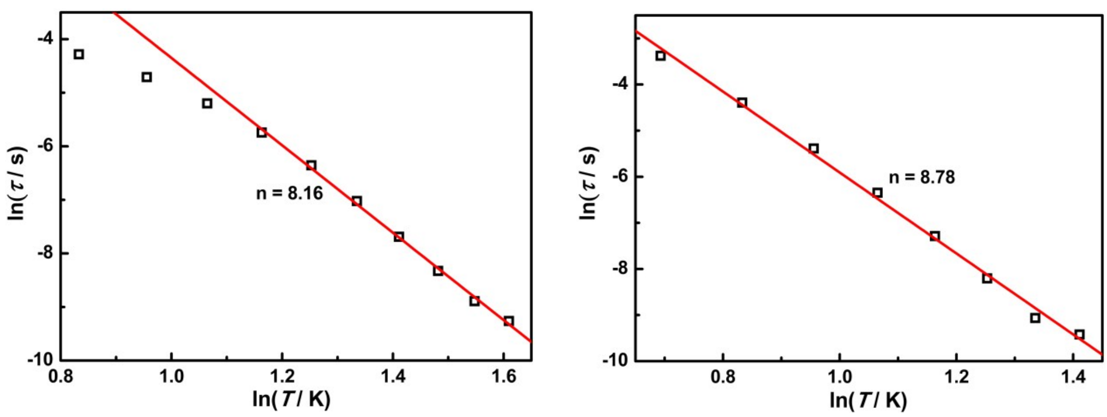
Fig. S11 The Cole-Cole plots for complexes **1** (a) and **2** (b). The solid lines are the best fits to a generalized Debye model.

Table S3 Cole-Cole parameters of **1** under 1200Oe dc field.

T / K	χ_S / cm^{-3}mol^{-1}	χ_T / cm^{-3}mol^{-1}	τ / s	α	R
2.3	1.93E-01	5.10E+00	1.38E-02	3.66E-01	2.60E-01
2.6	2.11E-01	4.52E+00	9.01E-03	3.16E-01	1.71E-01
2.9	2.37E-01	3.98E+00	5.52E-03	2.47E-01	1.00E-01
3.2	2.63E-01	3.57E+00	3.20E-03	1.70E-01	7.22E-02
3.5	2.57E-01	3.28E+00	1.74E-03	1.17E-01	8.07E-02
3.8	2.55E-01	3.04E+00	8.91E-04	7.22E-02	4.87E-02
4.1	2.49E-01	2.84E+00	4.57E-04	4.94E-02	4.10E-02
4.4	2.92E-01	2.68E+00	2.42E-04	3.19E-02	2.73E-02
4.7	4.37E-01	2.53E+00	1.38E-04	2.00E-02	1.72E-02
5.0	8.16E-01	2.40E+00	9.48E-05	7.86E-03	1.10E-02

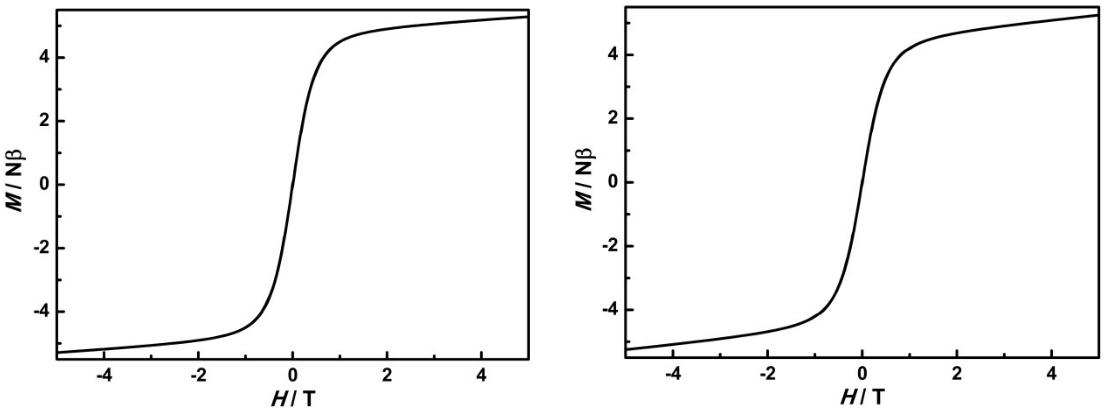
Table S4 Cole-Cole parameters of **2** under 500Oe dc field.

T / K	χ_S / cm^{-3}mol^{-1}	χ_T / cm^{-3}mol^{-1}	τ / s	α	R
2	1.04E+00	6.41E+00	3.42E-02	2.17E-01	4.90E-02
2.3	9.28E-01	5.39E+00	1.24E-02	1.73E-01	1.90E-02
2.6	8.61E-01	4.71E+00	4.57E-03	1.19E-01	3.22E-02
2.9	8.02E-01	4.21E+00	1.75E-03	8.87E-02	2.08E-02
3.2	7.67E-01	3.80E+00	6.84E-04	6.40E-02	2.32E-02
3.5	7.16E-01	3.48E+00	2.73E-04	7.58E-02	1.77E-02
3.8	7.71E-01	3.21E+00	1.16E-04	1.15E-01	1.05E-02
4.1	1.40E+00	2.99E+00	8.09E-05	1.49E-01	1.09E-02



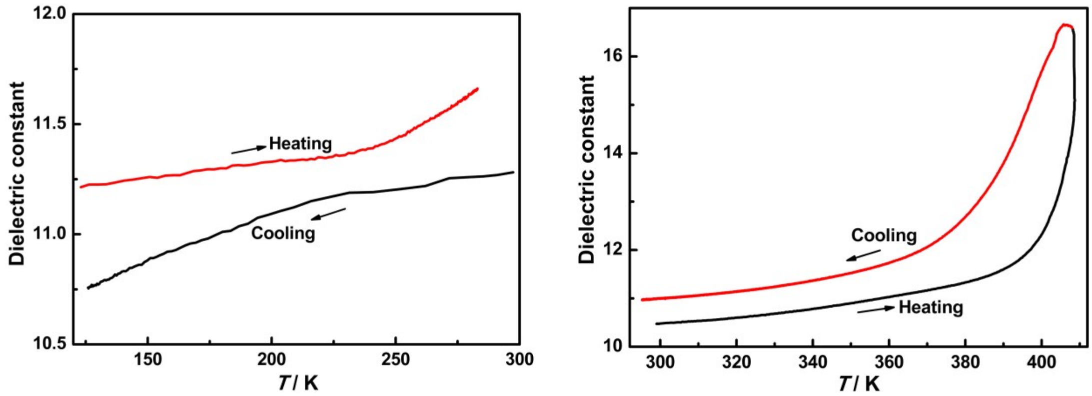
(a) (b)

Fig. S12 Lnτ vs. LnT plots for complexes **1** (a) and **2** (b). The red lines are the best fits to a power law.



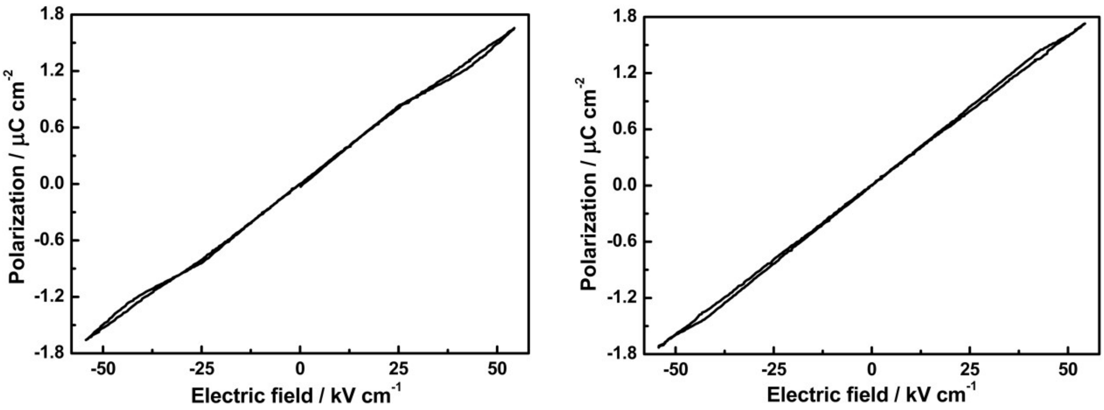
(a) (b)

Fig. S13 Field dependence of the magnetization at 2K for complexes **1** (a) and **2** (b).



(a) (b)

Fig. S14 Temperature dependence of the dielectric constant at 1MHz for complex **2**.



(a) (b)

Fig. S15 Selective P-E curves for complex **2** at 253K (a) and 273K (b).