Supporting information

Single molecule magnetic behaviour in lanthanide naphthalenesulfonate complexes

Guo Peng,*[a] Ying-Ying Zhang,[a] Bo Li,*[b] Xiao-Fan Sun,[c] Hong-Ling Cai,[c] De-Jing Li,[d] Zhi-Gang Gu,[d] and George E. Kostakis [e]

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

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

[c]Collaborative Innovation Center of Advanced Microstructures, Lab of Solid State Microstructures, School of Physics, Nanjing University, Nanjing 210093, P. R. China

[d]State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, 350002 Fuzhou, P. R. China

[e]Department of Chemistry, School of Life Sciences, University of Sussex, Brighton, BN1 9QJ, UK

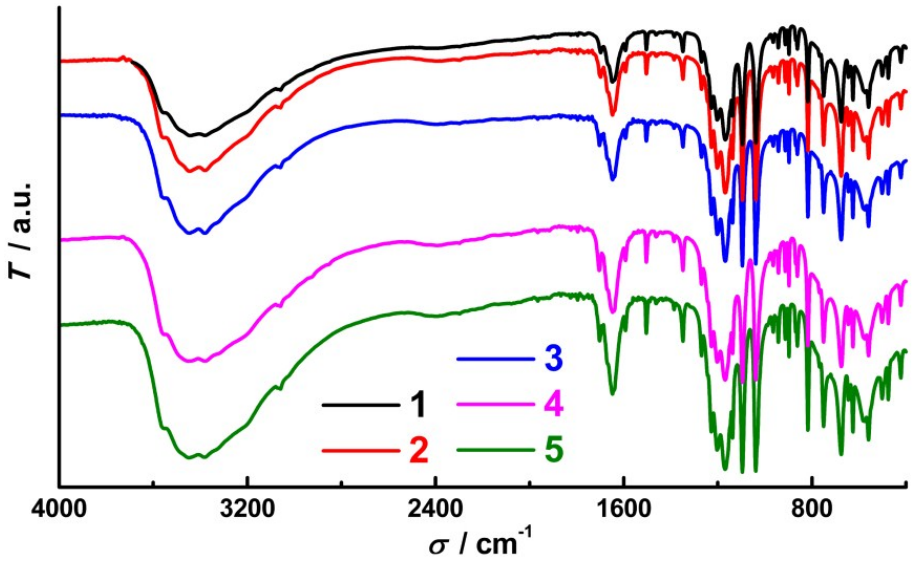


Fig. S1 IR spectra for complexes **1-5**.

Table S1 Continuous shape measures (CShM) for complexes **1-4**.

	1-Tb	**2-Dy**	**3-Er**	**4-Yb**
OP-8	29.156	29.056	29.473	28.868
HPY-8	23.875	23.835	23.515	23.889
HBPY-8	16.641	16.663	16.311	16.507
CU-8	10.209	10.281	10.03	10.082
SAPR-8	**0.619**	**0.619**	**0.639**	**0.621**
TDD-8	1.311	1.329	1.296	1.28
JGBF-8	14.862	14.904	14.872	15.045
JETBPY-8	28.707	28.643	28.785	28.534
JBTPR-8	1.787	1.75	1.828	1.738
BTPR-8	1.131	1.107	1.203	1.091
JSD-8	3.702	3.644	3.614	3.655
TT-8	10.995	11.043	10.763	10.864
ETBPY-8	24.297	24.397	24.445	24.311

OP-8=Octagon, HPY-8=Heptagonal pyramid, HBPY-8=Hexagonal bipyramid, CU-8=Cube, SAPR-8=Square antiprism, TDD-8=Triangular dodecahedron, JGBF-8=Johnson gyrobifastigium J26, JETBPY-8=Johnson elongated triangular bipyramid J14, JBTPR-8=Biaugmented trigonal prism J50, BTPR-8=Biaugmented trigonal prism, JSD-8=Snub diphenoid J84, TT-8=Triakis tetrahedron, ETBPY-8=Elongated trigonal bipyramid.

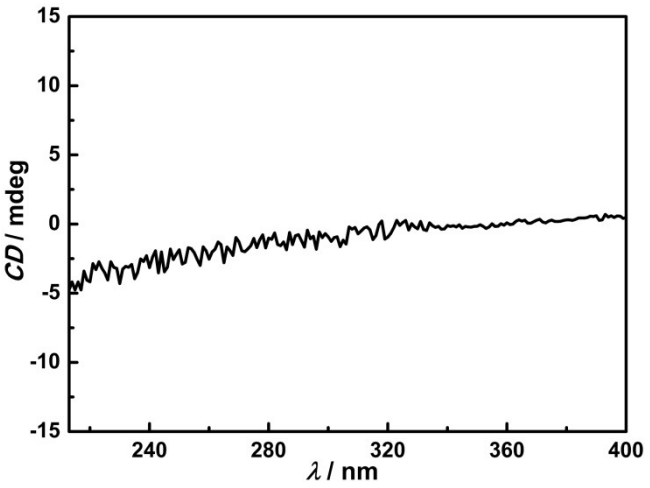


Fig. S2 Solid-state CD spectra of bulk sample for **2**.

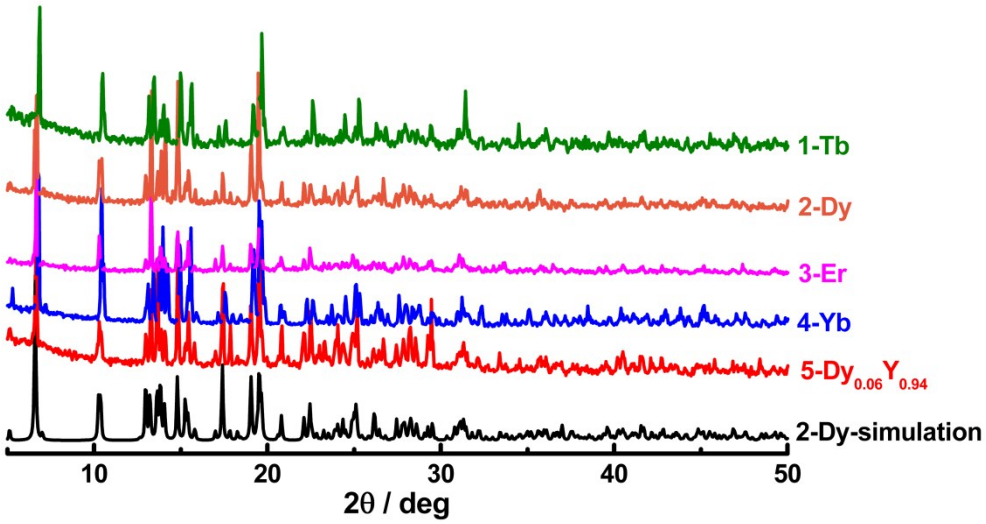


Fig. S3 Experimental and simulated PXRD patterns for complexes **1**-**5**.

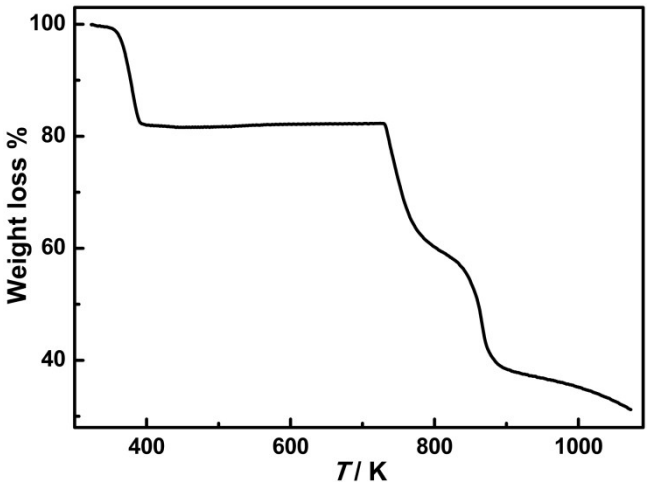


Fig. S4 TGA curve for **2**.

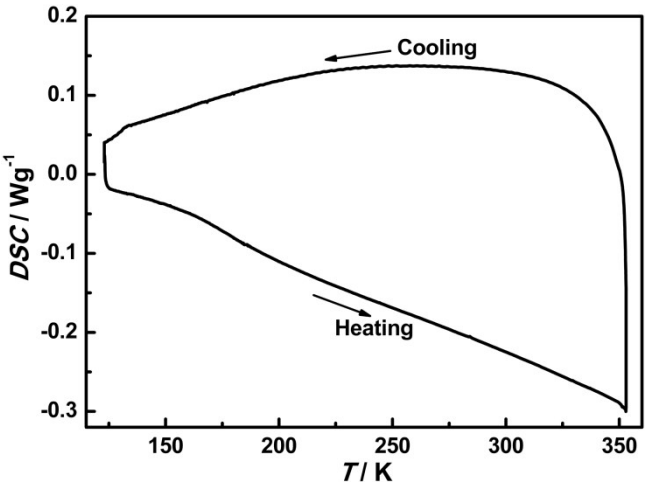


Fig. S5 DSC curve for **2**.

Table S2 Static magnetic data for **1**-**4**.

	Ground state of Ln^{III}	Expected χT at 300K (cm^3Kmol^{-1})	Measured χT at 300K (cm^3Kmol^{-1})	Saturation magnetization (Nβ)	Measured magnetization at 2K and 7T (Nβ)
1-Tb	$^7F_6$	11.82	11.52	9	4.65
2-Dy	$^6H_{15/2}$	14.17	13.75	10	5.09
3-Er	$^4I_{15/2}$	11.48	11.52	9	5.37
4-Yb	$^2F_{7/2}$	2.57	2.53	4	1.64

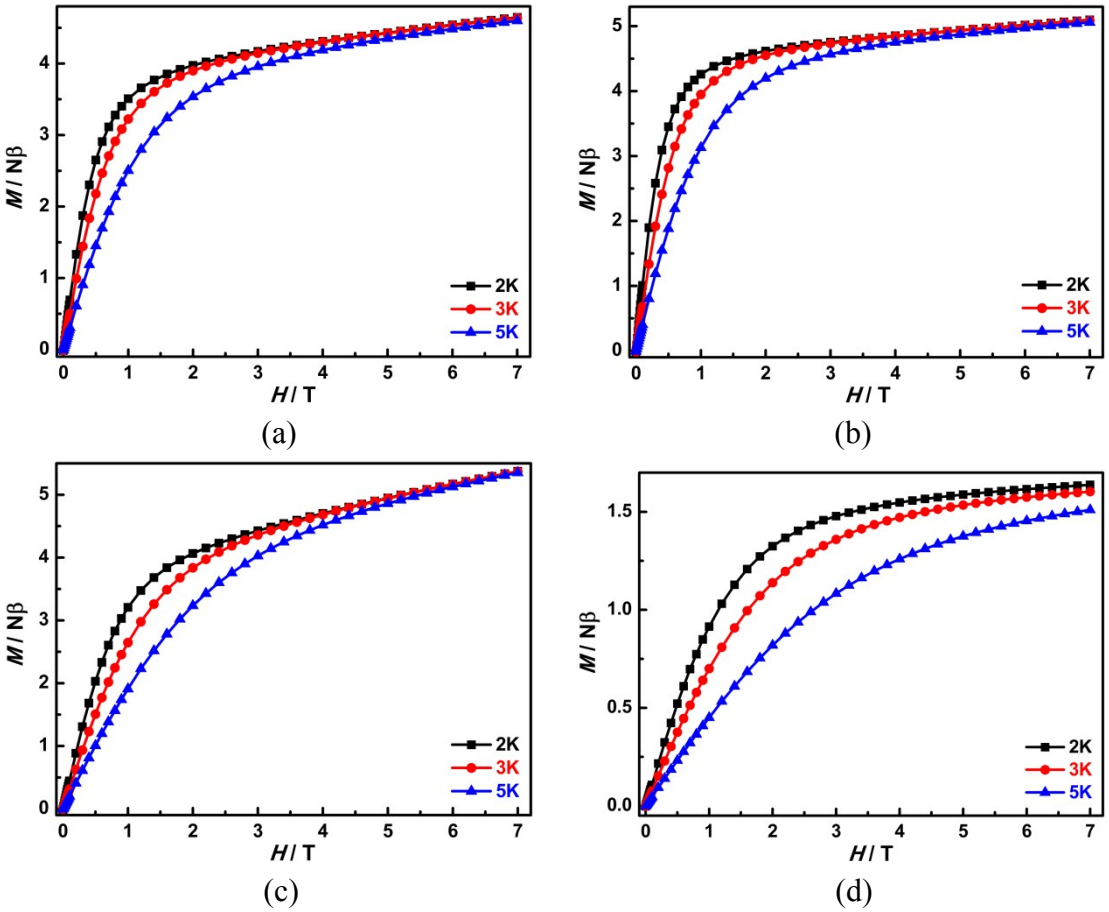


Fig. S6 *M* vs. *H* plots for **1** (a), **2** (b), **3** (c) and **4** (d).

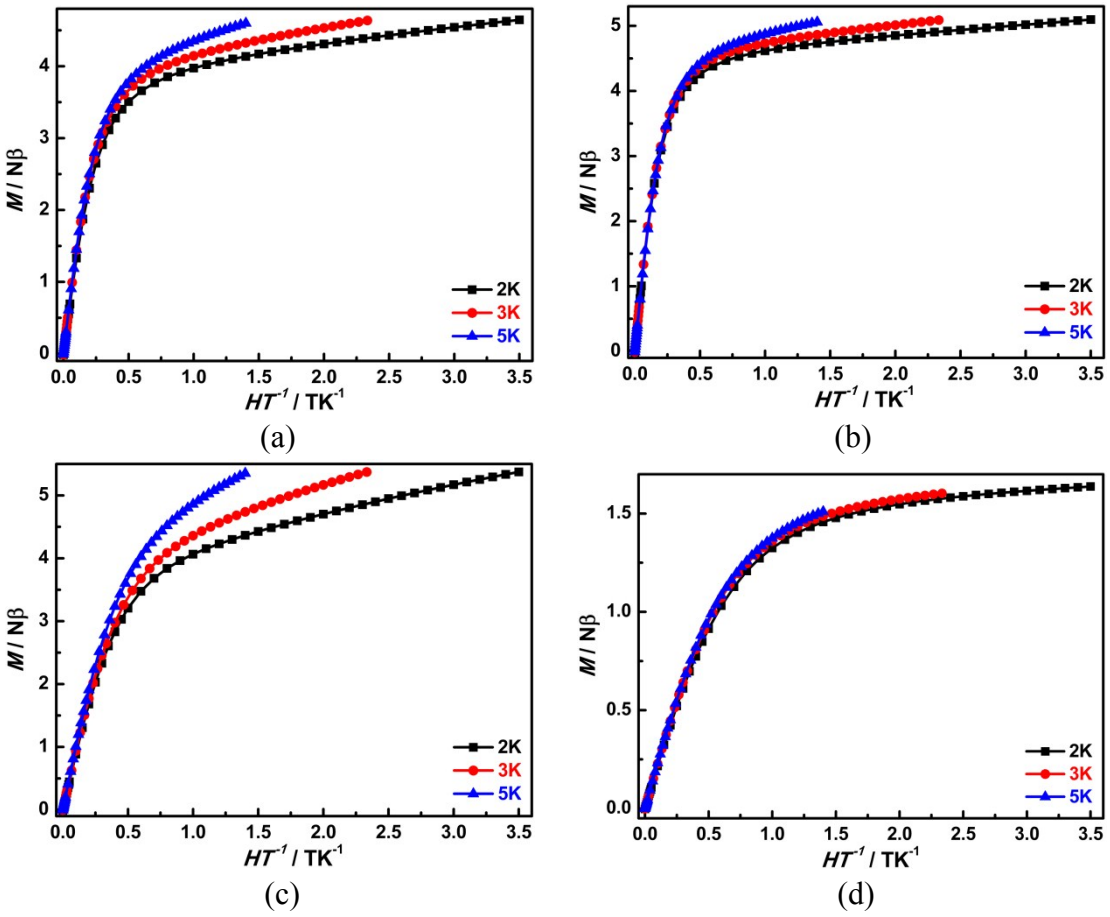


Fig. S7 *M* vs. HT^{-1} plots for **1** (a), **2** (b), **3** (c) and **4** (d).

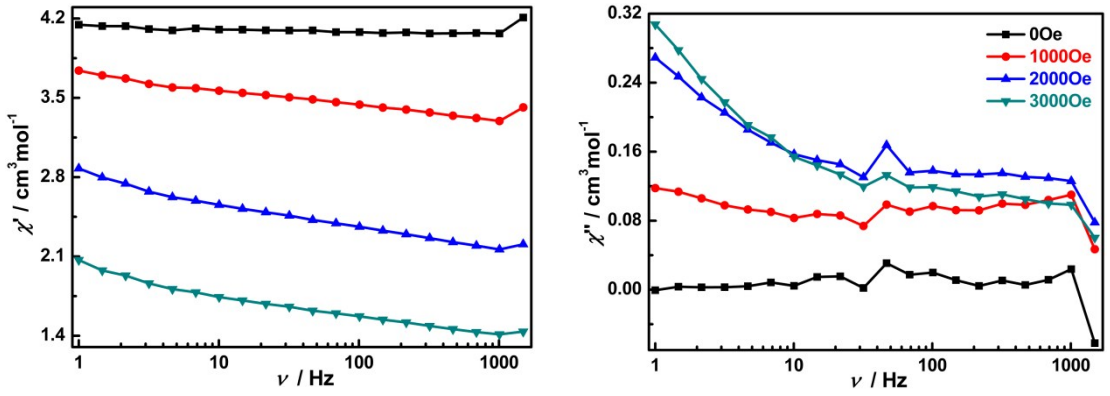
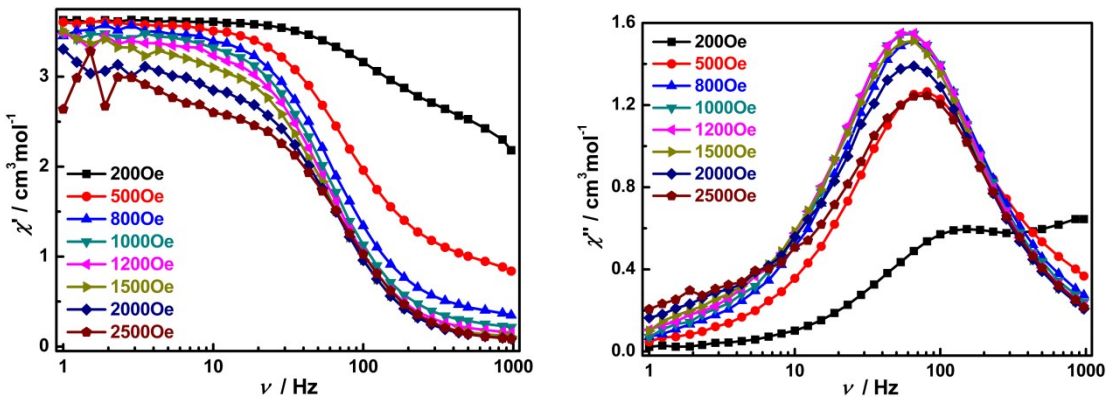


Fig. S8 Frequency dependence of in-phase (a) and out-of-phase (b) ac susceptibility data under different dc fields at 2 K for **1**.

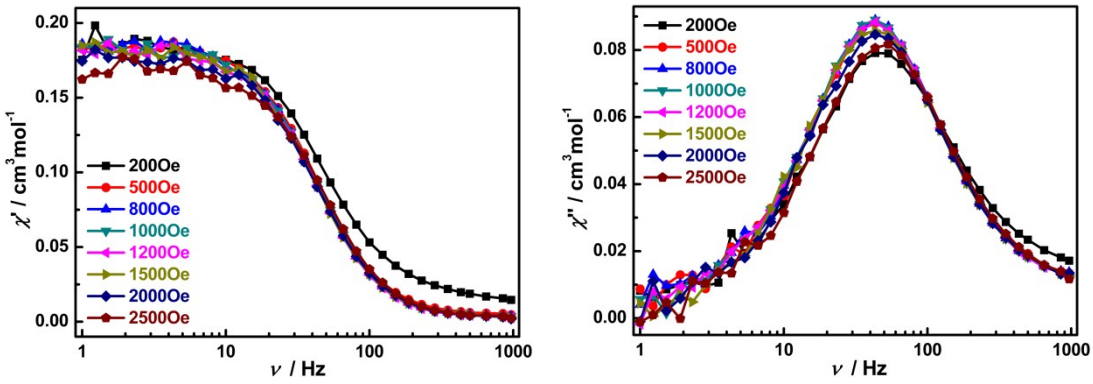


(a) (b)

Fig. S9 Frequency dependence of in-phase (a) and out-of-phase (b) ac susceptibility data under different dc fields at 4 K for **2**.

Table S3 Cole-Cole parameters of **2** under 1000 Oe dc field.

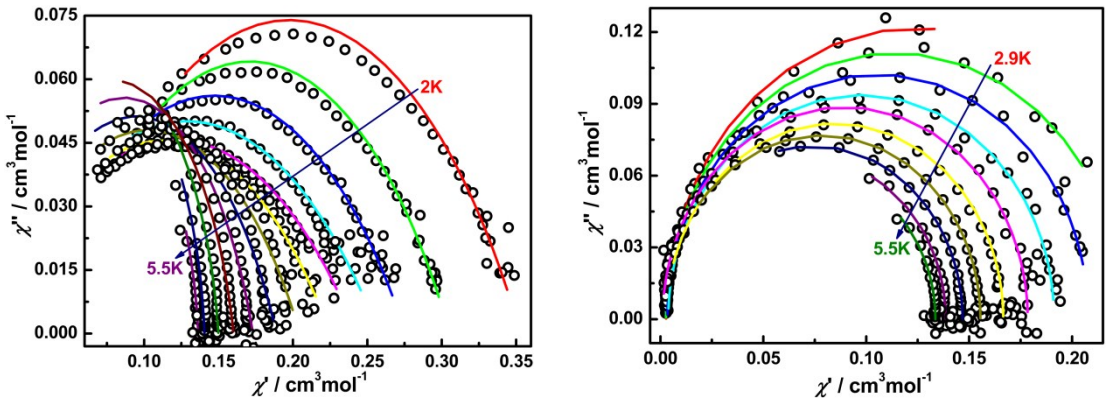
T / K	χ_S / cm^{-3}mol^{-1}	χ_T / cm^{-3}mol^{-1}	τ / s	α	R
2	3.33E-01	8.69E+00	3.19E-01	2.24E-01	9.62E-02
2.3	3.11E-01	7.73E+00	2.64E-01	2.25E-01	1.28E-01
2.6	3.00E-01	6.32E+00	1.54E-01	1.89E-01	1.89E-01
2.9	2.88E-01	5.15E+00	6.88E-02	1.30E-01	9.40E-02
3.2	2.53E-01	4.50E+00	2.93E-02	9.42E-02	1.32E-01
3.5	2.18E-01	4.00E+00	1.15E-02	7.74E-02	7.31E-02
3.8	1.88E-01	3.67E+00	4.69E-03	6.66E-02	5.08E-02
4.1	1.65E-01	3.36E+00	1.94E-03	5.12E-02	2.19E-02
4.4	1.51E-01	3.14E+00	8.31E-04	4.08E-02	2.30E-02
4.7	1.59E-01	2.94E+00	3.65E-04	3.21E-02	1.93E-02
5	2.34E-01	2.77E+00	1.68E-04	2.48E-02	1.27E-02
5.3	5.00E-01	2.62E+00	8.73E-05	2.58E-02	9.86E-03
5.5	9.98E-01	2.52E+00	7.27E-05	9.31E-03	5.97E-03



(a) (b)

Fig. S10 Frequency dependence of in-phase (a) and out-of-phase (b) ac susceptibility

data under different dc fields at 4 K for **5**.



(a) (b)

Fig. S11 The Cole-Cole plots for **5** under 0 (a) and 1000 Oe (b) dc fields. The solid lines are the best fits to a generalized Debye model.

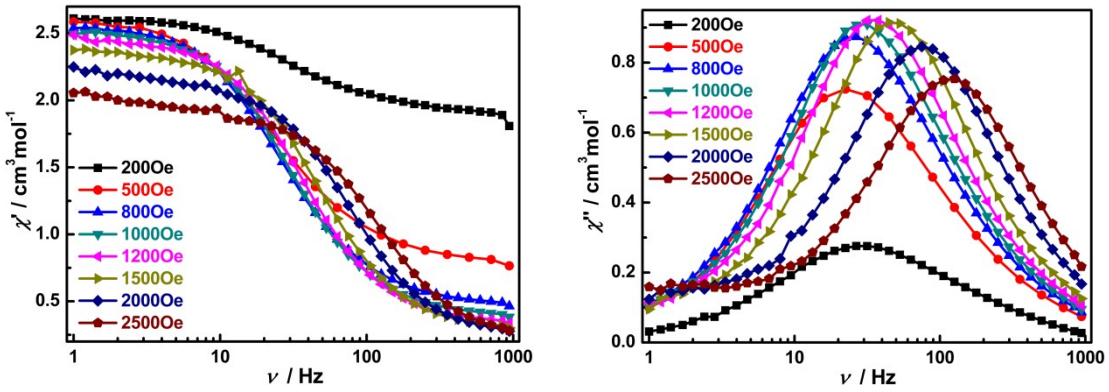
Table S4 Cole-Cole parameters of **5** under 0 Oe dc field.

T / K	χ_S / cm^{-3}mol^{-1}	χ_T / cm^{-3}mol^{-1}	τ / s	α	R
2	4.22E-02	3.53E-01	6.73E-04	4.34E-01	8.49E-04
2.3	3.67E-02	3.06E-01	6.40E-04	4.33E-01	3.22E-04
2.6	1.90E-02	2.76E-01	5.51E-04	4.75E-01	3.61E-04
2.9	1.39E-11	2.58E-01	4.78E-04	5.28E-01	4.37E-04
3.2	1.57E-11	2.43E-01	5.34E-04	5.42E-01	3.34E-04
3.5	2.13E-11	2.25E-01	5.21E-04	5.10E-01	2.16E-04
3.8	3.03E-11	2.05E-01	4.35E-04	4.42E-01	1.00E-03
4.1	5.28E-11	1.89E-01	3.42E-04	3.67E-01	8.33E-04
4.4	9.80E-11	1.73E-01	2.35E-04	2.72E-01	7.98E-04
4.7	1.81E-10	1.60E-01	1.47E-04	1.85E-01	4.20E-04
5	3.62E-10	1.50E-01	8.43E-05	1.20E-01	4.72E-04
5.3	6.60E-10	1.41E-01	4.51E-05	7.29E-02	2.83E-04
5.5	8.78E-10	1.36E-01	2.72E-05	9.25E-02	1.40E-04

Table S5 Cole-Cole parameters of **5** under 1000 Oe dc field.

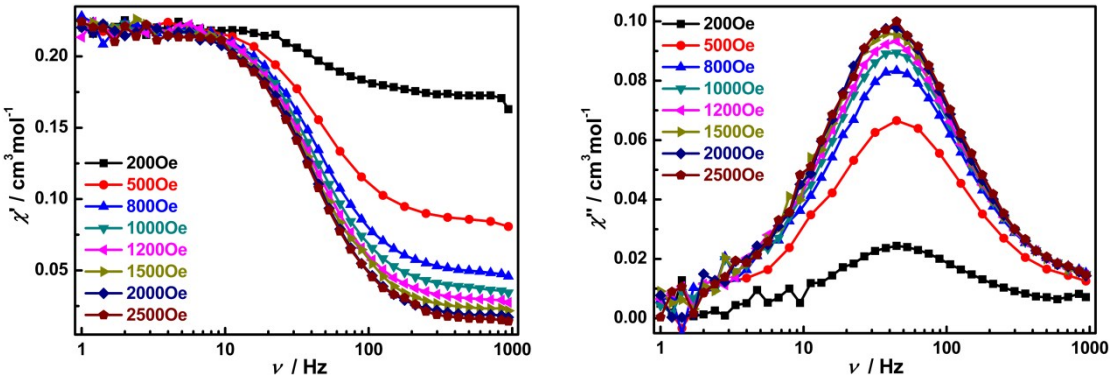
T / K	χ_S / cm^{-3}mol^{-1}	χ_T / cm^{-3}mol^{-1}	τ / s	α	R
2.3	3.52E-03	1.21E-01	3.42E-01	9.46E-10	5.36E-04
2.6	2.65E-03	2.16E-01	3.28E-01	1.32E-09	5.59E-04
2.9	2.76E-03	2.46E-01	1.48E-01	2.10E-09	2.85E-04
3.2	2.71E-03	2.25E-01	5.04E-02	2.26E-09	3.38E-04
3.5	3.36E-03	2.08E-01	1.81E-02	1.50E-08	2.93E-04
3.8	3.82E-03	1.91E-01	6.90E-03	8.20E-22	4.69E-04

4.1	1.08E-03	1.78E-01	2.70E-03	3.55E-22	4.93E-04
4.4	2.93E-03	1.67E-01	1.12E-03	1.31E-21	2.72E-04
4.7	1.85E-03	1.55E-01	4.68E-04	1.50E-21	2.57E-04
5	2.11E-03	1.47E-01	2.09E-04	2.76E-21	1.67E-04
5.3	3.70E-03	1.39E-01	9.86E-05	2.88E-21	1.26E-04
5.5	9.52E-03	1.34E-01	6.49E-05	2.67E-33	1.94E-04



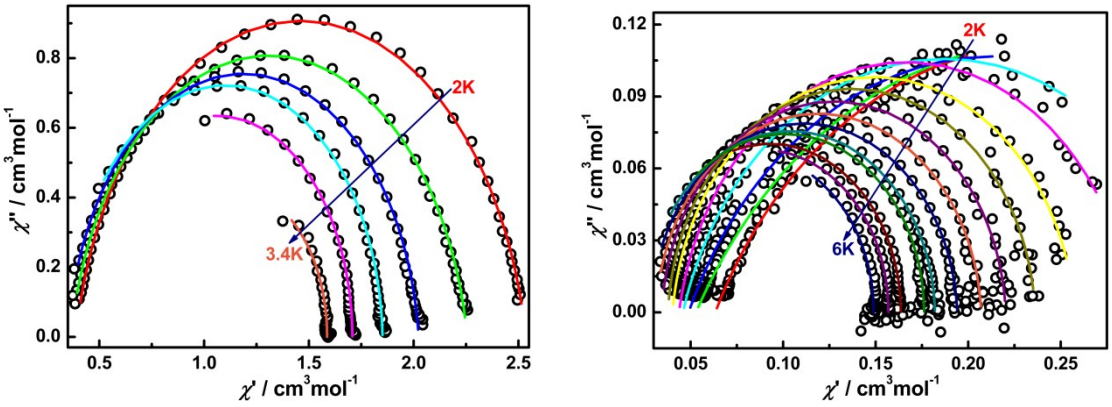
(a) (b)

Fig. S12 Frequency dependence of in-phase (a) and out-of-phase (b) ac susceptibility data under different dc fields at 2 K for **3**.



(a) (b)

Fig. S13 Frequency dependence of in-phase (a) and out-of-phase (b) ac susceptibility data under different dc fields at 4 K for **4**.



(a) (b)

Fig. S14 The Cole-Cole plots for **3** (a) and **4** (b) under 1000 Oe dc field. The solid lines are the best fits to a generalized Debye model.

Table S6 Cole-Cole parameters of **3** under 1000 Oe dc field.

T / K	χ_S / cm^{-3}mol^{-1}	χ_T / cm^{-3}mol^{-1}	τ / s	α	R
2	3.88E-01	2.54E+00	5.06E-03	1.07E-01	6.98E-03
2.3	3.65E-01	2.26E+00	3.28E-03	9.97E-02	5.20E-03
2.6	3.50E-01	2.02E+00	1.49E-03	6.49E-02	7.96E-03
2.9	3.51E-01	1.85E+00	5.05E-04	2.41E-02	6.22E-03
3.1	4.26E-01	1.71E+00	1.75E-04	6.15E-03	5.71E-03
3.4	7.55E-01	1.59E+00	8.55E-05	6.07E-09	4.74E-03

Table S7 Cole-Cole parameters of **4** under 1000 Oe dc field.

T / K	χ_S / cm^{-3}mol^{-1}	χ_T / cm^{-3}mol^{-1}	τ / s	α	R
2	6.33E-02	4.23E-01	2.66E-01	2.91E-01	6.25E-04
2.3	5.29E-02	4.36E-01	2.86E-01	3.24E-01	6.86E-04
2.6	4.89E-02	3.79E-01	1.60E-01	2.69E-01	4.85E-04
2.9	4.58E-02	3.28E-01	7.21E-02	1.82E-01	5.00E-04
3.1	4.38E-02	2.89E-01	3.14E-02	1.03E-01	4.97E-04
3.4	4.02E-02	2.58E-01	1.46E-02	6.53E-02	4.30E-04
3.7	3.78E-02	2.36E-01	7.00E-03	3.92E-02	5.24E-04
4	3.44E-02	2.20E-01	3.56E-03	3.46E-02	5.57E-04
4.3	3.12E-02	2.07E-01	1.89E-03	3.71E-02	4.91E-04
4.6	2.82E-02	1.94E-01	1.03E-03	3.23E-02	2.31E-04
4.9	2.61E-02	1.82E-01	5.94E-04	1.94E-02	2.24E-04
5.1	2.62E-02	1.76E-01	3.62E-04	4.52E-03	3.98E-04
5.4	2.25E-02	1.64E-01	2.27E-04	1.53E-03	2.61E-04
5.7	2.14E-02	1.57E-01	1.49E-04	1.22E-17	2.06E-04
6	1.75E-02	1.49E-01	9.79E-05	1.72E-17	3.24E-04

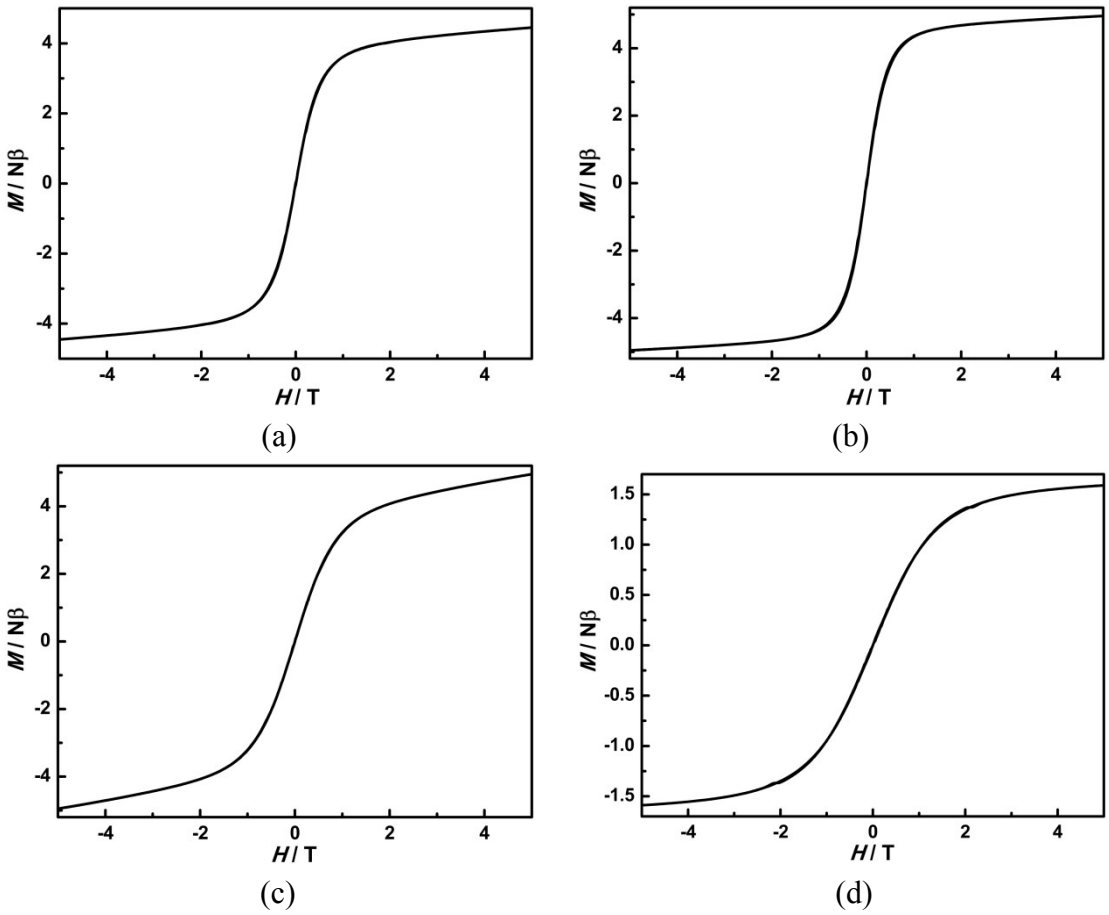


Fig. S15 Field dependence of the magnetization at 2 K for **1** (a), **2** (b), **3** (c) and **4** (d).

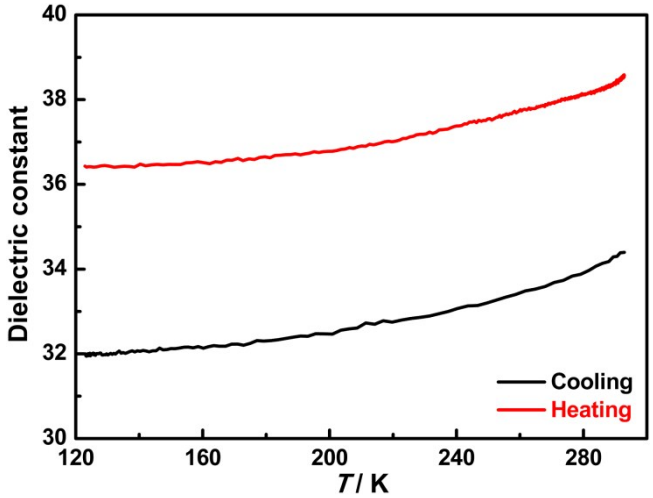


Fig. S16 Temperature dependence of the dielectric constant at 1 MHz for **2**.

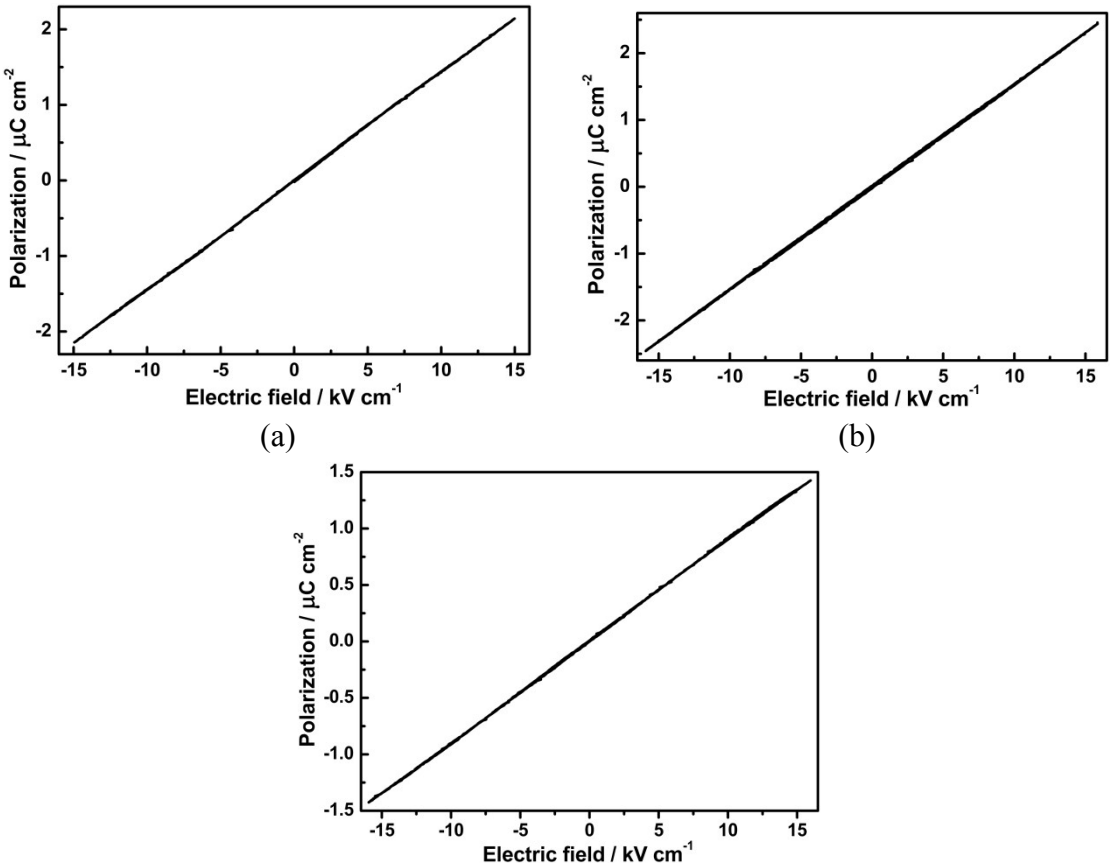


Fig. S17 Selective P-E curves for **2** at 223 (a), 296 (b) and 333 K (c).