Observation of field-induced single-ion magnet behavior in an octahedral dysprosium complex with strong ligand field

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Supporting Information

Table S1 The results of the continuous shape measure (CSM) analyses for **1** by using SHAPE software.

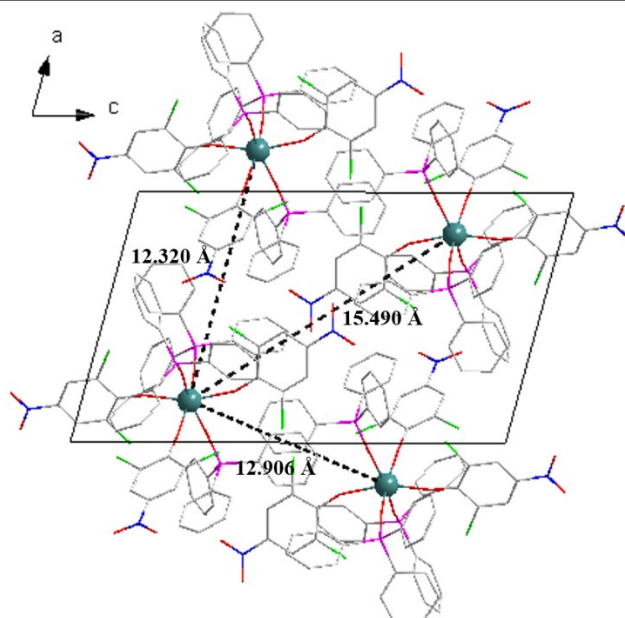| CSM	Hexagon	Pentagonal pyramid	Octahedron	Trigonal prism
1	32.280	21.074	2.461	7.507

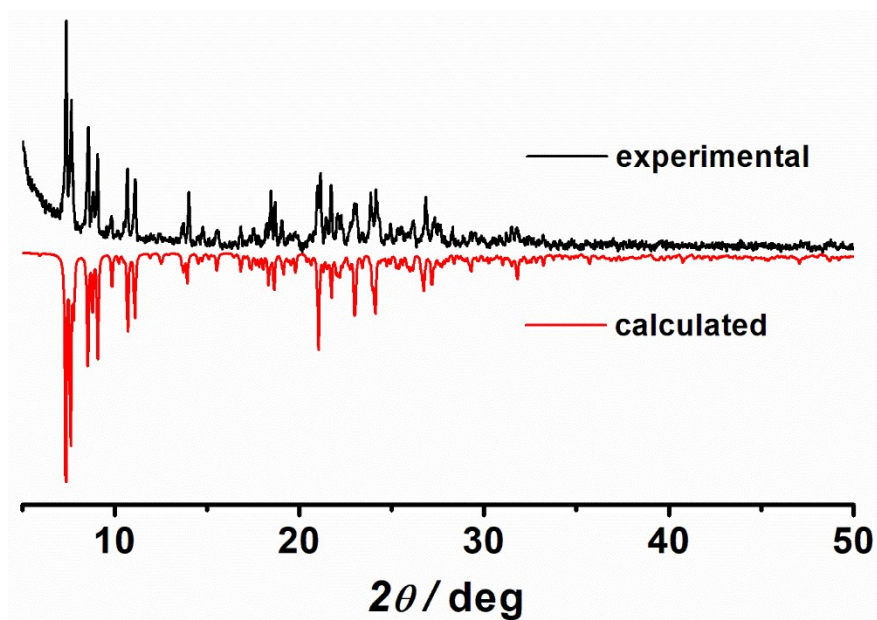**Figure S1** Crystal packing of **1** along the b axis. The H atoms are omitted for clarity.

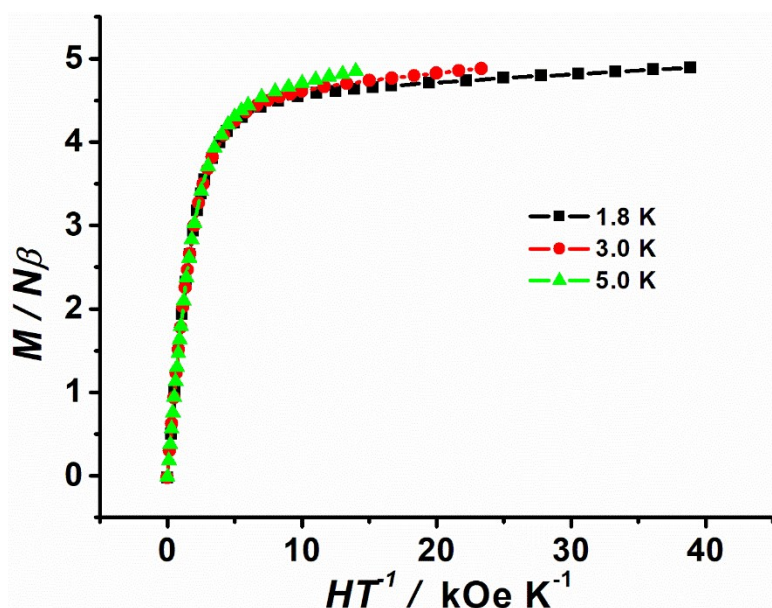**Figure S2** The XRD patterns for complex **1**.

Figure S3 Variable-temperature, variable-field dc magnetization data of **1**. The solid lines are a guide for the eye.

Table S2 Crystal field parameters for **1** fitted from $\chi_M T$ vs. T and M vs. H simultaneously.

	B_0^2	B_0^4	B_2^4
1	-275	321	-695

Table S3 Energy levels and *g* for **1** simulated from crystal field parameters in Table S2.

KDs	E/cm^{-1}	*g*
		1
1	0	0.2038
		0.5845
		18.5065
2	175	2.2847
		6.0090
		10.7762
3	232	0.0087
		0.0181
		19.6678
4	293	3.0319
		3.9220
		6.0918
5	436	0.0983
		0.17141

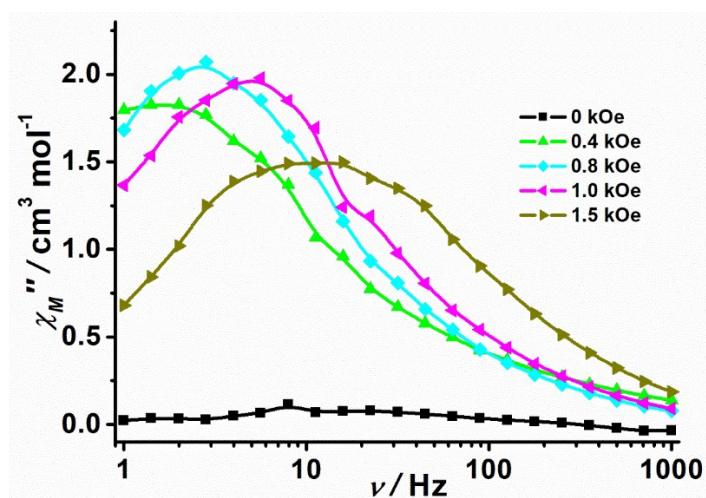|		9.7457
6	501	0.0056
		0.0060
		14.7840
7	705	0.0001
		0.0047
		14.4986
8	722	0.0012
		0.0049
		14.5466

Figure S4 Frequency dependence of out-of-phase ($\chi_M{''}$) ac susceptibility at 1.8 K under the different applied static fields from 0 to 1.5 kOe for **1**. The solid lines are for eye guide.
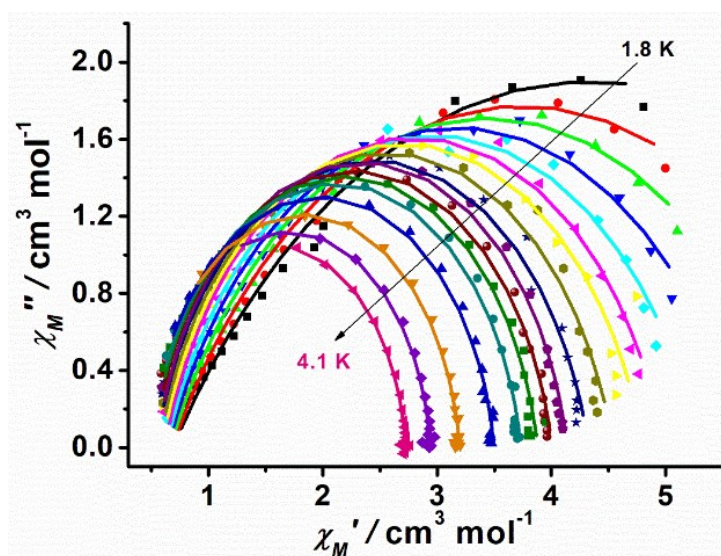

Figure S5 Cole-Cole plot obtained from the ac susceptibility under 0.4 kOe dc field.

Table S4 The parameters obtained by fitting Cole-Cole plot under 0.4 kOe dc field for **1**.

| T / K	χ_S	χ_T	τ	a
1.8	0.692	7.96	0.1264	0.39
1.9	0.684	6.79	0.06484	0.33
2.0	0.664	6.19	0.04015	0.29
2.1	0.644	5.70	0.02535	0.26
2.2	0.630	5.30	0.01725	0.23
2.3	0.616	4.99	0.01175	0.19
2.4	0.591	4.81	0.008418	0.18
2.5	0.566	4.54	0.005945	0.16
2.6	0.544	4.33	0.004328	0.15
2.7	0.553	4.14	0.003198	0.12
2.8	0.518	4.01	0.002389	0.12
2.9	0.511	3.88	0.001817	0.11
3.0	0.497	3.73	0.001399	0.11
3.2	0.476	3.50	0.000860	0.09
3.5	0.466	3.20	0.000438	0.08
3.8	0.469	2.94	0.000241	0.06
4.1	0.422	2.73	0.000136	0.06
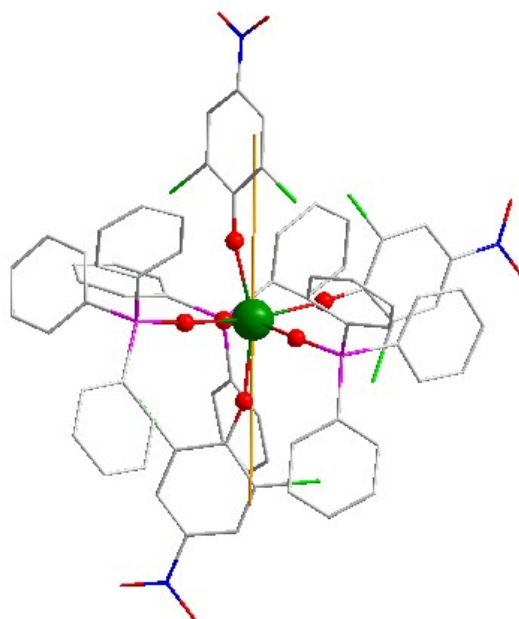
Figure S6 The orientation of the magnetic easy axes (yellow) obtained according to an electrostatic model for **1**.