

Supporting Information

Anion Effects on the Structures and Magnetic Properties of Binuclear Lanthanide Single-Molecule Magnets

Fen Yang, Qi Zhou, Guang Zeng, Guanghua Li, Lu Gao, Zhan Shi and Shouhua Feng*

State Key Laboratory of Inorganic Synthesis & Preparative Chemistry, College of Chemistry, Jilin University, Changchun 130012, P. R. China

RECEIVED DATE (to be automatically inserted after your manuscript is accepted if required according to the journal that you are submitting your paper to)

* To whom correspondence should be addressed. E-mail: zshi@mail.jlu.edu.cn. Phone: +86-431-85168662. Fax: +86-431-85168624.

Table S1. Selected bond lengths (Å) for compounds **1-4**.

Compound 1		Compound 3	
Dy1-O1	2.187(5)	Gd1-O1	2.232(2)
Dy1-O2	2.329(4)	Gd1-O2	2.377(8)
Dy1-O2#1	2.385(3)	Gd1-O2#1	2.395(2)
Dy1-O6	2.420(4)	Gd1-O6	2.457(2)
Dy1-O10	2.430(5)	Gd1-O10	2.460(2)
Dy1-O3	2.481(5)	Gd1-O3	2.508
Dy1-O9	2.510(5)	Gd1-O4	2.534
Dy1-O7	2.516(5)	Gd1-O9	2.536
Dy1-O4	2.526(5)	Gd1-O7	2.538
Dy1...Dy1#1	3.914(5)	Gd1...Gd1#1	3.969(7)
Dy1-O2-Dy1#1	112.26(1)	Gd1-O1-Gd1#1	112.55(8)

Compound 2		Compound 4	
Dy1-O1	2.135(3)	Gd1-O1	2.160(2)
Dy1-O2#1	2.300(3)	Gd1-O2#1	2.328(2)
Dy1-O2	2.361(3)	Gd1-O2	2.378(2)
Dy1-Cl2	2.609(8)	Gd1-Cl2	2.644(1)
Dy1-Cl1	2.642(4)	Gd1-Cl1	2.655(0)
Dy1-Cl3	2.674(3)	Gd1-Cl3	2.699(9)
Dy1...Dy1#1	3.836(8)	Gd1...Gd1#1	3.883 (6)
Dy1-O2-Dy1#1	110.81(1)	Gd1-O2-Gd1#1	111.21(8)

^a Symmetry transformations used to generate equivalent atoms: for **1** and **3**: #1 -x-1/2,y+1/2,-z+1/2; for **2** and **4**: #1 -x,-y,-z.

Table S2. Relaxation fitting parameters from least-squares fitting of the data for compound **1** to a distribution of single relaxation processes with a generalized Debye model.^a

T (K)	τ (s)	χ_s (emu mol ⁻¹)	χ_T (emu mol ⁻¹)	α
5.0	0.00542	0.123	3.58	0.0479
5.5	0.00376	0.122	3.27	0.0268
6.0	0.00265	0.127	3.01	0.0102
6.5	0.00191	0.126	2.79	7.80E-4
7.0	0.00140	0.122	2.68	0
7.5	0.00106	0.134	2.47	0
8.0	7.93E-4	0.146	2.33	0
8.5	6.27E-4	0.160	2.21	0
9.0	4.98E-4	0.190	2.10	0

^a Refs. K. S. Cole and R. H. Cole, *J. Chem. Phys.*, 1941, **9**, 341; S. M. Aubin, Z. Sun, L. Pardi, J. Krzystek, K. Folting, L. C. Brunel, A. L. Rheingold, G. Christou and D. N. Hendrickson, *Inorg. Chem.*, 1999, **38**, 5329.

Table S3. Relaxation fitting parameters from least-squares fitting of the data for compound **2** to a distribution of single relaxation processes with a generalized Debye model.

T (K)	τ (s)	χ_s (emu mol $^{-1}$)	χ_T (emu mol $^{-1}$)	α
12.0	0.00421	0.141	1.85	0.0622
13.0	0.00293	0.163	1.71	0.0360
14.0	0.00212	0.171	1.60	0.0332
15.0	0.00162	0.194	1.50	0.0120
16.0	0.00125	0.222	1.41	0.00879
17.0	9.59E-4	0.215	1.34	0.00298
18.0	7.92E-4	0.248	1.27	0
19.0	6.51E-4	0.270	1.21	0
20.0	5.37E-4	0.289	1.16	0
21.0	4.47E-4	0.322	1.11	0
22.0	3.73E-4	0.356	1.06	0

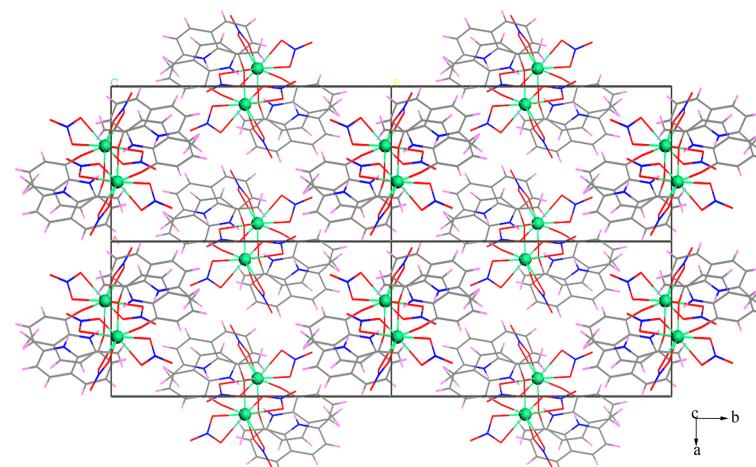


Fig. S1. Packing arrangement of **1** along the crystallographic *c* axis.

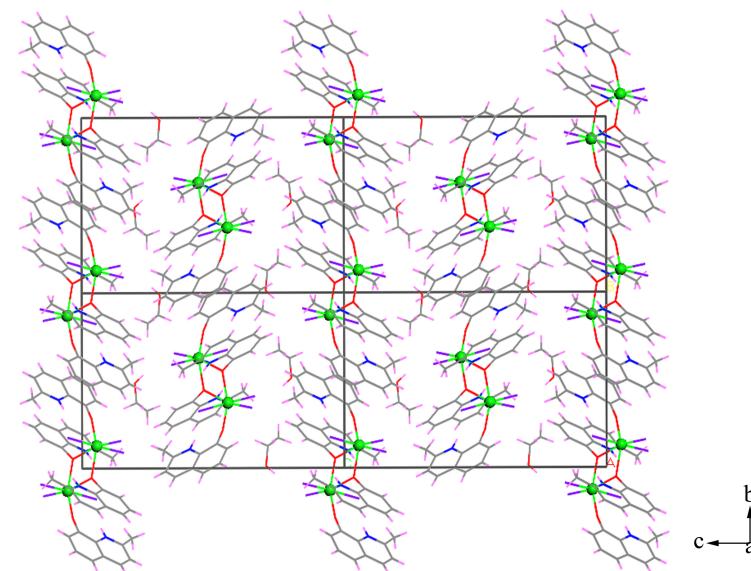


Fig. S2. Packing arrangement of **2** along the crystallographic *a* axis.

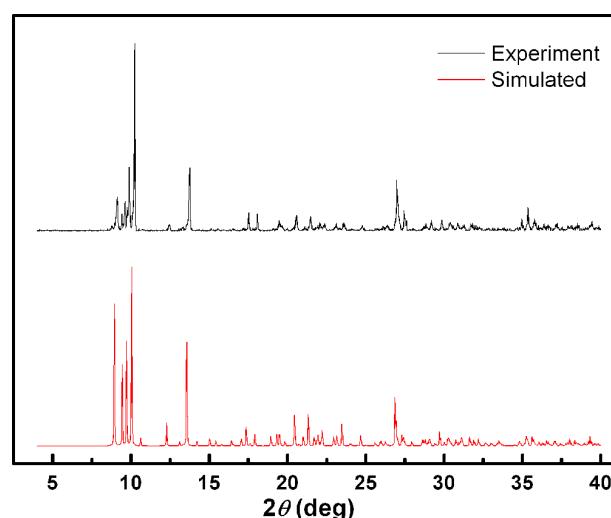


Fig. S3. XRPD pattern for compound 1.

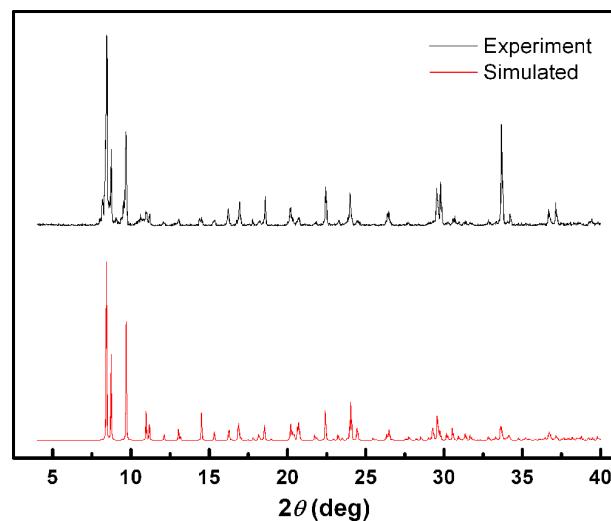


Fig. S4. XRPD pattern for compound 2.

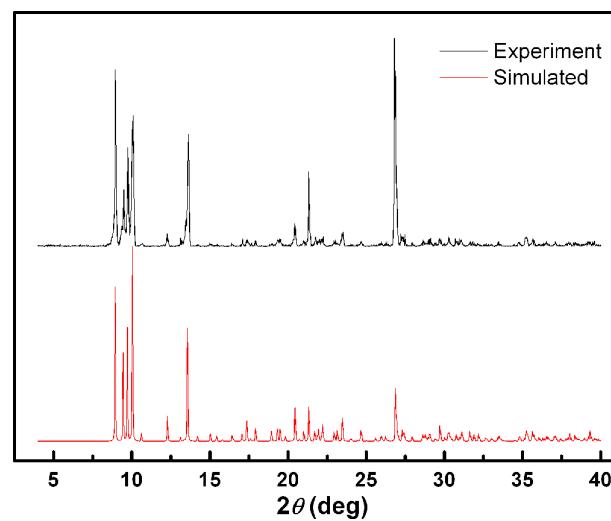


Fig. S5. XRPD pattern for compound 3.

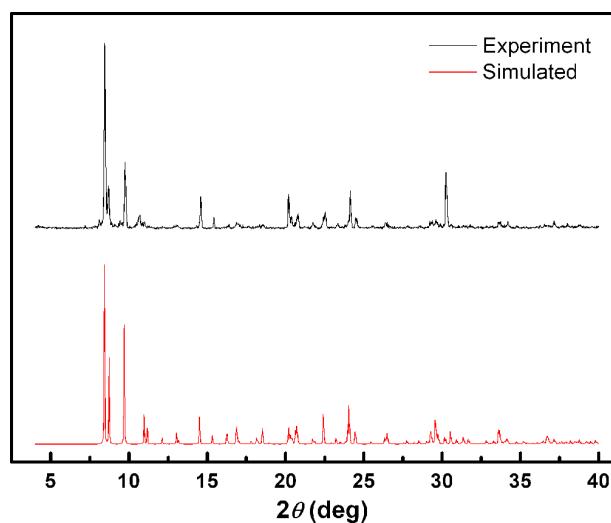


Fig. S6. XRPD pattern for compound 4.

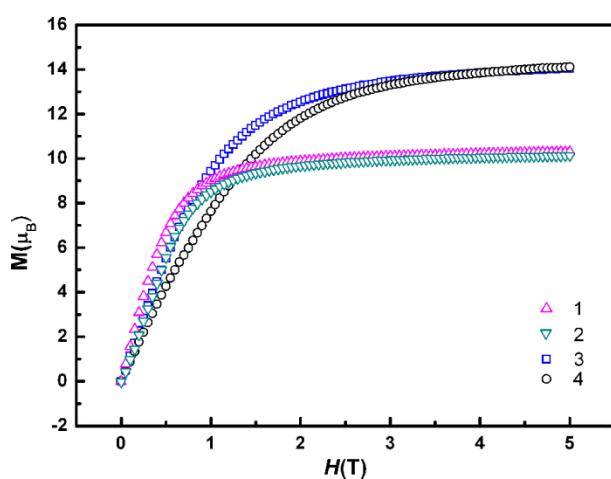


Fig. S7. Field dependence of the magnetization for compounds 1-4 at 2K.

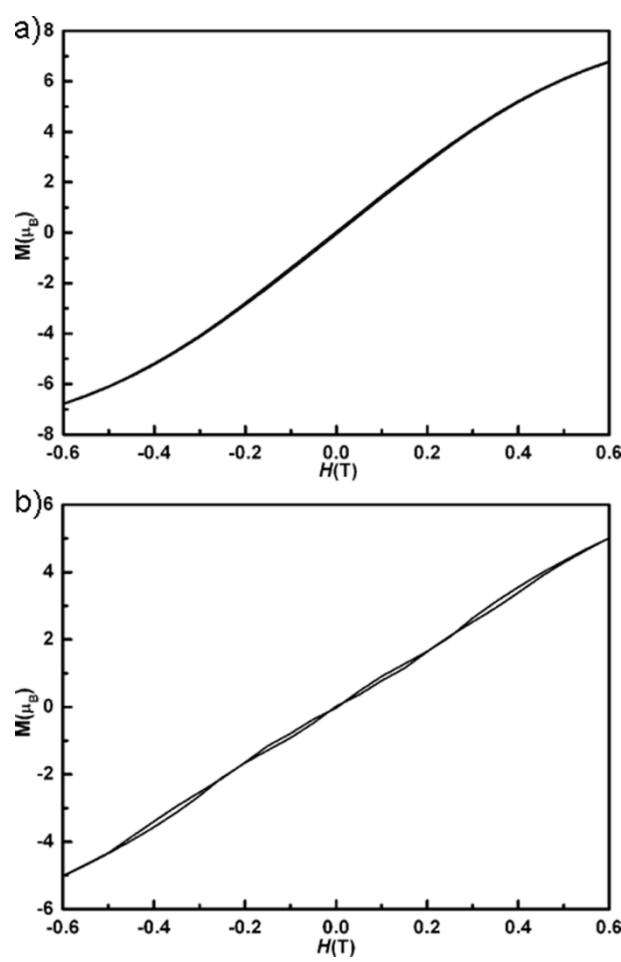


Fig. S8. Hysteresis loops for compounds **1(a)** and **2(b)** at 2 K.