

Supporting Information

## Acetato-bridged dinuclear lanthanide complexes with single molecule magnet behaviour for the Dy<sub>2</sub> species

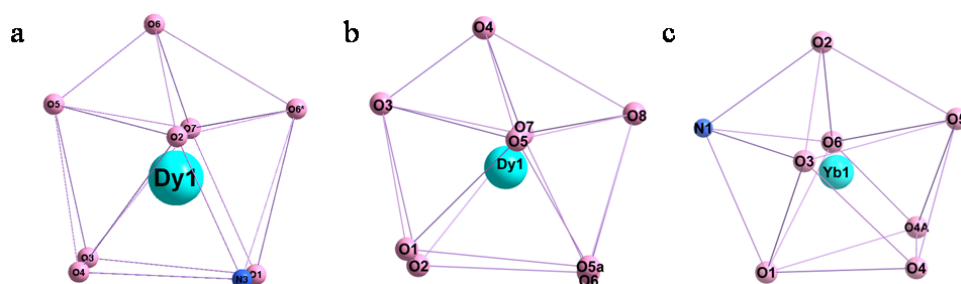
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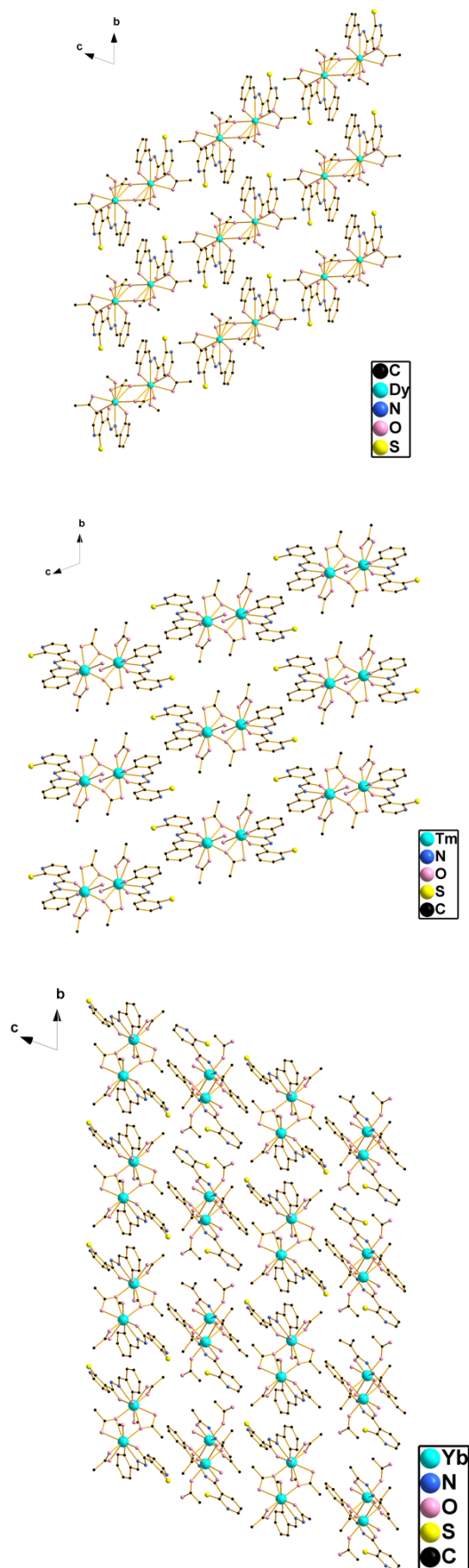
<sup>b</sup> University of Chinese Academy of Sciences, Beijing 100049, China

**Table S1.** Lanthanide geometry analysis by SHAPE 2.1 software.

Ln	Capped square antiprism ( $C_{4v}$ )	Tricapped trigonal prism ( $D_{3h}$ )	Square antiprism ( $D_{4d}$ )	Triangular dodecahedron ( $D_{2d}$ )
Sm(1)	2.092	2.792	#	#
Gd(2)	1.970	2.666	#	#
Dy(3)	1.917	2.645	#	#
Tm(4)	2.095	3.329	#	#
Yb1(5)	#	#	3.969	1.690
Yb2(5)	2.033	2.707	#	#
Dy(6)	2.097	2.824	#	#



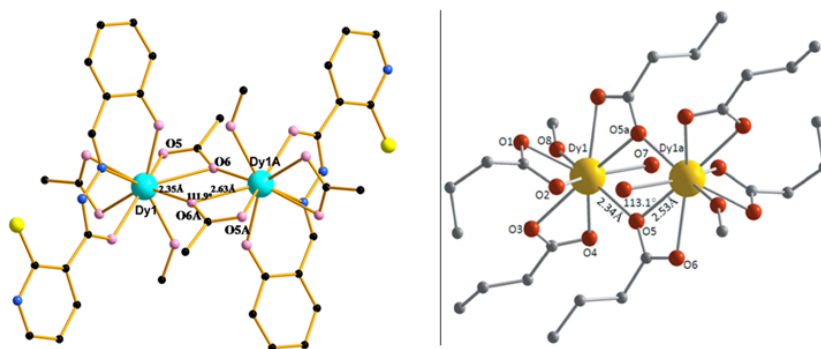
**Fig. S1** Coordination polyhedra observed of (a) Dy1, (b) Dy1, (c) Yb1 in complexes **3**, **6** and **5** respectively.



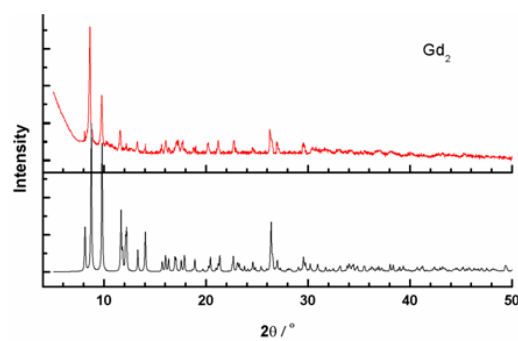
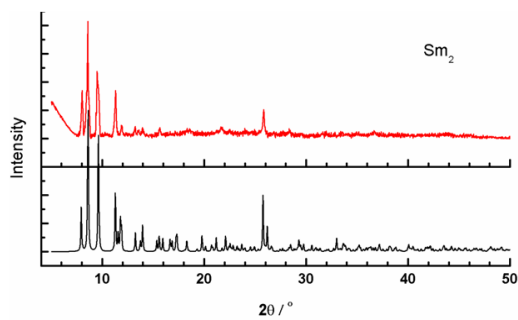
**Fig. S2** Molecular packing diagram of complexes **3**, **4**, **5** along *a* axis.

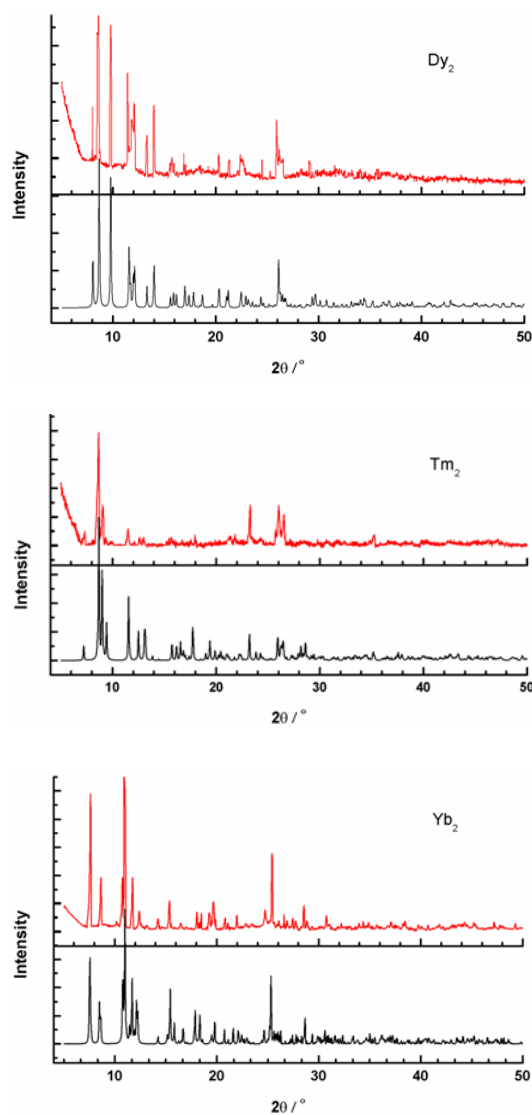
**Table S2.** Ln–Ln distances in molecular packing diagram of complexes **3**, **4**, **5** along *a* axis.

Complex	<b>3</b>	<b>4</b>	<b>5</b>
shortest intermolecular Ln–Ln distances for in parallel lines (Å)	12.6992	10.1025	8.4974
shortest intermolecular Ln–Ln distances for between parallel lines (Å)	10.6225	10.9065	10.5314

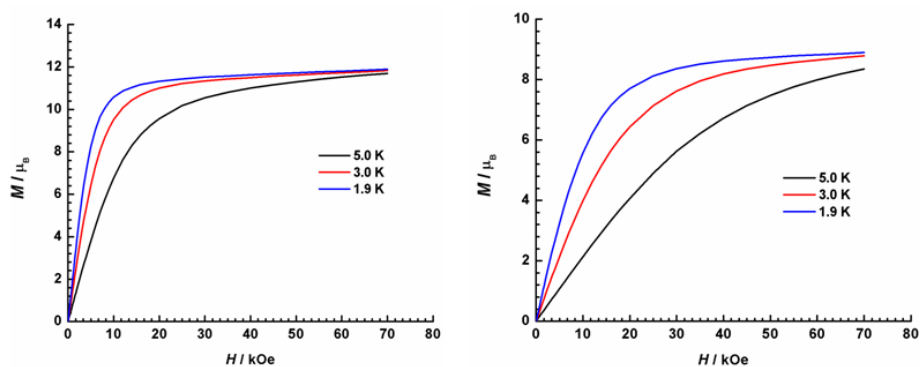


**Fig. S3** The molecular structure of complexes **3** (left) and **6** (right, refs 14a). Hydrogen atoms are omitted for clarity.

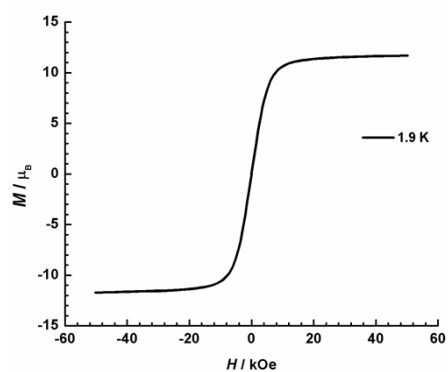




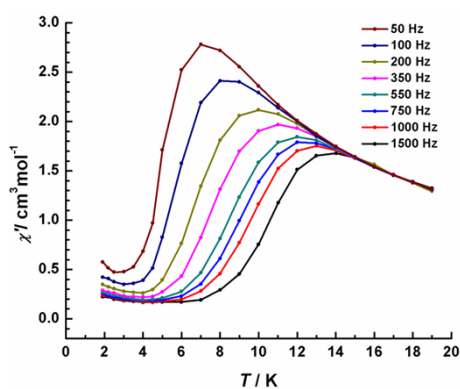
**Fig. 4** The experimental XRD patterns (red) and the calculated XRD patterns of single crystal X-ray diffraction data (black) for complexes **1-5**.



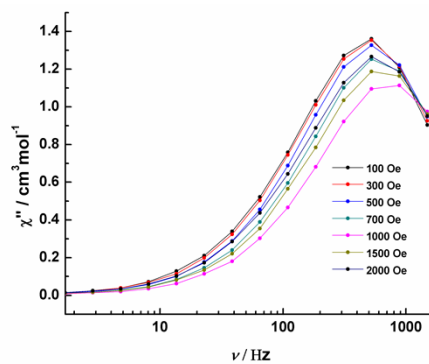
**Fig. S5** Field dependence of magnetizations of **3** (left) and **5** (right) at different temperatures below 5 K.



**Fig. S6** Hysteresis loops for **3** at 1.9 K.



**Fig. S7** Temperature dependence of the in-phase ( $\chi'$ ) of the ac susceptibility for **3** under zero-dc field. The solid lines are guides for the eyes.



**Fig. S8** Frequency dependence of the out-of-phase ( $\chi''$ ) parts of the ac susceptibility for **3** under various magnetic field at 9 K. The solid lines are guides for the eye.

**Table S4** Relaxation fitting parameters from the least-square fitting of the Cole-Cole plots according to the generalized Debye model for **3**.

Temperature / K	$\chi_S / \text{cm}^3\text{mol}^{-1}\text{K}$	$\chi_T / \text{cm}^3\text{mol}^{-1}\text{K}$	$\tau / \text{s}$	$\alpha$
1.9	0.23697	9.56297	1.13E-01	0.24943
2.2	0.22369	8.71436	9.66E-02	0.23217
2.5	0.21126	7.87979	7.46E-02	0.20992
3.0	0.18547	6.82012	4.48E-02	0.18191
3.5	0.16649	6.01678	2.56E-02	0.16465
4.0	0.14639	5.38099	2.56E-02	0.15326
4.5	0.13844	4.79735	8.48E-03	0.11009
5.0	0.11335	4.47684	5.15E-03	0.14714
6.0	0.08540	3.80817	2.18E-03	0.13750
7.0	0.05798	3.31482	1.03E-03	0.12850
8.0	0.04878	2.93787	5.59E-04	0.12114
9.0	0.07068	2.63777	3.27E-04	0.11032
10.0	0.07707	2.39497	1.85E-04	0.11620
11.0	0.22482	2.18837	1.06E-04	0.09961
12.0	0.34635	2.02223	1.02E-04	0.10292
13.0	0.85480	1.87351	7.39E-05	0.04674