Supporting Information

Multifunctional Properties Existing in Ln-Nitronyl Nitroxide Single-Chain Magnets

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Table S1. Selected bond lengths [Å] and angles [°] for compound **1**.

1			
N(1)-C(1)	1.314(2)	C(2)-C(3)	1.343(3)
N(1)-C(9)	1.361(2)	C(3)-C(4)	1.415(2)
N(2)-O(1)	1.2749(17)	C(4)-C(5)	1.406(3)
N(2)-C(10)	1.3388(18)	C(4)-C(9)	1.417(2)
N(2)-C(12)	1.496(2)	C(5)-C(6)	1.350(3)
N(3)-O(2)	1.2772(16)	C(6)-C(7)	1.405(2)
N(3)-C(10)	1.3340(19)	C(7)-C(8)	1.368(2)
N(3)-C(11)	1.5017(18)	C(8)-C(9)	1.415(2)
C(1)-C(2)	1.407(3)	C(8)-C(10)	1.4679(19)
C(1)-N(1)-C(9)	116.95(15)	N(1)-C(1)-C(2)	124.06(19)
O(1)-N(2)-C(10)	125.65(13)	C(3)-C(2)-C(1)	119.70(17)
O(1)-N(2)-C(12)	122.64(13)	N(1)-C(9)-C(8)	118.73(13)
C(10)-N(2)-C(12)	111.27(12)	N(1)-C(9)-C(4)	122.90(14)
O(2)-N(3)-C(10)	125.18(13)	N(3)-C(10)-N(2)	109.85(12)
O(2)-N(3)-C(11)	122.32(12)	N(3)-C(10)-C(8)	124.54(12)
C(10)-N(3)-C(11)	111.71(11)	N(2)-C(12)-C(11)	100.98(12)

Table S2. Selected bond lengths [Å] and angles [°] for complexes **2** and **3**.

2 Tb		**3** Dy	
Tb(1)-O(1)	2.378(7)	Dy(1)-O(1)	2.361(5)
Tb(1)-O(2)	2.333(6)	Dy(1)-O(2)	2.316(5)
Tb(1)-O(3)	2.345(6)	Dy(1)-O(3)	2.337(5)
Tb(1)-O(4)	2.393(7)	Dy(1)-O(4)	2.362(5)
Tb(1)-O(5)	2.392(6)	Dy(1)-O(5)	2.376(5)
Tb(1)-O(6)	2.363(6)	Dy(1)-O(6)	2.322(5)
Tb(1)-O(7)	2.386(7)	Dy(1)-O(7)	2.335(5)
Tb(1)-O(8)	2.358(7)	Dy(1)-O(8)	2.384(5)
Tb(2)-O(9)	2.389(7)	Dy(2)-O(9)	2.385(5)
Tb(2)-O(10)	2.371(6)	Dy(2)-O(10)	2.353(5)
Tb(2)-O(11)	2.350(6)	Dy(2)-O(11)	2.369(5)
Tb(2)-O(12)	2.387(7)	Dy(2)-O(12)	2.311(5)
Tb(2)-O(13)	2.326(6)	Dy(2)-O(13)	2.341(5)
Tb(2)-O(14)	2.368(6)	Dy(2)-O(14)	2.350(5)
Tb(2)-O(15)	2.366(6)	Dy(2)-O(15)	2.367(5)
Tb(2)-O(16)	2.357(7)	Dy(2)-O(16)	2.323(4)
O(1)-N(2)	1.291(10)	N(2)-O(1)	1.275(7)
O(9)-N(5)	1.287(10)	N(3)-O(2)	1.296(7)
N(6)-O(10)#1	1.278(9)	O(10)-N(6)	1.278(7)
N(3)-O(2)#2	1.291(10)	N(5)-O(9)	1.274(7)
O(2)-Tb(1)-O(1)	137.3(2)	O(2)#1-Dy(1)-O(1)	137.37(19)
O(10)-Tb(2)-O(9)	139.8(2)	O(10)-Dy(2)-O(9)#2	139.80(18)
O(3)-Tb(1)-O(4)	72.2(2)	O(3)-Dy(1)-O(4)	73.62(17)
O(6)-Tb(1)-O(5)	72.2(2)	O(6)-Dy(1)-O(5)	72.65(17)
O(8)-Tb(1)-O(7)	73.3(2)	O(7)-Dy(1)-O(8)	72.01(17)
O(11)-Tb(2)-O(12)	72.2(2)	O(12)-Dy(2)-O(11)	72.95(17)
O(13)-Tb(2)-O(14)	73.3(2)	O(13)-Dy(2)-O(14)	73.56(17)
O(16)-Tb(2)-O(15)	73.6(2)	O(16)-Dy(2)-O(15)	72.37(17)

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

Table S3. SHAPE analysis for complexes **2** and **3**.

Complex	SAPR-8	TDD-8	BTPR-8
2 Tb1	2.035	**0.390**	1.907
Tb2	1.988	**0.265**	2.367
3 Dy1	2.101	**0.372**	1.924
Dy2	2.037	**0.246**	2.401

SAPR-8: Square antiprism; TDD-8: Triangular dodecahedron; BTPR-8: Biaugmented trigonal prism

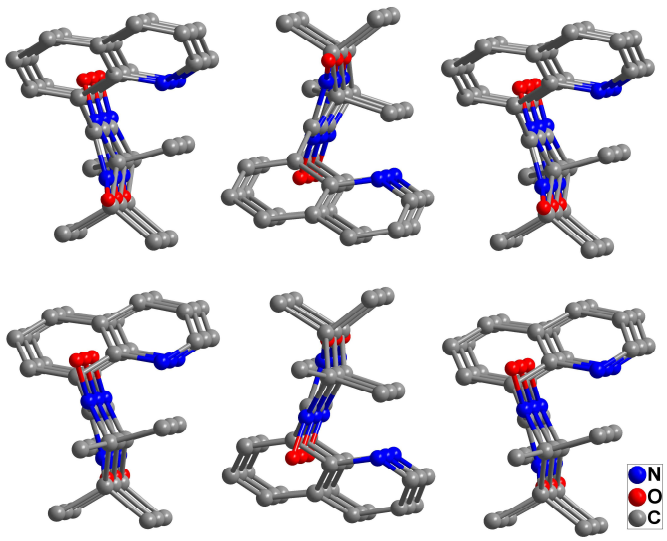

Figure S1. Packing diagram of complex **1** and all of the hydrogen atoms are omitted for clarity.

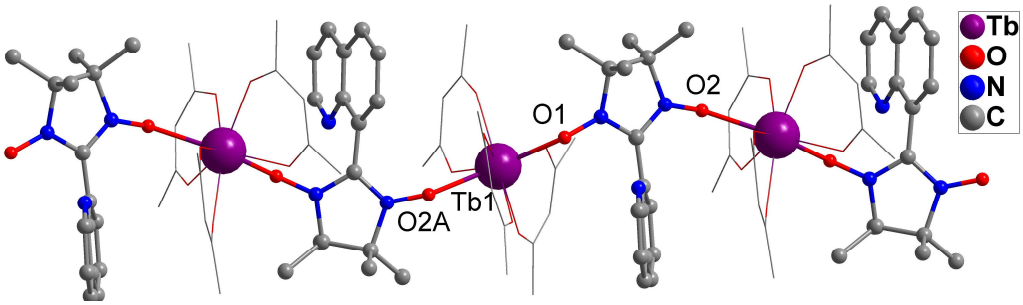

Figure S2. Single-crystal X-ray diffraction structure of complex **2**, in which H and F atoms are omitted for clarity.

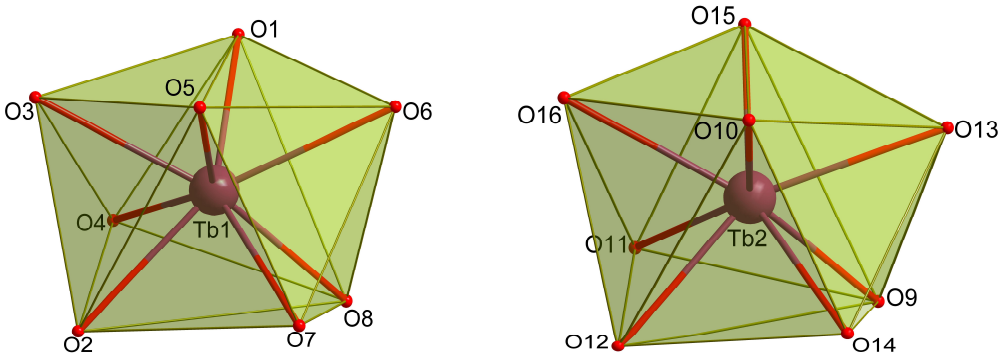

Figure S3. The coordination polyhedron of Tb(III) ions in complex **2**.

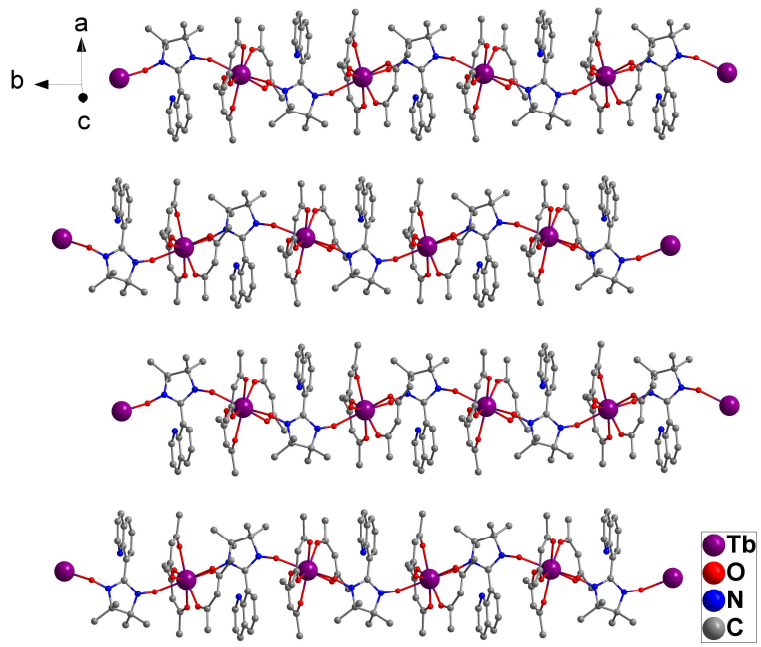

Figure S4. Packing diagram of complex **2** and all of the hydrogen and fluorine atoms are omitted for clarity.

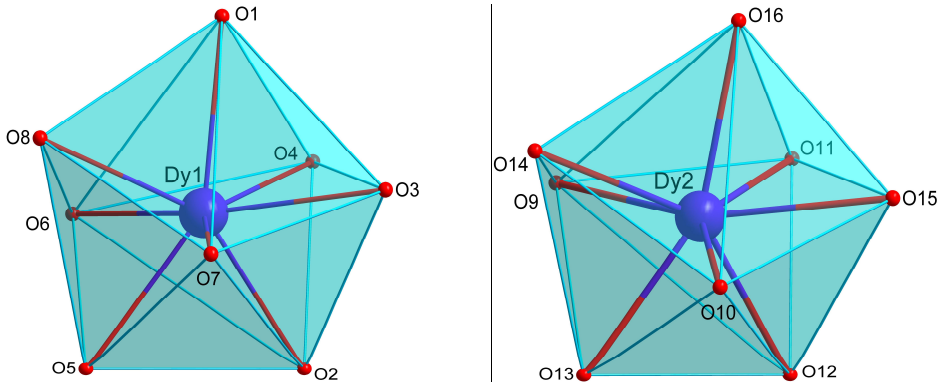

Figure S5. The coordination polyhedron of Dy(III) ions in complex **3**.

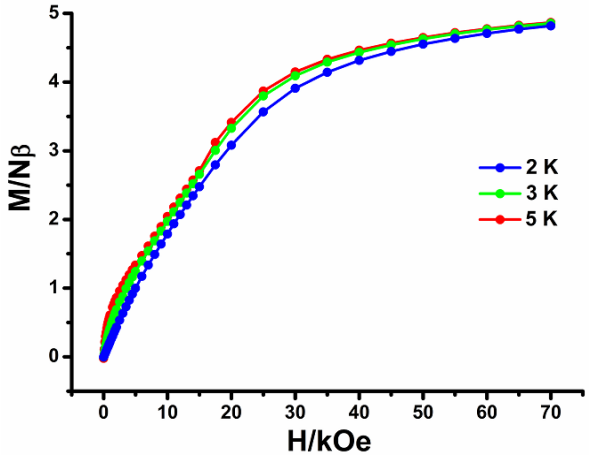

Figure S6. *M* versus *H* plot of complex **2** at 2.0 K.

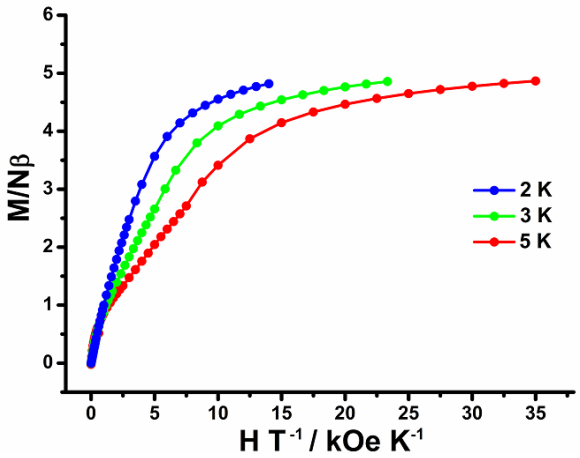

Figure S7. Plots of the reduced magnetization M versus HT^{-1} for compound **2**.

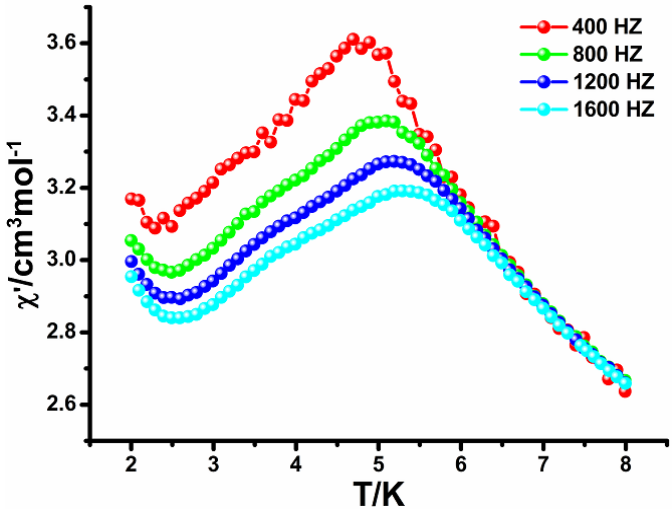

Figure S8. Temperature dependence of χ' for **2** in zero dc field with an oscillation of 3 Oe.

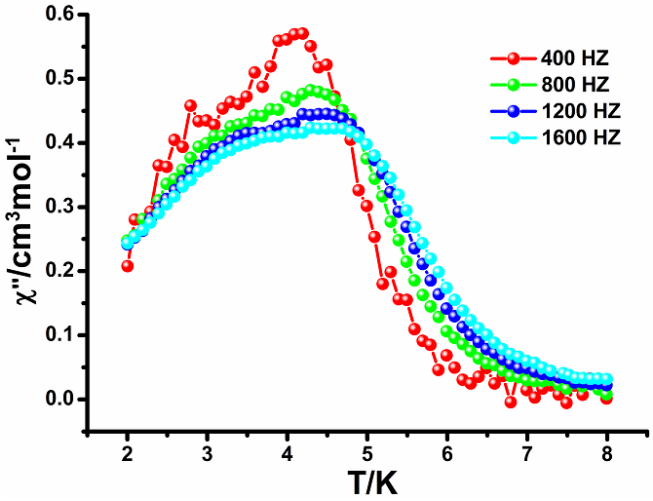

Figure S9. Temperature dependence of χ'' for **2** in zero dc field with an oscillation of 3 Oe.

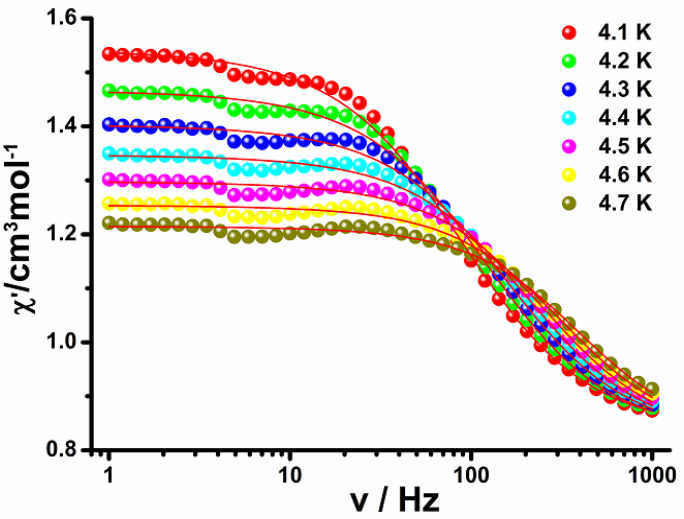

Figure S10. Frequency dependence of χ' for **2** under zero dc field in the temperature range 4.3-5.0 K. The solid line represents the fitting result.

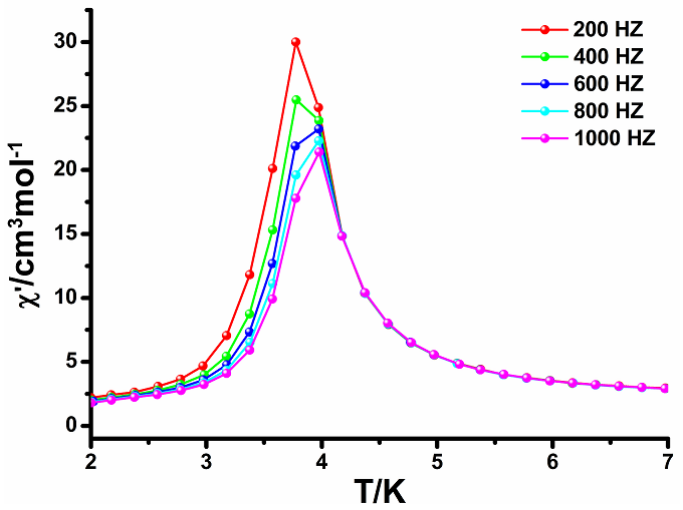

Figure S11. Temperature dependence of χ' for **3** in zero dc field with an oscillation of 3 Oe.

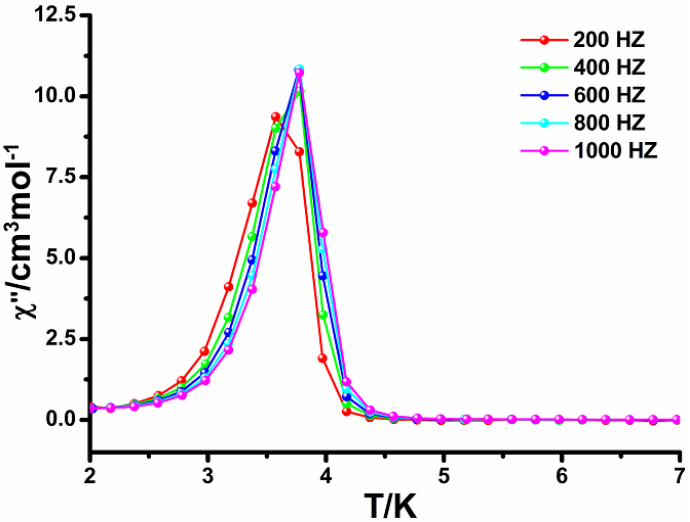

Figure S12. Temperature dependence of χ'' for **3** in zero dc field with an oscillation of 3 Oe.

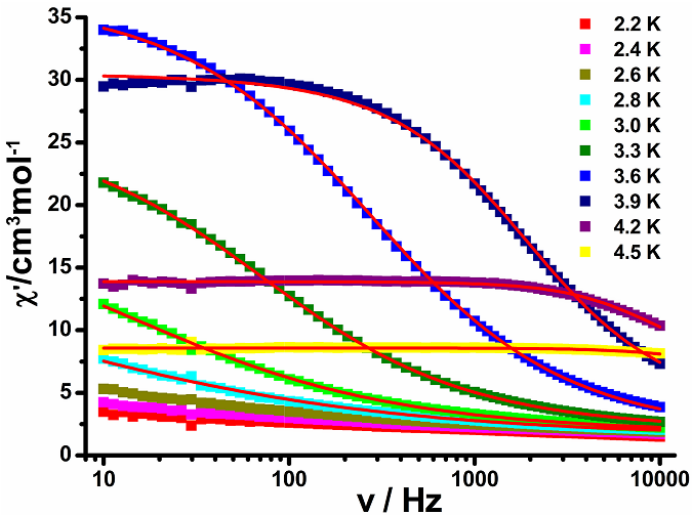

Figure S13. Frequency dependence of χ' for **3** under zero dc field in the temperature range 2.2 K-4.5 K. The solid line represents the fitting result.

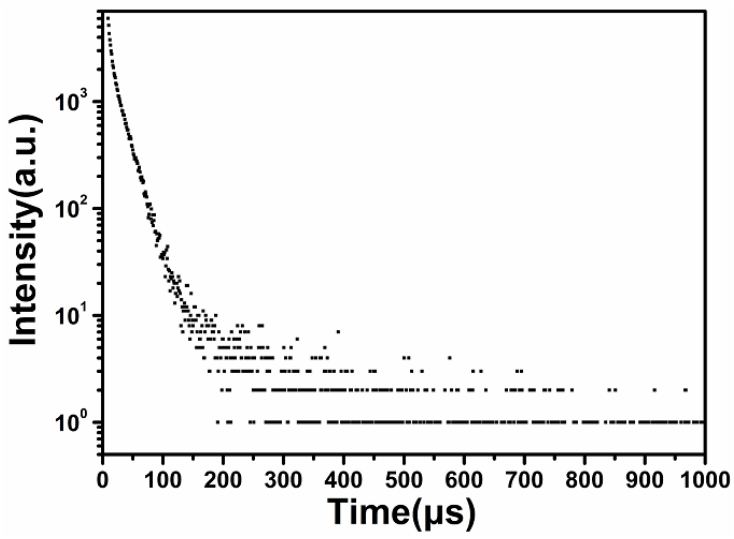

Figure S14. Luminescence decay of complex **2**.

Table S4. Selected parameters from the fitting result of the Cole-Cole plots for compound **2** under 0 Oe.

***Temp.* (K)**	***τ***	***α***	**residual**
4.1 K	0.0018	0.1990	3.53E-4
4.2 K	0.0013	0.1886	1.93E-5
4.3 K	0.00101	0.1794	1.66E-5
4.4 K	7.88E-4	0.1688	7.48E-6
4.5 K	6.21E-4	0.1580	5.27E-6
4.6 K	4.99E-4	0.1491	4.23E-6
4.7 K	4.05E-4	0.1403	4.05E-4