Supporting Information

Functionalized nitronyl nitroxide biradical bridged one-dimensional lanthanide chains: slow magnetic relaxation in the Tb and Dy analogues

Hongdao Li, Juan Sun, Meng Yang, Zan Sun, Jing Xie, Yue Ma, Licun Li*

Department of Chemistry, Key Laboratory of Advanced Energy Materials Chemistry and Tianjin Key Laboratory of Metal and Molecule-based Material Chemistry, Nankai University, Tianjin 300071, China

Table S1 Selected bond lengths [Å] and angles [°] for complexes **1** and **2**.

1 Gd		**2** Tb	
Gd(1)-O(6)	2.354(2)	Tb(1)-O(6)	2.353(4)
Gd(1)-O(1)	2.369(3)	Tb(1)-O(1)	2.339(4)
Gd(1)-O(2)	2.372(3)	Tb(1)-O(2)	2.364(4)
Gd(1)-O(3)	2.376(3)	Tb(1)-O(3)	2.352(5)
Gd(1)-O(4)	2.376(3)	Tb(1)-O(4)	2.349(4)
Gd(1)-O(5)	2.380(3)	Tb(1)-O(5)	2.349(4)
Gd(1)-O(7)	2.406(3)	Tb(1)-O(7)	2.400(4)
Gd(1)-N(1)	2.524(3)	Tb(1)-N(1)	2.515(5)
N(5)-O(7)	1.293(4)	N(5)-O(7)	1.293(6)
N(6)-O(8)	1.271(4)	N(6)-O(8)	1.269(7)
N(3)-O(9)	1.190(9)	N(3)-O(9)	1.249(1)
N(4)-O(10)	1.214(7)	N(4)-O(10)	1.219(10)
O(1)-Gd(1)-O(2)	70.74(9)	O(1)-Tb(1)-O(2)	74.06(15)
O(3)-Gd(1)-O(4)	73.09(9)	O(3)-Tb(1)-O(4)	70.84(16)
O(6)-Gd(1)-O(5)	74.06(9)	O(6)-Tb(1)-O(5)	73.31(15)
O(7)-Gd(1)-N(1)	98.07(9)	O(7)-Tb(1)-N(1)	98.36(16)
N(5)-O(7)-Gd(1)	136.4(2)	N(5)-O(7)-Tb(1)	136.6(4)

Table S2 Selected bond lengths [Å] and angles [°] for complexes **3** and **4**.

3 Dy		**4** Nd	
Dy(1)-O(6)	2.347(3)	Nd(1)-O(6)	2.419(3)
Dy(1)-O(1)	2.335(3)	Nd(1)-O(1)	2.426(3)
Dy(1)-O(2)	2.344(3)	Nd(1)-O(2)	2.419(3)
Dy(1)-O(3)	2.347(3)	Nd(1)-O(3)	2.423(3)
Dy(1)-O(4)	2.346(3)	Nd(1)-O(4)	2.428(3)

Dy(1)-O(5)	2.332(3)	Nd(1)-O(5)	2.404(3)
Dy(1)-O(7)	2.392(3)	Nd(1)-O(7)	2.467(3)
Dy(1)-N(1)	2.503(4)	Nd(1)-N(1)#1	2.577(4)
N(5)-O(7)	1.295(4)	N(5)-O(7)	1.289(4)
N(6)-O(8)	1.262(5)	N(6)-O(8)	1.258(5)
N(3)-O(9)	1.222(1)	N(3)-O(9)	1.386(11)
N(4)-O(10)	1.233(7)	N(4)-O(10)	1.318(11)
O(1)-Dy(1)-O(2)	71.18(11)	O(1)-Nd(1)-O(2)	69.55(11)
O(3)-Dy(1)-O(4)	73.70(11)	O(3)-Nd(1)-O(4)	71.63(11)
O(6)-Dy(1)-O(5)	74.28(11)	O(6)-Nd(1)-O(5)	72.66(11)
O(7)-Dy(1)-N(1)	98.30(11)	O(7)-Nd(1)-N(1)#1	97.58(11)
N(5)-O(7)-Dy(1)	136.8(3)	N(5)-O(7)-Nd(1)	136.9(3)

Symmetry transformations used to generate equivalent atoms: #1 x, - y + 1/2, z + 1/2 for **4**

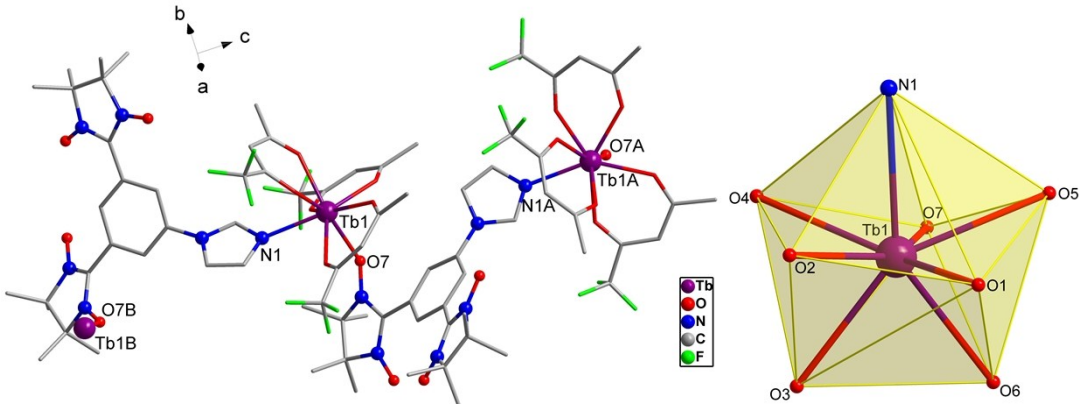

Figure S1 (left) Crystal structure of complex **2** with the atom-labeling. All of the hydrogen and dichloromethane solvent molecules are omitted for clarity. (right) The coordination polyhedron of the Tb ion.

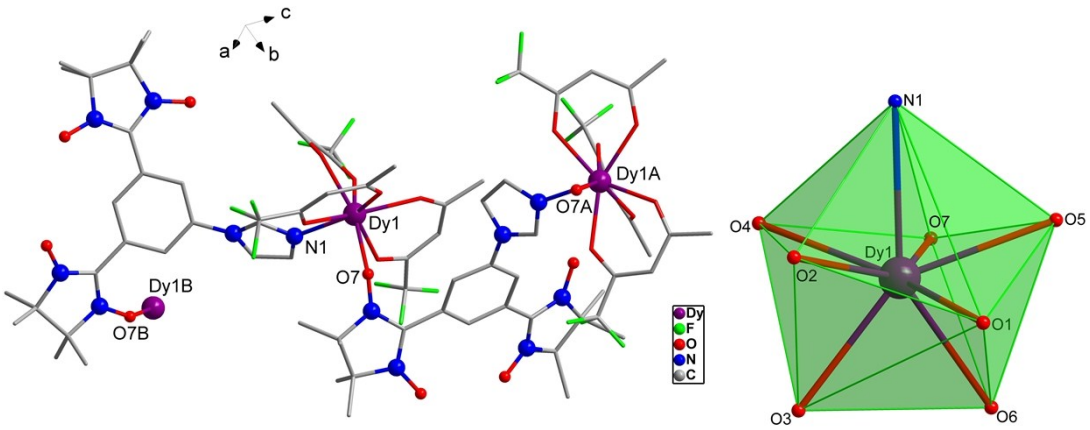

Figure S2 (left) Crystal structure of complex **3** with the atom-labeling. All of the hydrogen and dichloromethane solvent molecules are omitted for clarity. (right) The coordination polyhedron of the Dy ion.

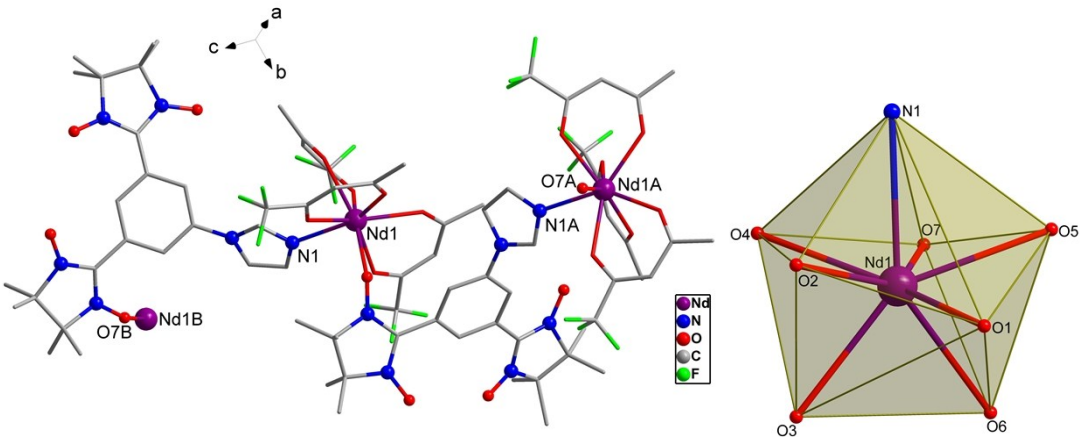

Figure S3 (left) Crystal structure of complex **4** with the atom-labeling. All of the hydrogen and dichloromethane solvent molecules are omitted for clarity. (right) The coordination polyhedron of the Nd ion.

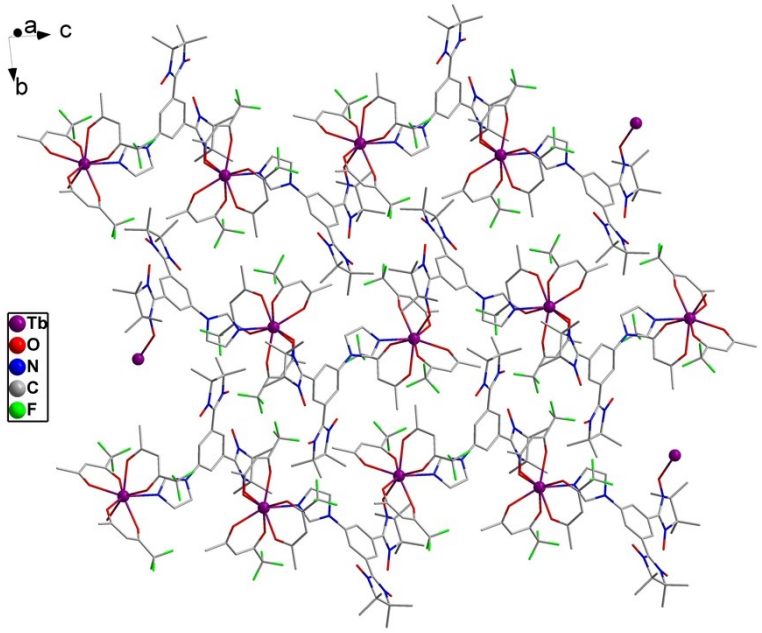

Figure S4 Packing of the chains in crystal for complex **2**. All of the hydrogen atoms and dichloromethane solvent molecules are omitted for clarity.

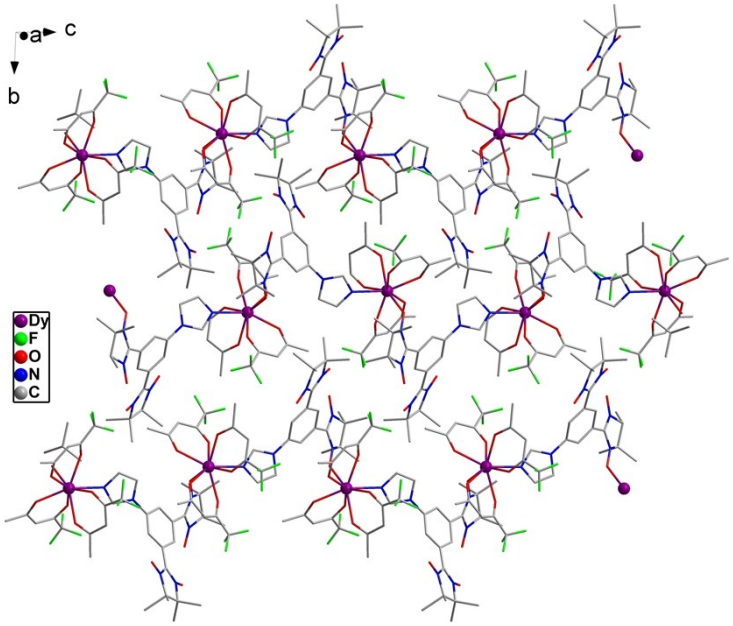

Figure S5 Packing of the chains in crystal for complex **3**. All of the hydrogen atoms and dichloromethane solvent molecules are omitted for clarity.

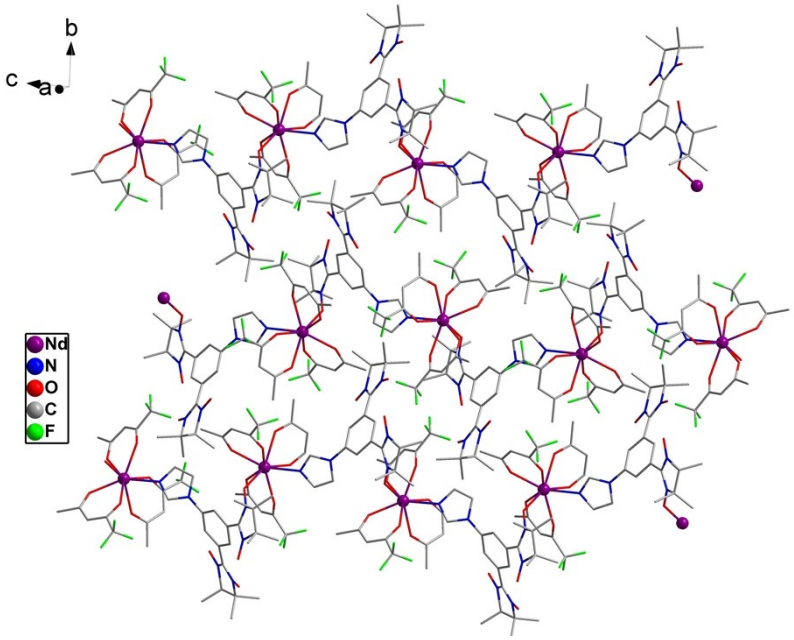

Figure S6 Packing of the chains in crystal for complex **4**. All of the hydrogen atoms and dichloromethane solvent molecules are omitted for clarity.

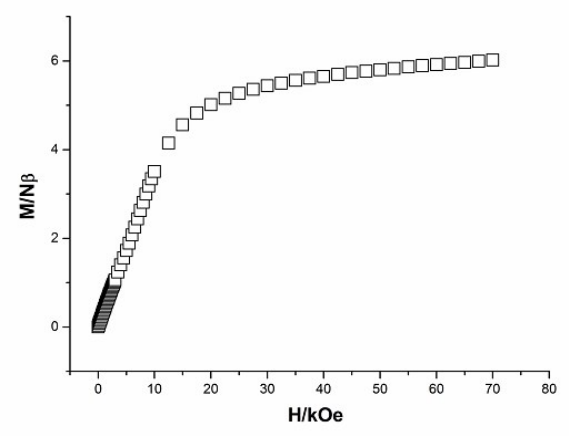

Figure S7 *M* versus *H* plot of complex **2** at 2.0K.

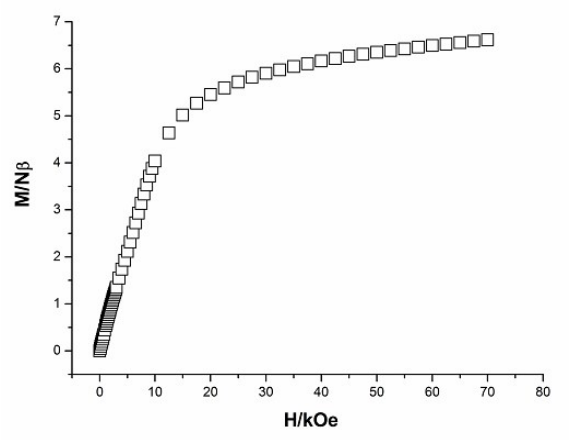

Figure S8 *M* versus *H* plot of complex **3** at 2.0K.

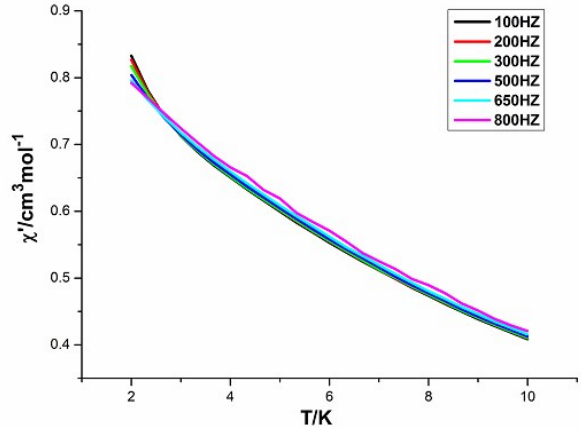

Figure S9 Temperature dependence of the in-phase of the ac magnetic susceptibilities for **2** in zero dc field with an oscillation of 3 Oe.

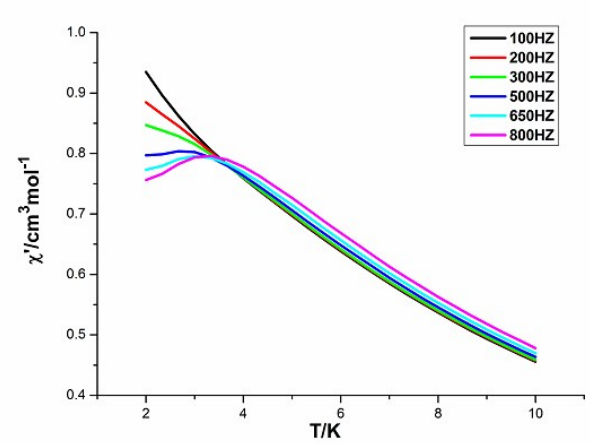

Figure S10 Temperature dependence of the in-phase of the ac magnetic susceptibilities for **3** in zero dc field with an oscillation of 3 Oe.

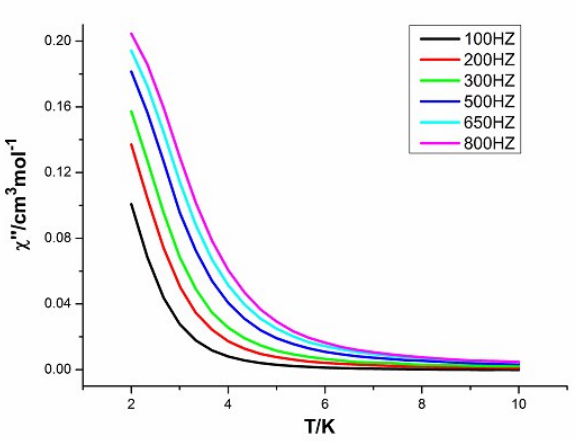

Figure S11 Temperature dependence of the out-of-phase of the ac magnetic susceptibilities for **3** in zero dc field with an oscillation of 3 Oe.

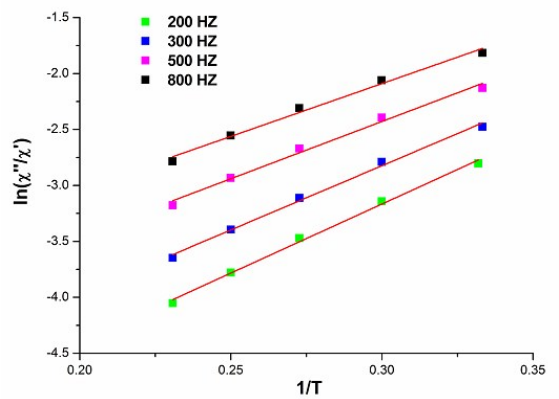

Figure S12 Natural logarithm of of χ''/χ' versus 1/T of **3** (the solid lines represent the fitting results).