Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information for

Luminescent, Magnetic and Ferroelectric Properties of Noncentrosymmetric Chain-Like Complexes Composed of Nine-Coordinate Lanthanide Ions

Xi-Li Li,*[a] Chun-Lai Chen,[a] Hong-Ping Xiao,[b] Ai-Ling Wang,[a] Cai-Ming Liu,*[c] Xianjun Zheng,[a] Li-Jun Gao,[a] Xiao-Gang Yang[a] and Shao-Ming Fang*[a]

[a]Henan Provincial Key Laboratory of Surface and Interface Sciences, Zhengzhou University of Light Industry, Zhengzhou 450002, P. R. China

[b]School of Chemistry and Materials Engineering, Wenzhou University, Wenzhou 325027, P. R. China

[c]Beijing National Laboratory for Molecular Sciences, Institution of Chemistry, Chinese Academy of Science, Center for Molecular Sciences, Beijing 100190, P. R. China

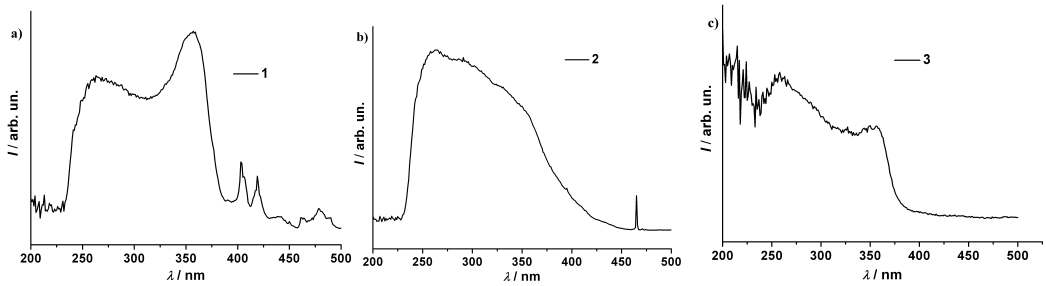


Fig. S1 The solid-state excitation spectrum for complexes **1** (a), **2** (b) and **3** (c) monitored by the respective emissions of $^4G_{5/2} \rightarrow {}^6H_{9/2}$, $^5D_0 \rightarrow {}^7F_2$ and $^5D_4 \rightarrow {}^7F_5$ at room temperature.

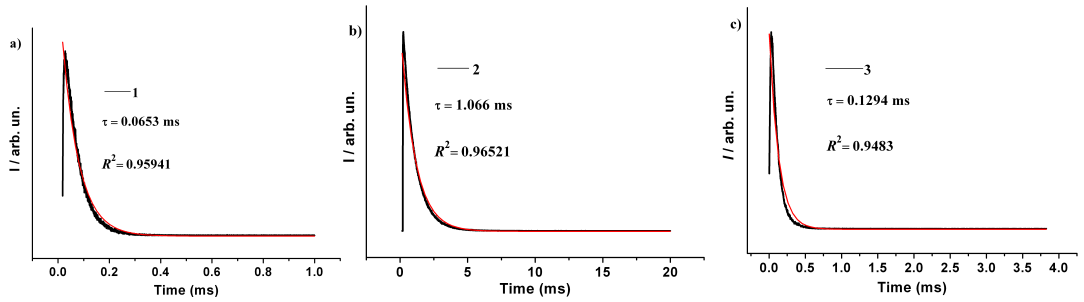


Fig. S2 The solid-state luminescent lifetime measurements for complexes **1** (a), **2** (b) and **3** (c) at room temperature.

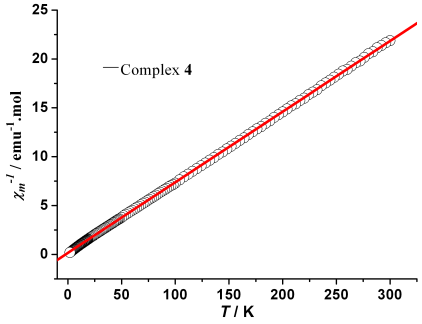


Fig. S3 The plot of χ_m^{-1} *vs.* *T* for Dy^{3+} complex **4.** The red line represents the best theoretic fitting.

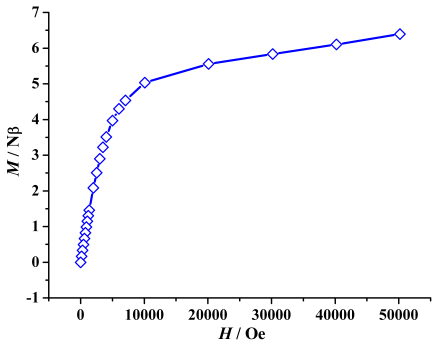
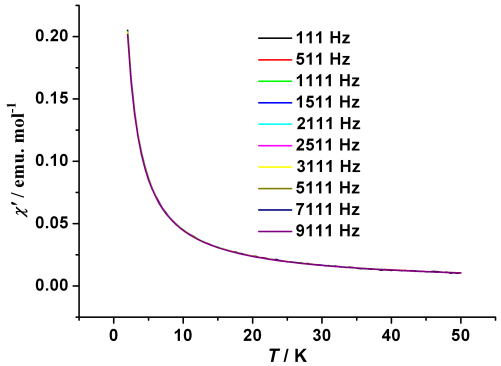


Fig. S4 The plot of *M* vs. *H* for complex **4** at 2 K.



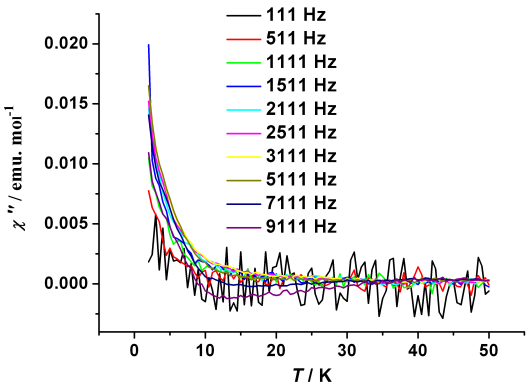


Fig. S5 Temperature-dependence of ac susceptibilities of in-phase (top) and out-of-phase (bottom) for **4** at the indicated frequency under H_{dc} = 0 and H_{ac} = 2.5 Oe.

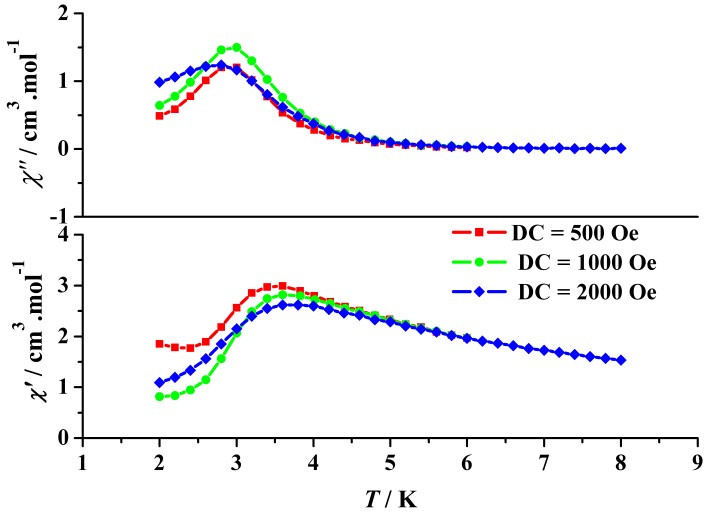


Fig. S6 AC susceptibilities measured at 250 Hz in a 2.5 Oe ac magnetic field with different dc-fields for **4.**

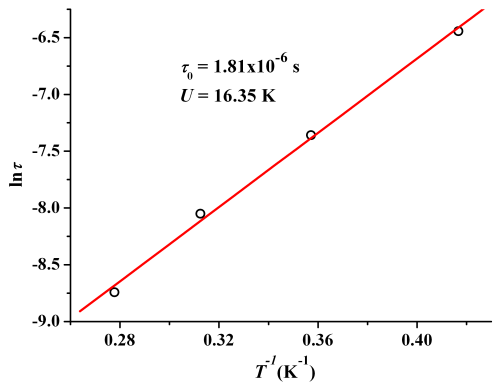


Fig. S7 The plot of ln(τ) vs.1/T under H_{dc} = 2000 Oe for **4** and the fitting results by

the Arrhénius law (red solid line).

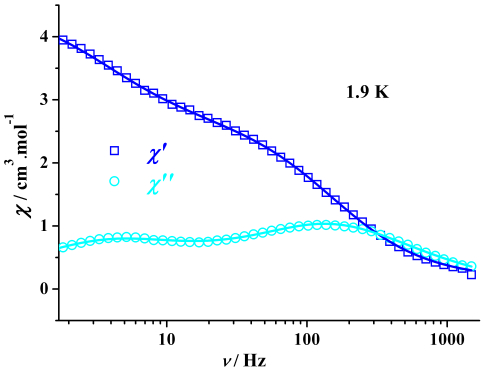


Fig. S8. Frequency dependence of the in-phase (χ', top) and out-of-phase (χ″, bottom) ac susceptibility of **4** at 1.9 K. the solid lines represent the best fitting with the sum of two modified Debye functions.

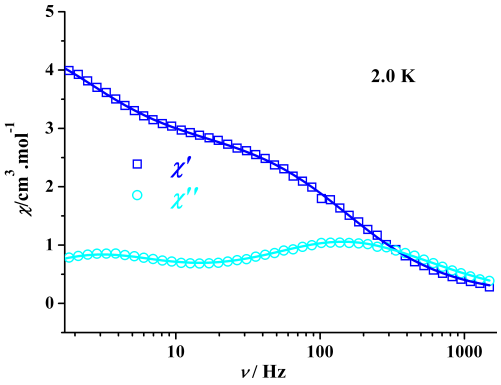


Fig. S9. Frequency dependence of the in-phase (χ', top) and out-of-phase (χ″, bottom) ac susceptibility of **4** at 2.0 K. the solid lines represent the best fitting with the sum of two modified Debye functions.

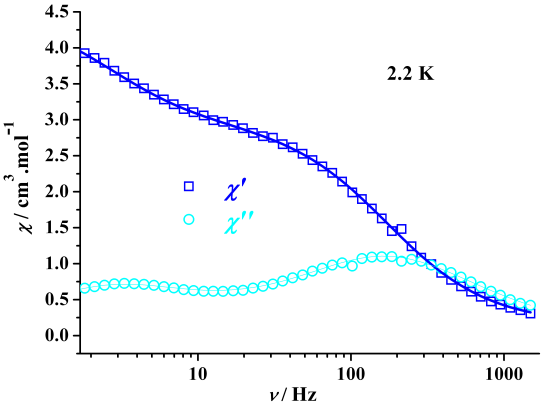


Fig. S10. Frequency dependence of the in-phase (χ', top) and out-of-phase (χ″, bottom) ac susceptibility of **4** at 2.2 K. the solid lines represent the best fitting with the sum of two modified Debye functions.

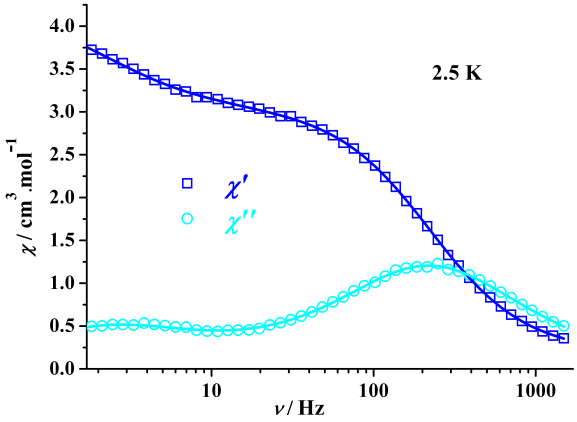


Fig. S11. Frequency dependence of the in-phase (χ', top) and out-of-phase (χ″, bottom) ac susceptibility of **4** at 2.5 K. the solid lines represent the best fitting with the sum of two modified Debye functions.

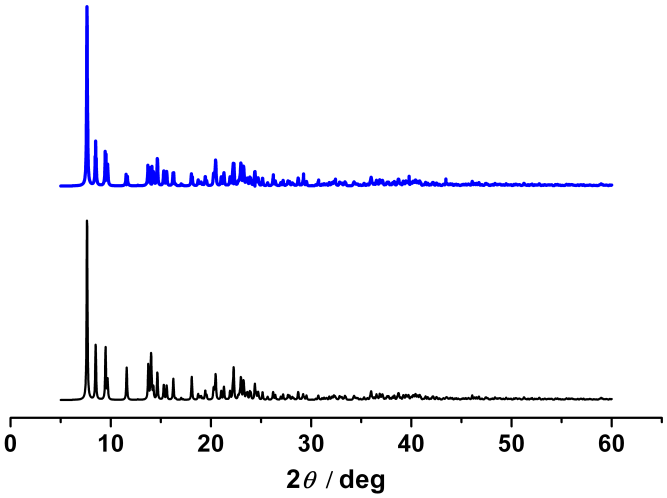


Fig. S12. The simulative (black) and experimental (blue) powder X-ray diffraction patterns for **4**.

Table S1. Selected bond lengths (Å) and angles (º) for **1**–**4**.

Complex **1**					
Sm1-O1	2.377(6)	Sm1-O2	2.383(5)	Sm1-O3	2.403(5)
Sm1-O4	2.407(5)	Sm1-O5	2.463(5)	Sm1-O6	2.372(5)
Sm1-N2	2.682(6)	Sm1-N3	2.607(6)	Sm1-N1(A)	2.624(6)
O6-Sm1-O1	95.03(19)	O1-Sm1-O3	132.98(18)	O3-Sm1-O4	67.86(18)
O6-Sm1-N3	136.90(2)	N3-Sm1-N2	61.6(2)	N1(A)-Sm1-N2	144.45(17)

Complex **2**					
Eu1-O1	2.436(8)	Eu1-O2	2.339(6)	Eu1-O3	2.337(7)
Eu1-O4	2.393(7)	Eu1-O5	2.473(8)	Eu1-O6	2.379(7)
Eu1-N2	2.673(8)	Eu1-N3	2.627(8)	Eu1-N1(A)	2.657(8)
O6-Eu1-O1	93.7(3)	O1-Eu1-O3	134.3(2)	O3-Eu1-O4	67.2(2)
O6-Eu1-N3	138.2(3)	N3-Eu1-N2	61.3(2)	N1(A)-Eu1-N2	143.3(2)
Complex **3**					
Tb1-O1	2.461(9)	Tb1-O2	2.289(7)	Tb1-O3	2.253(9)
Tb1-O4	2.386(8)	Tb1-O5	2.460(10)	Tb1-O6	2.336(8)
Tb1-N2	2.668(10)	Tb1-N3	2.585(10)	Tb1-N1(A)	2.596(9)
O6-Tb1-O1	92.9(3)	O1-Tb1-O3	133.9(2)	O3-Tb1-O4	70.6(3)
O6-Tb1-N3	137.3(3)	N3-Tb1-N2	62.2(3)	N1(A)-Tb1-N2	143.7(3)
Complex **4**					
Dy1-O1	2.578(7)	Dy1-O2	2.367(6)	Dy1-O3	2.278(6)
Dy1-O4	2.342(6)	Dy1-O5	2.536(6)	Dy1-O6	2.302(6)
Dy1-N2	2.697(6)	Dy1-N3	2.565(7)	Dy1-N1(A)	2.606(6)
O6-Dy1-O1	91.4(2)	O1-Dy1-O3	133.50(19)	O3- Dy1-O4	72.1(2)
O6-Dy1-N3	136.6(2)	N3-Dy1-N2	62.2(2)	N1(A)-Dy1-N2	143.8(2)
Symmetry code: A $x, -y, 0.5 + z$					

Table S2. Relaxation Fitting Parameters from Least-Squares Fitting of $\chi(\omega)$ Data of **4**.

T(K)	χ_2(cm^3.mol^{-1})	χ_1(cm^3.mol^{-1})	χ_0(cm^3.mol^{-1})	τ_1(s)	α_1	τ_2(s)	α_2
1.9	4.52014	2.66445	0.13338	0.00103	0.183	0.04381	0.198
2.0	4.69748	2.89267	0.11685	0.00101	0.201	0.06211	0.128
2.2	4.51441	2.95578	0.12751	0.00091	0.179	0.05993	0.143
2.5	4.22166	3.06421	0.15662	0.00071	0.129	0.06905	0.144