Supporting Information

Slow magnetic relaxation and selective luminescent probe in 2p−3d−4f heterotrispin chain

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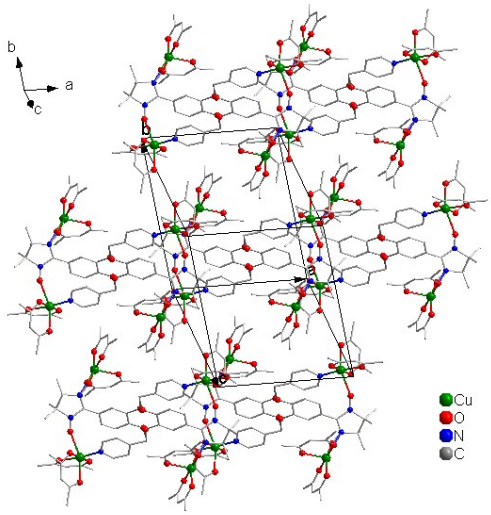

Fig. S1 Packing arrangement of **1** (H and F atoms are omitted for clarity).

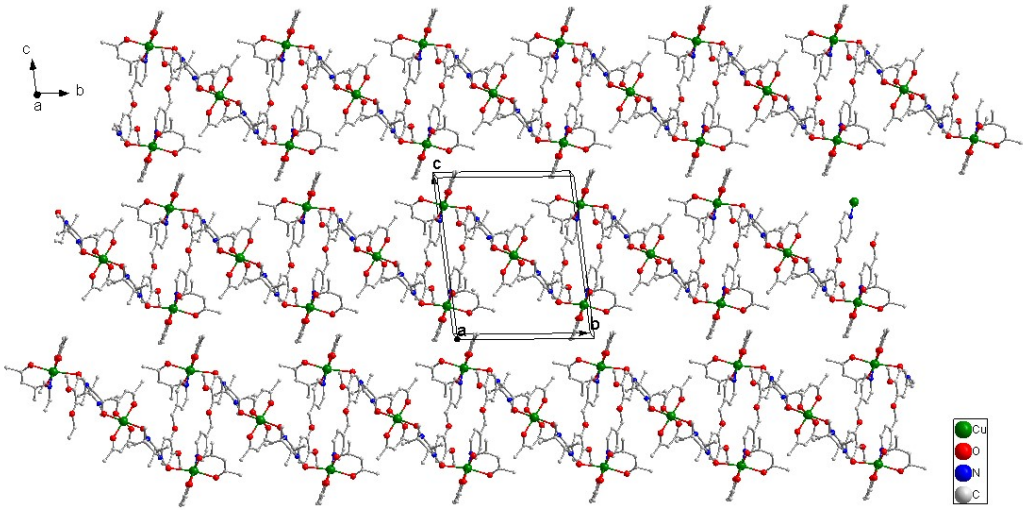

Fig. S2 Packing arrangement of **2** (H and F atoms are omitted for clarity).

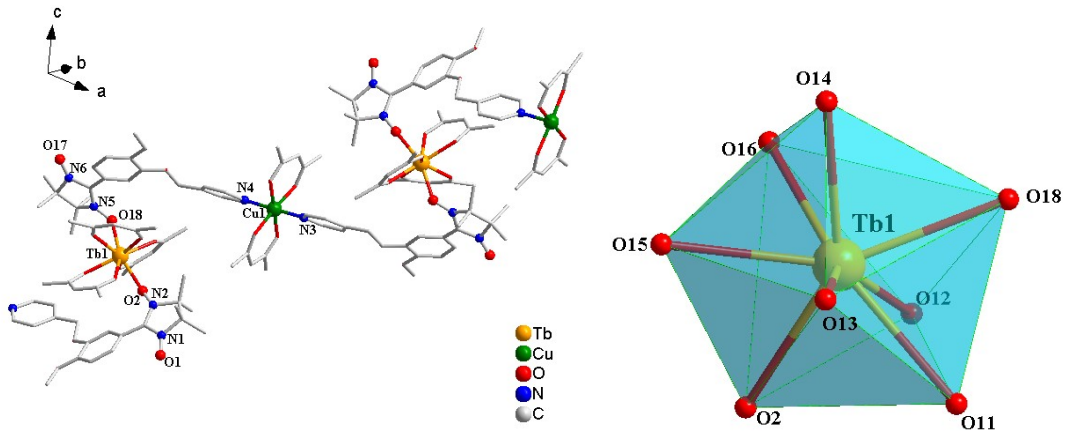

Fig. S3 (left) One-dimensional chain of **4**. (right) coordination polyhedron of a Tb^{III} ion (fluorine and hydrogen atoms are omitted).

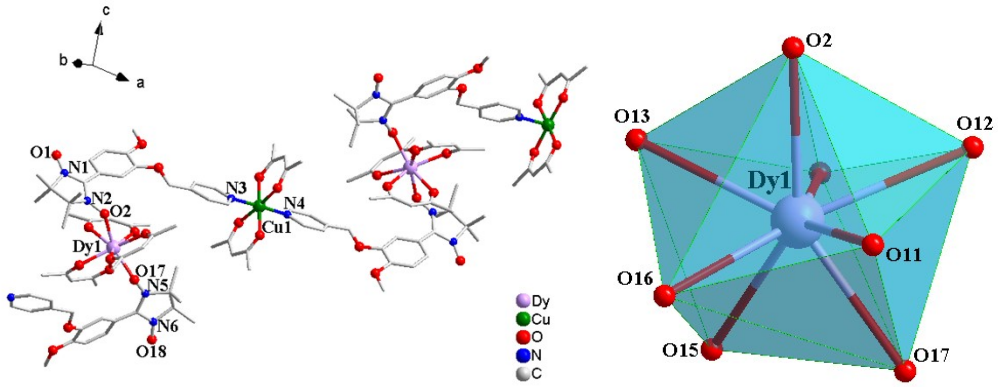

Fig. S4 (left) One-dimensional chain of **5**. (right) coordination polyhedron of a Dy^{III} ion (fluorine and hydrogen atoms are omitted).

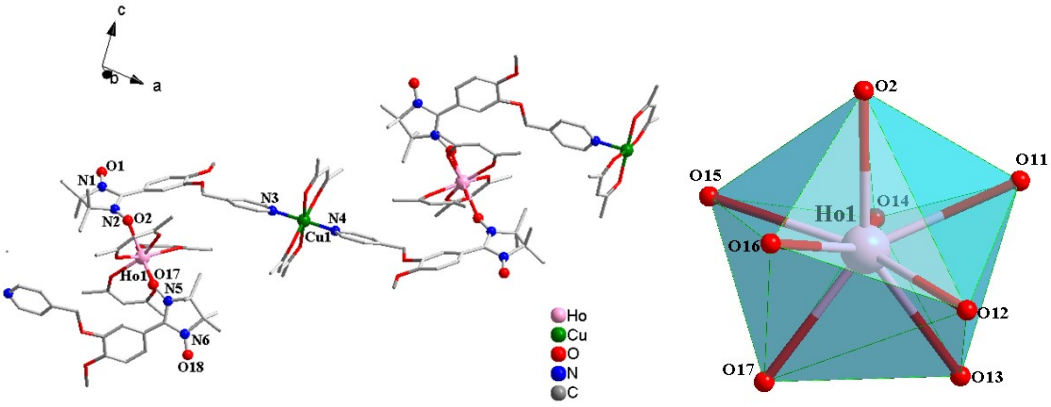

Fig. S5 (left) One-dimensional chain of **6**. (right) coordination polyhedron of a Ho^{III} ion (fluorine and hydrogen atoms are omitted).

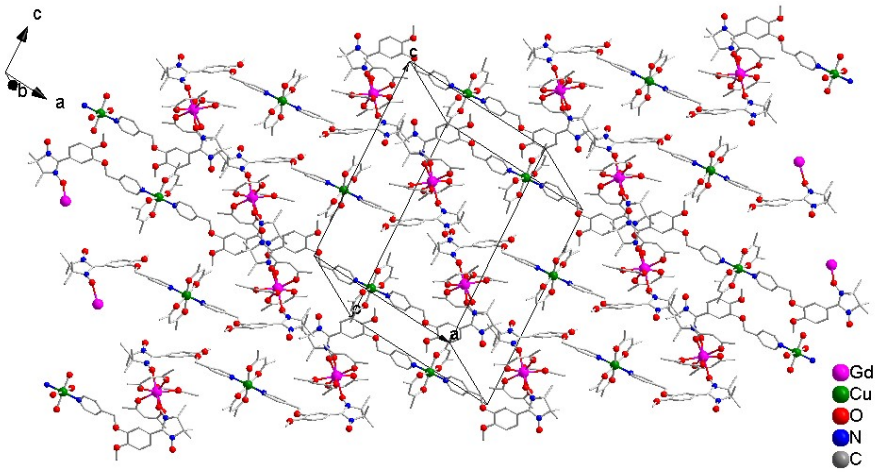

Fig. S6 Packing arrangement of **3** (H and F atoms are omitted for clarity).

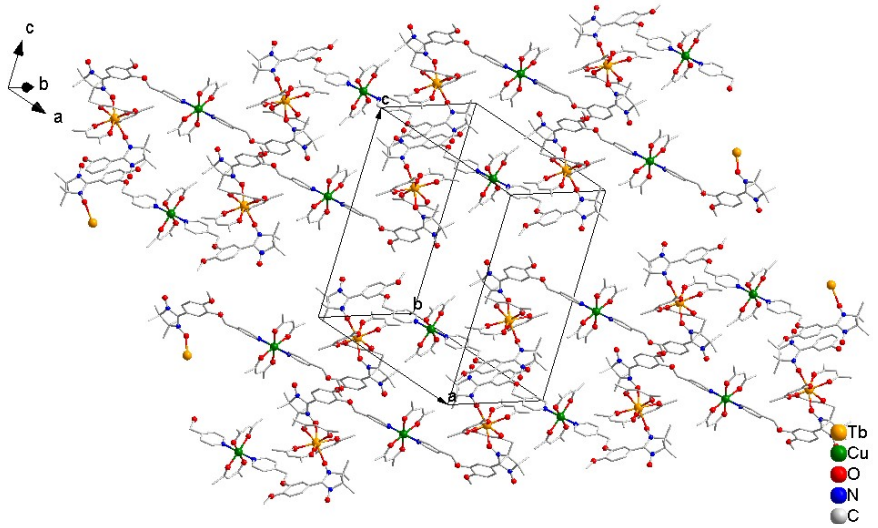

Fig. S7 Packing arrangement of **4** (H and F atoms are omitted for clarity).

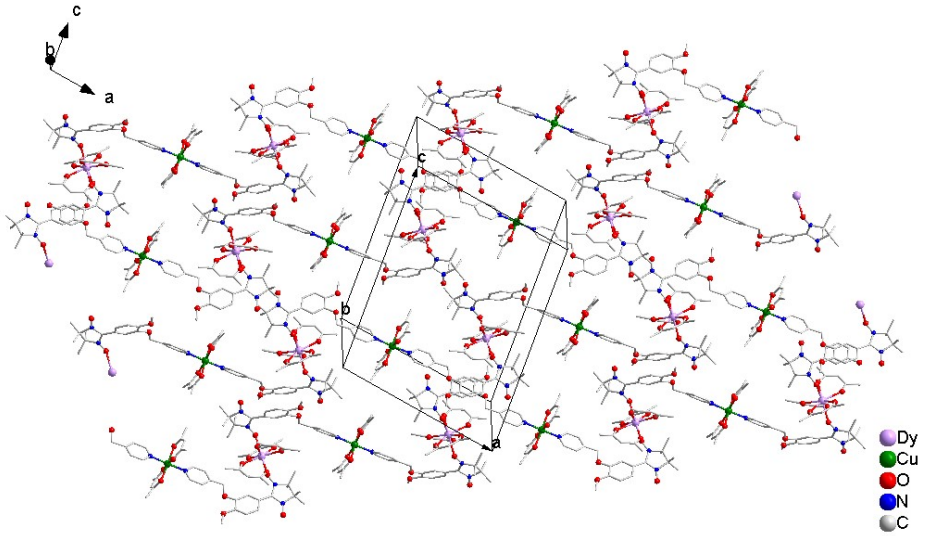

Fig. S8 Packing arrangement of **5** (H and F atoms are omitted for clarity).

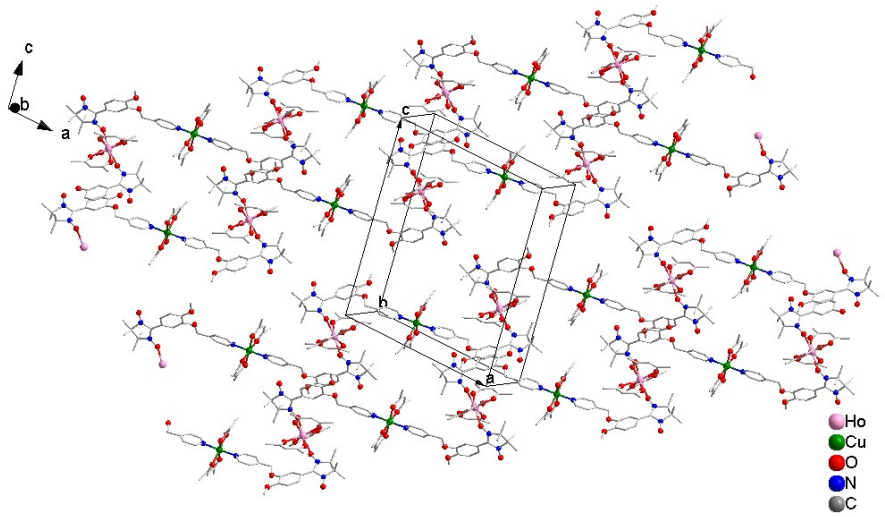

Fig. S9 Packing arrangement of **6** (H and F atoms are omitted for clarity).

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

Bond distances			
Cu (2)-O(2)	1.945(4)	Cu (1)-O(5)	1.942(4)
Cu (2)-O(3)	1.981(4)	Cu (1)-O(8)	2.193(5)
Cu (2)-N(3)	2.019(5)	Cu (1)-O(9)	1.900(4)
Cu (2)-O(6)	1.955(4)	Cu (1)-O(10)	1.913(4)
Cu (2)-O(7)	2.214(5)	O (12)-N(1)	2.232(7)
Cu(2)-O(12)	2.6123(7)	O (5)-N(2)	1.270(7)
Cu (1)-O(4)	1.989(4)		
Angles			
O(2)-Cu (2)-O(3)	91.06(17)	O(5)- Cu (1)-O(4)	160.65(18)
O(2)- Cu (2)-N(3)	90.15(18)	O(5)- Cu (1)-O(8)	107.58(18)
O(2)- Cu (2)-O(6)	177.21(17)	O(9)- Cu (1)-O(4)	90.16(18)
O(2)- Cu (2)-O(7)	91.71(17)	O(9)- Cu (1)-O(5)	94.17(19)
O(3)- Cu (2)-N(3)	173.48(19)	O(9)- Cu (1)-O(8)	91.7(2)
O(3)- Cu (2)-O(7)	86.66(18)	O(9)- Cu (1)-O(10)	177.3(2)
N(3)- Cu (2)-O(7)	99.71(18)	O(10)- Cu (1)-O(4)	92.18(17)
O(6)- Cu (2)-O(3)	86.29(17)	O(10)- Cu (1)-O(5)	83.16(18)
O(6)- Cu (2)-N(3)	92.39(19)	O(10)- Cu (1)-O(8)	89.4(2)
O(6)- Cu (2)-O(7)	89.01(19)	N(2)- O (5)-Cu(1)	119.2(4)
O(4)- Cu (1)-O(8)	91.08(18)		

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

Bond distances			
Cu (1)-O(2)	1.957(3)	Cu (2)-O(8)	1.942(3)
Cu (1)-O(4)	2.249(4)	O(1)-N(1)	1.285(5)

Cu (1)-O(6)	1.952(3)	O (10)-N(3)	1.273(5)
Cu (1)-N(2)	2.021(4)	Cu (2)-O(7)	1.947(3)
Cu (2)-O(1)	2.369(3)		
Angles			
O(2)-Cu (1)-O(4)	90.40(13)	O(7)- Cu (2)-O(1)#1	87.00(13)
O(2)- Cu (1)-N(2)	91.03(15)	O(7)- Cu (2)-O(1)	93.00(13)
O(6)- Cu (1)-O(2)	177.48(14)	O(7)#1- Cu (2)-O(1)	87.00(13)
O(6)- Cu (1)-O(4)	88.59(14)	O(7)#1- Cu (2)-O(1)#1	93.00(13)
O(6)- Cu (1)-O(9)	85.76(14)	O(7)- Cu (2)-O(7)#1	180.00(16)
O(6)- Cu (1)-N(2)	91.24(15)	O(8)#1- Cu (2)-O(1)#1	92.94(13)
O(9)- Cu (1)-O(2)	92.00(14)	O(8)#1- Cu (2)-O(1)	87.06(13)
O(9)- Cu (1)-O(4)	93.64(14)	O(8)- Cu (2)-O(7)#1	86.93(14)
O(9)- Cu (1)-N(2)	176.72(15)	O(8)- Cu (2)-O(7)	93.07(14)
N(2)- Cu (1)-O(4)	87.59(15)	O(8)#1- Cu (2)-O(7)#1	93.07(14)
O(1)#1- Cu (2)-O(1)	180.0	O(8)#1- Cu (2)-O(7)	86.93(14)
O(8)#1-Cu(2)-O(8)	180.0	N(1)-O(1)-Cu(2)	143.83(3)

Table S3 Selected bond lengths [Å] and angles [°] for **3**.

Bond distances			
Gd (1)-O(13)	2.428(5)	Cu (1)-O(7)	1.999(7)
Gd (1)-O(14)	2.407(5)	Cu (1)-N(3)	1.984(6)
Gd (1)-O(15)	2.352(6)	Cu (1)-N(4)	1.993(6)
Gd (1)-O(12)	2.359(5)	Cu (1)-O(6)	2.259(7)
Gd (1)-O(16)	2.407(6)	Cu (1)-O(8)	2.232(7)
Gd (1)-O(18)	2.350(6)	O (12)-N(6)	1.318(8)
Gd (1)-O(2)	2.372(5)	O (2)-N(2)	1.309(8)
Gd (1)-O(17)	2.420(6)	O (11)-N(5)	1.258(10)
Cu (1)-O(5)	2.011(6)	O (1)-N(1)	1.262(8)
Angles			
O(14)-Gd (1)-O(13)	72.7(2)	O(18)-Gd (1)-O(13)	147.5(2)
O(14)-Gd (1)-O(17)	128.3(2)	O(18)-Gd (1)-O(14)	74.9(2)
O(15)-Gd (1)-O(13)	76.92(19)	O(18)-Gd (1)-O(15)	135.6(2)
O(15)-Gd (1)-O(14)	149.3(2)	O(18)-Gd (1)-O(12)	94.9(2)
O(15)-Gd (1)-O(12)	98.89(18)	O(18)-Gd (1)-O(16)	73.3(2)
O(15)-Gd (1)-O(16)	72.56(19)	O(18)-Gd (1)-O(2)	99.6(2)
O(15)-Gd (1)-O(2)	95.86(19)	O(18)-Gd (1)-O(17)	72.7(2)
O(15)-Gd (1)-O(17)	71.3(2)	O(17)-Gd (1)-O(13)	132.1(2)
O(12)-Gd (1)-O(13)	77.32(19)	O(5)-Cu (1)-O(6)	86.8(3)
O(12)-Gd (1)-O(14)	70.40(19)	O(5)-Cu (1)-O(8)	91.7(3)
O(12)-Gd (1)-O(16)	147.54(19)	N(3)-Cu (1)-O(5)	92.1(3)
O(12)-Gd (1)-O(2)	140.7(2)	N(3)-Cu (1)-O(7)	89.5(3)

O(12)-Gd (1)-O(17)	73.4(2)	N(3)-Cu (1)-O(6)	88.1(3)
O(16)-Gd (1)-O(13)	128.16(19)	N(3)-Cu (1)-O(8)	87.9(3)
O(16)-Gd (1)-O(14)	131.37(19)	N(3)-Cu (1)-O(4)	178.6(3)
O(16)-Gd (1)-O(17)	74.2(2)	O(7)-Cu (1)-O(5)	178.1(3)
O(2)-Gd (1)-O(13)	70.87(18)	O(7)-Cu (1)-O(6)	94.2(3)
O(2)-Gd (1)-O(14)	78.41(19)	O(7)-Cu (1)-O(8)	87.4(3)
O(2)-Gd (1)-O(16)	71.77(19)	O(8)-Cu (1)-O(6)	175.7(2)
O(2)-Gd (1)-O(17)	145.8(2)	N(4)-Cu (1)-O(5)	89.2(3)
N(6) -O(12) -Gd(1)	134.7(5)	N(4)-Cu (1)-O(7)	89.1(3)
N(2)-O(2)-Gd(1)	134.7(5)	N(4)-Cu (1)-O(6)	92.4(3)
N(4)-Cu (1)-O(8)	91.7(3)		

Table S4 Selected bond lengths [Å] and angles [°] for **4**.

Bond distances			
Tb (1)-O(13)	2.330(5)	Cu (1)-O(7)	2.267(6)
Tb (1)-O(14)	2.398(6)	Cu (1)-N(3)	1.996(6)
Tb (1)-O(15)	2.379(5)	Cu (1)-N(4)	1.990(6)
Tb (1)-O(12)	2.406(5)	Cu (1)-O(6)	2.011(6)
Tb (1)-O(16)	2.344(5)	Cu (1)-O(8)	2.022(6)
Tb (1)-O(18)	2.347(5)	O (18)-N(5)	1.304(7)
Tb (1)-O(2)	2.364(5)	O (2)-N(2)	1.306(7)
Tb (1)-O(11)	2.393(5)	O (17)-N(6)	1.262(8)
Cu (1)-O(5)	2.248(6)	O (1)-N(1)	1.265(8)
Angles			
O(14)-Tb (1)-O(13)	72.6(2)	O(18)-Tb (1)-O(11)	70.51(17)
O(11)-Tb (1)-O(12)	72.88 (17)	O(18)-Tb (1)-O(14)	73.68(18)
O(15)-Tb (1)-O(13)	73.18(18)	O(18)-Tb (1)-O(15)	147.56(18)
O(15)-Tb (1)-O(14)	73.99(19)	O(18)-Tb (1)-O(12)	77.29(16)
O(15)-Tb (1)-O(12)	128.51(17)	O(18)-Tb (1)-O(16)	98.81(17)
O(15)-Tb (1)-O(16)	73.13(17)	O(18)-Tb (1)-O(2)	140.81(17)
O(15)-Tb (1)-O(2)	71.61(17)	O(18)-Tb (1)-O(13)	94.68(18)
O(11)-Tb (1)-O(14)	128.26(18)	O(11)-Tb (1)-O(13)	74.41(18)
O(12)-Tb (1)-O(13)	147.15(18)	O(5)-Cu (1)-O(6)	87.1(2)
O(12)-Tb (1)-O(14)	132.44(18)	O(5)-Cu (1)-O(8)	92.0(2)
O(12)-Tb (1)-O(16)	76.87(17)	N(3)-Cu (1)-O(5)	88.2(2)
O(12)-Tb (1)-O(2)	70.94(16)	N(3)-Cu (1)-O(7)	88.6(2)
O(16)-Tb (1)-O(11)	149.43(17)	N(3)-Cu (1)-O(6)	90.0(2)
O(16)-Tb (1)-O(13)	135.98(19)	N(3)-Cu (1)-O(8)	91.7(2)
O(16)-Tb (1)-O(14)	71.43(19)	N(4)-Cu (1)-O(8)	89.3(2)
O(2)-Tb (1)-O(11)	78.54(17)	O(7)-Cu (1)-O(5)	176.4(2)
O(2)-Tb (1)-O(13)	99.64(18)	O(7)-Cu (1)-O(6)	94.5(2)

O(2)-Tb (1)-O(14)	145.48(18)	O(7)-Cu (1)-O(8)	86.5(2)
O(2)-Tb (1)-O(16)	95.77(17)	O(8)-Cu (1)-O(6)	178.0(2)
O(15)-Tb (1)-O(11)	130.78(16)	N(4)-Cu (1)-O(5)	91.3(2)
N(5) -O(18) -Tb(1)	135.5(4)	N(4)-Cu (1)-O(7)	92.0(2)
N(2)-O(2)-Tb(1)	134.5(4)	N(4)-Cu (1)-O(6)	88.9 (2)
N(4)-Cu (1)-O(8)	89.3(2)		

Table S5 Selected bond lengths [Å] and angles [°] for **5**.

Bond distances			
Dy (1)-O(12)	2.404(6)	Cu (1)-O(7)	2.242(7)
Dy (1)-O(17)	2.335(6)	Cu (1)-N(3)	1.987(6)
Dy (1)-O(11)	2.404(6)	Cu (1)-N(4)	1.992(7)
Dy (1)-O(2)	2.354(6)	Cu (1)-O(6)	2.017(7)
Dy (1)-O(13)	2.392(6)	Cu (1)-O(8)	2.002(7)
Dy (1)-O(14)	2.328(6)	O (17)-N(5)	1.313(8)
Dy (1)-O(16)	2.324(6)	O (2)-N(2)	1.307(8)
Dy (1)-O(15)	2.401(7)	O (18)-N(6)	1.251(10)
Cu (1)-O(6)	2.017(7)	O (1)-N(1)	1.254(9)
Angles			
O(17)- Dy (1)-O(12)	77.2(2)	O(16)- Dy (1)-O(17)	95.3(2)
O(17)- Dy (1)-O(11)	70.55(19)	O(16)- Dy (1)-O(11)	74.6(2)
O(17)- Dy (1)-O(2)	140.4(2)	O(16)- Dy (1)-O(2)	99.2(2)
O(17)- Dy (1)-O(13)	148.1(2)	O(16)- Dy (1)-O(13)	73.3(2)
O(17)- Dy (1)-O(15)	73.5(2)	O(16)- Dy (1)-O(14)	136.3(2)
O(11)- Dy (1)-O(12)	73.1(2)	O(16)- Dy (1)-O(15)	73.4(2)
O(2)- Dy (1)-O(12)	70.81(19)	O(15)- Dy (1)-O(12)	131.7(2)
O(2)- Dy (1)-O(11)	78.18(19)	O(15)- Dy (1)-O(11)	128.5(2)
O(2)- Dy (1)-O(13)	71.5(2)	O(5)-Cu (1)-O(6)	87.0(3)
O(2)- Dy (1)-O(15)	146.0(2)	O(6)-Cu (1)-O(7)	91.9(3)
O(13)- Dy (1)-O(12)	127.7(2)	N(3)-Cu (1)-O(5)	87.9(3)
O(13)- Dy (1)-O(11)	130.89(19)	N(3)-Cu (1)-O(7)	88.0(3)
O(13)- Dy (1)-O(15)	74.6(2)	N(3)-Cu (1)-O(8)	89.8(3)
O(14)- Dy (1)-O(12)	76.1(2)	N(3)-Cu (1)-O(4)	178.5(3)
O(14)- Dy (1)-O(17)	98.2(2)	N(4)-Cu (1)-O(6)	89.4(3)
O(14)- Dy (1)-O(11)	148.9(2)	O(7)-Cu (1)-O(5)	175.7(2)
O(14)- Dy (1)-O(2)	96.2(2)	O(8)-Cu (1)-O(6)	177.9(3)
O(14)- Dy (1)-O(13)	73.4(2)	O(5)-Cu (1)-O(8)	94.1(3)
O(14)- Dy (1)-O(15)	71.2(2)	O(8)-Cu (1)-O(7)	87.2(3)
O(16)- Dy (1)-O(12)	147.5(2)	N(4)-Cu (1)-O(5)	92.4(3)
N(5) -O(17) - Dy (1)	135.7(5)	N(4)-Cu (1)-O(7)	91.7(3)
N(2)-O(2)- Dy (1)	135.0(5)	N(4)-Cu (1)-O(8)	88.7(3)

N(3)-Cu (1)-O(6)	92.1(3)		

Table S6 Selected bond lengths [Å] and angles [°] for **6**.

Bond distances			
Ho (1)-O(16)	2.376(4)	Cu (1)-O(8)	2.027(5)
Ho (1)-O(17)	2.321(4)	Cu (1)-N(4)	1.996(5)
Ho (1)-O(11)	2.371(4)	Cu (1)-O(6)	2.000(5)
Ho (1)-O(12)	2.329(5)	Cu (1)-O(7)	2.253(6)
Ho (1)-O(2)	2.337(4)	Cu (1)-O(5)	2.238(6)
Ho (1)-O(15)	2.374(5)	O (17)-N(5)	1.309(6)
Ho (1)-O(14)	2.314(5)	O (2)-N(2)	1.313(6)
Ho (1)-O(13)	2.391(5)	O (18)-N(6)	1.267(8)
Cu (1)-N(3)	1.995(5)	O (1)-N(1)	1.267(7)
Angles			
O(16)- Ho (1)-O(13)	131.30(17)	O(15)- Ho (1)-O(13)	128.05(16)
O(17)- Ho (1)-O(16)	77.33(15)	O(14)- Ho (1)-O(16)	147.46(17)
O(17)- Ho (1)-O(11)	147.44(15)	O(14)- Ho (1)-O(17)	94.58(16)
O(17)- Ho (1)-O(12)	98.70(16)	O(14)- Ho (1)-O(11)	73.24(16)
O(17)- Ho (1)-O(2)	140.62(16)	O(14)- Ho (1)-O(12)	136.74(18)
O(17)- Ho (1)-O(15)	70.53(15)	O(14)- Ho (1)-O(2)	99.33(16)
O(17)- Ho (1)-O(13)	73.14(16)	O(14)- Ho (1)-O(15)	73.86(17)
O(11)- Ho (1)-O(16)	128.42(15)	O(14)- Ho (1)-O(13)	73.40(18)
O(11)- Ho (1)-O(15)	130.58(15)	O(8)-Cu (1)-O(7)	86.8(2)
O(11)- Ho (1)-O(13)	74.43(16)	O(8)-Cu (1)-O(5)	92.0(2)
O(12)- Ho (1)-O(16)	75.79(16)	N(3)-Cu (1)-O(4)	178.9(2)
O(12)- Ho (1)-O(11)	73.58(16)	N(3)-Cu (1)-O(6)	89.9(2)
O(12)- Ho (1)-O(2)	95.93(15)	N(3)-Cu (1)-O(7)	87.9(2)
O(12)- Ho (1)-O(15)	149.22(16)	N(3)-Cu (1)-O(5)	88.4(2)
O(12)- Ho (1)-O(13)	71.54(17)	N(4)-Cu (1)-O(8)	89.3(2)
O(2)- Ho (1)-O(16)	71.18(15)	O(6)-Cu (1)-O(8)	177.9(2)
O(2)- Ho (1)-O(11)	71.91(15)	O(6)-Cu (1)-O(7)	94.6(2)
O(2)- Ho (1)-O(15)	78.28(15)	O(6)-Cu (1)-O(5)	86.8(2)
O(2)- Ho (1)-O(13)	146.21(16)	O(5)-Cu (1)-O(7)	176.12(19)
O(15)- Ho (1)-O(16)	73.73(17)	N(4)-Cu (1)-O(6)	89.0(2)
N(5) -O(17) - Ho (1)	135.3(4)	N(4)-Cu (1)-O(7)	92.1(2)
N(2)-O(2)- Ho (1)	135.1(4)	N(4)-Cu (1)-O(5)	91.6(2)
N(3)-Cu (1)-O(8)	91.8(2)		

Table S7 SHAPE Analysis for the Ln Coordination Spheres

Compound	SAPR-8	**TDD-8**	JBTPR-8	BTPR-8	JSD-8
Gd	2.867	**0.126**	3.158	2.695	2.601
Tb	2.829	**0.122**	3.144	2.648	2.657
Dy	2.911	**0.121**	3.165	2.691	2.572
Ho	2.790	**0.105**	3.154	2.666	2.638

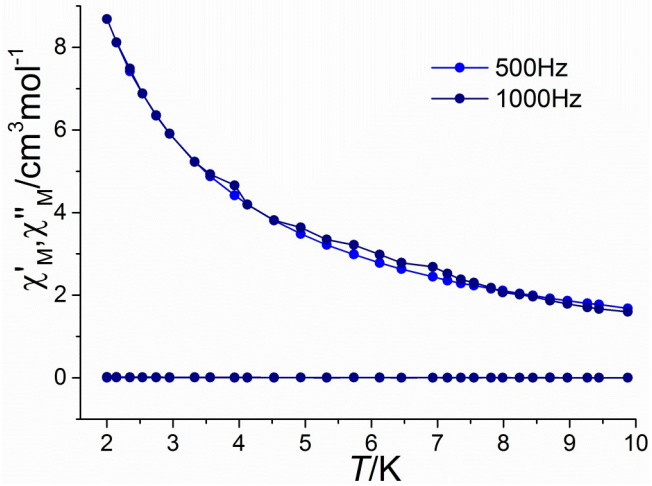

Fig. S10 Temperature dependence of the in-phase and out-of-phase components of the ac magnetic susceptibility for complex **3** in zero dc fields with an oscillation of 3Oe.

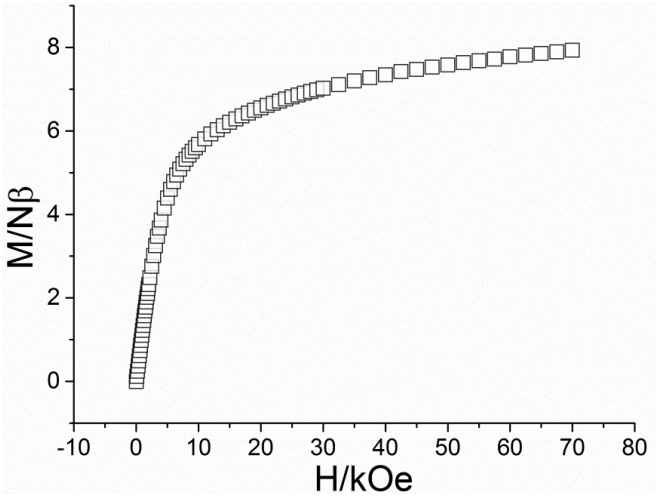

Fig. S11 The M vs. H plots of complex **4.**

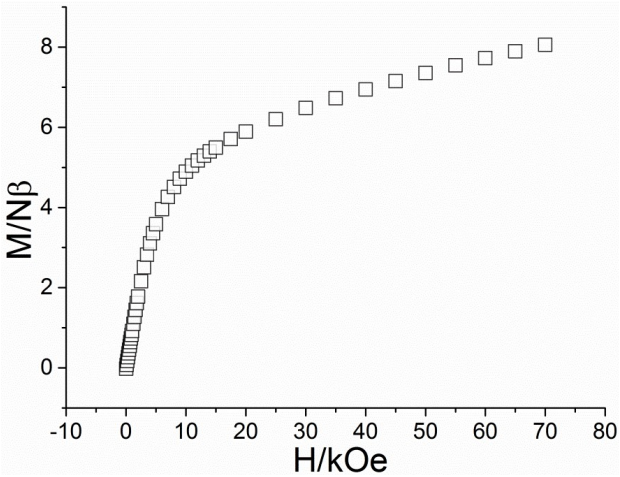

Fig. S12 The M vs. H plots of complex **5.**

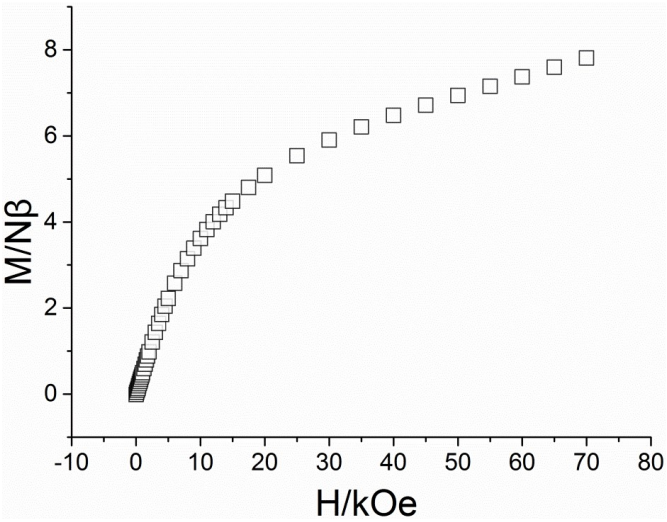

Fig. S13 The M vs. H plots of complex **6.**

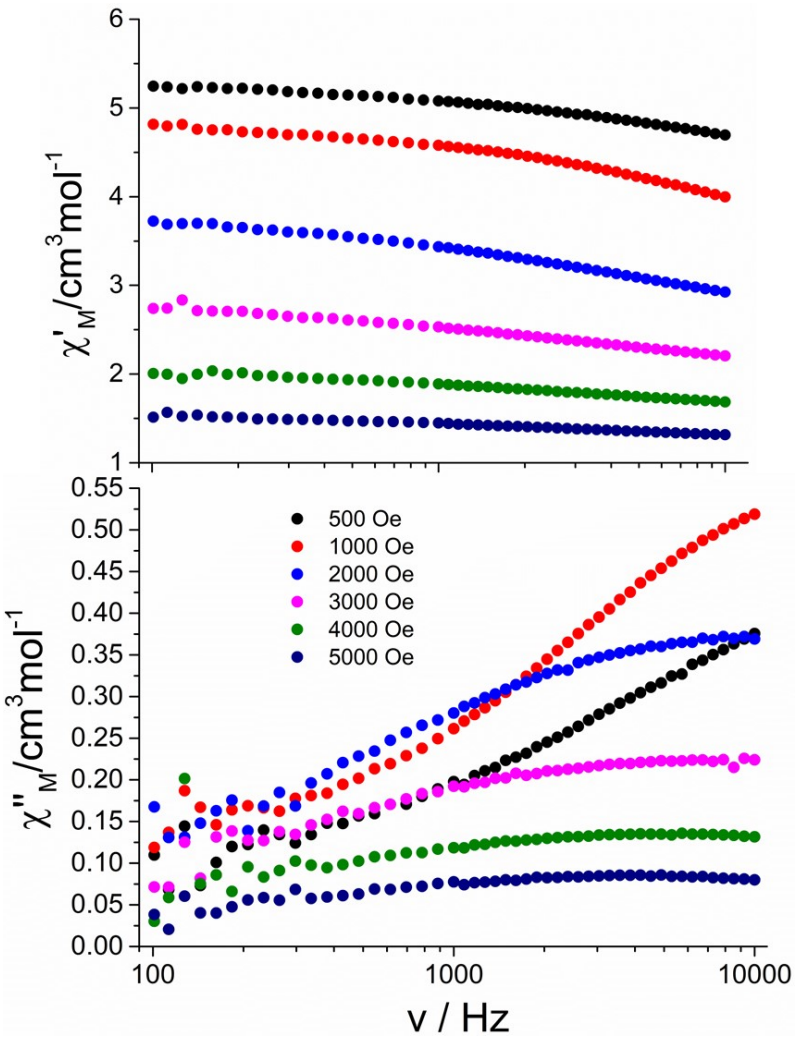

Fig. S14 Frequency dependence of the χ′ (top) and χ″ (bottom) components of the ac susceptibility, between 500 and 5000 Oe and between 100 and 10000 Hz, for **5** at 2 K.

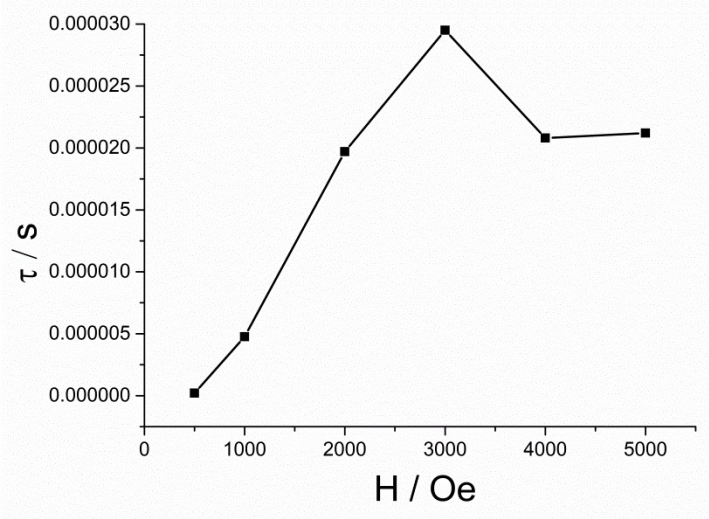

Fig. S15 The τ *versus* H plot for complex **5** at 2.0 K under the applied dc field

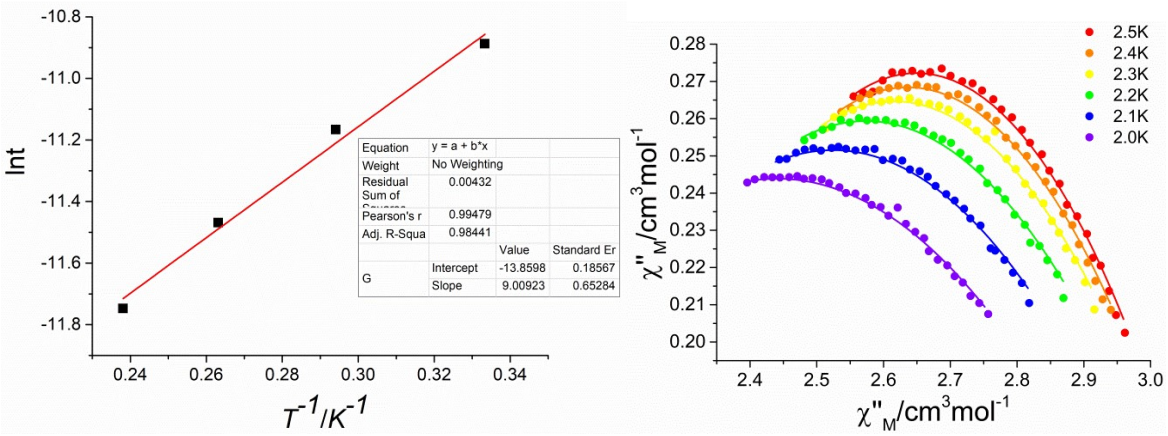

Fig. 16 (left) Plots of lnτ versus T^{-1} fitting to the Arrhenius law for complex **5**. (right) Cole–Cole plots for complex **5**(The solid lines represent the fitting result).

Table S8 Best fitted parameters (χ_T, χ_S, τ and α) with the extended Debye model for complex **5** under 3000 dc field in the temperature range 2.0–2.5 K.

T/K	χ_S /cm^{3}mol^{-1}	χ_T /cm^{3}mol^{-1}	τ/s	α	R
2.0	1.68421	3.22059	2.32×10^{-5}	0.60914	2.62×10^{-4}
2.1	1.78127	3.25671	2.55×10^{-5}	0.58085	2.33×10^{-4}
2.2	1.82891	3.27394	2.40×10^{-5}	0.55883	2.77×10^{-4}
2.3	1.97851	3.25183	2.84×10^{-5}	0.49825	2.75×10^{-4}
2.4	2.02687	3.24463	2.75×10^{-5}	0.47131	2.13×10^{-4}
2.5	2.15925	3.21221	2.91×10^{-5}	0.41217	2.17×10^{-4}

Table S9 Magnetic relaxation parameters for β-diketone Dy(III) complexes possessing triangular dodecahedron (D_{2d}) coordination spheres.

Complex	U_{eff}/k_B (K)	τ_0 (s)	α	H_{dc} (Oe)	Ref.
$[Dy_4(hfac)_8(IMPhThio)_2(OH)_4][Dy(hfac)_3(NITPhThio)_2]$	32	2.96×10^{-9}	0.50-0.15	5000	31a
$[Dy(hfac)_3(tmphen)]$	35.09	9.16×10^{-9}	0.20-0.41	3500	31b
$[Dy(thd)_2(NO_3)(TPPO)_2]$	20.7	1.59×10^{-6}	0.12-0.23	1000	31c
$[Dy(9Accm)_2(NO_3)(dmf)_2]$	23	1.3×10^{-6}	0.3-0.4	1000	31d
$[Dy_2Cu_2(hfac)_{10}(NIT3py)_2(H_2O)_2]$	13.14	1.77×10^{-6}	--	2000	31e
$\{[Cu(hfac)_2][(NIT\text{-}4\text{-}OMe\text{-}4PyPh)]_2[Ln(hfac)_3]\}_n$	25	9.56×10^{-7}	0.37-0.52	3000	This work

NITPhThio = (2-(benzo[d]thiophen-2-yl)-4,4,5,5-tetramethylimidazolin-1-oxyl-3-oxide; IMPhThio = 2-(benzo[d]thiophen-2-yl)-4,4,5,5-tetramethylimidazolin-1-oxyl; mphen = 3,4,7,8-tetramethyl-1,10-phenanthroline; thd = 2,2,6,6-tetramethyl-3,5-heptanedione; TPPO = triphenylphosphane oxide; 9Accm =

1,7-di-9-anthracene-6-heptadiene-3,5-dione; NIT-3py = 2-(3-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl-3-oxide.

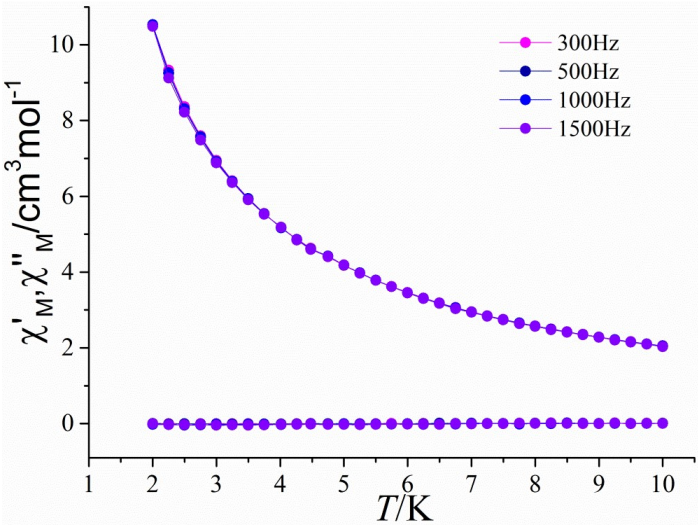

Fig. S17 Temperature dependence of the in-phase and out-of-phase components of the ac magnetic susceptibility for complex **4** in zero dc fields with an oscillation of 3Oe.

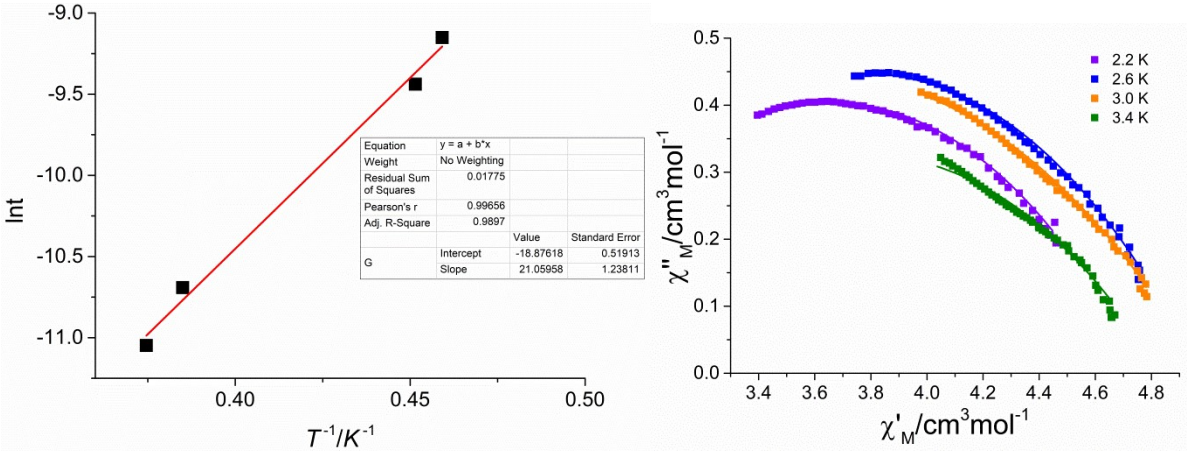

Fig. S18 (left) Plots of lnτ *versus* T^{-1} fitting to the Arrhenius law for complex **4**. (right)Cole–Cole plots for complex **4** (The solid lines represent the fitting result).

Table S10 Best fitted parameters (χ_T, χ_S, τ and α) with the extended Debye model for complex **4** under 3000 dc field in the temperature of 2.2,2.6,3.0 and 3.4 K.

T/K	χ_S /cm^{3}mol^{-1}	χ_T /cm^{3}mol^{-1}	τ/s	α	R
2.2	2.47019	4.79773	3.93×10^{-5}	0.57582	3.39×10^{-4}
2.6	2.66141	4.90636	1.83×10^{-5}	0.51504	2.67×10^{-4}
3.0	2.16028	4.94562	3.90×10^{-6}	0.59319	2.82×10^{-4}
3.4	1.99236	4.87279	1.21×10^{-6}	0.67206	8.71×10^{-4}

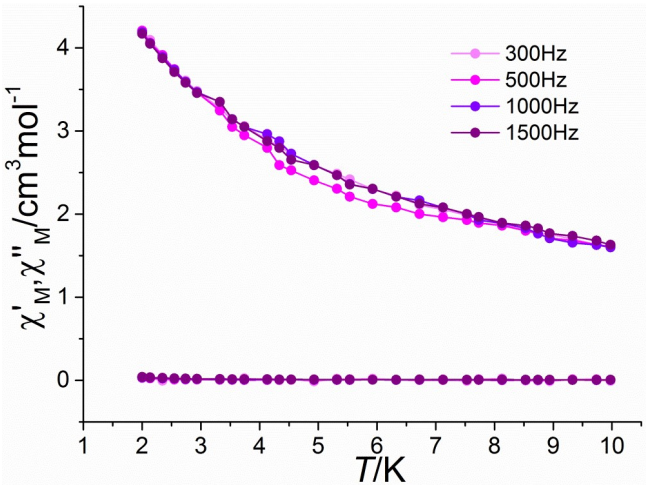

Fig. S19 Temperature dependence of the in-phase and out-of-phase components of the ac magnetic susceptibility for complex **6** in zero dc fields with an oscillation of 3Oe.

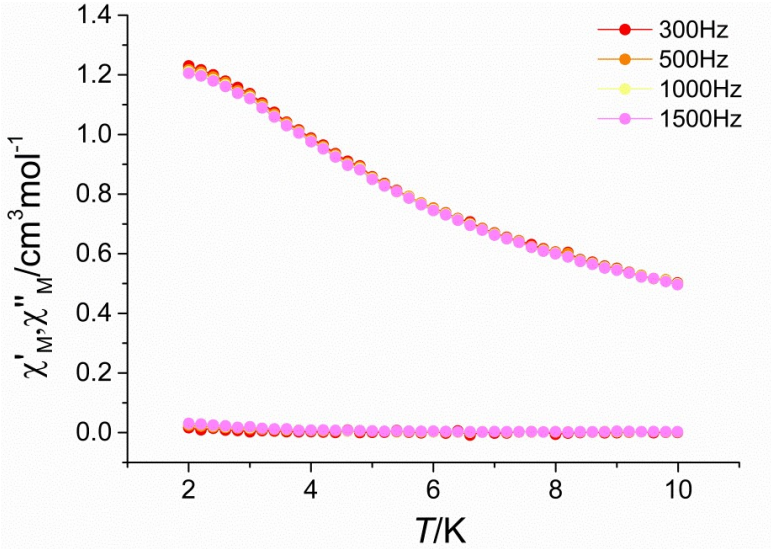

Fig. S20 Temperature dependence of the in-phase and out-of-phase components of the ac magnetic susceptibility for complex **6** under 3000 Oe dc fields with an oscillation of 3Oe.

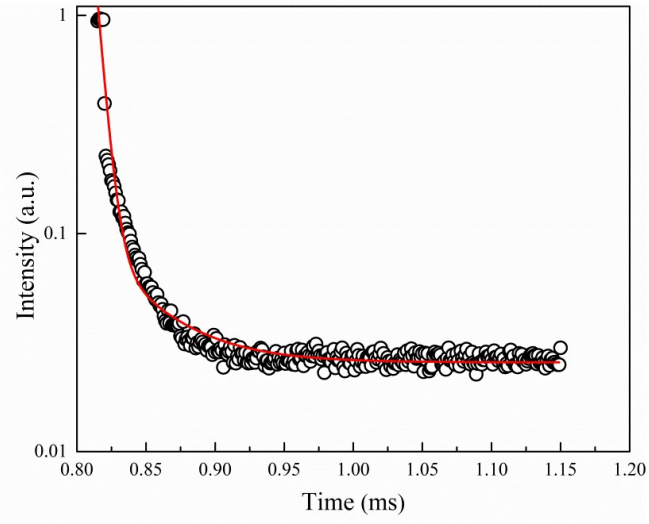

Fig. S21 The fluorescence decay of complex **4** (solid-lines: fitting curves).

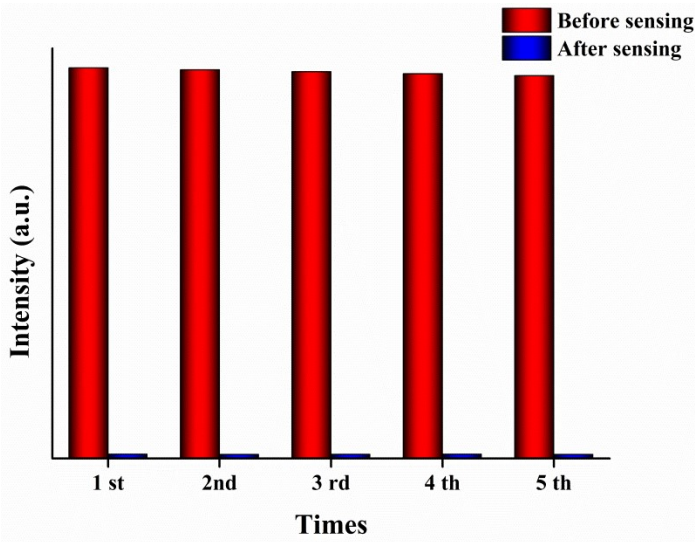

Fig. S22 The luminescence intensity ($^5D_4$–$^7F_5$) of five recyclable experiments of sensing for Fe^{3+} ion in aqueous solution

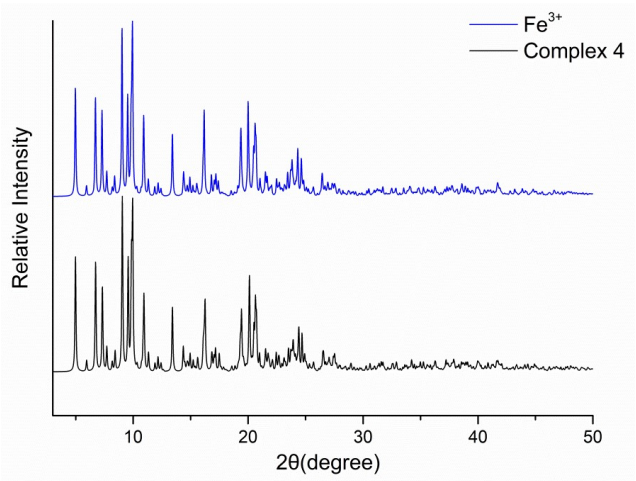

Fig. S23 PXRD patterns of complex **4** after soaking in Fe^{3+} ion.

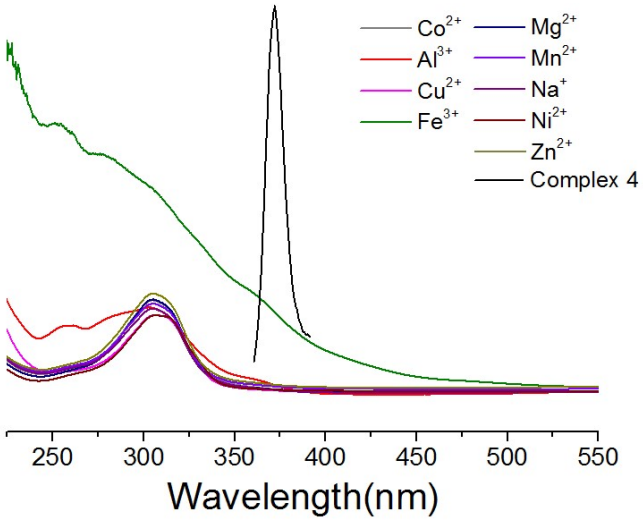

Fig. S24 The UV-vis absorption spectra of metal anions aqueous solution with the same concentration of analytes (0.01 M) and the excitation spectra of complex **4**.

Table S11 Diverse properties for reported nitronyl nitroxide-based multifunctional molecular materials

Complex	Diverse properties			Ref.
$[Tb(acac)_3NIT2Py \cdot 0.5H_2O]$	Luminescence	SMM behavior		38 a
$Ln(hfac)_3(NITPhOCF_3)_2$ (LnIII = Tb, Dy)	Thermodynamics	Slow magnetic relaxation		38 b
$[\{Ln(hfac)_3\}_3\{Cu(hfac)_2\}\{NIT\text{-}Ph(OMe)_2\}_4]_n$ (LnIII = Gd, Tb)	Magnetocaloric effect	Slow magnetic relaxation		38 c
$[Ln(hfac)_3(8\text{-}QNNIT)]_n$ (LnIII = Tb, Dy)	Optical property	SCM behavior	Thermodynamics	38 d
$\{[Cu(hfac)_2][(NIT\text{-}4\text{-}OMe\text{-}4PyPh)]_2[Tb(hfac)_3]\}_n$	luminescent probe	Slow magnetic relaxation		This work