Supporting Materials for

Rhodamine-based field-induced single molecule magnets in Yb(III) and Dy(III) series

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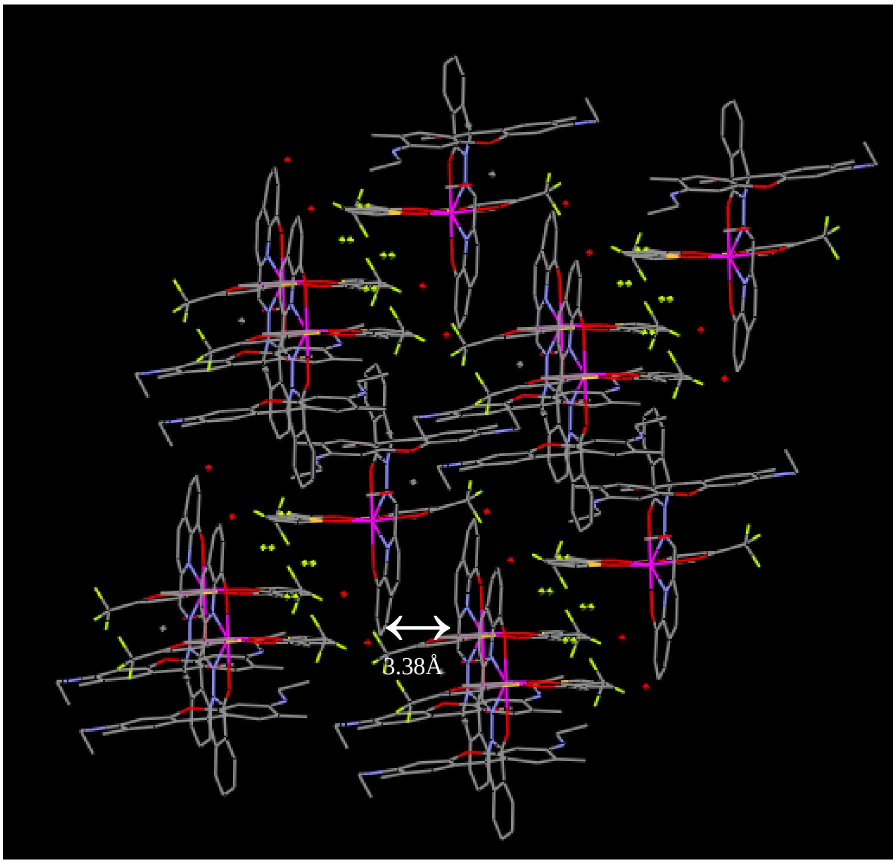
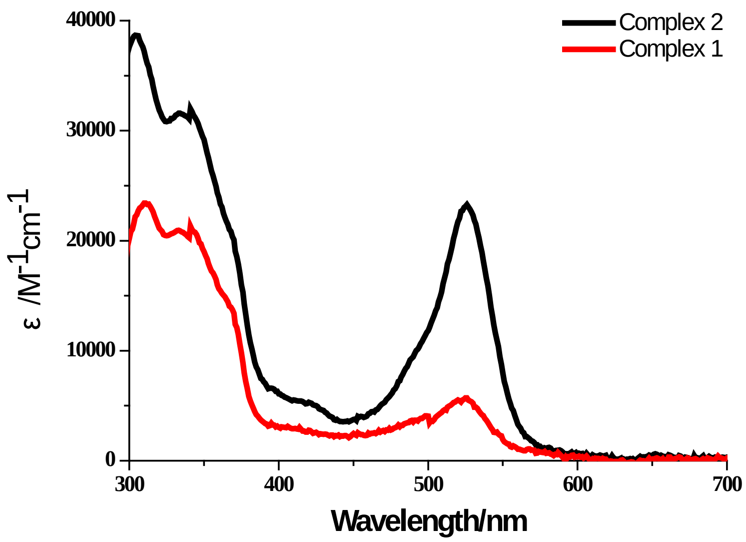


Figure S1. Crystal packing diagram of complex 3 showing the face-to-face π…π stacking interactions. Megenta: Yb, Gray: C, Blue: N, Red: O, Yellow: F.



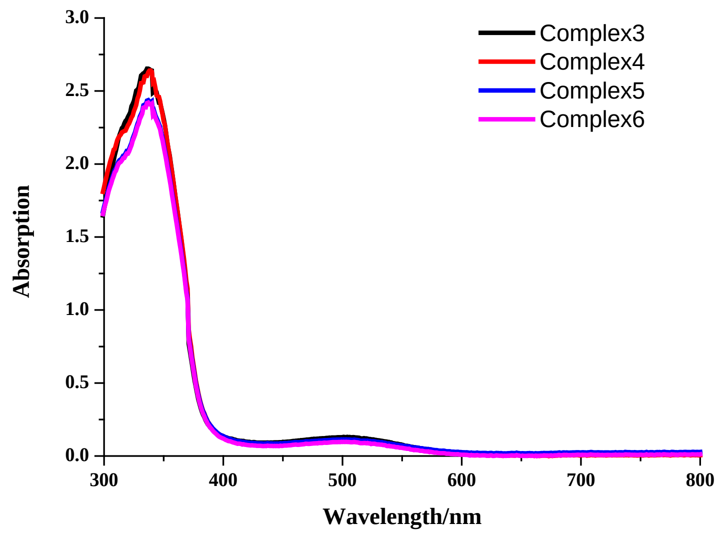


Figure S2. Uv-vis spectra of compounds **1-2** in CH_3CN(RT) and Uv spectra of compounds 3-6 in CH_3CN(RT,$5*10^{-6}$ M)

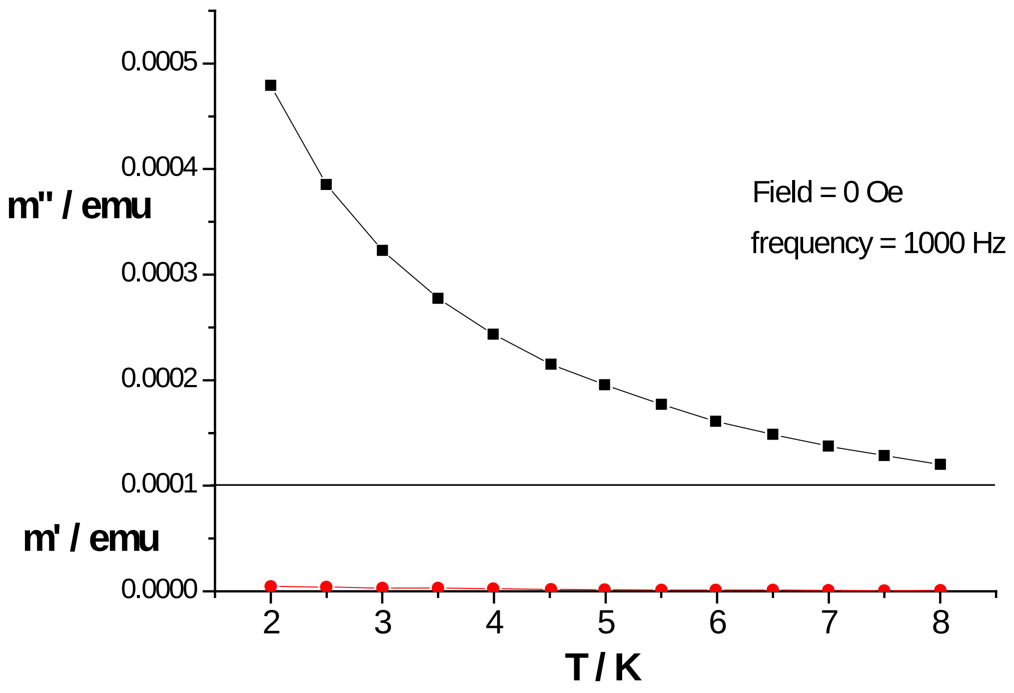


Figure S3. Temperature dependence of m ′ and m″ of **1** under zero static field with a 3.0 G oscillating field at frequency of 1.0 kHz.

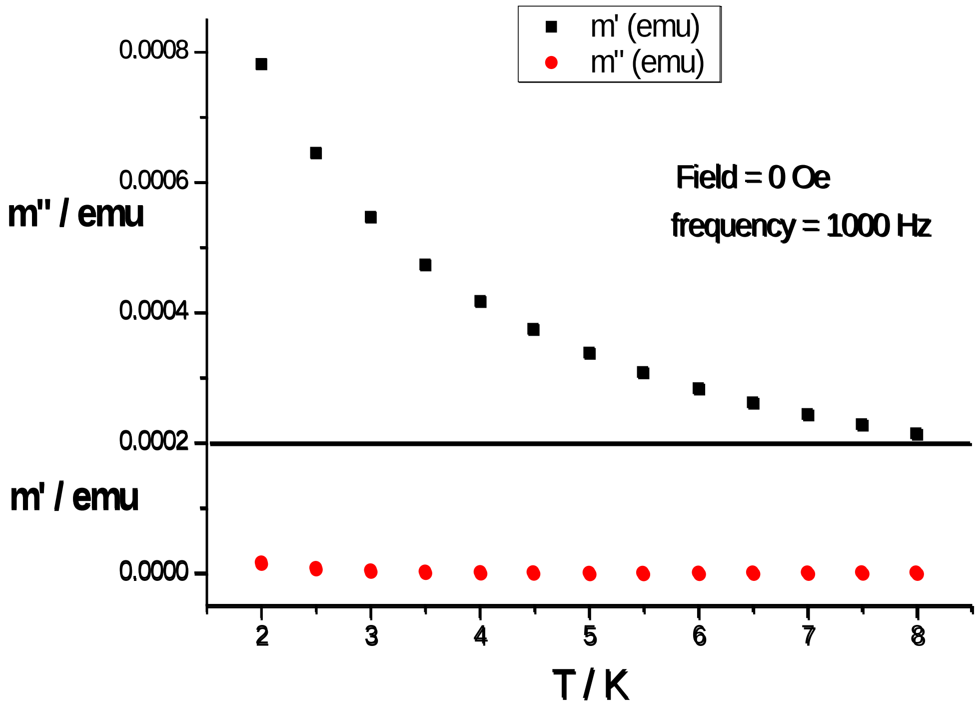


Figure S4. Temperature dependence of m′ and m″ of **3** under zero static field with a 3.0 G oscillating field at frequency of 1.0 kHz.

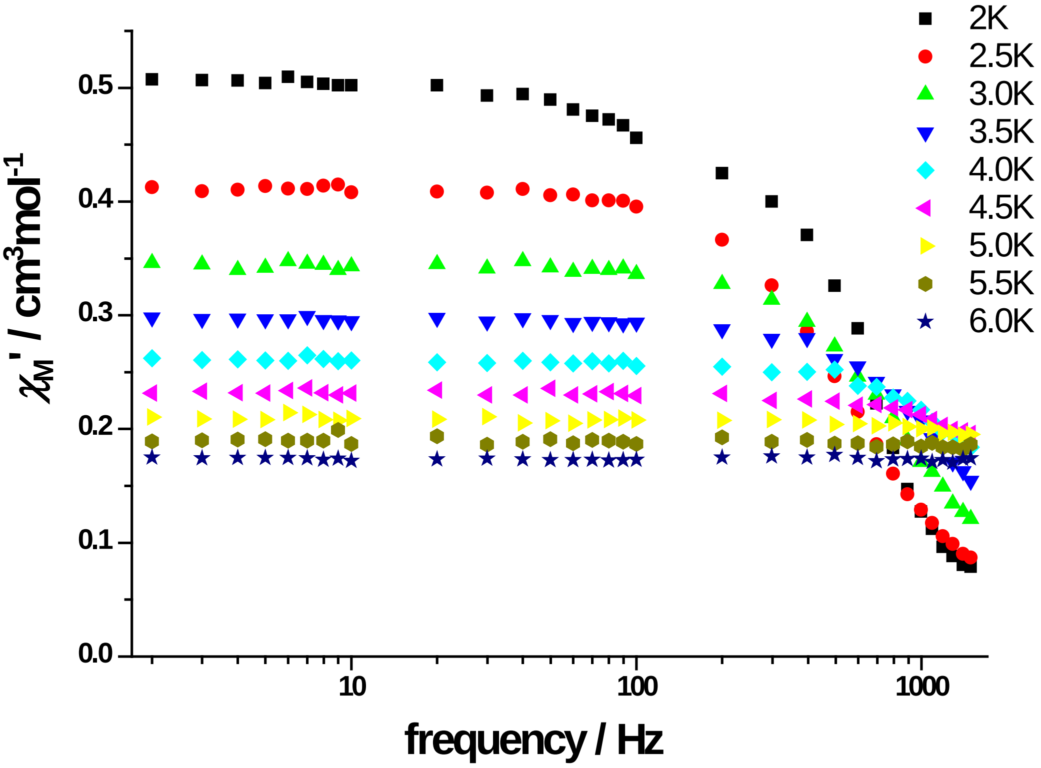


Figure S5. The in-phase ac susceptibility of compound **1** under 1000 Oe static field with a 3.0 G oscillating field at frequencies in the range of 1 Hz to 1.5 kHz.

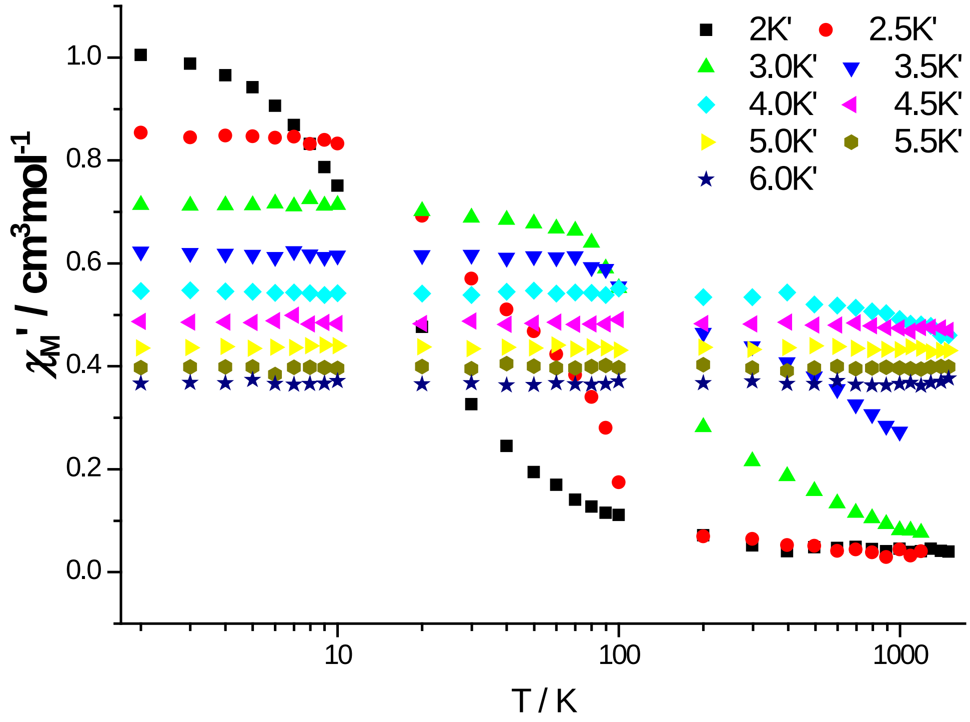


Figure S6. The in-phase ac susceptibility of compound **3** under 1000 Oe static field with a 3.0 G oscillating field at frequencies in the range of 1 Hz to 1.5 kHz.

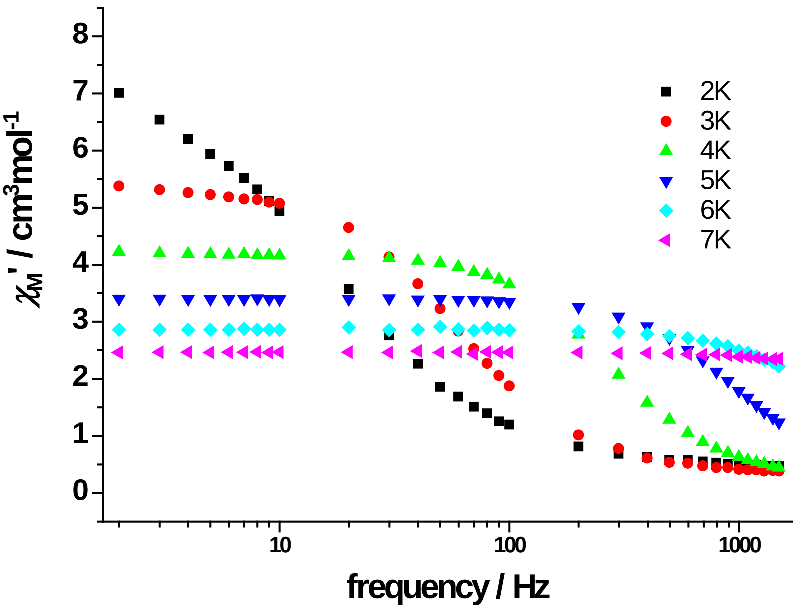
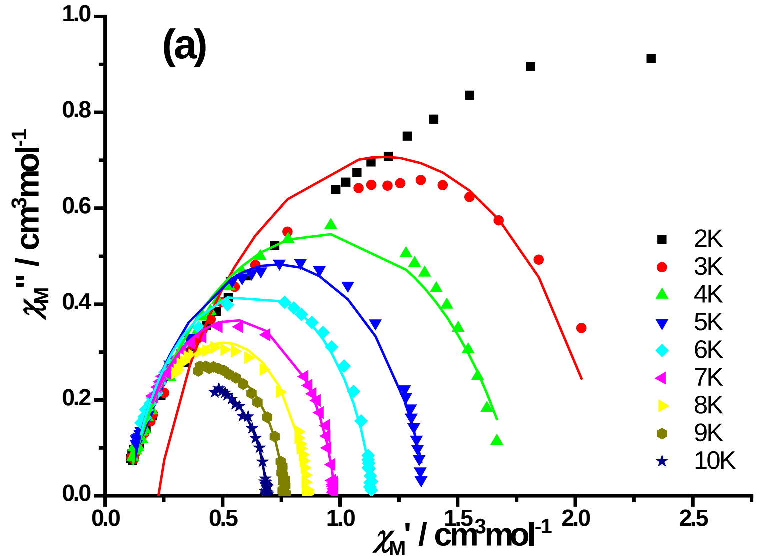


Figure S7. The in-phase ac susceptibility of compound **4** under 1000 Oe static field with a 3.0 G oscillating field at frequencies in the range of 1 Hz to 1.5 kHz.



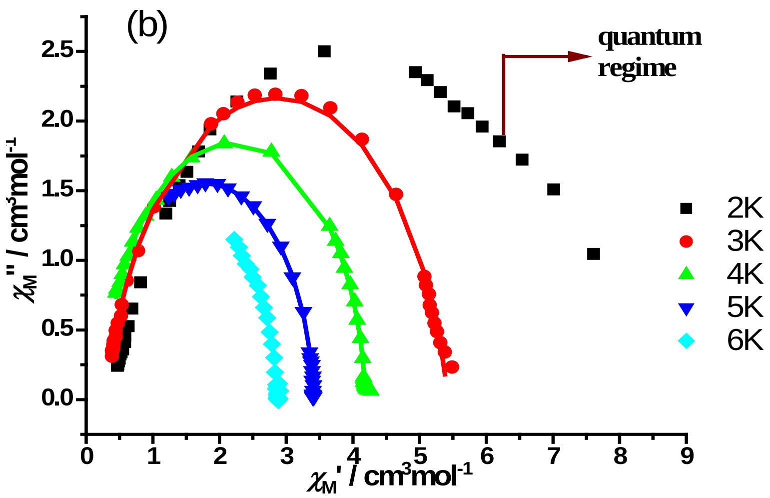


Figure S8. Cole−Cole plots for **2** (a) and **4** (b) obtained using the ac susceptibility data at a 1 kOe dc field.

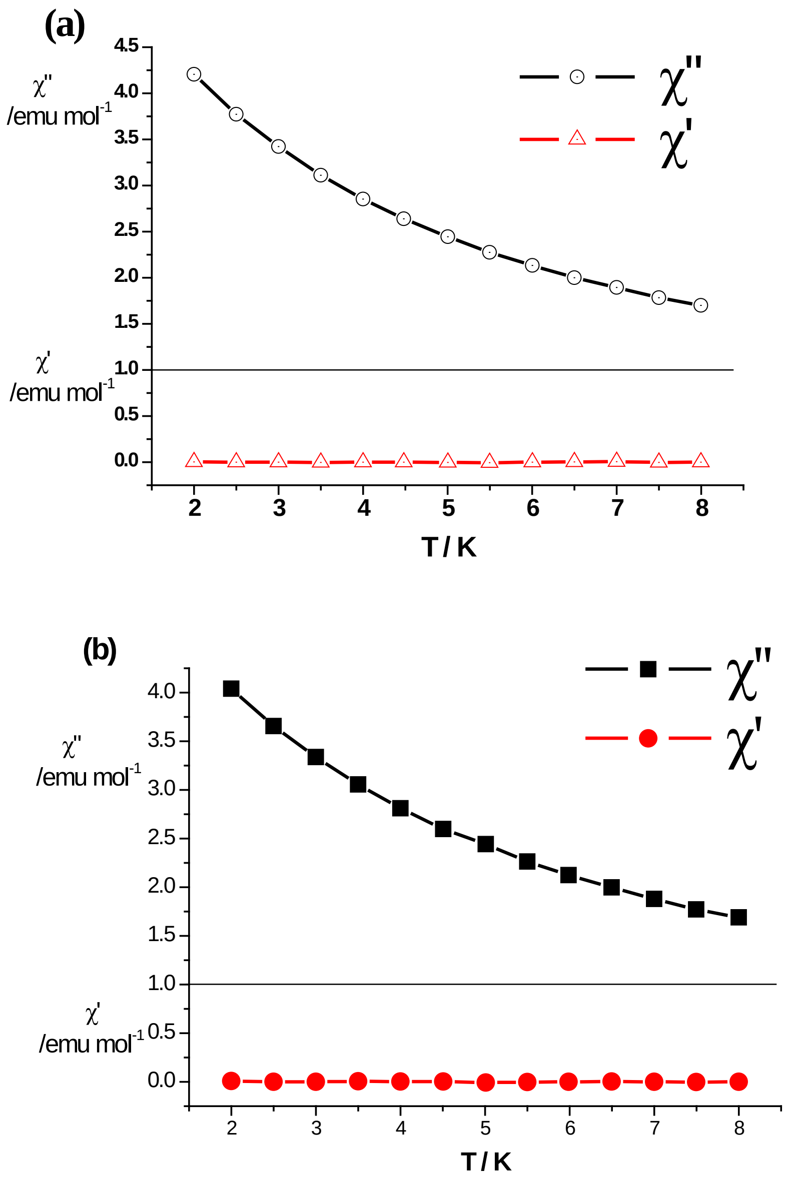


Figure S9. (a) Temperature dependence of ac signals of **5** under zero static field with a 3.0 Oe oscillating field at frequency of 1.0 kHz. (b) Temperature dependence of ac signals of **5** under 1000 Oe static field with a 3.0 Oe oscillating field at frequency of 1.0 kHz.

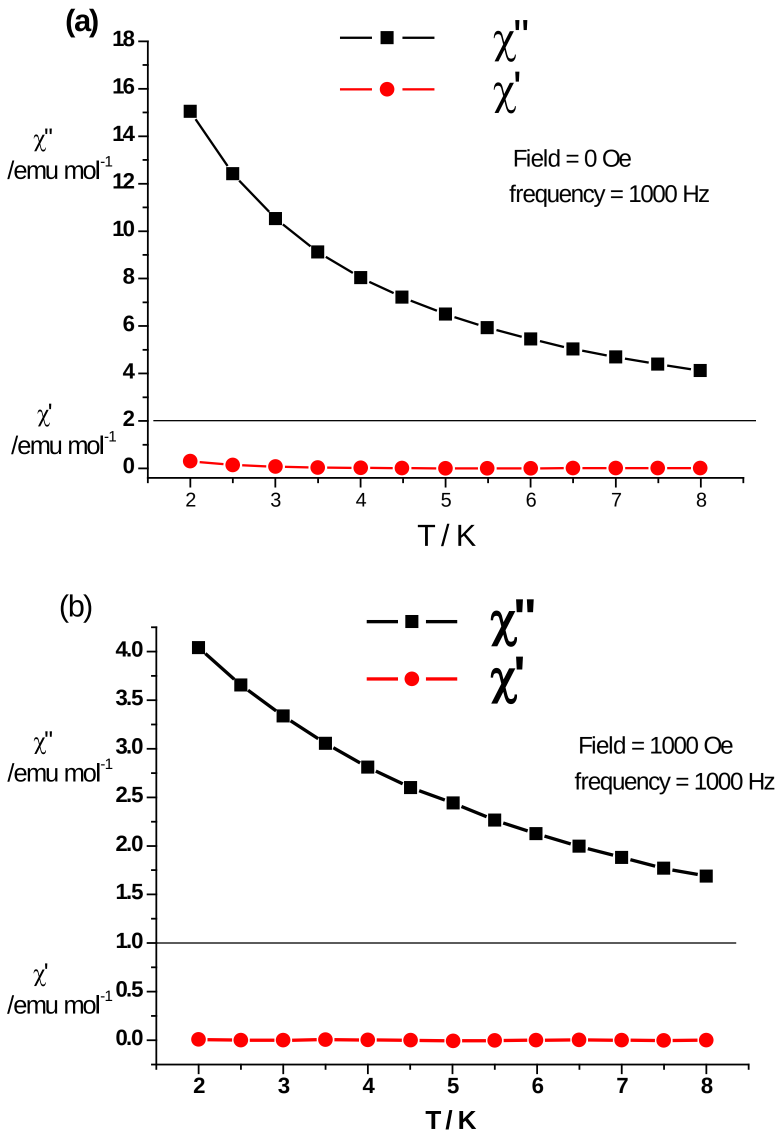


Figure S10. (a)Temperature dependence of ac signals of **6** under zero static field with a 3.0 G oscillating field at frequency of 1.0 kHz. (b) Temperature dependence of ac signals of **6** under 1000 Oe static field with a 3.0 Oe oscillating field at frequency of 1.0 kHz.

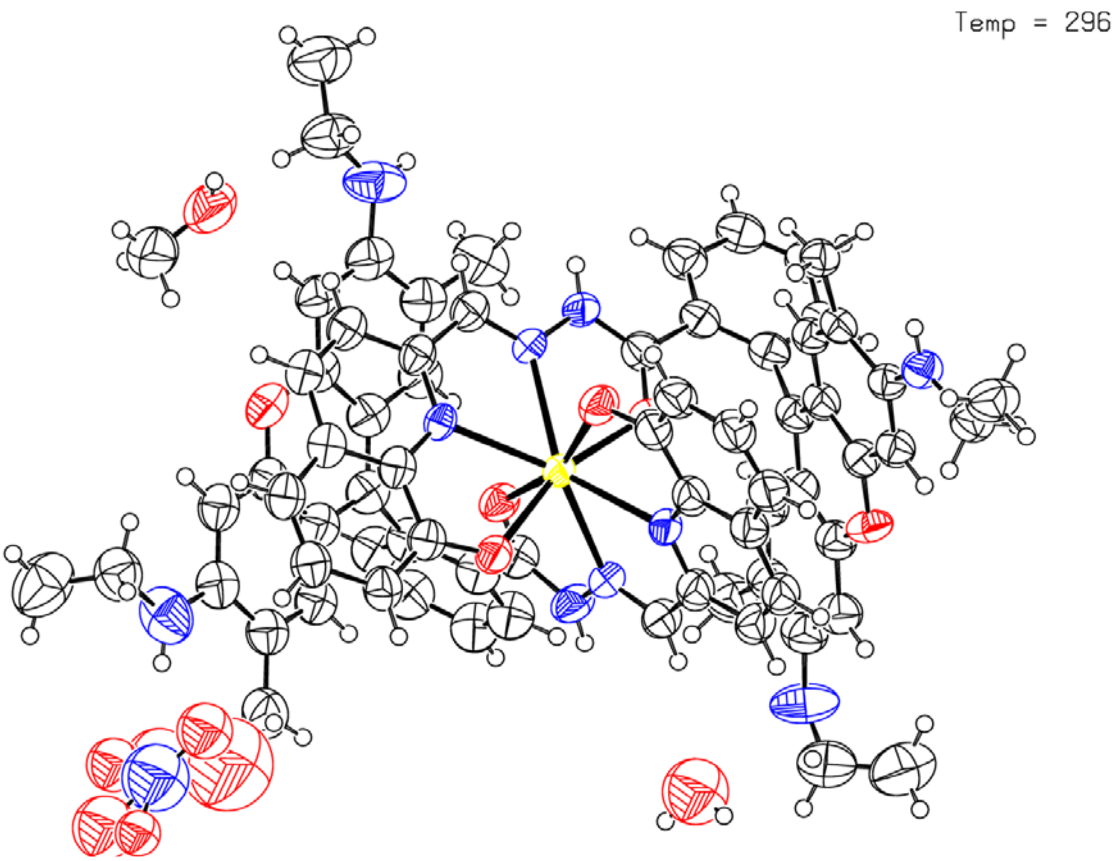


Figure S11. The ORTEP style image of the complex **1**

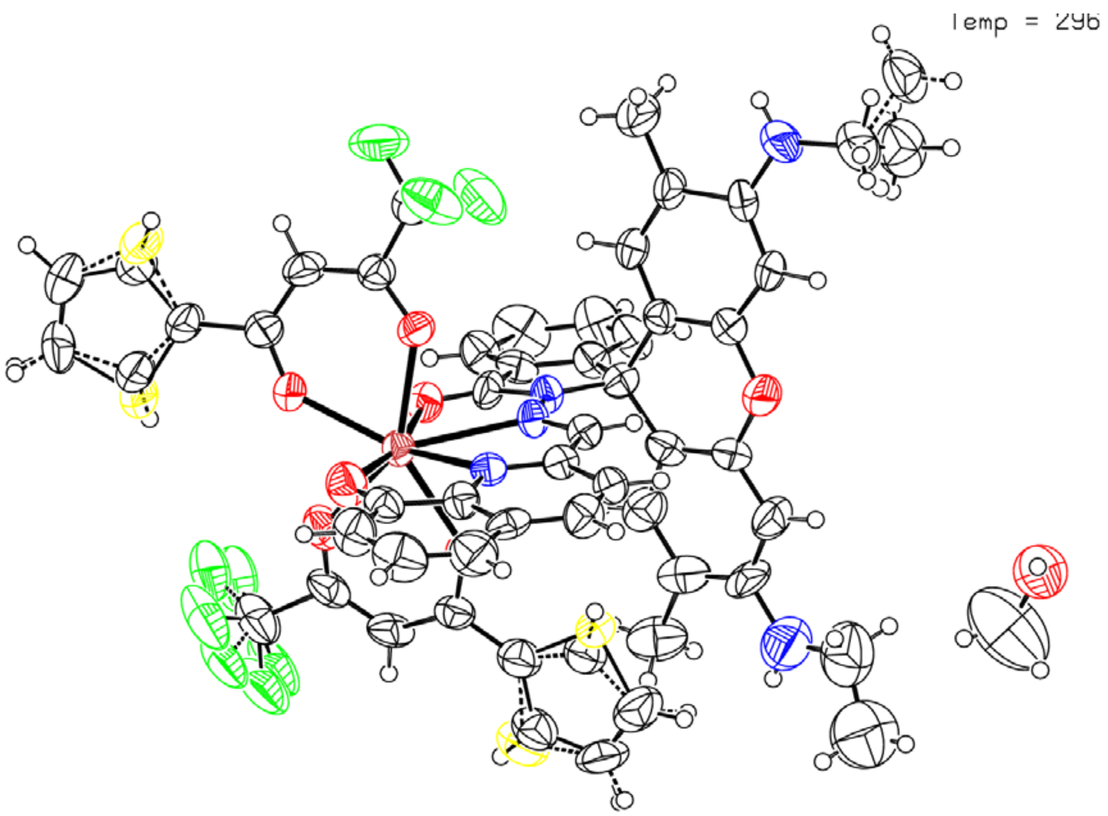


Figure S12. The ORTEP style image of the complex **3**

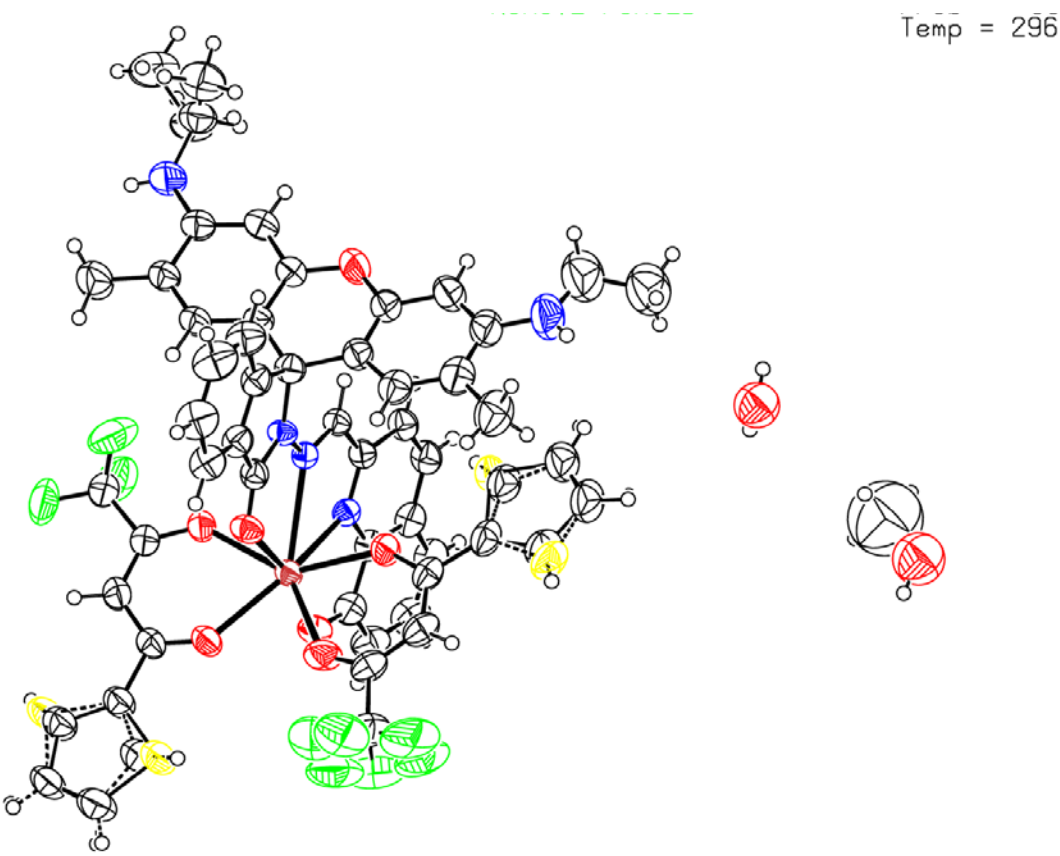


Figure S13. The ORTEP style image of the complex **4**.

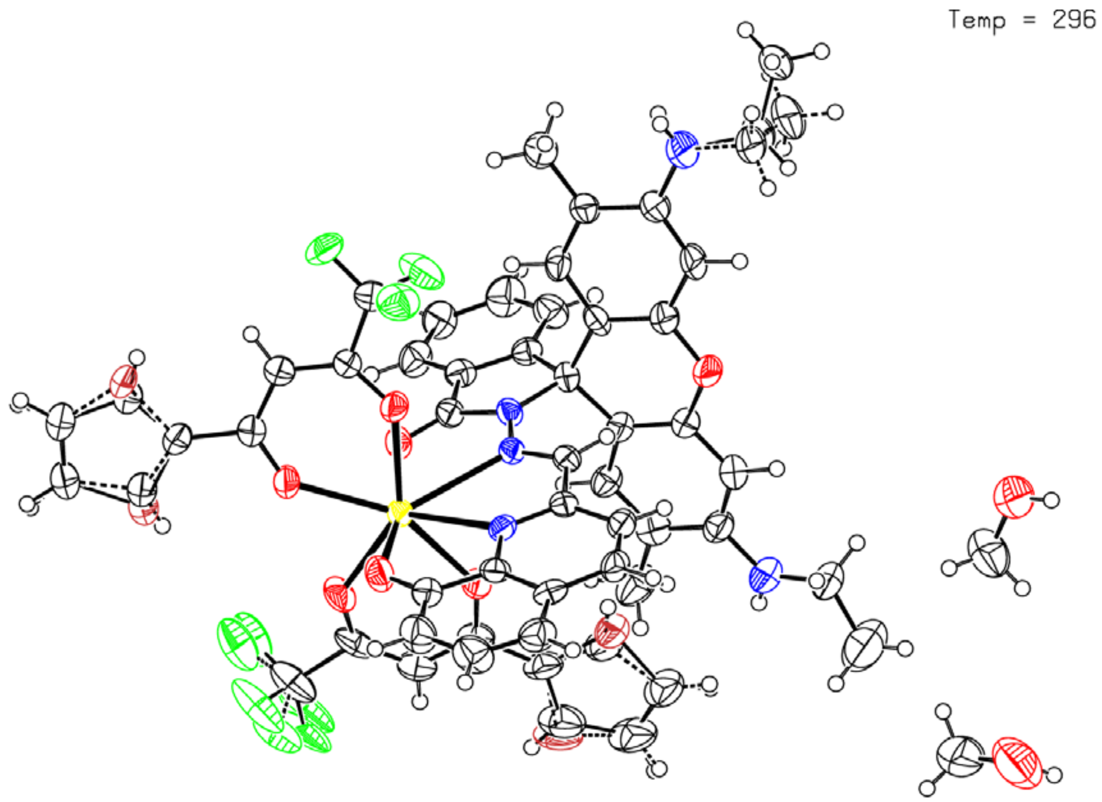


Figure S14. The ORTEP style image of the complex **5**.

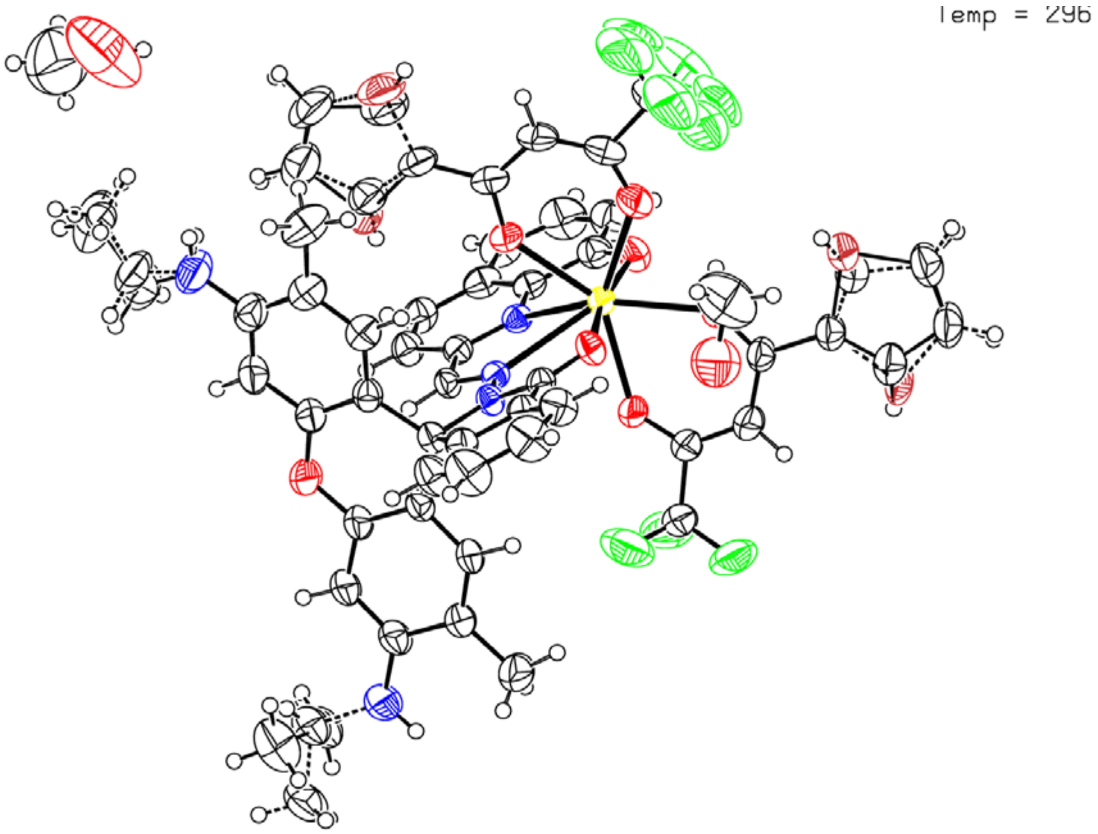


Figure S15. The ORTEP style image of the complex **6**

Table S1. The parameters of χ_T, χ_S, τ, and α used in the analyses by Debye model for complex **1** and **3** under 1000 Oe field.

	1				**3**			
Temp	2.0 K	2.5K	3.0K	3.5K	2.0 K	2.5K	3.0K	3.5K
χ_T	2.23	2.20	2.17	2.14	2.67	2.39	2.33	2.29
χ_S	1.76	1.81	1.84	1.87	3.68	3.68	1.63	1.68
τ(s)	5×10^{-4}	2.8×10^{-4}	1.7×10^{-4}	1.1×10^{-4}	9.3×10^{-3}	1.86×10^{-3}	4.3×10^{-4}	1.3×10^{-4}
α	0.035	0.048	0.031	0.021	0.090	0.062	0.020	0.08

Table S2. The parameters of χ_T, χ_S, τ, and α used in the analyses by Debye model for complex **2**, **4** under 1000 Oe field.

	4				**2**							
Temp (K)	2.0	3.0	4.0	5.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0
χ_T	21.4	20.15	19.55	19.22	2.34	1.71	1.52	1.42	1.33	1.26	1.50	1.43
χ_S	13.6	14.96	15.60	15.88	0.027	0.05	0.24	0.35	0.44	0.50	0.86	0.94
τ(s)	0.011	2.7×10^{-3}	5.7×10^{-4}	1.6×10^{-4}	0.021	7×10^{-3}	2.4×10^{-3}	1×10^{-3}	4.8×10^{-4}	2.4×10^{-4}	1.4×10^{-4}	1.0×10^{-4}
α	0.28[a]	0.12	0.04	0.03	0.35	0.27	0.18	0.15	0.136	0.124	0.109	0.068

a: the data at 2 K is not reliable because the system enters the quantum regime.

Table S3. Comparison of Bond Distance(Å) and Bond Angles(°) for Complexes 1-6.

	Complex **1**		
Yb(1)-O(1)	2.235(6)	Yb(1)-N(10)	2.392(7)
Yb(1)-O(4)	2.264(6)	Yb(1)-N(5)	2.402(6)
Yb(1)-O(5)	2.307(6)	Yb(1)-N(9)	2.442(8)
Yb(1)-O(2)	2.338(6)	Yb(1)-N(4)	2.460(7)
O(1)-Yb(1)-O(4)	96.9(2)	N(10)-Yb(1)-N(5)	140.1(2)
O(1)-Yb(1)-O(5)	91.1(2)	O(1)-Yb(1)-N(9)	83.1(2)
O(4)-Yb(1)-O(5)	161.6(2)	O(4)-Yb(1)-N(9)	133.1(2)
O(1)-Yb(1)-O(2)	162.3(2)	O(5)-Yb(1)-N(9)	64.2(2)
O(4)-Yb(1)-O(2)	91.7(2)	O(2)-Yb(1)-N(9)	79.8(2)
O(5)-Yb(1)-O(2)	85.3(2)	N(10)-Yb(1)-N(9)	64.4(3)
O(1)-Yb(1)-N(10)	85.6(2)	N(5)-Yb(1)-N(9)	137.2(2)
O(4)-Yb(1)-N(10)	68.8(3)	O(1)-Yb(1)-N(4)	132.6(2)
O(5)-Yb(1)-N(10)	128.6(2)	O(4)-Yb(1)-N(4)	81.3(2)
O(2)-Yb(1)-N(10)	83.2(2)	O(5)-Yb(1)-N(4)	81.1(2)
O(1)-Yb(1)-N(5)	69.2(2)	O(2)-Yb(1)-N(4)	63.9(2)
O(4)-Yb(1)-N(5)	83.6(2)	N(10)-Yb(1)-N(4)	134.7(2)
O(5)-Yb(1)-N(5)	83.8(2)	N(5)-Yb(1)-N(4)	63.5(2)
O(2)-Yb(1)-N(5)	127.3(2)	N(9)-Yb(1)-N(4)	131.5(2)
	Complex **3**		
Yb(1)-O(3)	2.234(11)	Yb(1)-O(6)	2.301(10)
Yb(1)-O(7)	2.250(9)	Yb(1)-O(2)	2.404(9)
Yb(1)-O(4)	2.271(8)	Yb(1)-N(5)	2.427(10)
Yb(1)-O(5)	2.273(9)	Yb(1)-N(4)	2.562(10)
O(3)-Yb(1)-O(7)	101.6(4)	O(6)-Yb(1)-O(2)	84.9(4)
O(3)-Yb(1)-O(4)	95.8(4)	O(3)-Yb(1)-N(5)	67.7(4)
O(7)-Yb(1)-O(4)	139.7(3)	O(7)-Yb(1)-N(5)	72.0(3)
O(3)-Yb(1)-O(5)	85.1(4)	O(4)-Yb(1)-N(5)	81.9(3)
O(7)-Yb(1)-O(5)	142.0(3)	O(5)-Yb(1)-N(5)	142.1(4)
O(4)-Yb(1)-O(5)	75.0(3)	O(6)-Yb(1)-N(5)	130.1(4)
O(3)-Yb(1)-O(6)	87.4(4)	O(2)-Yb(1)-N(5)	125.9(3)
O(7)-Yb(1)-O(6)	71.9(4)	O(3)-Yb(1)-N(4)	129.5(3)
O(4)-Yb(1)-O(6)	145.5(4)	O(7)-Yb(1)-N(4)	66.7(3)
O(5)-Yb(1)-O(6)	71.1(4)	O(4)-Yb(1)-N(4)	74.2(3)
O(3)-Yb(1)-O(2)	166.0(3)	O(5)-Yb(1)-N(4)	135.3(3)
O(7)-Yb(1)-O(2)	87.0(3)	O(6)-Yb(1)-N(4)	128.4(4)
O(4)-Yb(1)-O(2)	84.1(3)	O(2)-Yb(1)-N(4)	64.0(3)
O(5)-Yb(1)-O(2)	81.4(3)	N(5)-Yb(1)-N(4)	62.0(3)

Complex **4**

Dy(1)-O(5)	2.273(4)	Dy(1)-O(3)	2.349(4)
Dy(1)-O(1)	2.313(4)	Dy(1)-O(6)	2.464(4)
Dy(1)-O(4)	2.314(4)	Dy(1)-N(5)	2.484(4)
Dy(1)-O(2)	2.345(4)	Dy(1)-N(4)	2.600(4)
O(5)-Dy(1)-O(1)	85.92(16)	O(3)-Dy(1)-O(6)	85.97(16)
O(5)-Dy(1)-O(4)	101.04(16)	O(5)-Dy(1)-N(5)	66.87(14)
O(1)-Dy(1)-O(4)	142.31(15)	O(1)-Dy(1)-N(5)	141.85(15)
O(5)-Dy(1)-O(2)	96.09(16)	O(4)-Dy(1)-N(5)	72.00(14)
O(1)-Dy(1)-O(2)	72.62(14)	O(2)-Dy(1)-N(5)	83.81(14)
O(4)-Dy(1)-O(2)	141.53(14)	O(3)-Dy(1)-N(5)	129.03(16)
O(5)-Dy(1)-O(3)	88.00(17)	O(6)-Dy(1)-N(5)	124.13(13)
O(1)-Dy(1)-O(3)	72.87(16)	O(5)-Dy(1)-N(4)	127.89(14)
O(4)-Dy(1)-O(3)	70.44(15)	O(1)-Dy(1)-N(4)	135.27(14)
O(2)-Dy(1)-O(3)	144.84(15)	O(4)-Dy(1)-N(4)	67.14(14)
O(5)-Dy(1)-O(6)	168.71(13)	O(2)-Dy(1)-N(4)	75.12(13)
O(1)-Dy(1)-O(6)	83.19(15)	O(3)-Dy(1)-N(4)	128.18(15)
O(4)-Dy(1)-O(6)	85.92(15)	O(6)-Dy(1)-N(4)	62.97(12)
O(2)-Dy(1)-O(6)	83.49(15)	N(5)-Dy(1)-N(4)	61.18(13)

Complex **5**

Tb(1)-O(1)	2.274(8)	Tb(1)-O(4)	2.349(7)
Tb(1)-O(5)	2.331(7)	Tb(1)-O(2A)	2.480(7)
Tb(1)-O(6)	2.337(7)	Tb(1)-N(1)	2.502(8)
Tb(1)-O(7)	2.343(7)	Tb(1)-N(2)	2.611(8)
O(1)-Tb(1)-O(5)	86.9(3)	O(4)-Tb(1)-O(2A)	82.5(3)
O(1)-Tb(1)-O(6)	88.7(3)	O(1)-Tb(1)-N(1)	66.6(3)
O(5)-Tb(1)-O(6)	72.6(3)	O(5)-Tb(1)-N(1)	142.7(3)
O(1)-Tb(1)-O(7)	100.9(3)	O(6)-Tb(1)-N(1)	129.2(3)
O(5)-Tb(1)-O(7)	142.4(3)	O(7)-Tb(1)-N(1)	71.4(3)
O(6)-Tb(1)-O(7)	70.8(3)	O(4)-Tb(1)-N(1)	83.4(3)
O(1)-Tb(1)-O(4)	95.5(3)	O(2A)-Tb(1)-N(1)	123.6(3)
O(5)-Tb(1)-O(4)	73.1(3)	O(1)-Tb(1)-N(2)	127.3(3)
O(6)-Tb(1)-O(4)	145.1(3)	O(5)-Tb(1)-N(2)	134.4(3)
O(7)-Tb(1)-O(4)	141.0(3)	O(6)-Tb(1)-N(2)	128.7(3)
O(1)-Tb(1)-O(2A)	169.0(3)	O(7)-Tb(1)-N(2)	67.7(3)
O(5)-Tb(1)-O(2A)	82.2(3)	O(4)-Tb(1)-N(2)	74.2(3)
O(6)-Tb(1)-O(2A)	86.8(3)	O(2A)-Tb(1)-N(2)	62.6(2)
O(7)-Tb(1)-O(2A)	87.2(3)	N(1)-Tb(1)-N(2)	61.0(3)

Complex **6**

Ho(1)-O(6)	2.25(3)	Ho(1)-O(1)	2.33(2)

Ho(1)-O(2)	2.29(2)	Ho(1)-O(7)	2.45(2)
Ho(1)-O(4)	2.31(2)	Ho(1)-N(5)	2.48(3)
Ho(1)-O(3)	2.32(3)	Ho(1)-N(4)	2.59(3)
O(6)-Ho(1)-O(2)	86.0(10)	O(1)-Ho(1)-O(7)	83.1(9)
O(6)-Ho(1)-O(4)	101.3(10)	O(6)-Ho(1)-N(5)	67.1(9)
O(2)-Ho(1)-O(4)	142.1(9)	O(2)-Ho(1)-N(5)	142.1(9)
O(6)-Ho(1)-O(3)	88.4(10)	O(4)-Ho(1)-N(5)	72.1(9)
O(2)-Ho(1)-O(3)	72.6(10)	O(3)-Ho(1)-N(5)	129.5(9)
O(4)-Ho(1)-O(3)	70.6(9)	O(1)-Ho(1)-N(5)	83.2(8)
O(6)-Ho(1)-O(1)	96.0(9)	O(7)-Ho(1)-N(5)	124.4(8)
O(2)-Ho(1)-O(1)	73.3(9)	O(6)-Ho(1)-N(4)	128.2(9)
O(4)-Ho(1)-O(1)	141.0(8)	O(2)-Ho(1)-N(4)	134.8(9)
O(3)-Ho(1)-O(1)	145.2(9)	O(4)-Ho(1)-N(4)	67.3(8)
O(6)-Ho(1)-O(7)	168.1(8)	O(3)-Ho(1)-N(4)	128.1(9)
O(2)-Ho(1)-O(7)	82.4(9)	O(1)-Ho(1)-N(4)	74.4(8)
O(4)-Ho(1)-O(7)	86.5(9)	O(7)-Ho(1)-N(4)	63.0(8)
O(3)-Ho(1)-O(7)	85.7(9)	N(5)-Ho(1)-N(4)	61.4(8)