Supporting Information

Three New heterometallic Zn^{II}–Ln^{III} complexes with Windmill-like Framework and Field-Induced SMMs behavior

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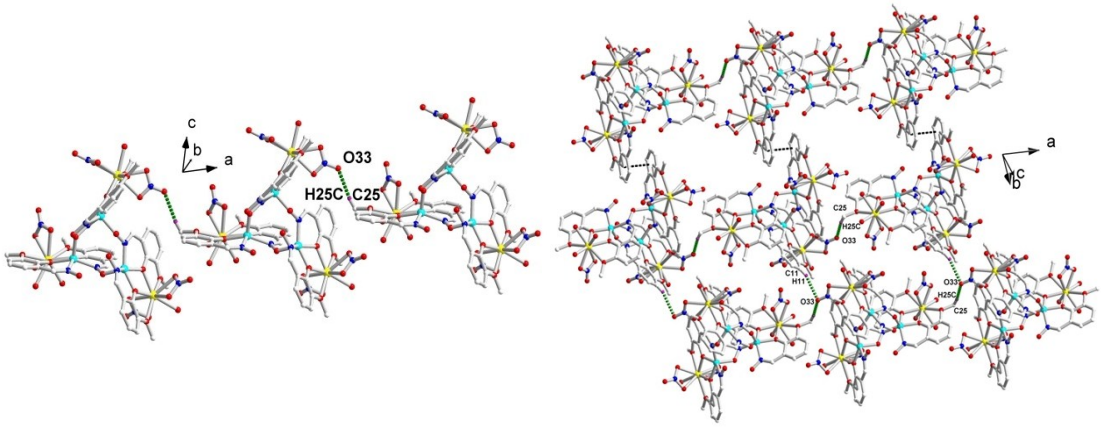

Fig. S1 Weak C–H···O interactions of **1** along the a axis (left) and the two-dimensional supramolecular network of complex **1** (right).

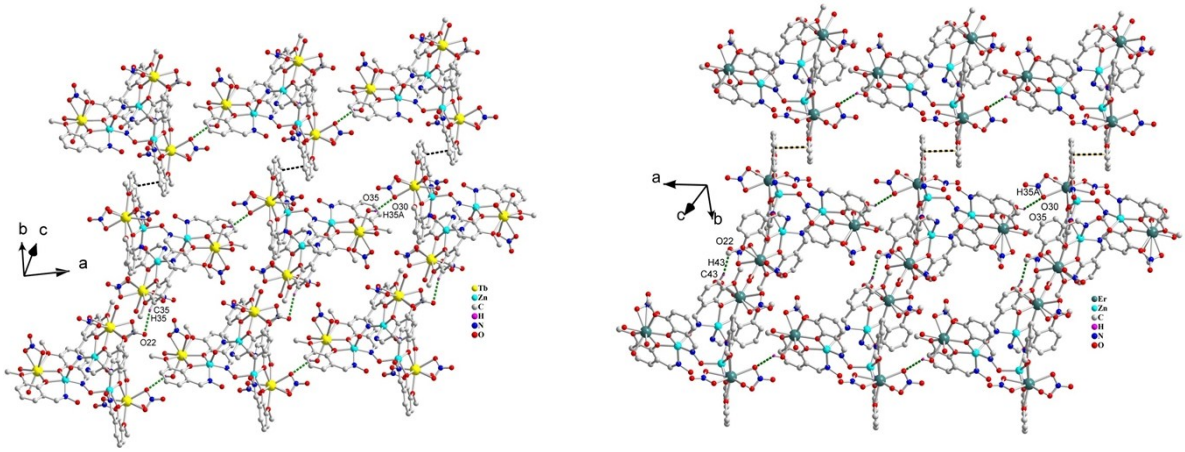

Fig. S2 The two-dimensional supramolecular network of complex **2** (left) and **3** (right).

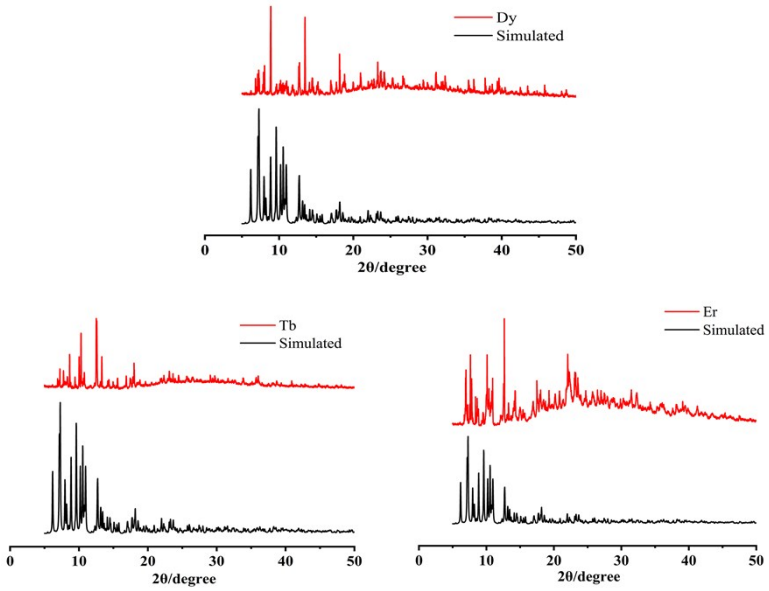

Fig. S3 Powder XRD patterns of complexes **1-3**.

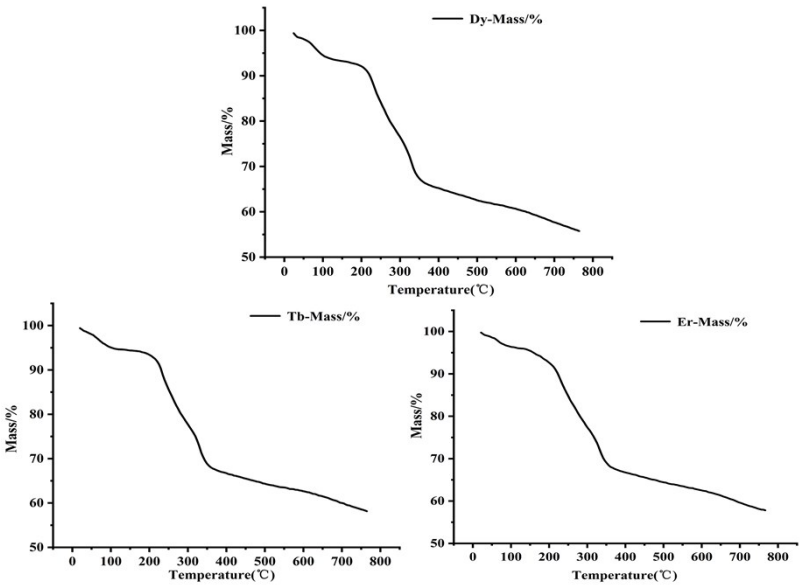

Figure S4. Thermogravimetric analysis of complexes **1-3**.

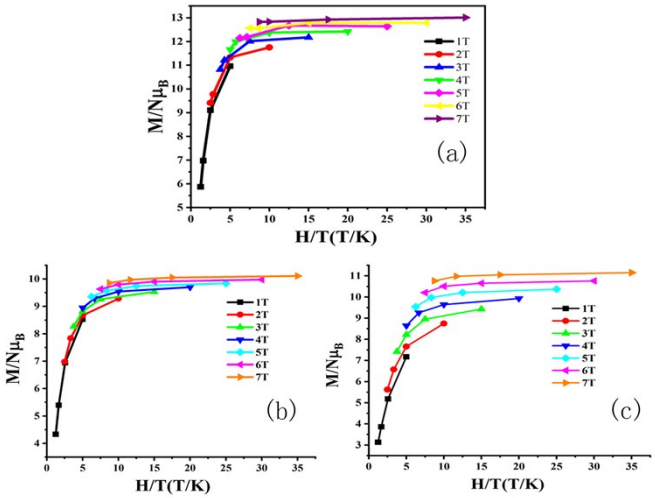

Fig. S5 Field dependence of magnetizations of **1** (a), **2** (b), **3** (c). Solid lines are guides for the eyes.

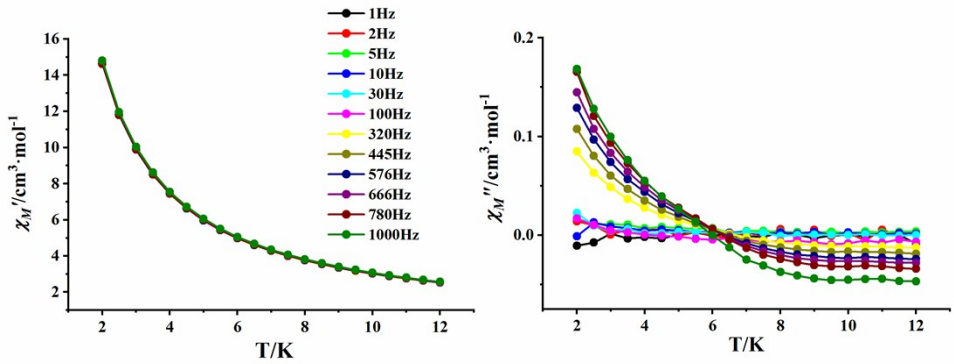

Fig. S6 The temperature-dependent of in-phase χ'_M (left) and out-of-phase χ''_M (right) components of the ac susceptibility for complex **1** measured under 0 Oe applied dc field. The solid lines are guides for the eyes.

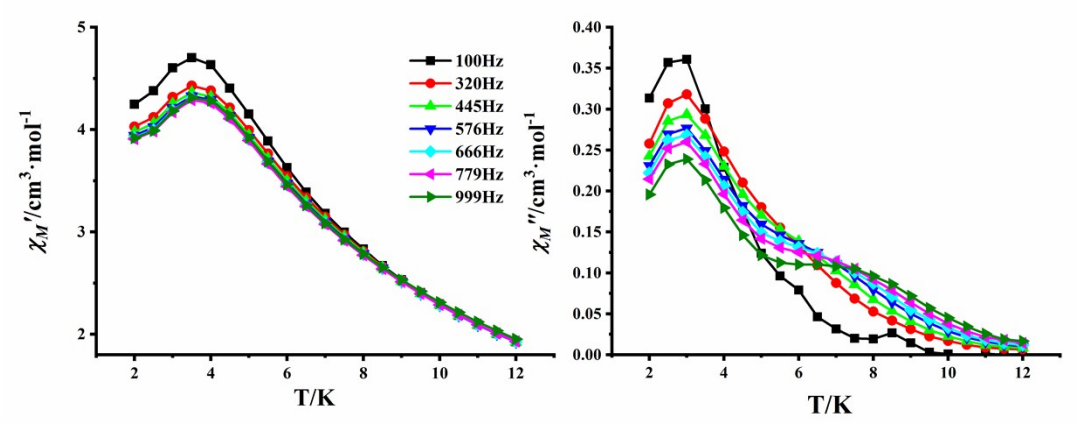

Fig. S7 The temperature-dependent of in-phase χ'_M (left) and out-of-phase χ''_M (right) components of the ac susceptibility for complex **2** measured under 2000 Oe applied dc field. The solid lines are guides for the eyes.

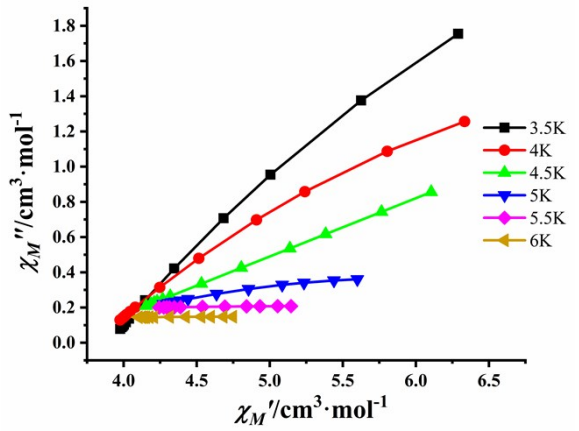

Fig. S8 The Cole–Cole plots fitting of complex **2** between 3.5 K and 6.0 K

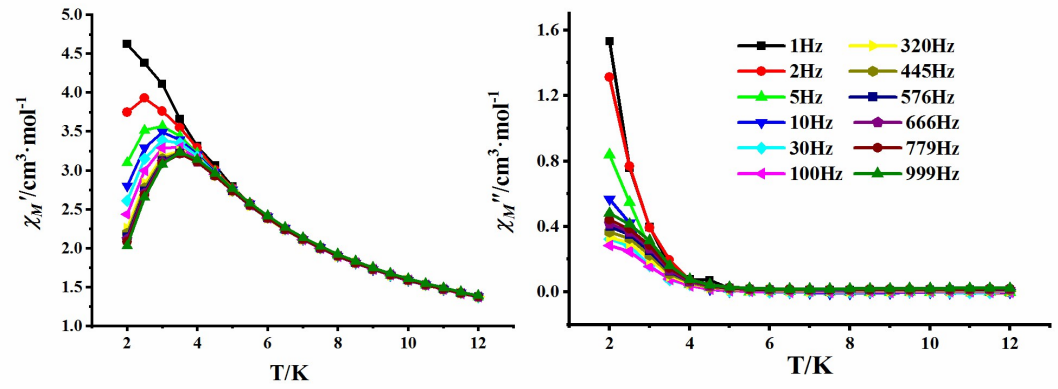

Fig. S9 The temperature-dependent of in-phase χ'_M (left) and out-of-phase χ''_M (right) components of the ac susceptibility for complex **3** measured under 2000 Oe applied dc field. The solid lines are guides for the eyes.

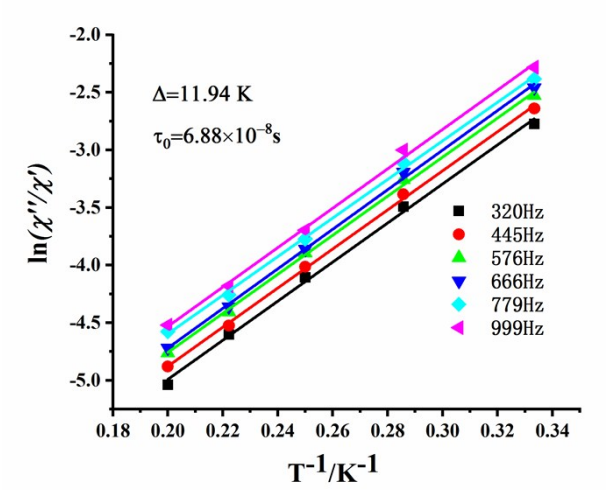

Fig. S10 Magnetization relaxation time ln(χ''/χ') vs T^{-1} plots for **3**. The solid line is fitted with the Debye model.

Table S1. Crystal data and structure refinement for complexes **1−3.**

Complex	**1**	**2**	**3**
Empirical formula	$C_{48}H_{55}N_{12}O_{41}Dy_3Zn_3$	$C_{48}H_{55}N_{12}O_{41}Tb_3Zn_3$	$C_{48}H_{55}N_{12}O_{41}Er_3Zn_3$
Formula weight	2139.65	2128.91	2153.93
Temperature(K)	298(2)	298(2)	298(2)
Crystal system	Triclinic	Triclinic	Triclinic
Space group	*P*-1	*P*-1	*P*-1
a(Å)	15.0890(14)	15.0276(13)	14.9778(12)
b(Å)	16.3063(15)	16.2205(14)	16.2400(14)
c(Å)	19.7970(18)	19.6624(17)	19.6798(17)
α(°)	87.765(3)	87.720(2)	87.674(2)
β(°)	72.711(2)	72.5750(10)	72.8900(10)
γ(°)	85.128(3)	85.635(2)	85.783(2)
V(Å3)	4633.6(7)	4558.9(7)	4561.8(7)
Z	2	2	2
μ (mm^{-1})	3.234	3.156	3.588
R_{int}	0.0940	0.0251	0.0317
Data /parameters	16004/973	15862/973	1587/973
GOOF (F^2)	0.724	0.690	0.641
R_1[I >2σ(I)]	0.0688	0.0357	0.0347
wR_2 (all data)	0.2090	0.1115	0.1050

Table.S2 Selected bond distances and angles for **1**

Zn(1)-O(18) 1.969(15)	Zn(1)-O(8) 2.043(14)	Zn(1)-O(11)2.043(15)	Zn(1)-N(2) 2.09(2)	Zn(1)-N(1) 2.11(2)	O(18)-Zn(1)-O(8) 108.8(6)
Zn(1)-Dy(2) 3.525(3)	Zn(2)-O(12)1.998(16)	Zn(2)-O(2) 2.041(14)	Zn(2)-O(5) 2.069(18)	Zn(2)-N(4) 2.09(2)	O(18)-Zn(1)-O(11) 114.9(6)
Zn(2)-N(3) 2.10(2)	Zn(2)-Dy(1) 3.510(3)	Zn(3)-O(6) 1.964(17)	Zn(3)-O(14)2.055(15)	Zn(3)-O(17) 2.083(15)	O(8)-Zn(1)-O(11) 75.0(6)
Zn(3)-N(6) 2.09(2)	Zn(3)-N(5) 2.09(2)	Zn(3)-Dy(3) 3.522(3)	Dy(1)-O(5) 2.253(16)	Dy(1)-O(2) 2.278(16)	O(18)-Zn(1)-N(2) 92.8(7)
Dy(1)-O(37) 2.417(17)	Dy(1)-O(4) 2.436(18)	Dy(1)-O(20) 2.457(19)	Dy(1)-O(22) 2.459(19)	Dy(1)-O(1) 2.470(15)	O(8)-Zn(1)-N(2) 86.4(7)
Dy(1)-O(19) 2.494(17)	Dy(1)-O(24) 2.498(19)	Dy(3)-O(32) 2.52(2)	Dy(3)-O(16) 2.513(18)	Dy(2)-O(11) 2.263(14)	O(11)-Zn(1)-N(2) 150.3(7)
Dy(2)-O(8) 2.289(15)	Dy(2)-O(35) 2.385(17)	Dy(2)-O(34) 2.389(17)	Dy(2)-O(36) 2.424(17)	Dy(2)-O(25) 2.424(18)	O(18)-Zn(1)-N(1) 103.1(7)
Dy(2)-O(26) 2.505(18)	Dy(2)-O(10) 2.510(18)	Dy(2)-O(7) 2.523(17)	Dy(3)-O(31) 2.462(19)	Dy(3)-O(14) 2.295(16)	O(8)-Zn(1)-N(1) 147.7(7)
Dy(3)-O(17) 2.309(14)	Dy(3)-O(38) 2.326(17)	Dy(3)-O(28) 2.35(2)	Dy(3)-O(29) 2.409(19)	Dy(3)-O(13) 2.435(19)	O(11)-Zn(1)-N(1) 87.1(7)
O(8)-Zn(1)-Dy(2) 37.9(4)	O(11)-Zn(1)-Dy(2) 37.2(4)	N(2)-Zn(1)-Dy(2) 121.6(6)	N(1)-Zn(1)-Dy(2) 120.5(6)	O(12)-Zn(2)-O(5) 117.6(6)	
O(12)-Zn(2)-N(4) 102.8(7)	O(12)-Zn(2)-O(2) 106.4(6)	O(2)-Zn(2)-N(4) 150.4(7)	O(5)-Zn(2)-N(4) 87.7(7)	O(12)-Zn(2)-N(3) 92.2(7)	
O(2)-Zn(2)-N(3) 86.7(7)	O(5)-Zn(2)-N(3) 148.1(7)	N(4)-Zn(2)-N(3) 96.9(8)	O(12)-Zn(2)-Dy(1) 112.4(5)	O(2)-Zn(2)-Dy(1) 38.0(4)	
O(5)-Zn(2)-Dy(1) 37.5(4)	N(4)-Zn(2)-Dy(1) 123.8(6)	N(3)-Zn(2)-Dy(1) 122.8(6)	O(6)-Zn(3)-O(14) 102.6(7)	O(6)-Zn(3)-O(17) 120.2(8)	
O(14)-Zn(3)-O(17) 76.8(6)	O(6)-Zn(3)-N(6) 104.8(7)	O(14)-Zn(3)-N(6) 152.4(7)	O(17)-Zn(3)-N(6) 86.9(7)	O(6)-Zn(3)-N(5) 92.2(8)	
O(14)-Zn(3)-N(5) 84.7(8)	O(17)-Zn(3)-N(5) 145.3(8)	N(6)-Zn(3)-N(5) 97.1(8)	O(6)-Zn(3)-Dy(3) 113.0(5)	O(14)-Zn(3)-Dy(3) 38.3(5)	
O(17)-Zn(3)-Dy(3) 38.9(4)	N(6)-Zn(3)-Dy(3) 124.3(6)	N(5)-Zn(3)-Dy(3) 119.9(6)	O(5)-Dy(1)-O(2) 66.8(6)	O(5)-Dy(1)-O(37) 141.0(6)	
O(2)-Dy(1)-O(37) 143.4(6)	O(5)-Dy(1)-O(4) 66.0(6)	O(2)-Dy(1)-O(4) 131.8(5)	O(37)-Dy(1)-O(4) 83.3(6)	O(5)-Dy(1)-O(20) 74.7(6)	
O(2)-Dy(1)-O(20) 102.9(6)	O(37)-Dy(1)-O(20) 73.9(6)	O(4)-Dy(1)-O(20) 73.8(6)	O(5)-Dy(1)-O(22) 123.5(7)	O(2)-Dy(1)-O(22) 119.0(6)	
O(37)-Dy(1)-O(22) 70.5(7)	O(4)-Dy(1)-O(22) 80.5(6)	O(20)-Dy(1)-O(22) 138.0(7)	O(5)-Dy(1)-O(1) 132.2(6)	O(2)-Dy(1)-O(1) 66.0(6)	
O(37)-Dy(1)-O(1) 85.1(6)	O(4)-Dy(1)-O(1) 155.2(6)	O(20)-Dy(1)-O(1) 123.6(6)	O(22)-Dy(1)-O(1) 75.0(6)	O(5)-Dy(1)-O(19) 103.9(6)	
O(2)-Dy(1)-O(19)	O(37)-Dy(1)-O(19)	O(4)-Dy(1)-O(19)	O(22)-Dy(1)-O(19)	O(5)-Dy(1)-O(24)	

75.5(6)	74.1(6)	125.6(6)	132.5(7)	77.9(6)
O(2)-Dy(1)-O(24) 83.0(6)	O(37)-Dy(1)-O(24) 120.1(7)	O(4)-Dy(1)-O(24) 78.1(6)	O(20)-Dy(1)-O(24)146.7(6)	O(22)-Dy(1)-O(24)50.6(7)
O(1)-Dy(1)-O(24) 89.0(6)	O(19)-Dy(1)-O(24) 155.3(7)	O(14)-Dy(3)-Zn(3) 33.7(4)	O(17)-Dy(3)-Zn(3)34.5(4)	O(38)-Dy(3)-Zn(3)169.1(6)
O(28)-Dy(3)-Zn(3) 93.6(5)	O(5)-Dy(1)-Zn(2) 34.0(4)	O(2)-Dy(1)-Zn(2) 33.5(3)	O(37)-Dy(1)-Zn(2) 166.0(4)	O(4)-Dy(1)-Zn(2) 98.4(4)
O(20)-Dy(1)-Zn(2) 93.1(5)	O(22)-Dy(1)-Zn(2) 123.5(6)	O(1)-Dy(1)-Zn(2) 98.2(4)	O(19)-Dy(1)-Zn(2)94.0(5)	O(24)-Dy(1)-Zn(2)73.7(5)
N(2)-Zn(1)-N(1) 97.3(9)	O(10)-Dy(2)-O(7) 143.4(6)	O(11)-Dy(2)-O(8) 66.3(5)	O(11)-Dy(2)-O(8) 66.3(5)	O(8)-Dy(2)-O(35)74.9(6)
O(11)-Dy(2)-O(34) 139.2(7)	O(8)-Dy(2)-O(34) 149.0(6)	O(35)-Dy(2)-O(34) 77.2(6)	O(11)-Dy(2)-O(36)75.1(5)	O(8)-Dy(2)-O(36)109.1(6)
O(35)-Dy(2)-O(36) 69.5(6)	O(34)-Dy(2)-O(36) 72.6(7)	O(11)-Dy(2)-O(25) 121.1(6)	O(8)-Dy(2)-O(25) 118.5(6)	O(35)-Dy(2)-O(25)124.7(6)
O(34)-Dy(2)-O(25) 68.3(7)	O(36)-Dy(2)-O(25) 132.3(7)	O(11)-Dy(2)-O(26) 75.5(6)	O(8)-Dy(2)-O(26) 76.6(6)	O(35)-Dy(2)-O(26)142.5(6)
O(34)-Dy(2)-O(26) 120.9(6)	O(36)-Dy(2)-O(26) 144.2(6)	O(25)-Dy(2)-O(26) 53.2(6)	O(11)-Dy(2)-O(10)65.6(5)	O(8)-Dy(2)-O(10) 128.9(5)
O(35)-Dy(2)-O(10) 141.7(6)	O(34)-Dy(2)-O(10) 81.9(7)	O(36)-Dy(2)-O(10) 73.8(6)	O(25)-Dy(2)-O(10)74.5(6)	O(26)-Dy(2)-O(10)75.7(6)
O(11)-Dy(2)-O(7) 128.4(5)	O(8)-Dy(2)-O(7) 65.5(5)	O(35)-Dy(2)-O(7) 69.8(6)	O(34)-Dy(2)-O(7) 92.4(7)	O(36)-Dy(2)-O(7) 138.7(6)
O(26)-Dy(2)-O(7) 76.6(6)	O(11)-Dy(2)-Zn(1) 33.1(4)	O(8)-Dy(2)-Zn(1) 33.3(4)	O(35)-Dy(2)-Zn(1)95.8(4)	O(34)-Dy(2)-Zn(1)165.8(5)
O(36)-Dy(2)-Zn(1) 93.4(4)	O(25)-Dy(2)-Zn(1) 125.1(5)	O(26)-Dy(2)-Zn(1) 72.0(4)	O(10)-Dy(2)-Zn(1)96.9(4)	O(7)-Dy(2)-Zn(1) 96.8(4)
O(25)-Dy(2)-O(7) 69.9(6)	O(14)-Dy(3)-O(17) 67.9(6)	O(14)-Dy(3)-O(38) 141.8(7)	O(17)-Dy(3)-O(38)145.0(7)	O(14)-Dy(3)-O(28)100.4(7)
O(17)-Dy(3)-O(28) 79.4(7)	O(38)-Dy(3)-O(28) 77.0(8)	O(14)-Dy(3)-O(29) 73.9(6)	O(17)-Dy(3)-O(29)110.8(7)	O(38)-Dy(3)-O(29)74.4(7)
O(28)-Dy(3)-O(29) 53.6(6)	O(14)-Dy(3)-O(13) 65.5(6)	O(17)-Dy(3)-O(13) 130.5(6)	O(38)-Dy(3)-O(13)84.4(7)	O(28)-Dy(3)-O(13)124.4(7)
O(29)-Dy(3)-O(13) 71.0(6)	O(14)-Dy(3)-O(31) 121.0(7)	O(17)-Dy(3)-O(31) 118.6(7)	O(38)-Dy(3)-O(31)67.8(8)	O(28)-Dy(3)-O(31)138.4(7)
O(29)-Dy(3)-O(31) 130.4(7)	O(13)-Dy(3)-O(31) 74.3(6)	O(14)-Dy(3)-O(16) 130.8(5)	O(17)-Dy(3)-O(16)64.5(5)	O(38)-Dy(3)-O(16)87.1(7)
O(28)-Dy(3)-O(16)82.8(7)	O(29)-Dy(3)-O(16) 135.1(6)	O(13)-Dy(3)-O(16) 148.3(6)	O(31)-Dy(3)-O(16)74.2(6)	O(14)-Dy(3)-O(32)79.0(6)
O(17)-Dy(3)-O(32)75.6(6)	O(38)-Dy(3)-O(32) 120.0(7)	O(28)-Dy(3)-O(32) 153.2(7)	O(29)-Dy(3)-O(32)146.5(6)	O(13)-Dy(3)-O(32)80.1(6)
O(29)-Dy(3)-Zn(3)95.6(5)	O(13)-Dy(3)-Zn(3) 96.7(4)	O(31)-Dy(3)-Zn(3) 123.0(5)	O(16)-Dy(3)-Zn(3)97.4(4)	O(32)-Dy(3)-Zn(3)70.9(5)

Table. S3 Selected bond distances and angles for **2**

Tb(1)-O(5) 2.284(7)	Tb(1)-O(2) 2.282(7)	Tb(1)-O(38) 2.393(8)	Tb(1)-O(4) 2.455(7)	Tb(1)-O(30) 2.452(9)	O(5)-Tb(1)-O(2) 67.2(2)
Tb(1)-O(32) 2.467(10)	Tb(1)-O(1) 2.470(8)	Tb(1)-O(33) 2.499(10)	Tb(1)-O(29) 2.499(10)	Tb(1)-Zn(1) 3.4997(12)	O(5)-Tb(1)-O(38) 144.1(3)
Tb(3)-O(11) 2.289(7)	Tb(3)-O(8) 2.337(8)	Tb(3)-O(35) 2.359(9)	Tb(3)-O(36) 2.394(10)	Tb(3)-O(27) 2.434(9)	O(2)-Tb(1)-O(38) 140.1(3)
Tb(3)-O(34) 2.438(9)	Tb(3)-O(26) 2.492(9)	Tb(3)-O(10) 2.526(8)	Tb(3)-O(7) 2.545(8)	Tb(3)-Zn(3) 3.5206(13)	O(5)-Tb(1)-O(4) 65.4(2)
Tb(2)-O(14) 2.302(7)	Tb(2)-O(17) 2.307(7)	Tb(2)-O(20) 2.364(12)	Tb(2)-O(37) 2.382(9)	Tb(2)-O(23) 2.482(9)	O(2)-Tb(1)-O(4) 132.0(2)
Tb(2)-O(19) 2.482(10)	Tb(2)-O(24) 2.480(9)	Tb(2)-O(13) 2.496(9)	Tb(2)-O(16) 2.491(8)	Tb(2)-Zn(2) 3.5177(12)	O(38)-Tb(1)-O(4) 86.2(3)
Zn(1)-O(12) 1.976(7)	Zn(1)-O(2) 2.049(7)	Zn(1)-O(5) 2.049(7)	Zn(1)-N(4) 2.069(9)	Zn(1)-N(3) 2.098(9)	O(5)-Tb(1)-O(30) 102.4(3)
Zn(3)-O(15) 1.993(7)	Zn(3)-O(8) 2.029(7)	Zn(3)-O(11) 2.029(7)	Zn(3)-N(2) 2.055(9)	Zn(3)-N(1) 2.097(9)	O(2)-Tb(1)-O(30) 75.9(3)
Zn(2)-O(3) 1.988(8)	Zn(2)-O(17) 2.024(7)	Zn(2)-O(14) 2.063(7)	Zn(2)-N(5) 2.070(10)	Zn(2)-N(6) 2.102(9)	O(38)-Tb(1)-O(30) 73.1(3)
O(4)-Tb(1)-O(30) 121.3(3)	O(5)-Tb(1)-O(32) 118.0(3)	O(2)-Tb(1)-O(32) 123.3(3)	O(38)-Tb(1)-O(32) 71.2(4)	O(4)-Tb(1)-O(32) 75.0(3)	
O(30)-Tb(1)-O(32) 139.3(3)	O(5)-Tb(1)-O(1) 132.2(3)	O(2)-Tb(1)-O(1) 66.0(2)	O(38)-Tb(1)-O(1) 82.1(3)	O(4)-Tb(1)-O(1) 155.9(3)	
O(30)-Tb(1)-O(1) 75.1(3)	O(32)-Tb(1)-O(1) 81.3(3)	O(5)-Tb(1)-O(33) 82.8(3)	O(2)-Tb(1)-O(33) 76.6(3)	O(38)-Tb(1)-O(33) 120.7(3)	
O(4)-Tb(1)-O(33) 90.5(3)	O(30)-Tb(1)-O(33) 147.2(3)	O(32)-Tb(1)-O(33) 51.1(3)	O(1)-Tb(1)-O(33) 77.7(3)	O(5)-Tb(1)-O(29) 74.5(3)	
O(2)-Tb(1)-O(29) 103.4(3)	O(38)-Tb(1)-O(29) 75.6(4)	O(4)-Tb(1)-O(29) 70.7(3)	O(30)-Tb(1)-O(29) 51.2(3)	O(32)-Tb(1)-O(29) 133.2(4)	
O(1)-Tb(1)-O(29) 125.7(3)	O(33)-Tb(1)-O(29) 155.0(3)	O(5)-Tb(1)-Zn(1) 33.93(18)	O(2)-Tb(1)-Zn(1) 33.91(16)	O(38)-Tb(1)-Zn(1) 166.0(2)	
O(4)-Tb(1)-Zn(1) 98.10(18)	O(30)-Tb(1)-Zn(1) 93.5(2)	O(32)-Tb(1)-Zn(1) 122.8(3)	O(1)-Tb(1)-Zn(1) 98.32(18)	O(33)-Tb(1)-Zn(1) 72.7(2)	
O(29)-Tb(1)-Zn(1) 93.2(3)	O(11)-Tb(3)-O(8) 66.3(2)	O(11)-Tb(3)-O(35) 113.1(4)	O(8)-Tb(3)-O(35) 75.4(3)	O(11)-Tb(3)-O(36) 139.7(4)	
O(8)-Tb(3)-O(36) 147.6(3)	O(35)-Tb(3)-O(36) 75.3(4)	O(11)-Tb(3)-O(27) 120.4(3)	O(8)-Tb(3)-O(27) 118.1(3)	O(35)-Tb(3)-O(27) 125.8(4)	
O(36)-Tb(3)-O(27) 70.3(4)	O(11)-Tb(3)-O(34) 73.3(3)	O(8)-Tb(3)-O(34) 108.7(3)	O(35)-Tb(3)-O(34) 69.9(3)	O(36)-Tb(3)-O(34) 73.4(4)	
O(27)-Tb(3)-O(34) 133.0(3)	O(11)-Tb(3)-O(26) 75.7(3)	O(8)-Tb(3)-O(26) 76.9(3)	O(35)-Tb(3)-O(26) 143.6(3)	O(36)-Tb(3)-O(26) 122.0(4)	
O(27)-Tb(3)-O(26)	O(34)-Tb(3)-O(26)	O(11)-Tb(3)-O(10)	O(8)-Tb(3)-O(10)	O(35)-Tb(3)-O(10)	

52.2(3)	142.4(3)	65.4(2)	128.2(2)	142.2(3)
O(36)-Tb(3)-O(10) 84.0(3)	O(27)-Tb(3)-O(10) 73.4(3)	O(34)-Tb(3)-O(10) 74.0(3)	O(26)-Tb(3)-O(10) 74.2(3)	O(11)-Tb(3)-O(7) 128.0(2)
O(8)-Tb(3)-O(7) 64.5(3)	O(35)-Tb(3)-O(7) 69.2(3)	O(36)-Tb(3)-O(7) 92.2(4)	O(27)-Tb(3)-O(7) 71.7(3)	O(34)-Tb(3)-O(7) 138.9(3)
O(26)-Tb(3)-O(7) 77.9(3)	O(10)-Tb(3)-O(7) 144.1(3)	O(11)-Tb(3)-Zn(3) 33.00(17)	O(8)-Tb(3)-Zn(3) 33.39(18)	O(35)-Tb(3)-Zn(3) 96.0(3)
O(36)-Tb(3)-Zn(3) 165.0(3)	O(27)-Tb(3)-Zn(3) 124.3(2)	O(34)-Tb(3)-Zn(3) 92.1(2)	O(26)-Tb(3)-Zn(3) 72.2(2)	O(10)-Tb(3)-Zn(3) 96.31(18)
O(7)-Tb(3)-Zn(3) 96.13(19)	O(14)-Tb(2)-O(17) 66.7(3)	O(14)-Tb(2)-O(20) 79.0(4)	O(17)-Tb(2)-O(20) 97.6(4)	O(14)-Tb(2)-O(37) 146.6(4)
O(17)-Tb(2)-O(37) 141.3(4)	O(20)-Tb(2)-O(37) 79.0(5)	O(14)-Tb(2)-O(23) 76.2(3)	O(17)-Tb(2)-O(23) 79.3(3)	O(20)-Tb(2)-O(23) 154.1(4)
O(37)-Tb(2)-O(23) 119.3(4)	O(14)-Tb(2)-O(19) 110.7(3)	O(17)-Tb(2)-O(19) 75.1(3)	O(20)-Tb(2)-O(19) 51.0(4)	O(37)-Tb(2)-O(19) 73.1(4)
O(23)-Tb(2)-O(19) 147.5(3)	O(14)-Tb(2)-O(24) 118.1(3)	O(17)-Tb(2)-O(24) 120.5(3)	O(20)-Tb(2)-O(24) 141.6(4)	O(37)-Tb(2)-O(24) 68.7(4)
O(23)-Tb(2)-O(24) 50.7(3)	O(19)-Tb(2)-O(24) 131.0(3)	O(14)-Tb(2)-O(13) 64.9(3)	O(17)-Tb(2)-O(13) 130.1(2)	O(20)-Tb(2)-O(13) 84.6(4)
O(37)-Tb(2)-O(13) 88.3(4)	O(23)-Tb(2)-O(13) 78.3(3)	O(19)-Tb(2)-O(13) 133.9(3)	O(24)-Tb(2)-O(13) 74.5(3)	O(14)-Tb(2)-O(16) 129.1(3)
O(17)-Tb(2)-O(16) 65.3(3)	O(20)-Tb(2)-O(16) 123.0(3)	O(37)-Tb(2)-O(16) 84.1(4)	O(23)-Tb(2)-O(16)79.4(3)	O(19)-Tb(2)-O(16) 72.0(3)
O(24)-Tb(2)-O(16) 74.7(3)	O(13)-Tb(2)-O(16) 149.0(3)	O(14)-Tb(2)-Zn(2) 34.06(18)	O(17)-Tb(2)-Zn(2) 33.08(18)	O(20)-Tb(2)-Zn(2) 91.9(3)
O(37)-Tb(2)-Zn(2) 169.0(3)	O(23)-Tb(2)-Zn(2) 71.3(2)	O(19)-Tb(2)-Zn(2) 96.3(3)	O(24)-Tb(2)-Zn(2) 122.0(2)	O(13)-Tb(2)-Zn(2) 97.24(18)
O(16)-Tb(2)-Zn(2) 95.71(18)	O(12)-Zn(1)-O(2) 118.4(3)	O(12)-Zn(1)-O(5) 106.2(3)	O(2)-Zn(1)-O(5) 76.1(3)	O(12)-Zn(1)-N(4) 102.8(3)
O(2)-Zn(1)-N(4) 85.4(3)	O(5)-Zn(1)-N(4) 150.5(3)	O(12)-Zn(1)-N(3) 92.7(3)	O(2)-Zn(1)-N(3) 147.2(3)	O(5)-Zn(1)-N(3) 85.7(3)
N(4)-Zn(1)-N(3) 98.4(3)	O(12)-Zn(1)-Tb(1) 112.9(2)	O(2)-Zn(1)-Tb(1) 38.4(2)	O(5)-Zn(1)-Tb(1) 38.47(19)	N(4)-Zn(1)-Tb(1) 122.6(2)
N(3)-Zn(1)-Tb(1) 122.1(3)	O(15)-Zn(3)-O(8) 108.1(3)	O(15)-Zn(3)-O(11) 114.9(3)	O(8)-Zn(3)-O(11) 77.2(3)	O(15)-Zn(3)-N(2) 103.3(3)
O(8)-Zn(3)-N(2) 148.4(3)	O(11)-Zn(3)-N(2) 86.3(3)	O(15)-Zn(3)-N(1) 93.3(3)	O(8)-Zn(3)-N(1) 84.7(3)	O(11)-Zn(3)-N(1) 150.0(3)
N(2)-Zn(3)-N(1) 97.4(3)	O(15)-Zn(3)-Tb(3) 116.3(3)	O(8)-Zn(3)-Tb(3) 39.3(2)	O(11)-Zn(3)-Tb(3) 37.9(2)	N(2)-Zn(3)-Tb(3) 120.5(2)
N(1)-Zn(3)-Tb(3) 121.1(2)	O(3)-Zn(2)-O(17) 103.0(3)	O(3)-Zn(2)-O(14) 120.5(3)	O(17)-Zn(2)-O(14) 76.7(3)	O(3)-Zn(2)-N(5) 104.5(3)
O(17)-Zn(2)-N(5) 152.3(4)	O(14)-Zn(2)-N(5) 86.1(3)	O(3)-Zn(2)-N(6) 92.3(3)	O(17)-Zn(2)-N(6) 83.5(3)	O(14)-Zn(2)-N(6)144.5(3)

N(5)-Zn(2)-N(6) 99.1(4)	O(3)-Zn(2)-Tb(2)113.2(3)	O(17)-Zn(2)-Tb(2)38.5(2)	O(14)-Zn(2)-Tb(2) 38.7(2)	N(5)-Zn(2)-Tb(2) 123.5(3)
N(6)-Zn(2)-Tb(2)119.0(3)				

Table. S4 Selected bond distances and angles for **3**

Er(1)-O(5) 2.252(8)	Er(1)-O(2) 2.306(8)	Er(1)-O(35) 2.349(10)	Er(1)-O(36) 2.380(10)	Er(1)-O(26) 2.407(9)	O(5)-Er(1)-O(2) 66.7(3)
Er(1)-O(37) 2.419(10)	Er(1)-O(25) 2.450(10)	Er(1)-O(4) 2.500(8)	Er(1)-O(1) 2.536(9)	Zn(3)-O(9) 2.004(8)	O(5)-Er(1)-O(35) 112.0(4)
Er(1)-Zn(2) 3.5009(15)	Er(2)-O(8) 2.242(8)	Er(2)-O(11) 2.259(8)	Er(2)-O(34) 2.389(9)	Er(2)-O(10) 2.426(8)	O(2)-Er(1)-O(35) 74.6(3)
Er(2)-O(31) 2.438(11)	Er(2)-O(7) 2.442(9)	Er(2)-O(30) 2.458(10)	Er(2)-O(32) 2.464(11)	Er(2)-O(28) 2.466(11)	O(5)-Er(1)-O(36) 140.5(4)
Zn(3)-O(14) 2.041(8)	Zn(3)-O(17) 2.057(8)	Er(2)-Zn(1) 3.4802(14)	Er(3)-O(14) 2.266(8)	Er(3)-O(17) 2.289(8)	O(2)-Er(1)-O(36) 146.5(4)
Er(3)-O(41) 2.335(9)	Er(3)-O(20) 2.357(11)	Er(3)-O(24) 2.446(10)	Er(3)-O(16) 2.457(9)	Er(3)-O(23) 2.447(10)	O(35)-Er(1)-O(36) 75.5(4)
Er(3)-O(21) 2.454(10)	Er(3)-O(13) 2.457(9)	Zn(3)-N(4) 2.069(11)	Zn(3)-N(3) 2.101(10)	Er(3)-Zn(3) 3.4972(14)	O(5)-Er(1)-O(26) 121.4(3)
Zn(1)-O(6) 1.982(8)	Zn(1)-O(8) 2.043(7)	Zn(1)-O(11) 2.035(8)	Zn(1)-N(1) 2.074(10)	Zn(1)-N(2) 2.088(10)	O(2)-Er(1)-O(26) 117.5(3)
Zn(2)-O(18) 1.995(8)	Zn(2)-O(2) 2.031(8)	Zn(2)-O(5) 2.033(8)	Zn(2)-N(5) 2.056(10)	Zn(2)-N(5) 2.056(10)	O(35)-Er(1)-O(26) 125.7(4)
O(5)-Er(1)-O(37) 73.5(3)	O(2)-Er(1)-O(37) 109.6(3)	O(35)-Er(1)-O(37) 69.9(3)	O(36)-Er(1)-O(37) 73.4(4)	O(26)-Er(1)-O(37) 132.6(3)	
O(5)-Er(1)-O(25) 76.9(3)	O(2)-Er(1)-O(25) 77.0(3)	O(35)-Er(1)-O(25) 143.1(3)	O(36)-Er(1)-O(25) 121.4(4)	O(26)-Er(1)-O(25) 51.9(3)	
O(37)-Er(1)-O(25) 143.3(3)	O(5)-Er(1)-O(4) 66.7(3)	O(2)-Er(1)-O(4) 129.6(3)	O(35)-Er(1)-O(4) 142.1(3)	O(36)-Er(1)-O(4) 83.8(4)	
O(26)-Er(1)-O(4) 73.3(3)	O(37)-Er(1)-O(4) 73.9(3)	O(25)-Er(1)-O(4) 74.8(3)	O(5)-Er(1)-O(1) 129.2(3)	O(2)-Er(1)-O(1) 65.3(3)	
O(35)-Er(1)-O(1) 69.7(3)	O(36)-Er(1)-O(1) 90.2(4)	O(26)-Er(1)-O(1) 70.0(3)	O(37)-Er(1)-O(1) 139.1(3)	O(25)-Er(1)-O(1) 77.2(3)	
O(4)-Er(1)-O(1) 142.6(3)	O(36)-Er(1)-O(26) 69.9(4)	O(32)-Er(2)-O(28) 153.9(3)	O(21)-Er(3)-O(13) 72.5(4)	O(23)-Er(3)-O(13) 74.4(3)	
O(5)-Er(1)-Zn(2) 33.20(19)	O(2)-Er(1)-Zn(2) 33.6(2)	O(35)-Er(1)-Zn(2) 95.2(3)	O(36)-Er(1)-Zn(2) 165.4(3)	O(26)-Er(1)-Zn(2) 124.5(2)	
O(37)-Er(1)-Zn(2) 93.0(2)	O(25)-Er(1)-Zn(2) 72.7(2)	O(4)-Er(1)-Zn(2) 97.7(2)	O(1)-Er(1)-Zn(2) 97.1(2)	N(3)-Zn(3)-Er(3) 118.8(3)	
O(8)-Er(2)-O(11) 67.0(3)	O(8)-Er(2)-O(34) 139.8(3)	O(11)-Er(2)-O(34) 144.5(3)	O(8)-Er(2)-O(10) 133.0(3)	O(11)-Er(2)-O(10) 66.5(3)	
O(34)-Er(2)-O(10) 85.4(3)	O(8)-Er(2)-O(31) 123.3(3)	O(11)-Er(2)-O(31) 117.8(3)	O(34)-Er(2)-O(31) 71.5(4)	O(10)-Er(2)-O(31) 74.7(3)	

O(8)-Er(2)-O(7) 67.0(3)	O(11)-Er(2)-O(7) 132.7(3)	O(34)-Er(2)-O(7) 81.5(3)	O(10)-Er(2)-O(7) 153.8(3)	O(31)-Er(2)-O(7) 79.7(3)
O(8)-Er(2)-O(30) 75.5(3)	O(11)-Er(2)-O(30) 103.1(3)	O(34)-Er(2)-O(30) 72.8(3)	O(10)-Er(2)-O(30) 121.7(3)	O(31)-Er(2)-O(30) 138.9(4)
O(7)-Er(2)-O(30) 75.6(3)	O(8)-Er(2)-O(32) 76.5(3)	O(11)-Er(2)-O(32) 81.6(3)	O(34)-Er(2)-O(32) 121.6(4)	O(10)-Er(2)-O(32) 90.5(3)
O(31)-Er(2)-O(32) 51.5(4)	O(7)-Er(2)-O(32) 77.4(3)	O(30)-Er(2)-O(32) 146.8(3)	O(8)-Er(2)-O(28) 103.3(4)	O(11)-Er(2)-O(28) 74.6(3)
O(34)-Er(2)-O(28) 75.7(4)	O(10)-Er(2)-O(28) 70.3(3)	O(31)-Er(2)-O(28) 133.2(4)	O(7)-Er(2)-O(28) 127.1(3)	O(30)-Er(2)-O(28) 52.3(3)
O(8)-Er(2)-Zn(1) 33.83(18)	O(11)-Er(2)-Zn(1) 33.8(2)	O(34)-Er(2)-Zn(1) 165.8(3)	O(10)-Er(2)-Zn(1) 99.2(2)	O(31)-Er(2)-Zn(1) 122.7(3)
O(7)-Er(2)-Zn(1) 99.0(2)	O(30)-Er(2)-Zn(1) 93.5(2)	O(32)-Er(2)-Zn(1) 72.1(2)	O(28)-Er(2)-Zn(1) 93.1(3)	O(6)-Zn(1)-O(8) 118.8(3)
O(6)-Zn(1)-O(11) 106.4(3)	O(14)-Er(3)-O(17) 67.3(3)	O(14)-Er(3)-O(41) 141.2(4)	O(17)-Er(3)-O(41) 144.1(4)	O(14)-Er(3)-O(20) 99.7(4)
O(17)-Er(3)-O(20) 77.3(4)	O(41)-Er(3)-O(20) 76.3(4)	O(14)-Er(3)-O(24) 79.6(3)	O(17)-Er(3)-O(24) 76.1(3)	O(41)-Er(3)-O(24) 121.9(4)
O(20)-Er(3)-O(24) 151.3(4)	O(14)-Er(3)-O(16) 132.0(3)	O(17)-Er(3)-O(16) 66.1(3)	O(41)-Er(3)-O(16) 86.0(4)	O(20)-Er(3)-O(16) 80.5(4)
O(24)-Er(3)-O(16) 79.1(3)	O(14)-Er(3)-O(23) 121.4(3)	O(17)-Er(3)-O(23) 119.4(3)	O(41)-Er(3)-O(23) 69.8(4)	O(20)-Er(3)-O(23) 138.8(4)
O(24)-Er(3)-O(23) 52.1(3)	O(16)-Er(3)-O(23) 74.6(3)	O(14)-Er(3)-O(21) 73.9(3)	O(17)-Er(3)-O(21) 108.6(4)	O(41)-Er(3)-O(21) 73.2(4)
O(20)-Er(3)-O(21) 53.2(4)	O(24)-Er(3)-O(21) 148.2(3)	O(16)-Er(3)-O(21) 132.2(4)	O(23)-Er(3)-O(21) 131.9(4)	O(14)-Er(3)-O(13) 66.0(3)
O(17)-Er(3)-O(13) 130.6(3)	O(41)-Er(3)-O(13) 84.8(4)	O(20)-Er(3)-O(13) 125.5(4)	O(24)-Er(3)-O(13) 80.8(3)	O(16)-Er(3)-O(13) 149.0(3)
O(8)-Zn(1)-O(11) 75.0(3)	O(14)-Er(3)-Zn(3) 33.6(2)	O(17)-Er(3)-Zn(3) 34.2(2)	O(41)-Er(3)-Zn(3) 167.3(3)	O(20)-Er(3)-Zn(3) 92.6(3)
O(24)-Er(3)-Zn(3) 70.8(2)	O(16)-Er(3)-Zn(3) 98.5(2)	O(23)-Er(3)-Zn(3) 122.8(2)	O(21)-Er(3)-Zn(3) 95.2(3)	O(13)-Er(3)-Zn(3) 96.90(19)
O(6)-Zn(1)-N(1) 102.3(4)	O(8)-Zn(1)-N(1) 86.7(3)	O(11)-Zn(1)-N(1) 150.8(4)	O(6)-Zn(1)-N(2) 93.3(4)	O(8)-Zn(1)-N(2) 145.9(4)
O(11)-Zn(1)-N(2) 85.3(4)	N(1)-Zn(1)-N(2) 98.4(4)	O(6)-Zn(1)-Er(2) 113.3(3)	O(8)-Zn(1)-Er(2) 37.7(2)	O(11)-Zn(1)-Er(2) 38.1(2)
N(1)-Zn(1)-Er(2) 123.1(3)	N(2)-Zn(1)-Er(2) 121.1(3)	O(18)-Zn(2)-O(2) 108.1(4)	O(18)-Zn(2)-O(5) 116.1(3)	O(2)-Zn(2)-O(5) 76.2(3)
O(18)-Zn(2)-N(5) 102.7(4)	O(2)-Zn(2)-N(5) 148.8(4)	O(5)-Zn(2)-N(5) 86.2(4)	O(18)-Zn(2)-N(6) 92.9(4)	O(2)-Zn(2)-N(6) 85.3(4)
O(5)-Zn(2)-N(6) 149.2(4)	N(5)-Zn(2)-N(6) 97.9(4)	O(18)-Zn(2)-Er(1) 116.7(3)	O(2)-Zn(2)-Er(1) 38.9(2)	O(5)-Zn(2)-Er(1) 37.3(2)
N(5)-Zn(2)-Er(1) 120.4(3)	N(6)-Zn(2)-Er(1) 121.2(3)	O(9)-Zn(3)-O(14) 104.7(4)	O(9)-Zn(3)-O(17) 121.6(4)	O(14)-Zn(3)-O(17) 76.0(3)

O(9)-Zn(3)-N(4) 103.8(4)	O(14)-Zn(3)-N(4) 151.1(4)	O(17)-Zn(3)-N(4) 85.3(4)	O(9)-Zn(3)-N(3) 92.6(4)	O(14)-Zn(3)-N(3) 83.8(4)
O(17)-Zn(3)-N(3) 143.5(4)	N(4)-Zn(3)-N(3) 99.3(4)	O(9)-Zn(3)-Er(3) 114.3(3)	O(14)-Zn(3)-Er(3) 37.9(2)	O(17)-Zn(3)-Er(3) 38.7(2)
N(4)-Zn(3)-Er(3) 122.9(3)				

Table. S5 SHAPE analyses for **1-3.**

Complex 1	CSAPR-9	MFF-9	**Complex 2**	CSAPR-9	MFF-9	**Complex 3**	CSAPR-9	MFF-9
Dy1	1.797	1.826	Tb1	2.094	2.025	Er1	0.991	1.438
Dy2	1.159	1.568	Tb2	1.926	2.240	Er2	1.875	1.830
Dy3	1.680	2.023	Tb3	1.090	1.531	Er3	1.475	1.851

CSAPR-9 Capped square antiprism；MFF-9 Muffin

Table S6. Relaxation distribution and times fitted from Cole-Cole data for **1**

T(K)	α	τ(s)
4K	0.549	0.153220E-02
4.5K	0.562	0.866696E-03
5K	0.537	0.629100E-03
5.5K	0.481	0.571864E-03
6K	0.384	0.584498E-03
6.5K	0.343	0.478468E-03
7K	0.315	0.367573E-03
7.5K	0.295	0.264255E-03

Table S7. Relaxation distribution and times fitted from Cole-Cole data for **2**

T(K)	α	τ(s)
3.5K	0.498	0.233437E+01
4K	0.587	0.130393E+01
4.5K	0.796	0.123458E+15
5K	0.819	0.572144E+00
5.5K	0.949	0.426134E+00
6K	0.961	0.404486E+00