

Synthesis, Structure and Properties of 2D Lanthanide Coordination Polymers Based on *N*-heterocyclic Arylpolycarboxylate Ligands

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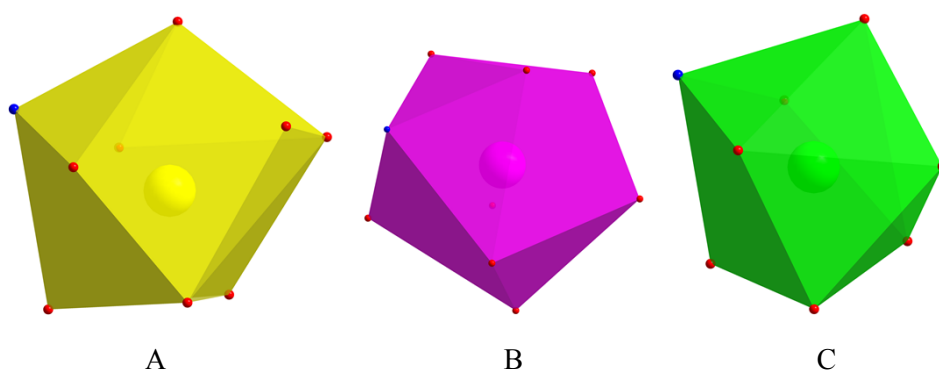


Fig.S1 Geometric configuration of 1(A), 3(B) and 7(C).

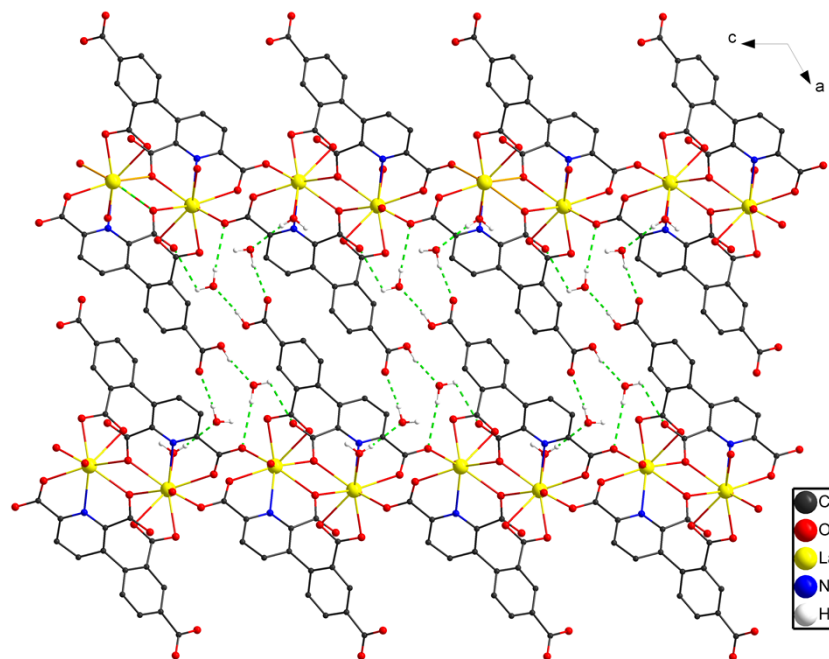


Fig.S2 Three-dimensional framework via hydrogen bonding interaction of 1.

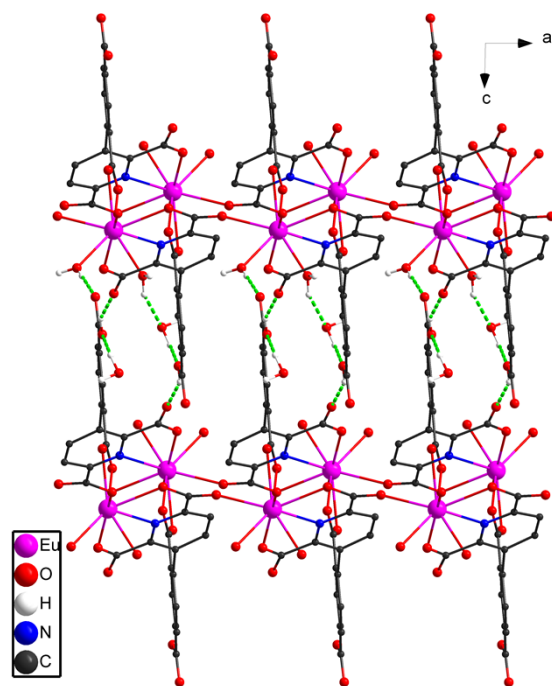


Fig.S3 Three-dimensional framework via hydrogen bonding interaction of 3.

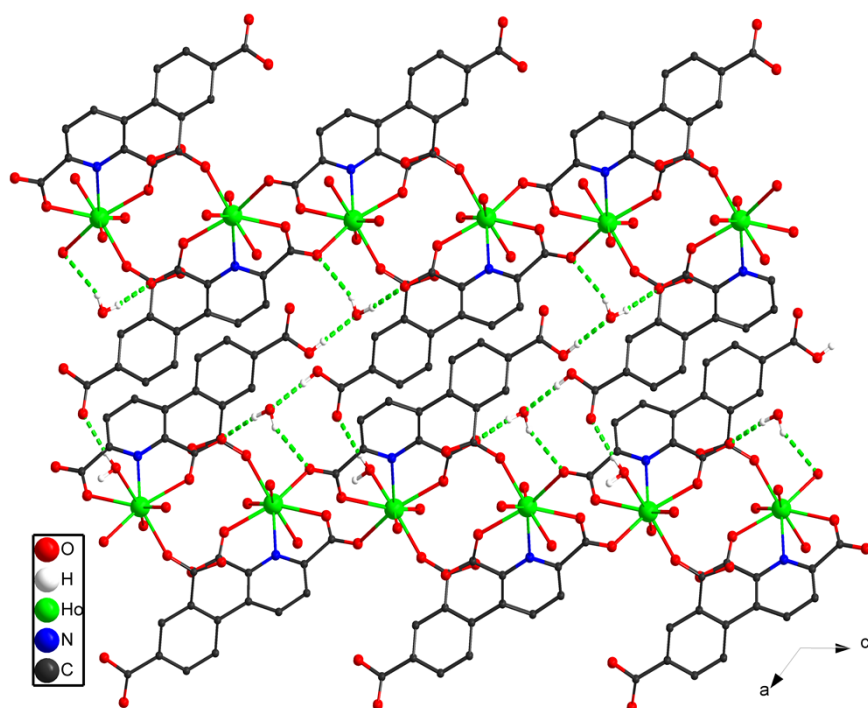
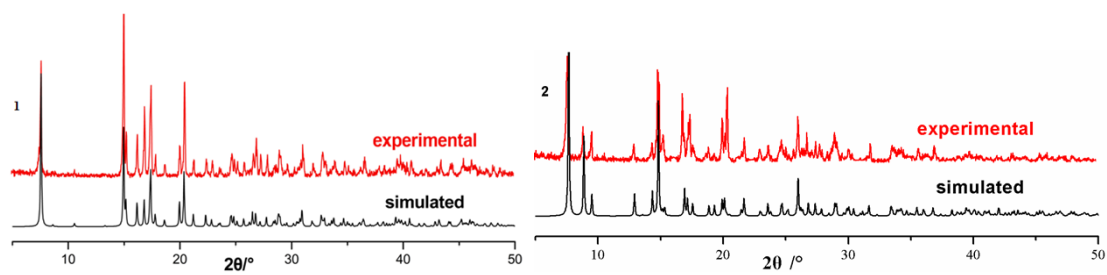


Fig. S4 Three-dimensional framework via hydrogen bonding interaction of 7.



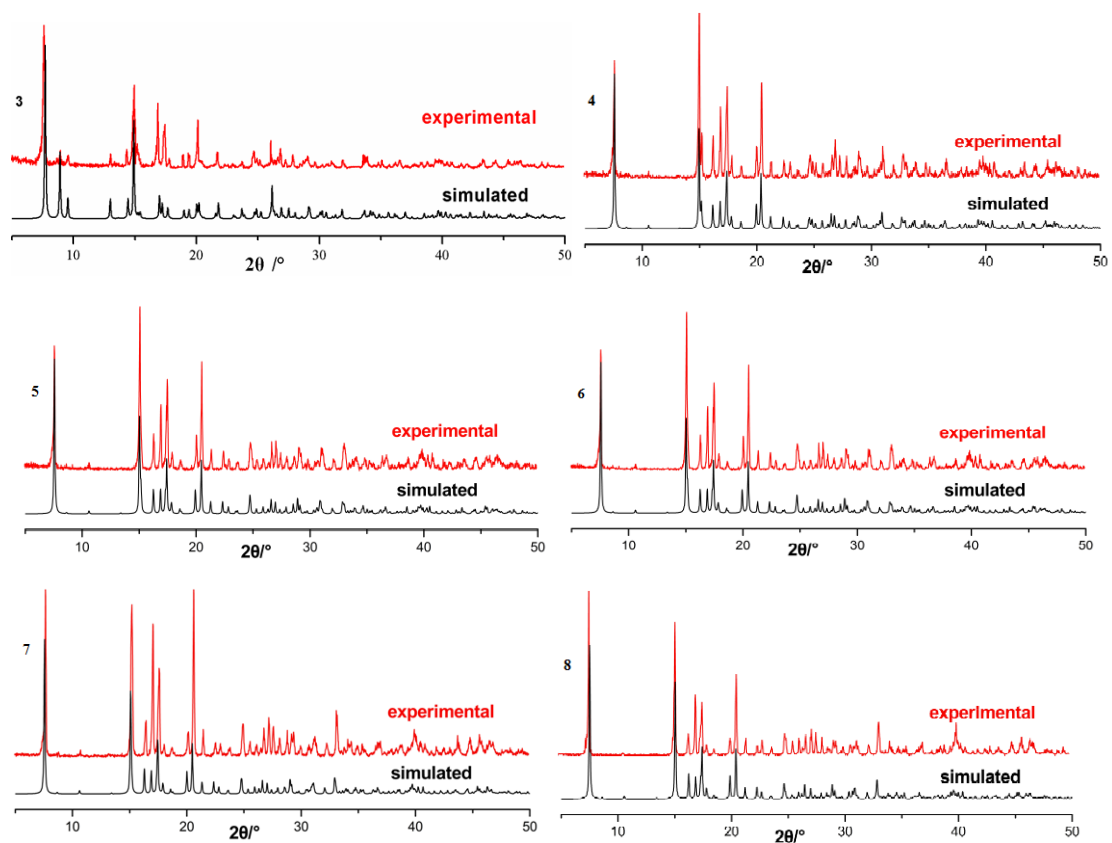


Fig.S5 The simulated and experimental PXRD patterns of 1-8.

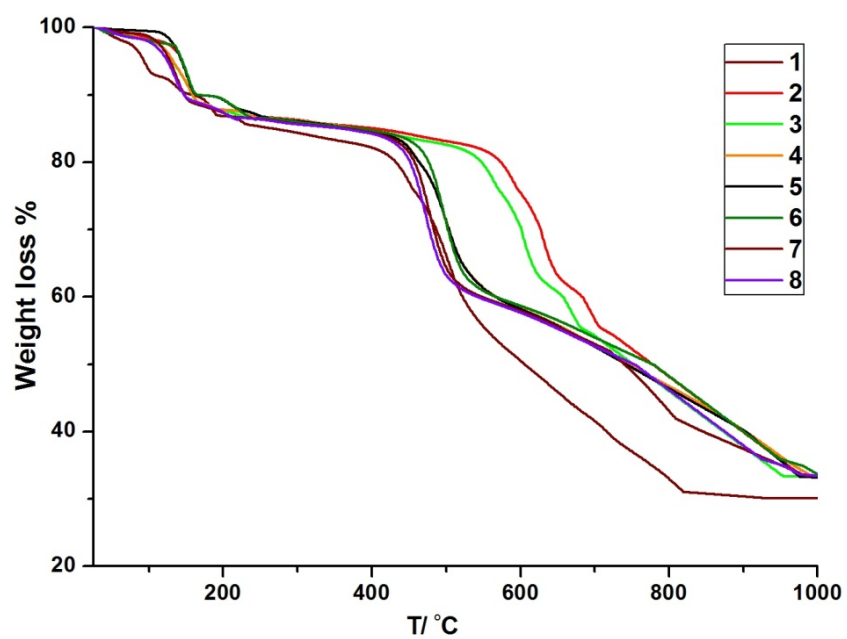


Fig. S6 TGA curves of 1-8.

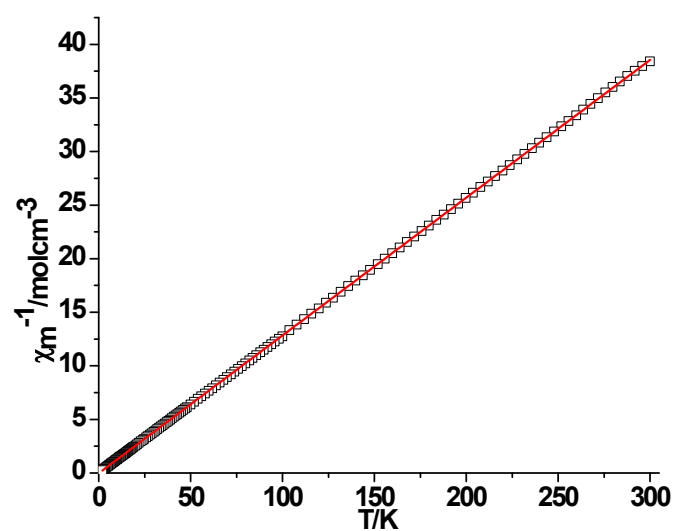


Fig. S7 χ_m^{-1} vs. T curve for 4.

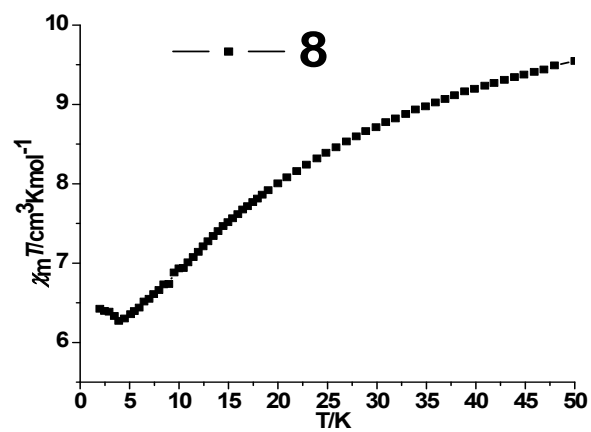


Fig. S8 Plot of $\chi_m T$ vs. T for 8 in the temperature range from 2 to 50 K.

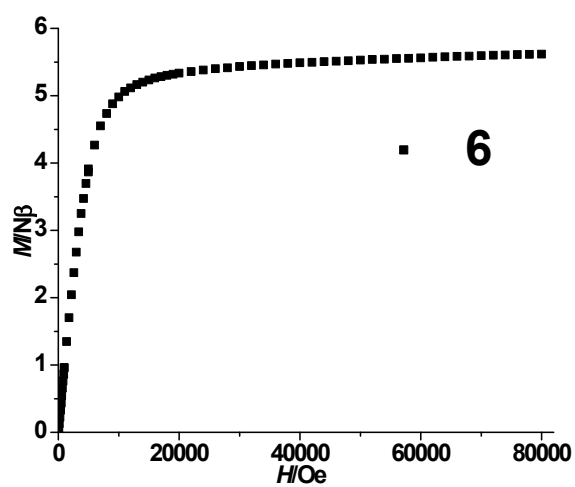


Fig. S9 M vs. H curve of 6.

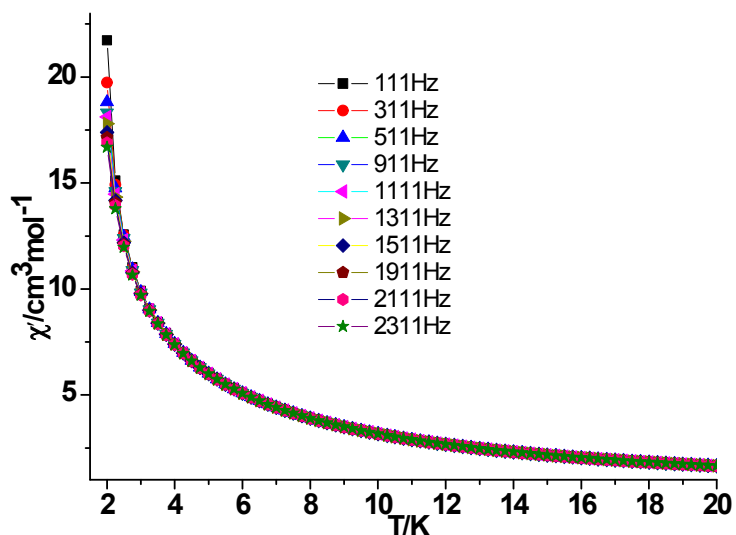


Fig. S10 Temperature dependence of the in-phase (χ') ac susceptibility components at different frequencies for **6** at zero dc field.

Eq.1:

$$\chi_{sm} = \frac{2N\beta}{3kTx} \frac{2.143x + 7.347 + (42.92x + 1.641)e^{-3.5x} + (283.7x - 0.6571)e^{-8x} + (620.6x - 1.94)e^{-13.5x} + (1122x - 2.835)e^{-20x} + (1813x - 3.556)e^{-27.5x}}{3 + 4e^{-3.5x} + 5e^{-8x} + 6e^{-13.5x} + 7e^{-20x} + 8e^{-27.5x}}$$

$$x = \lambda/kT$$

N is Avogadro's number;

k is Boltzmann constant;

β is Bohr magneton.

Table S1. Bond lengths [\AA] and angles [deg] for **1-8**.

La			
O(9)-La(1)	2.593(3)	La(1)-O(2)	2.543(2)
O(10)-La(1)	2.604(2)	La(1)-O(6)	2.564(2)
O(4)-La(1)#1	2.474(2)	La(1)-O(2)#3	2.621(2)
La(1)-O(3)	2.525(2)	La(1)-O(5)	2.666(2)
La(1)-N(1)	2.693(2)		
O(4)#2-La(1)-O(3)	70.27(7)	O(6)-La(1)-O(2)#3	102.98(7)

O(4)#2-La(1)-O(2)	147.60(7)	O(9)-La(1)-O(2)#3	134.86(8)
O(3)-La(1)-O(2)	121.47(7)	O(10)-La(1)-O(2)#3	72.25(7)
O(4)#2-La(1)-O(6)	76.15(7)	O(4)#2-La(1)-O(5)	115.46(7)
O(3)-La(1)-O(6)	93.74(7)	O(3)-La(1)-O(5)	134.51(7)
O(2)-La(1)-O(6)	128.06(7)	O(2)-La(1)-O(5)	79.12(7)
O(4)#2-La(1)-O(9)	124.46(9)	O(6)-La(1)-O(5)	49.97(7)
O(3)-La(1)-O(9)	71.30(8)	O(9)-La(1)-O(5)	69.78(8)
O(2)-La(1)-O(9)	87.27(9)	O(10)-La(1)-O(5)	142.66(7)
O(6)-La(1)-O(9)	68.01(9)	O(2)#3-La(1)-O(5)	71.61(7)
O(4)#2-La(1)-O(10)	75.37(8)	O(4)#2-La(1)-N(1)	123.93(7)
O(3)-La(1)-O(10)	82.69(8)	O(3)-La(1)-N(1)	61.69(7)
O(2)-La(1)-O(10)	76.54(7)	O(2)-La(1)-N(1)	59.88(7)
O(6)-La(1)-O(10)	150.79(8)	O(6)-La(1)-N(1)	131.59(8)
O(9)-La(1)-O(10)	135.88(8)	O(9)-La(1)-N(1)	64.77(8)
O(4)#2-La(1)-O(2)#3	92.92(7)	O(10)-La(1)-N(1)	71.64(7)
O(3)-La(1)-O(2)#3	152.85(7)	O(2)#3-La(1)-N(1)	117.45(7)
O(2)-La(1)-O(2)#3	63.11(8)	O(5)-La(1)-N(1)	118.40(7)

#1: -x,y+1/2,-z+3/2; #2: -x,y-1/2,-z+3/2; #3: -x,-y+1,-z+2; #4: -x,-y+2,-z+2

Sm			
Sm(1)-O(6)	2.382(4)	Sm(1)-O(8)#3	2.527(4)
Sm(1)-O(10)	2.475(5)	Sm(1)-O(8)	2.554(4)
Sm(1)-O(9)	2.477(4)	Sm(1)-N(1)	2.564(5)
Sm(1)-O(7)#1	2.496(4)	Sm(1)-O(4)#2	2.572(4)
Sm(1)-O(3)#2	2.503(4)	O(7)-Sm(1)#4	2.496(4)
O(6)-Sm(1)-O(10)	77.23(15)	O(7)#1-Sm(1)-O(8)	145.99(13)
O(6)-Sm(1)-O(9)	81.16(15)	O(3)#2-Sm(1)-O(8)	74.07(13)
O(10)-Sm(1)-O(9)	68.10(15)	O(8)#3-Sm(1)-O(8)	64.60(15)

O(6)-Sm(1)-O(7)#1	79.94(14)	O(6)-Sm(1)-N(1)	63.58(15)
O(10)-Sm(1)-O(7)#1	71.32(15)	O(10)-Sm(1)-N(1)	126.54(15)
O(9)-Sm(1)-O(7)#1	138.02(15)	O(9)-Sm(1)-N(1)	71.07(15)
O(6)-Sm(1)-O(3)#2	133.40(14)	O(7)#1-Sm(1)-N(1)	129.79(14)
O(10)-Sm(1)-O(3)#2	124.62(14)	O(3)#2-Sm(1)-N(1)	108.79(15)
O(9)-Sm(1)-O(3)#2	142.93(14)	O(8)#3-Sm(1)-N(1)	124.89(14)
O(7)#1-Sm(1)-O(3)#2	71.92(14)	O(8)-Sm(1)-N(1)	63.43(13)
O(6)-Sm(1)-O(8)#3	151.91(15)	O(6)-Sm(1)-O(4)#2	85.74(15)
O(10)-Sm(1)-O(8)#3	77.72(14)	O(10)-Sm(1)-O(4)#2	143.60(15)
O(9)-Sm(1)-O(8)#3	77.87(14)	O(9)-Sm(1)-O(4)#2	140.85(15)
O(7)#1-Sm(1)-O(8)#3	103.72(13)	O(7)#1-Sm(1)-O(4)#2	74.18(15)
O(3)#2-Sm(1)-O(8)#3	72.53(13)	O(3)#2-Sm(1)-O(4)#2	51.50(13)
O(6)-Sm(1)-O(8)	126.10(13)	O(8)#3-Sm(1)-O(4)#2	122.22(13)
O(10)-Sm(1)-O(8)	130.49(14)	O(8)-Sm(1)-O(4)#2	85.43(14)
O(9)-Sm(1)-O(8)	73.33(14)	N(1)-Sm(1)-O(4)#2	70.05(15)

#1: x+1,y,z; #2: -x+2,-y+1,-z+1; #3: -x+2,-y,-z+1; #4: x-1,y,z

Eu			
Eu(1)-O(3)	2.355(6)	Eu(1)-N(1)	2.533(7)
Eu(1)-O(9)	2.447(7)	Eu(1)-O(1)	2.545(6)
Eu(1)-O(10)	2.453(6)	Eu(1)-O(8)#2	2.558(6)
Eu(1)-O(2)#1	2.469(6)	Eu(1)-Eu(1)#3	4.2619(16)
Eu(1)-O(7)#2	2.481(6)	O(2)-Eu(1)#4	2.469(6)
Eu(1)-O(1)#3	2.514(6)		
O(3)-Eu(1)-O(9)	81.3(2)	O(10)-Eu(1)-O(1)	130.8(2)
O(3)-Eu(1)-O(10)	77.6(2)	O(2)#1-Eu(1)-O(1)	145.7(2)
O(9)-Eu(1)-O(10)	68.3(2)	O(7)#2-Eu(1)-O(1)	73.86(19)
O(3)-Eu(1)-O(2)#1	80.0(2)	O(1)#3-Eu(1)-O(1)	65.2(2)

O(9)-Eu(1)-O(2)#1	137.8(2)	N(1)-Eu(1)-O(1)	63.6(2)
O(10)-Eu(1)-O(2)#1	70.9(2)	O(3)-Eu(1)-O(8)#2	85.4(2)
O(3)-Eu(1)-O(7)#2	133.1(2)	O(9)-Eu(1)-O(8)#2	140.7(2)
O(9)-Eu(1)-O(7)#2	143.1(2)	O(10)-Eu(1)-O(8)#2	143.6(2)
O(10)-Eu(1)-O(7)#2	124.2(2)	O(2)#1-Eu(1)-O(8)#2	74.6(2)
O(2)#1-Eu(1)-O(7)#2	71.8(2)	O(7)#2-Eu(1)-O(8)#2	51.65(19)
O(3)-Eu(1)-O(1)#3	151.6(2)	O(1)#3-Eu(1)-O(8)#2	122.82(19)
O(9)-Eu(1)-O(1)#3	77.7(2)	N(1)-Eu(1)-O(8)#2	69.9(2)
O(10)-Eu(1)-O(1)#3	76.9(2)	O(1)-Eu(1)-O(8)#2	85.1(2)
O(2)#1-Eu(1)-O(1)#3	103.20(19)	O(3)-Eu(1)-Eu(1)#3	150.70(16)
O(7)#2-Eu(1)-O(1)#3	72.93(19)	O(9)-Eu(1)-Eu(1)#3	73.00(16)
O(3)-Eu(1)-N(1)	63.5(2)	O(10)-Eu(1)-Eu(1)#3	104.91(16)
O(9)-Eu(1)-N(1)	71.0(2)	O(2)#1-Eu(1)-Eu(1)#3	128.90(14)
O(10)-Eu(1)-N(1)	126.7(2)	O(7)#2-Eu(1)-Eu(1)#3	70.17(14)
O(2)#1-Eu(1)-N(1)	130.0(2)	O(1)#3-Eu(1)-Eu(1)#3	32.83(13)
O(7)#2-Eu(1)-N(1)	109.0(2)	N(1)-Eu(1)-Eu(1)#3	94.32(16)
O(1)#3-Eu(1)-N(1)	125.3(2)	O(1)-Eu(1)-Eu(1)#3	32.38(13)
O(3)-Eu(1)-O(1)	126.2(2)	O(8)#2-Eu(1)-Eu(1)#3	105.56(15)
O(9)-Eu(1)-O(1)	73.7(2)		

#1: x+1,y,z; #2: -x+1,-y,-z+2; #3: -x+1,-y-1,-z+2; #4: x-1,y,z

Gd			
Gd(1)-O(6)#1	2.297(3)	Gd(1)-O(9)	2.452(3)
Gd(1)-O(1)	2.344(3)	Gd(1)-O(3)	2.458(3)
Gd(1)-O(4)#2	2.384(2)	Gd(1)-N(1)	2.558(3)
Gd(1)-O(10)	2.423(3)	Gd(1)-O(11)	2.444(4)
O(6)#1-Gd(1)-O(1)	91.37(10)	O(11)-Gd(1)-O(9)	145.49(12)
O(6)#1-Gd(1)-O(4)#2	77.82(9)	O(6)#1-Gd(1)-O(3)	127.58(10)

O(1)-Gd(1)-O(4)#2	154.47(10)	O(1)-Gd(1)-O(3)	127.06(8)
O(6)#1-Gd(1)-O(10)	141.55(10)	O(4)#2-Gd(1)-O(3)	76.52(9)
O(1)-Gd(1)-O(10)	95.41(11)	O(10)-Gd(1)-O(3)	75.90(10)
O(4)#2-Gd(1)-O(10)	80.04(9)	O(11)-Gd(1)-O(3)	73.62(12)
O(6)#1-Gd(1)-O(11)	71.73(12)	O(9)-Gd(1)-O(3)	140.02(9)
O(1)-Gd(1)-O(11)	90.56(14)	O(6)#1-Gd(1)-N(1)	137.70(10)
O(4)#2-Gd(1)-O(11)	107.43(12)	O(1)-Gd(1)-N(1)	63.65(9)
O(10)-Gd(1)-O(11)	145.68(12)	O(4)#2-Gd(1)-N(1)	137.75(9)
O(6)#1-Gd(1)-O(9)	77.80(10)	O(10)-Gd(1)-N(1)	77.73(10)
O(1)-Gd(1)-O(9)	74.14(10)	O(11)-Gd(1)-N(1)	74.82(12)
O(4)#2-Gd(1)-O(9)	80.94(9)	O(9)-Gd(1)-N(1)	121.71(9)
O(10)-Gd(1)-O(9)	67.92(10)	O(3)-Gd(1)-N(1)	63.46(8)

#1: -x+2,-y+1,-z+2; #2: -x+2,y-1/2,-z+3/2; #3: -x+2,y+1/2,-z+3/2

Tb			
Tb(1)-O(6)#1	2.277(5)	Tb(1)-O(11)	2.427(5)
Tb(1)-O(3)	2.321(5)	Tb(1)-O(2)	2.436(5)
Tb(1)-O(1)#2	2.368(5)	Tb(1)-N(1)	2.527(5)
Tb(1)-O(9)	2.385(5)	Tb(1)-O(10)	2.402(6)
O(6)#1-Tb(1)-O(3)	90.9(2)	O(10)-Tb(1)-O(11)	145.8(2)
O(6)#1-Tb(1)-O(1)#2	77.55(19)	O(6)#1-Tb(1)-O(2)	127.78(19)
O(3)-Tb(1)-O(1)#2	154.53(18)	O(3)-Tb(1)-O(2)	127.16(16)
O(6)#1-Tb(1)-O(9)	141.87(18)	O(1)#2-Tb(1)-O(2)	76.64(17)
O(3)-Tb(1)-O(9)	96.18(19)	O(9)-Tb(1)-O(2)	75.26(18)
O(1)#2-Tb(1)-O(9)	80.28(17)	O(10)-Tb(1)-O(2)	73.4(2)
O(6)#1-Tb(1)-O(10)	71.9(2)	O(11)-Tb(1)-O(2)	139.72(18)
O(3)-Tb(1)-O(10)	90.5(2)	O(6)#1-Tb(1)-N(1)	137.76(19)
O(1)#2-Tb(1)-O(10)	107.0(2)	O(3)-Tb(1)-N(1)	63.58(17)

O(9)-Tb(1)-O(10)	145.0(2)	O(1)#2-Tb(1)-N(1)	138.12(17)
O(6)#1-Tb(1)-O(11)	77.49(18)	O(9)-Tb(1)-N(1)	77.36(18)
O(3)-Tb(1)-O(11)	74.86(18)	O(10)-Tb(1)-N(1)	75.0(2)
O(1)#2-Tb(1)-O(11)	80.46(18)	O(11)-Tb(1)-N(1)	121.93(17)
O(9)-Tb(1)-O(11)	68.48(17)	O(2)-Tb(1)-N(1)	63.67(16)

#1: -x+1,-y+2,-z+2; #2 -x+1,y-1/2,-z+3/2; #3: -x+1,y+1/2,-z+3/2

Dy			
Dy(1)-O(3)#1	2.263(2)	Dy(1)-O(10)	2.423(2)
Dy(1)-O(6)	2.322(2)	Dy(1)-O(7)	2.439(2)
Dy(1)-O(8)#2	2.357(2)	Dy(1)-N(1)	2.516(3)
Dy(1)-O(9)	2.393(2)	Dy(1)-O(11)	2.408(3)
O(3)#1-Dy(1)-O(6)	90.56(10)	O(11)-Dy(1)-O(10)	145.74(11)
O(3)#1-Dy(1)-O(8)#2	77.67(9)	O(3)#1-Dy(1)-O(7)	127.07(9)
O(6)-Dy(1)-O(8)#2	153.96(8)	O(6)-Dy(1)-O(7)	128.34(8)
O(3)#1-Dy(1)-O(9)	141.82(9)	O(8)#2-Dy(1)-O(7)	76.07(8)
O(6)-Dy(1)-O(9)	95.76(10)	O(9)-Dy(1)-O(7)	76.08(9)
O(8)#2-Dy(1)-O(9)	80.49(9)	O(11)-Dy(1)-O(7)	73.45(11)
O(3)#1-Dy(1)-O(11)	71.80(12)	O(10)-Dy(1)-O(7)	139.79(9)
O(6)-Dy(1)-O(11)	90.49(12)	O(3)#1-Dy(1)-N(1)	137.60(9)
O(8)#2-Dy(1)-O(11)	107.29(12)	O(6)-Dy(1)-N(1)	64.16(8)
O(9)-Dy(1)-O(11)	145.39(11)	O(8)#2-Dy(1)-N(1)	138.08(8)
O(3)#1-Dy(1)-O(10)	77.82(9)	O(9)-Dy(1)-N(1)	77.45(9)
O(6)-Dy(1)-O(10)	74.10(9)	O(11)-Dy(1)-N(1)	74.83(12)
O(8)#2-Dy(1)-O(10)	80.70(9)	O(10)-Dy(1)-N(1)	121.71(9)
O(9)-Dy(1)-O(10)	67.97(9)	O(7)-Dy(1)-N(1)	64.28(8)

#1: -x+1,-y,-z+1; #2: -x+1,y+1/2,-z+3/2; #3: -x+1,y-1/2,-z+3/2

Ho

Ho(1)-O(5)#1	2.258(3)	Ho(1)-O(2)#2	2.425(3)
Ho(1)-O(3)#2	2.306(3)	Ho(1)-N(1)#2	2.503(3)
Ho(1)-O(1)	2.336(3)	Ho(1)-O(9)	2.392(4)
Ho(1)-O(10)	2.377(3)	Ho(1)-O(11)	2.405(3)
O(5)#1-Ho(1)-O(3)#2	90.43(12)	O(9)-Ho(1)-O(11)	145.65(13)
O(5)#1-Ho(1)-O(1)	77.47(11)	O(5)#1-Ho(1)-O(2)#2	126.79(12)
O(3)#2-Ho(1)-O(1)	153.83(11)	O(3)#2-Ho(1)-O(2)#2	128.62(11)
O(5)#1-Ho(1)-O(10)	141.84(12)	O(1)-Ho(1)-O(2)#2	76.06(10)
O(3)#2-Ho(1)-O(10)	95.80(12)	O(10)-Ho(1)-O(2)#2	76.34(11)
O(1)-Ho(1)-O(10)	80.73(11)	O(9)-Ho(1)-O(2)#2	73.32(13)
O(5)#1-Ho(1)-O(9)	71.78(13)	O(11)-Ho(1)-O(2)#2	139.91(12)
O(3)#2-Ho(1)-O(9)	90.41(15)	O(5)#1-Ho(1)-N(1)#2	137.64(12)
O(1)-Ho(1)-O(9)	107.23(14)	O(3)#2-Ho(1)-N(1)#2	64.35(11)
O(10)-Ho(1)-O(9)	145.42(13)	O(1)-Ho(1)-N(1)#2	138.17(11)
O(5)#1-Ho(1)-O(11)	77.71(12)	O(10)-Ho(1)-N(1)#2	77.39(11)
O(3)#2-Ho(1)-O(11)	74.20(12)	O(9)-Ho(1)-N(1)#2	74.83(13)
O(1)-Ho(1)-O(11)	80.53(11)	O(11)-Ho(1)-N(1)#2	121.93(11)
O(10)-Ho(1)-O(11)	68.03(12)	O(2)#2-Ho(1)-N(1)#2	64.39(10)
#1: x,-y+1/2,z-1/2; #2: -x+1,y+1/2,-z+1/2; #3: -x+1,y-1/2,-z+1/2; #4: x,-y+1/2,z+1/2			

Er			
Er(1)-O(3)#1	2.262(5)	Er(1)-O(9)	2.392(5)
Er(1)-O(6)	2.303(5)	Er(1)-O(11)	2.415(4)
Er(1)-O(8)#2	2.346(4)	Er(1)-O(7)	2.439(4)
Er(1)-O(10)	2.370(4)	Er(1)-N(1)	2.507(5)
O(3)#1-Er(1)-O(6)	90.28(18)	O(8)#2-Er(1)-O(11)	80.21(15)
O(3)#1-Er(1)-O(8)#2	77.52(16)	O(10)-Er(1)-O(11)	68.50(15)
O(6)-Er(1)-O(8)#2	153.60(16)	O(9)-Er(1)-O(11)	145.73(16)

O(3)#1-Er(1)-O(10)	142.16(16)	O(3)#1-Er(1)-O(7)	126.40(17)
O(6)-Er(1)-O(10)	96.11(17)	O(6)-Er(1)-O(7)	129.12(16)
O(8)#2-Er(1)-O(10)	80.56(15)	O(8)#2-Er(1)-O(7)	75.82(14)
O(3)#1-Er(1)-O(9)	72.07(17)	O(10)-Er(1)-O(7)	76.16(16)
O(6)-Er(1)-O(9)	90.1(2)	O(9)-Er(1)-O(7)	73.19(17)
O(8)#2-Er(1)-O(9)	107.79(18)	O(11)-Er(1)-O(7)	139.91(15)
O(10)-Er(1)-O(9)	144.81(18)	O(3)#1-Er(1)-N(1)	137.67(17)
O(3)#1-Er(1)-O(11)	77.60(15)	O(6)-Er(1)-N(1)	64.70(16)
O(6)-Er(1)-O(11)	74.29(17)	O(8)#2-Er(1)-N(1)	138.03(14)
O(11)-Er(1)-N(1)	122.31(15)	O(10)-Er(1)-N(1)	77.21(16)
O(7)-Er(1)-N(1)	64.55(15)	O(9)-Er(1)-N(1)	74.31(18)

#1: -x,-y+2,-z+1; #2: -x,y-1/2,-z+3/2; #3: -x,y+1/2,-z+3/2