Supplementary Material (ESI) for CrystEngComm

Supplementary Information

A Series of Novel Chiral Lanthanide Coordination Polymers with Channels Constructed from 16Ln-Based Cage-like Building Units

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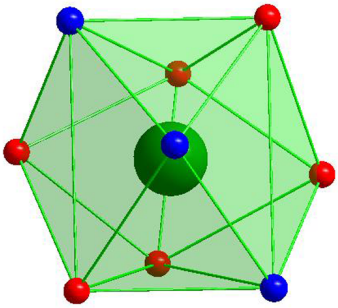

Fig. S1 The tricapped trigonal prism geometry of La center.

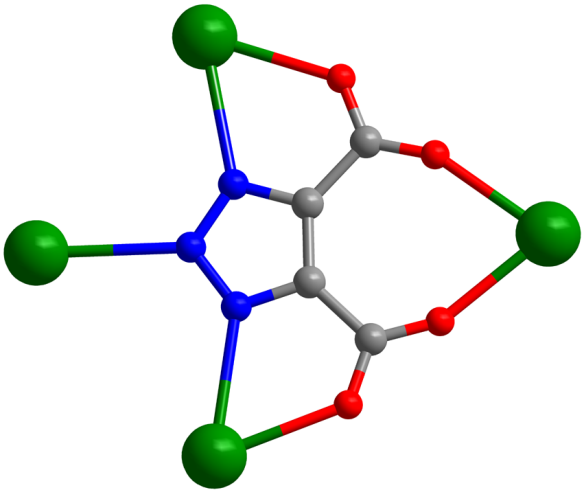

Fig. S2 Coordination mode of the tda^{3-} ligand.

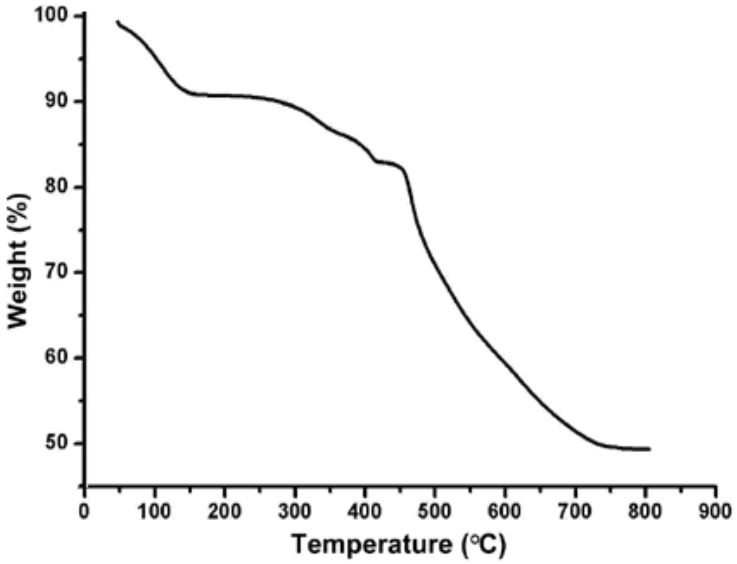

Fig. S3 TGA curve for complex **6.**

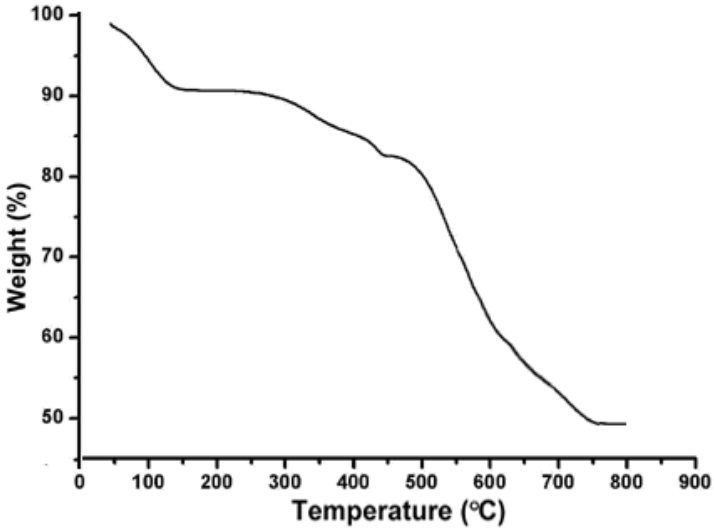

Fig. S4 TGA curve for complex **7**.

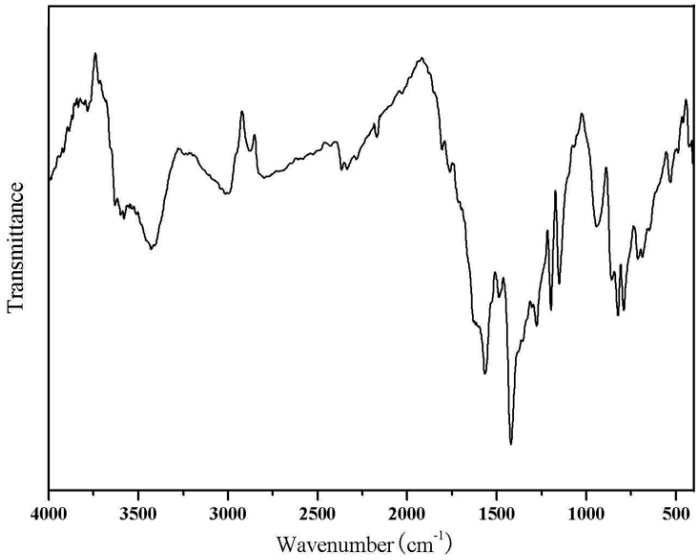

Fig. S5 Infrared spectrum of **1**.

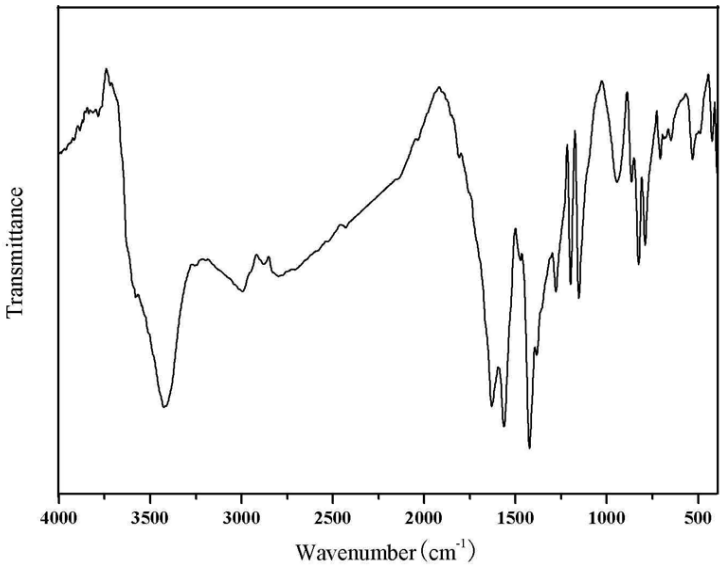

Fig. S6 Infrared spectrum of **2.**

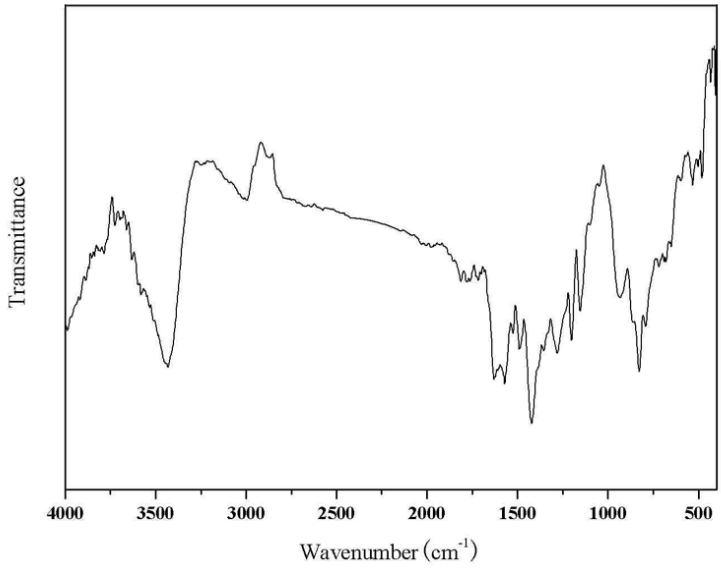

Fig. S7 Infrared spectrum of **3.**

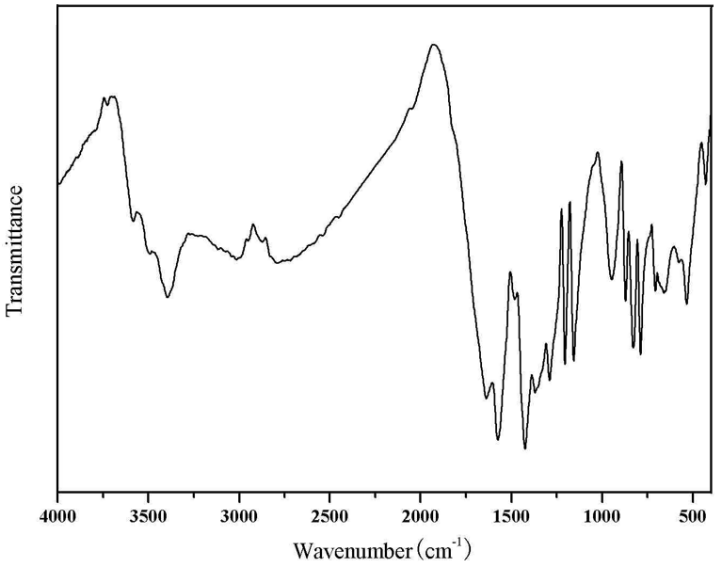

Fig. S8 Infrared spectrum of **4.**

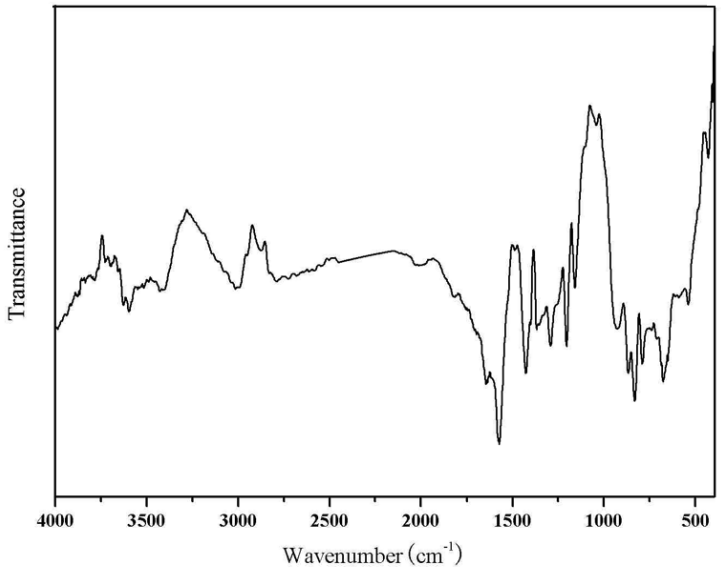

Fig. S9 Infrared spectrum of **5.**

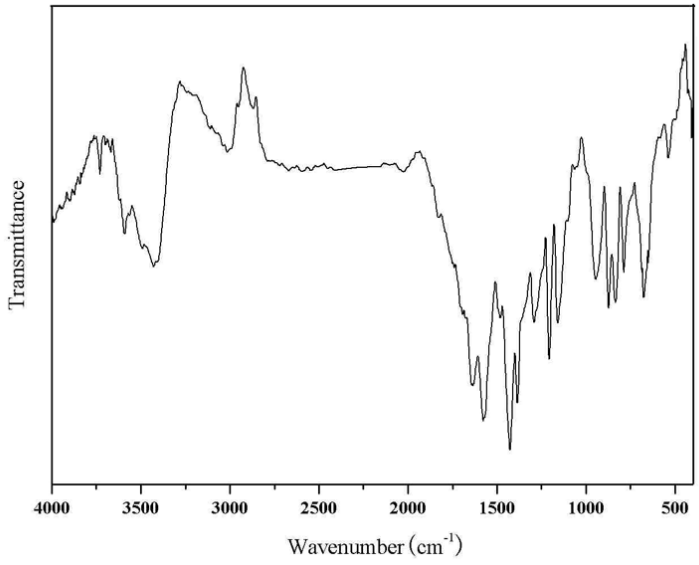

Fig. S10 Infrared spectrum of **6.**

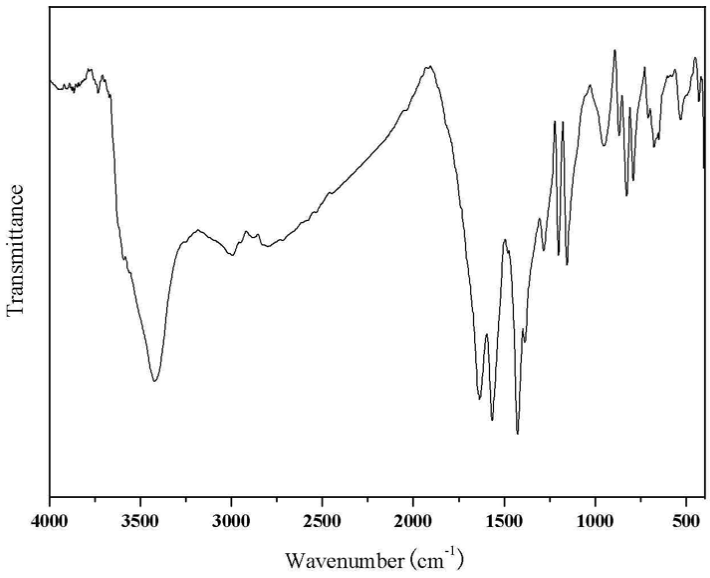

Fig. S11 Infrared spectrum of **7.**

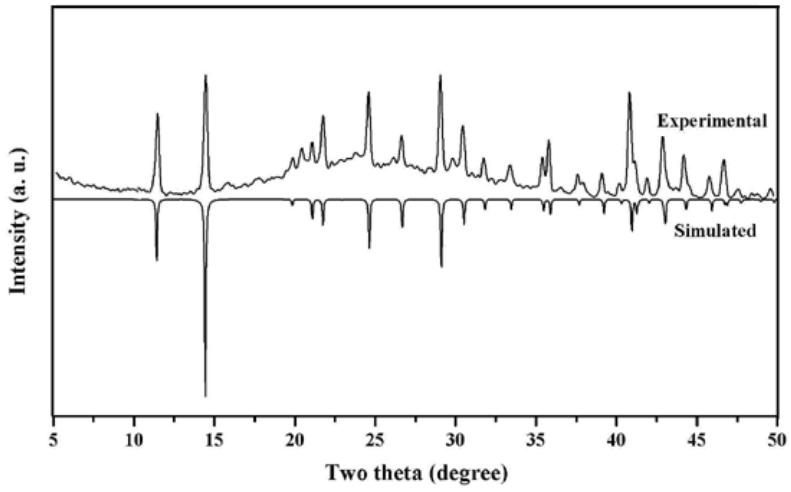

Fig. S12 Experimental and simulated XRD patterns for **1.**

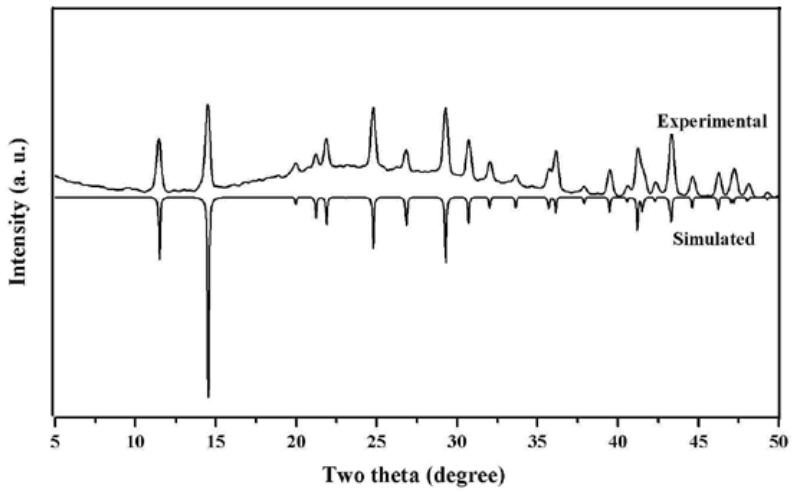

Fig. S13 Experimental and simulated XRD patterns for **2.**

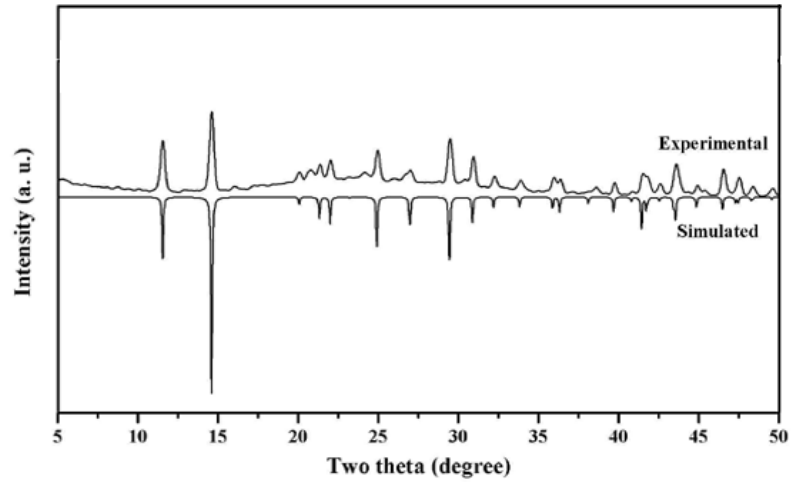

Fig. S14 Experimental and simulated XRD patterns for **3.**

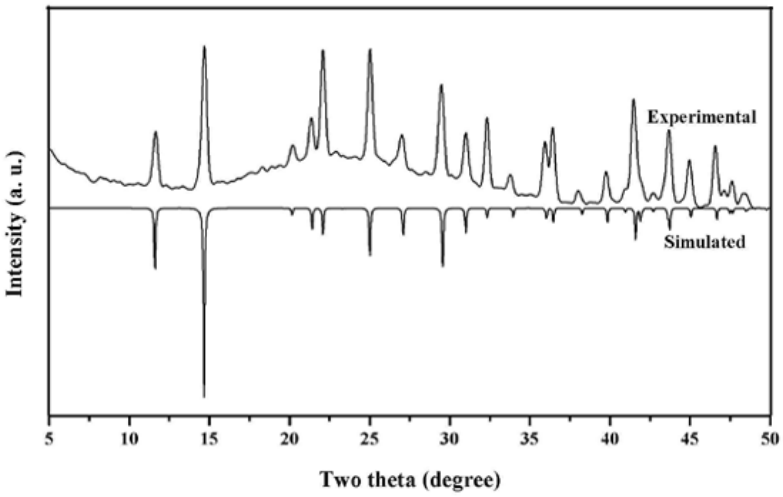

Fig. S15 Experimental and simulated XRD patterns for **4.**

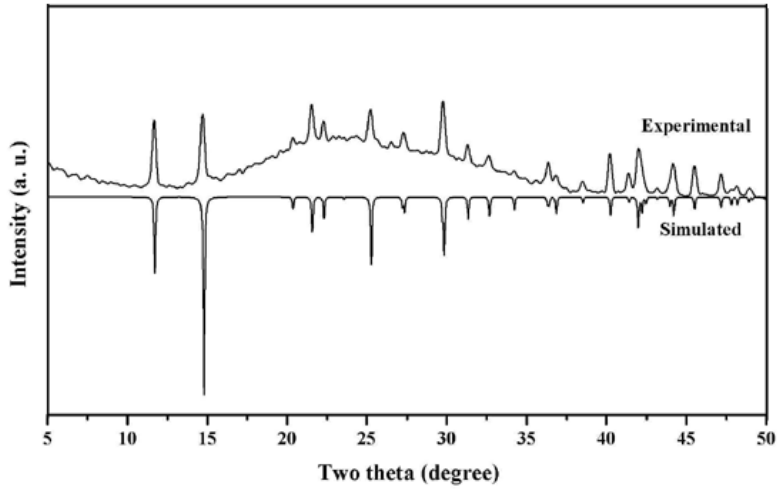

Fig. S16 Experimental and simulated XRD patterns for **5.**

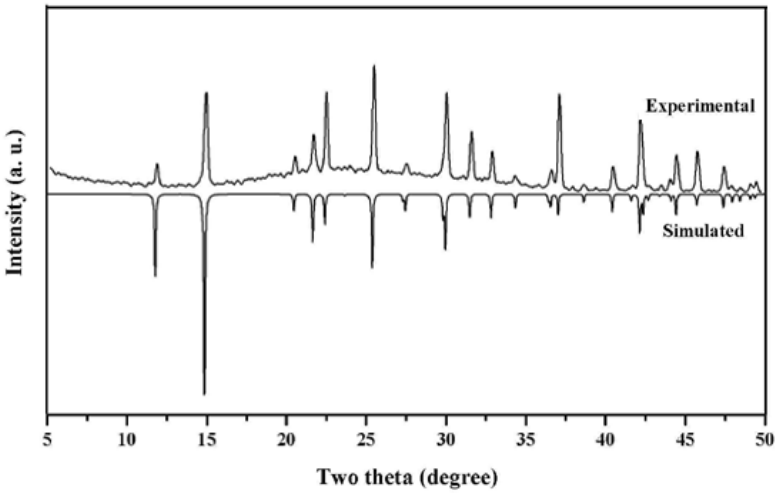

Fig. S17 Experimental and simulated XRD patterns for **6.**

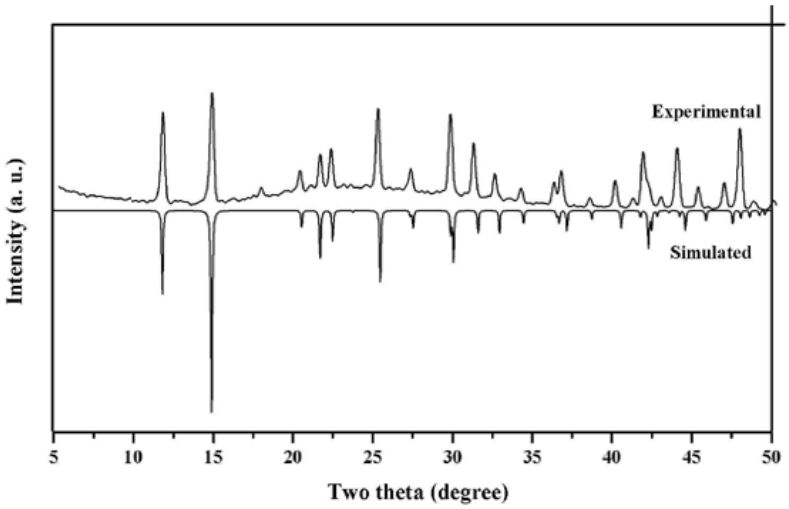

Fig. S18 Experimental and simulated XRD patterns for **7.**

Table S1 Selected bond lengths [Å] and angles [°] for complexes **1–7.**

		Compound **1**	
La(1)—O(1)	2.425(4)	La(1)—O(2)	2.503(4)
La(1)—N(2)	2.696(6)	La(1)—O(1W)	2.707(3)
La(1)—N(1)	2.711(5)		
O(1)#1—La(1)—O(1)	74.34(19)	O(1)#1—La(1)—O(2)	75.27(17)
O(1)—La(1)—O(2)	72.89(15)	O(2)—La(1)—O(2)#1	139.7(2)
O(1)—La(1)—N(2)	142.83(9)	O(2)—La(1)—N(2)	110.13(11)
O(1)#1—La(1)—O(1W)	76.45(12)	O(1)—La(1)—O(1W)	139.99(15)
O(2)—La(1)—O(1W)	124.43(11)	O(2)#1—La(1)—O(1W)	70.38(16)
N(2)—La(1)—O(1W)	70.51(9)	O(1W)—La(1)—O(1W)#2	141.02(18)
O(1)#1—La(1)—N(1)	80.74(15)	O(1)—La(1)—N(1)	131.93(15)
O(2)—La(1)—N(1)	61.21(13)	O(2)#1—La(1)—N(1)	134.48(15)
N(2)—La(1)—N(1)	71.44(10)	O(1W)—La(1)—N(1)	67.72(13)
O(1W)#2—La(1)—N(1)	99.60(11)	N(1)—La(1)—N(1)#1	142.9(2)
		Compound **2**	
Ce(1)—O(1)#1	2.408(4)	Ce(1)—O(2)	2.484(4)
Ce(1)—N(2)#4	2.669(6)	Ce(1)—O(1W)	2.687(3)
Ce(1)—N(1)	2.692(5)		
O(1)#1—Ce(1)—O(1)#2	75.05(19)	O(1)#1—Ce(1)—O(2)	75.56(17)
O(1)#2—Ce(1)—O(2)	72.70(15)	O(2)—Ce(1)—O(2)#3	139.7(2)
O(1)#1—Ce(1)—N(2)#4	142.48(9)	O(2)—Ce(1)—N(2)#4	110.16(11)
O(1)#1—Ce(1)—O(1W)#5	76.28(12)	O(1)#2—Ce(1)—O(1W)#5	140.50(14)
O(2)—Ce(1)—O(1W)#5	124.68(11)	O(2)#3—Ce(1)—O(1W)#5	70.32(15)
N(2)#4—Ce(1)—O(1W)#5	70.31(9)	O(1)#1—Ce(1)—O(1W)	140.50(15)
O(1W)#5—Ce(1)—O(1W)	140.62(17)	O(1)#1—Ce(1)—N(1)	80.51(15)
O(1)#2—Ce(1)—N(1)	132.24(15)	O(2)—Ce(1)—N(1)	61.69(13)
O(2)#3—Ce(1)—N(1)	134.01(15)	N(2)#4—Ce(1)—N(1)	71.34(10)
O(1W)#5—Ce(1)—N(1)	67.38(13)	O(1W)—Ce(1)—N(1)	99.73(11)
		Compound **3**	
Pr(1)—O(1)#1	2.389(5)	Pr(1)—O(2)	2.465(5)
Pr(1)—N(2)#4	2.643(7)	Pr(1)—O(1W)	2.666(3)
Pr(1)—N(1)	2.672(5)		
O(1)#1—Pr(1)—O(1)#2	75.5(2)	O(1)#1—Pr(1)—O(2)	75.64(19)
O(1)#2—Pr(1)—O(2)	72.59(17)	O(2)—Pr(1)—O(2)#3	139.5(3)
O(1)#1—Pr(1)—N(2)#4	142.25(10)	O(2)—Pr(1)—N(2)#4	110.24(13)
O(1)#1—Pr(1)—O(1W)	76.24(14)	O(1)#2—Pr(1)—O(1W)	140.76(16)
O(2)—Pr(1)—O(1W)	124.92(12)	O(2)#3—Pr(1)—O(1W)	70.27(17)
N(2)#4—Pr(1)—O(1W)	70.16(10)	O(1W)—Pr(1)—O(1W)#4	140.3(2)
O(1)#1—Pr(1)—N(1)	80.11(17)	O(1)#2—Pr(1)—N(1)	132.44(17)
O(2)—Pr(1)—N(1)	62.03(15)	O(2)#3—Pr(1)—N(1)	133.56(17)

N(2)#4—Pr(1)—N(1)	71.45(11)	O(1W)—Pr(1)—N(1)	67.13(15)
O(1W)#4—Pr(1)—N(1)	99.95(13)	N(1)—Pr(1)—N(1)#3	142.9(2)

Compound **4**

Nd(1)—O(1)	2.374(4)	Nd(1)—O(2)#2	2.455(4)
Nd(1)—N(2)#4	2.623(7)	Nd(1)—O(1W)	2.653(3)
Nd(1)—N(1)#2	2.657(5)		
O(1)#1—Nd(1)—O(1)	76.3(2)	O(1)#1—Nd(1)—O(2)#2	75.94(19)
O(1)—Nd(1)—O(2)#2	72.51(16)	O(2)#2—Nd(1)—O(2)#3	139.6(2)
O(1)#1—Nd(1)—N(2)#4	141.86(10)	O(2)#2—Nd(1)—N(2)#4	110.21(12)
O(1)#1—Nd(1)—O(1W)	75.92(13)	O(1)—Nd(1)—O(1W)	141.10(16)
O(2)#2—Nd(1)—O(1W)	125.14(12)	O(2)#3—Nd(1)—O(1W)	70.09(17)
N(2)#4—Nd(1)—O(1W)	70.11(10)	O(1W)—Nd(1)—O(1W)#5	140.23(19)
O(1)#1—Nd(1)—N(1)#2	79.92(16)	O(1)—Nd(1)—N(1)#2	132.66(16)
O(2)#2—Nd(1)—N(1)#2	62.24(15)	O(2)#3—Nd(1)—N(1)#2	133.36(17)
N(2)#4—Nd(1)—N(1)#2	71.37(11)	O(1W)—Nd(1)—N(1)#2	67.10(14)
O(1W)#5—Nd(1)—N(1)#2	99.89(12)	N(1)#2—Nd(1)—N(1)#3	142.7(2)

Compound **5**

Sm(1)—O(1)#1	2.341(5)	Sm(1)—O(2)	2.429(6)
Sm(1)—N(2)#4	2.572(8)	Sm(1)—N(1)	2.624(6)
Sm(1)—O(1W)	2.630(4)		
O(1)#1—Sm(1)—O(1)#2	78.2(2)	O(1)#1—Sm(1)—O(2)	76.5(2)
O(1)#2—Sm(1)—O(2)	72.9(2)	O(2)—Sm(1)—O(2)#3	140.2(3)
O(1)#1—Sm(1)—N(2)#4	140.91(12)	O(2)—Sm(1)—N(2)#4	109.89(16)
O(1)#1—Sm(1)—N(1)	78.71(19)	O(1)#2—Sm(1)—N(1)	133.5(2)
O(2)—Sm(1)—N(1)	62.79(18)	O(2)#3—Sm(1)—N(1)	132.3(2)
N(2)#4—Sm(1)—N(1)	71.48(13)	N(1)—Sm(1)—N(1)#3	143.0(3)
O(1)#1—Sm(1)—O(1W)	75.12(16)	O(1)#2—Sm(1)—O(1W)	141.2(2)
O(2)—Sm(1)—O(1W)	125.84(15)	O(2)#3—Sm(1)—O(1W)	69.1(2)
N(2)#4—Sm(1)—O(1W)	70.31(12)	N(1)—Sm(1)—O(1W)	67.01(18)
N(1)#3—Sm(1)—O(1W)	100.17(15)	O(1W)—Sm(1)—O(1W)#4	140.6(2)

Compound **6**

Eu(1)—O(1)#1	2.332(5)	Eu(1)—O(2)	2.418(5)
Eu(1)—N(2)#4	2.567(7)	Eu(1)—O(1W)	2.613(4)
Eu(1)—N(1)	2.617(6)		
O(1)#1—Eu(1)—O(1)#2	78.5(2)	O(1)#1—Eu(1)—O(2)	77.0(2)
O(1)#2—Eu(1)—O(2)	72.66(19)	O(2)—Eu(1)—O(2)#3	140.6(3)
O(1)#1—Eu(1)—N(2)#4	140.73(12)	O(2)—Eu(1)—N(2)#4	109.71(16)
O(1)#1—Eu(1)—O(1W)	74.97(15)	O(1)#2—Eu(1)—O(1W)	141.74(19)
O(2)—Eu(1)—O(1W)	125.93(14)	O(2)#3—Eu(1)—O(1W)	69.0(2)
N(2)#4—Eu(1)—O(1W)	70.14(12)	O(1W)—Eu(1)—O(1W)#4	140.3(2)
O(1)#1—Eu(1)—N(1)	78.67(19)	O(1)#2—Eu(1)—N(1)	133.59(19)
O(2)—Eu(1)—N(1)	63.09(17)	O(2)#3—Eu(1)—N(1)	131.86(19)
N(2)#4—Eu(1)—N(1)	71.43(13)	O(1W)—Eu(1)—N(1)	66.61(17)
O(1W)#4—Eu(1)—N(1)	100.41(14)	N(1)—Eu(1)—N(1)#3	142.9(3)

Compound **7**

Gd(1)—O(1)	2.318(5)	Gd(1)—O(2)	2.417(6)
Gd(1)—N(2)#2	2.547(8)	Gd(1)—O(1W)	2.602(4)
Gd(1)—N(1)	2.604(6)		
O(1)#1—Gd(1)—O(1)	79.3(2)	O(1)—Gd(1)—O(2)	77.4(2)
O(1)—Gd(1)—O(2)#1	72.6(2)	O(2)#1—Gd(1)—O(2)	140.7(3)
O(1)#1—Gd(1)—N(2)#2	140.35(12)	O(2)#1—Gd(1)—N(2)#2	109.64(17)
O(1)#1—Gd(1)—O(1W)#2	74.60(16)	O(1)—Gd(1)—O(1W)#2	142.1(2)
O(2)#1—Gd(1)—O(1W)#2	126.10(15)	O(2)—Gd(1)—O(1W)#2	68.8(2)
N(2)#2—Gd(1)—O(1W)#2	70.14(12)	O(1W)#2—Gd(1)—O(1W)	140.3(2)
O(1)#1—Gd(1)—N(1)#1	78.3(2)	O(1)—Gd(1)—N(1)#1	133.7(2)
O(2)#1—Gd(1)—N(1)#1	63.28(19)	O(2)—Gd(1)—N(1)#1	131.5(2)
N(2)#2—Gd(1)—N(1)#1	71.49(14)	O(1W)#2—Gd(1)—N(1)#1	66.50(19)
O(1W)—Gd(1)—N(1)#1	100.55(16)	N(1)#1—Gd(1)—N(1)	143.0(3)

Symmetry codes: #1: x-y,-y,-z+1/3, #2: -y+1,x-y-1,z-1/3, #3: -x+y+2,-x+1,z+1/3, #4 : -y,x-y-1,z-1/3, #5: -x+y+1,-x,z+1/3.