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Electronic Supplementary Information (ESI) for

Homochiral three-dimensional noncentrosymmetric lanthanide coordination polymers directed by chiral linkers: syntheses, crystal structures, and optical properties

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Figure S1. SEM-EDX data for **Ln(R)** and **Ln(S)** (Ln = La, Ce, and Pr).

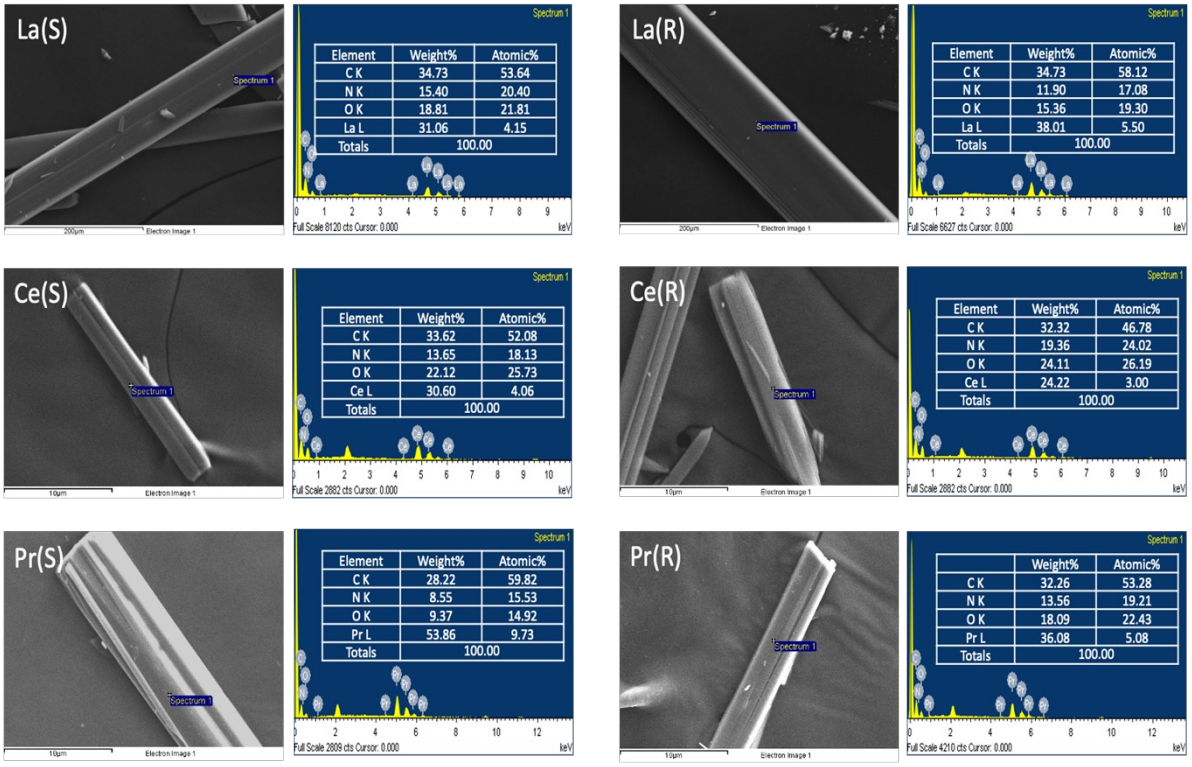

Figure S2. Calculated and experimental powder X-ray diffraction patterns for **Ln(R)** and **Ln(S)** (Ln = La, Ce, and Pr).

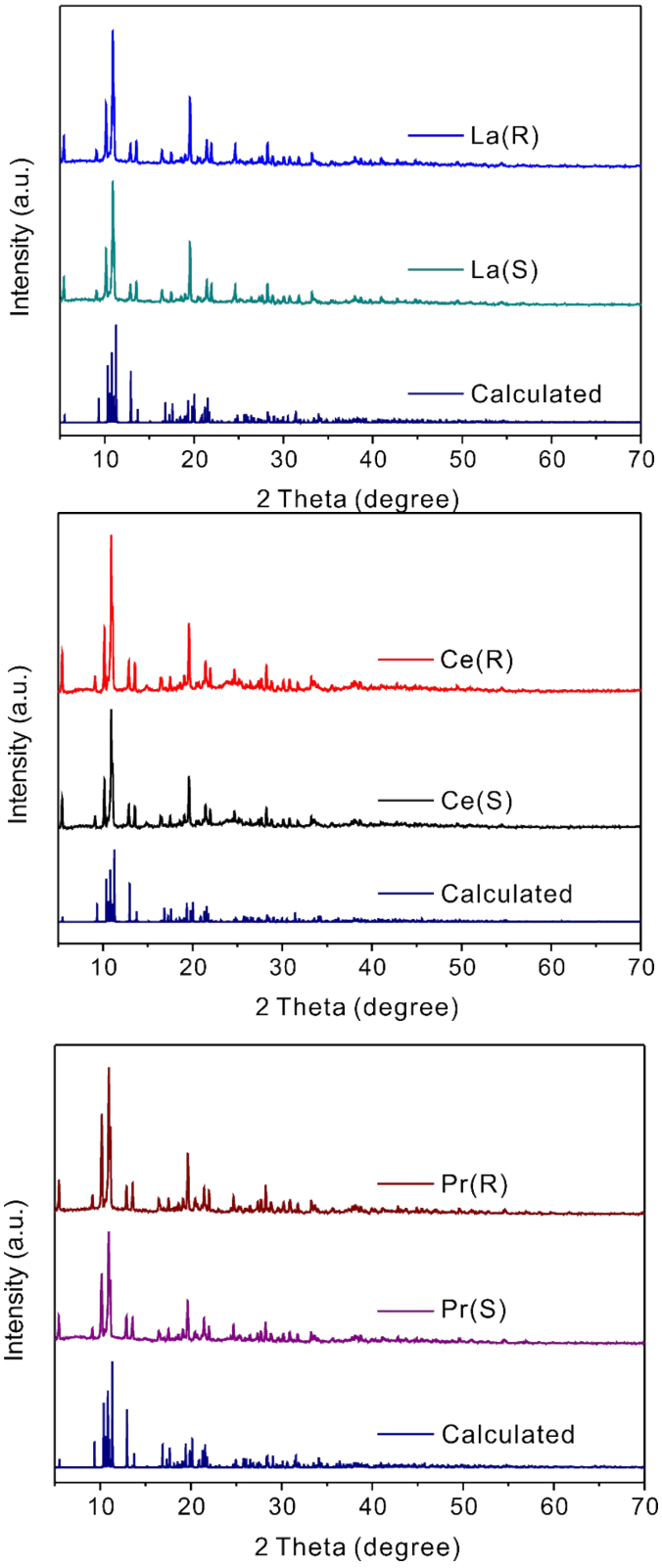

Figure S3. A diagram representing the hydrogen bonding network among the organic ligands (cyan, La; black, C; gray, H; blue, N; red, O; orange, hydrogen bonding).

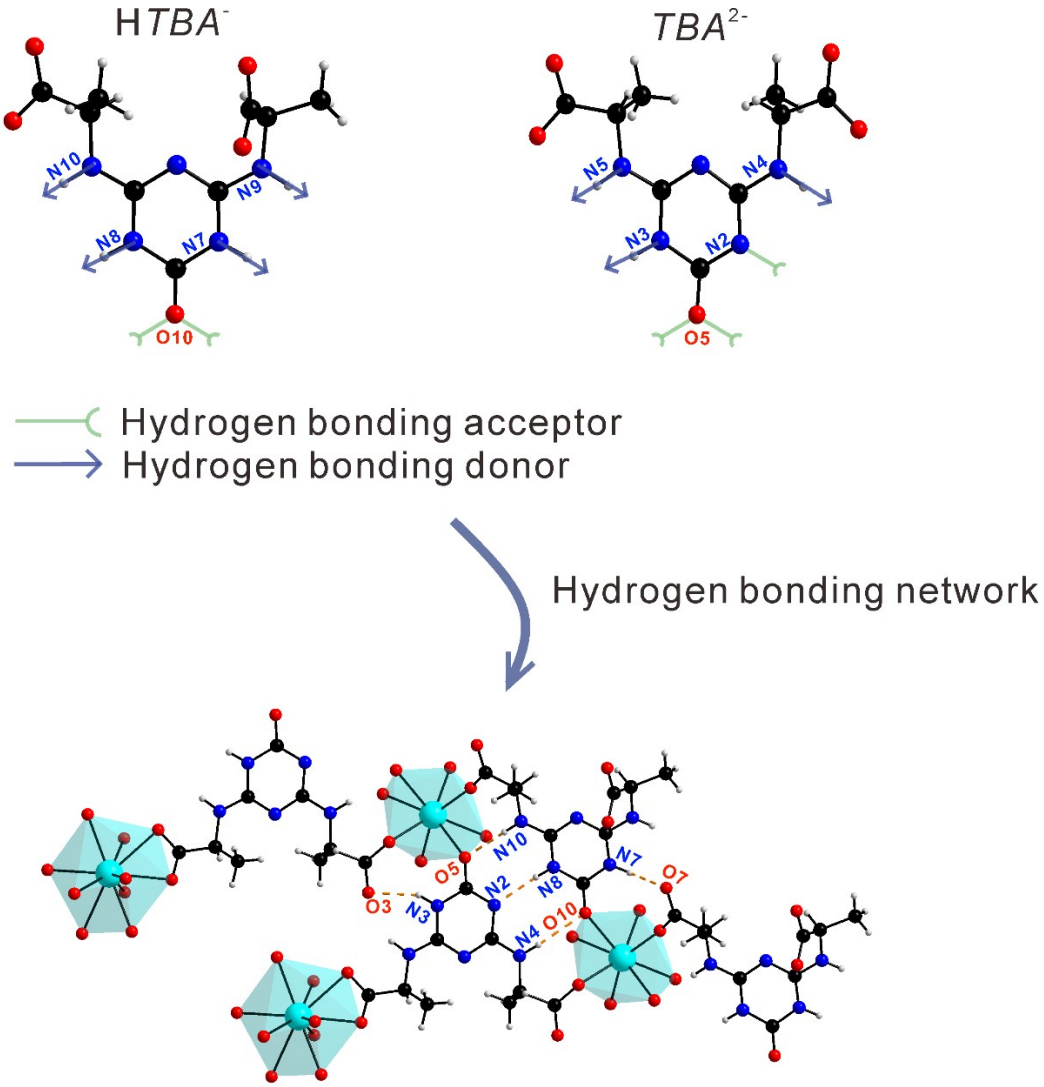

Figure S4. Thermogravimetric analysis diagrams and PXRD data after calcination for **La(R)**, **Ce(R)**, and **Pr(R)**.

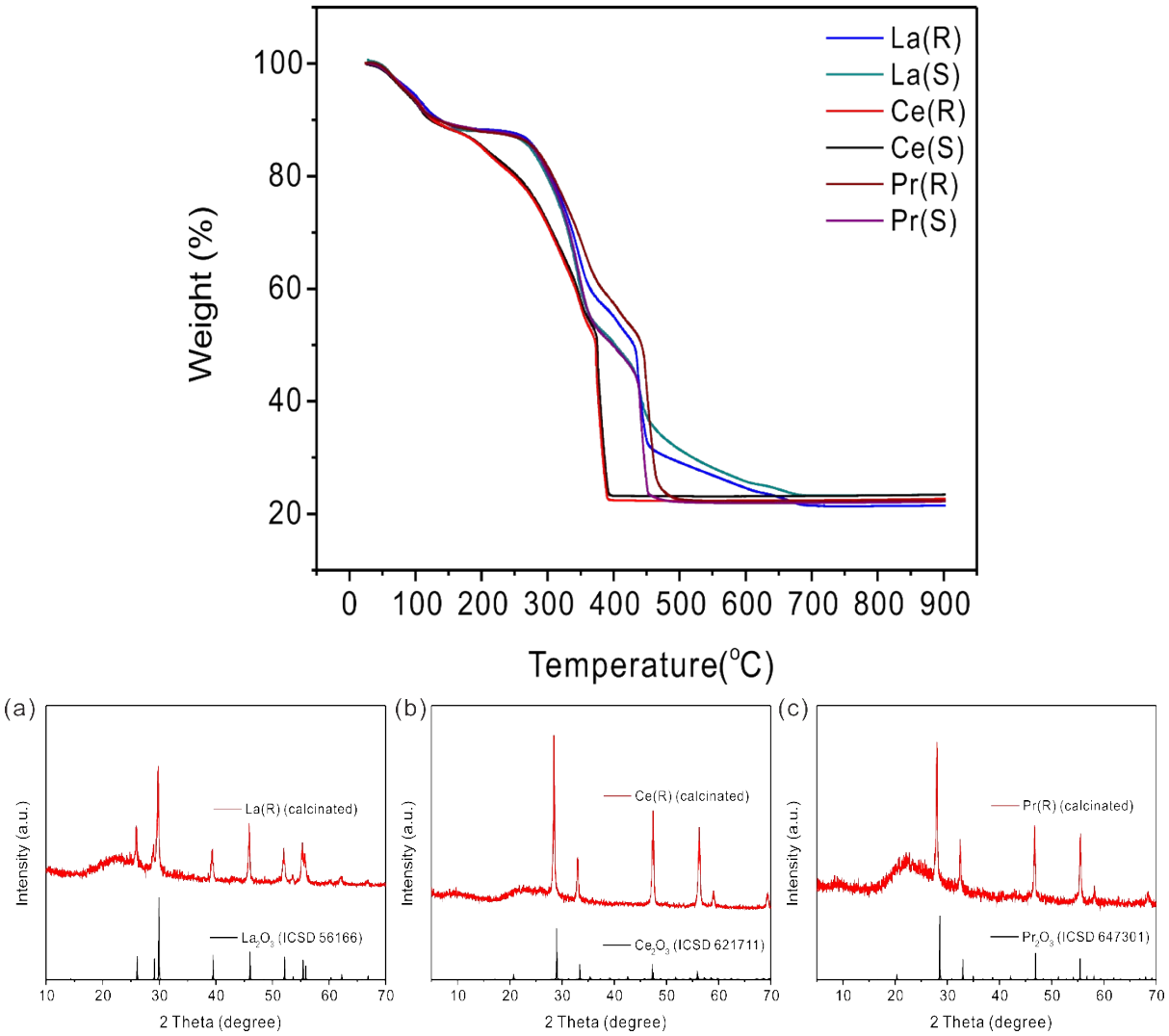

Figure S5. Infrared spectra for **Ln(R)** and **Ln(S)** (Ln = La, Ce, and Pr).

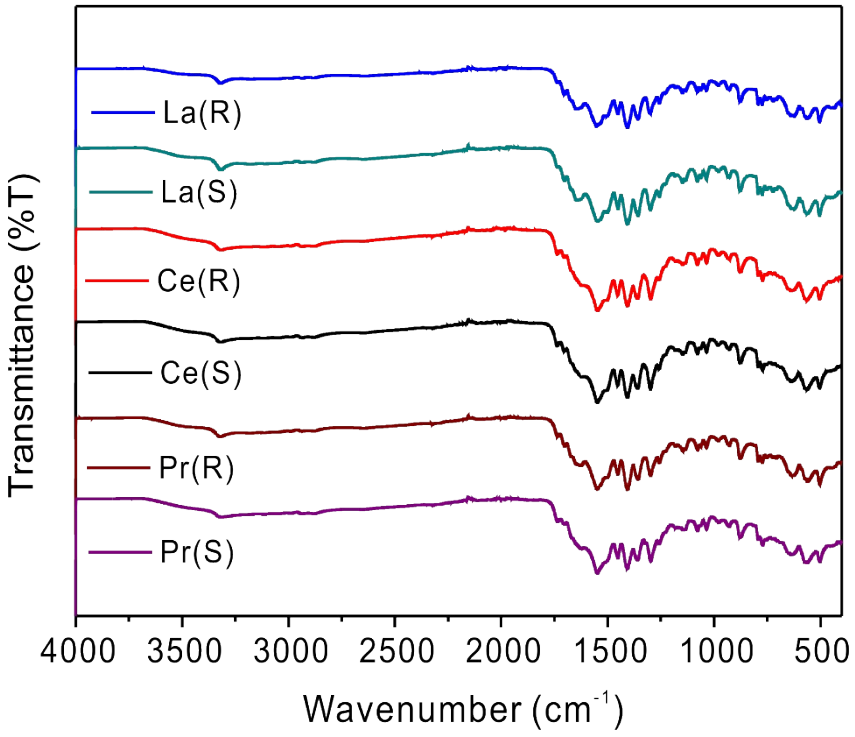

Figure S6. UV-vis spectra for (a and b) **Ln(R)** and **Ln(S)** (Ln = La, Ce, and Pr). (Inset) Magnified absorption peaks in the range of 400–650 nm for Pr(R) and Pr(S).

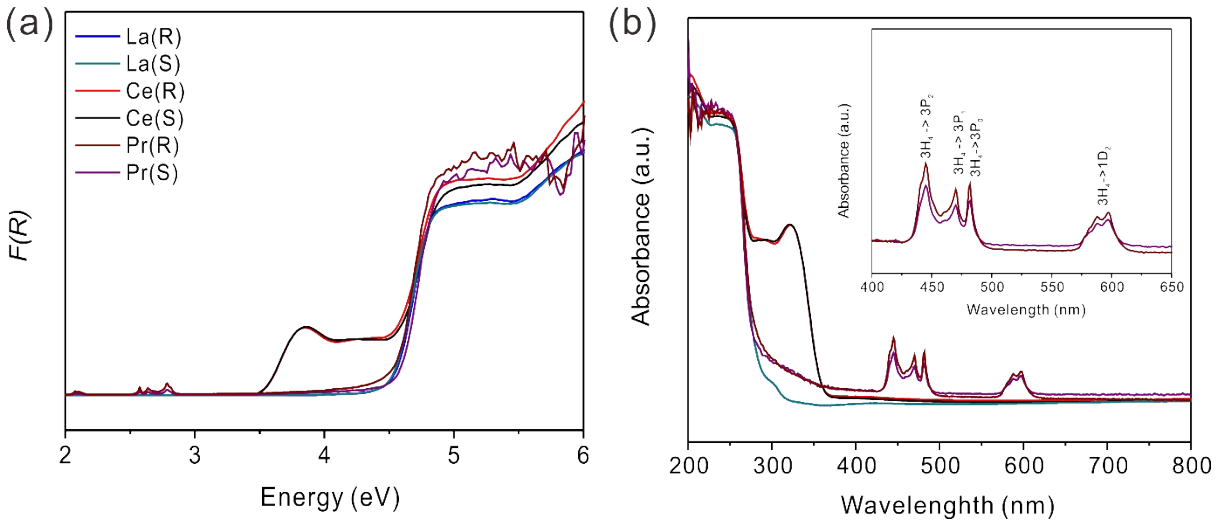

Figure S7. Ball-and-stick models of antiparallel environments of TBA^{2-} and HTBA^{-} ligand (black, C; gray, H; blue, N; red, O).

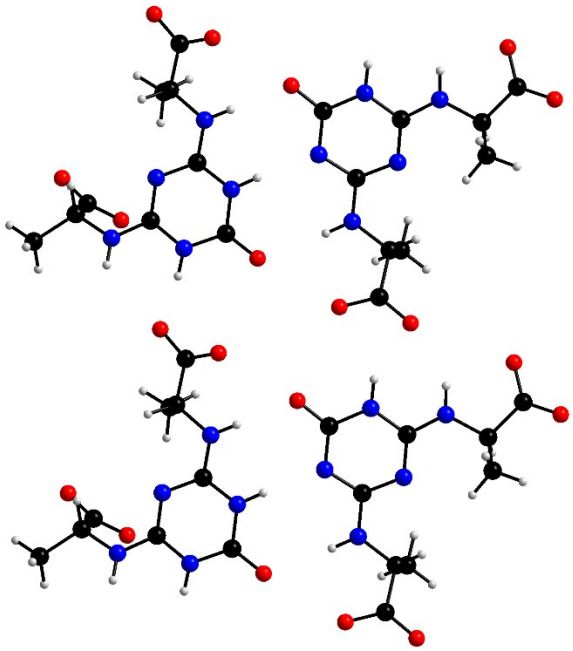

Table S1. Bond lengths [Å] and angles [°] for **La(R)**.

Selected bond distances (Å)			
La(1)-O(6)	2.389(3)	N(1)-C(3)	1.320(7)
La(1)-O(6)#1	2.389(3)	N(1)-C(2)	1.349(6)
La(1)-O(4)	2.415(4)	N(2)-C(1)	1.337(7)
La(1)-O(4)#1	2.415(4)	N(2)-C(2)	1.362(6)
La(1)-O(5)#2	2.583(4)	N(3)-C(3)	1.366(6)
La(1)-O(5)#3	2.583(4)	N(3)-C(1)	1.383(6)
La(1)-O(10)#4	2.624(3)	N(4)-C(2)	1.334(6)
La(1)-O(10)#5	2.624(3)	N(4)-C(7)	1.470(6)
La(2)-O(2)	2.542(4)	N(5)-C(3)	1.328(6)
La(2)-O(2)#6	2.542(4)	N(5)-C(4)	1.461(6)
La(2)-O(11)#6	2.572(4)	N(6)-C(11)	1.323(7)
La(2)-O(11)	2.572(4)	N(6)-C(12)	1.344(6)
La(2)-O(8)#7	2.592(4)	N(7)-C(10)	1.365(6)
La(2)-O(8)#8	2.592(4)	N(7)-C(11)	1.372(6)
La(2)-O(9)#7	2.600(4)	N(8)-C(10)	1.360(6)
La(2)-O(9)#8	2.600(4)	N(8)-C(12)	1.366(6)
La(2)-O(1)#6	2.724(3)	N(9)-C(11)	1.323(6)
La(2)-O(1)	2.724(3)	N(9)-C(16)	1.462(6)
O(1)-C(5)	1.256(7)	N(10)-C(12)	1.320(6)
O(2)-C(5)	1.251(7)	N(10)-C(13)	1.475(6)
O(3)-C(8)	1.247(6)	C(4)-C(5)	1.525(7)
O(4)-C(8)	1.268(6)	C(4)-C(6)	1.544(9)
O(5)-C(1)	1.248(6)	C(7)-C(8)	1.529(7)
O(6)-C(14)	1.276(6)	C(7)-C(9)	1.530(9)
O(7)-C(14)	1.243(7)	C(13)-C(14)	1.510(7)
O(8)-C(17)	1.261(6)	C(13)-C(15)	1.519(9)
O(9)-C(17)	1.252(6)	C(16)-C(18)	1.529(7)
O(10)-C(10)	1.237(6)	C(16)-C(17)	1.540(7)
Selected bond angle (°)			
O(6)-La(1)-O(6)#1	148.38(18)	O(11)-La(2)-O(1)	136.07(12)
O(6)-La(1)-O(4)	111.27(13)	O(8)#7-La(2)-O(1)	103.19(12)
O(6)#1-La(1)-O(4)	77.89(12)	O(8)#8-La(2)-O(1)	69.33(12)
O(6)-La(1)-O(4)#1	77.89(12)	O(9)#7-La(2)-O(1)	70.17(12)
O(6)#1-La(1)-O(4)#1	111.26(13)	O(9)#8-La(2)-O(1)	114.74(12)
O(4)-La(1)-O(4)#1	147.41(19)	O(1)#6-La(2)-O(1)	156.73(17)
O(6)-La(1)-O(5)#2	69.05(12)	C(5)-O(1)-La(2)	89.0(3)
O(6)#1-La(1)-O(5)#2	84.46(12)	C(5)-O(2)-La(2)	97.7(3)
O(4)-La(1)-O(5)#2	77.59(12)	C(8)-O(4)-La(1)	146.3(4)
O(4)#1-La(1)-O(5)#2	133.04(12)	C(1)-O(5)-La(1)#4	134.2(3)
O(6)-La(1)-O(5)#3	84.46(12)	C(14)-O(6)-La(1)	168.2(4)
O(6)#1-La(1)-O(5)#3	69.05(12)	C(17)-O(8)-La(2)#9	93.0(3)
O(4)-La(1)-O(5)#3	133.04(12)	C(17)-O(9)-La(2)#9	92.9(3)
O(4)#1-La(1)-O(5)#3	77.59(12)	C(10)-O(10)-La(1)#2	144.7(3)
O(5)#2-La(1)-O(5)#3	67.11(17)	C(3)-N(1)-C(2)	115.4(4)
O(6)-La(1)-O(10)#4	76.85(12)	C(1)-N(2)-C(2)	116.7(4)
O(6)#1-La(1)-O(10)#4	133.33(12)	C(3)-N(3)-C(1)	120.9(4)
O(4)-La(1)-O(10)#4	70.77(12)	C(2)-N(4)-C(7)	122.4(4)
O(4)#1-La(1)-O(10)#4	81.78(13)	C(3)-N(5)-C(4)	124.6(5)
O(5)#2-La(1)-O(10)#4	119.96(12)	C(11)-N(6)-C(12)	116.0(4)
O(5)#3-La(1)-O(10)#4	154.63(11)	C(10)-N(7)-C(11)	120.7(4)

O(6)-La(1)-O(10)#5	133.33(12)	C(10)-N(8)-C(12)	121.2(4)
O(6)#1-La(1)-O(10)#5	76.85(12)	C(11)-N(9)-C(16)	121.9(4)
O(4)-La(1)-O(10)#5	81.78(13)	C(12)-N(10)-C(13)	121.0(4)
O(4)#1-La(1)-O(10)#5	70.77(12)	O(5)-C(1)-N(2)	123.1(4)
O(5)#2-La(1)-O(10)#5	154.63(11)	O(5)-C(1)-N(3)	118.1(4)
O(5)#3-La(1)-O(10)#5	119.96(12)	N(2)-C(1)-N(3)	118.7(4)
O(10)#4-La(1)-O(10)#5	65.34(16)	N(4)-C(2)-N(1)	116.3(4)
O(2)-La(2)-O(2)#6	63.83(19)	N(4)-C(2)-N(2)	117.1(4)
O(2)-La(2)-O(11)#6	115.63(13)	N(1)-C(2)-N(2)	126.6(4)
O(2)#6-La(2)-O(11)#6	164.28(14)	N(1)-C(3)-N(5)	121.9(5)
O(2)-La(2)-O(11)	164.28(14)	N(1)-C(3)-N(3)	121.5(4)
O(2)#6-La(2)-O(11)	115.63(13)	N(5)-C(3)-N(3)	116.6(5)
O(11)#6-La(2)-O(11)	69.46(18)	N(5)-C(4)-C(5)	106.5(5)
O(2)-La(2)-O(8)#7	72.81(14)	N(5)-C(4)-C(6)	112.4(5)
O(2)#6-La(2)-O(8)#7	76.72(14)	C(5)-C(4)-C(6)	109.1(5)
O(11)#6-La(2)-O(8)#7	118.69(13)	O(2)-C(5)-O(1)	123.1(5)
O(11)-La(2)-O(8)#7	91.64(13)	O(2)-C(5)-C(4)	116.9(5)
O(2)-La(2)-O(8)#8	76.72(14)	O(1)-C(5)-C(4)	120.0(5)
O(2)#6-La(2)-O(8)#8	72.81(14)	N(4)-C(7)-C(8)	109.8(4)
O(11)#6-La(2)-O(8)#8	91.64(13)	N(4)-C(7)-C(9)	111.1(5)
O(11)-La(2)-O(8)#8	118.69(13)	C(8)-C(7)-C(9)	109.1(5)
O(8)#7-La(2)-O(8)#8	143.95(19)	O(3)-C(8)-O(4)	124.6(5)
O(2)-La(2)-O(9)#7	78.42(15)	O(3)-C(8)-C(7)	117.7(5)
O(2)#6-La(2)-O(9)#7	122.31(15)	O(4)-C(8)-C(7)	117.6(4)
O(11)#6-La(2)-O(9)#7	71.16(13)	O(10)-C(10)-N(8)	121.6(4)
O(11)-La(2)-O(9)#7	89.99(13)	O(10)-C(10)-N(7)	122.7(5)
O(8)#7-La(2)-O(9)#7	50.33(12)	N(8)-C(10)-N(7)	115.7(4)
O(8)#8-La(2)-O(9)#7	139.47(11)	N(6)-C(11)-N(9)	120.0(4)
O(2)-La(2)-O(9)#8	122.31(15)	N(6)-C(11)-N(7)	123.2(4)
O(2)#6-La(2)-O(9)#8	78.42(15)	N(9)-C(11)-N(7)	116.8(4)
O(11)#6-La(2)-O(9)#8	89.98(13)	N(10)-C(12)-N(6)	119.1(4)
O(11)-La(2)-O(9)#8	71.16(13)	N(10)-C(12)-N(8)	118.2(4)
O(8)#7-La(2)-O(9)#8	139.47(11)	N(6)-C(12)-N(8)	122.7(4)
O(8)#8-La(2)-O(9)#8	50.33(12)	N(10)-C(13)-C(14)	110.2(4)
O(9)#7-La(2)-O(9)#8	157.3(2)	N(10)-C(13)-C(15)	111.1(5)
O(2)-La(2)-O(1)#6	108.01(12)	C(14)-C(13)-C(15)	112.6(5)
O(2)#6-La(2)-O(1)#6	49.34(12)	O(7)-C(14)-O(6)	124.4(5)
O(11)#6-La(2)-O(1)#6	136.07(12)	O(7)-C(14)-C(13)	117.2(4)
O(11)-La(2)-O(1)#6	67.12(12)	O(6)-C(14)-C(13)	118.4(4)
O(8)#7-La(2)-O(1)#6	69.33(12)	N(9)-C(16)-C(18)	109.3(5)
O(8)#8-La(2)-O(1)#6	103.19(12)	N(9)-C(16)-C(17)	110.6(4)
O(9)#7-La(2)-O(1)#6	114.74(12)	C(18)-C(16)-C(17)	110.5(5)
O(9)#8-La(2)-O(1)#6	70.17(12)	O(9)-C(17)-O(8)	122.9(5)
O(2)-La(2)-O(1)	49.34(12)	O(9)-C(17)-C(16)	116.8(4)
O(2)#6-La(2)-O(1)	108.01(12)	O(8)-C(17)-C(16)	120.2(4)
O(11)#6-La(2)-O(1)	67.12(12)		

Symmetry operation: #1 -x+1,y,-z+1; #2 x,y-1,z; #3 -x+1,y-1,-z+1; #4 x,y+1,z; #5 -x+1,y+1,-z+1; #6 -x, y,-z; #7 x-1/2,y+3/2,z-1; #8 -x+1/2,y+3/2,-z+1;#9 x+1/2,y-3/2,z+1

Table S2. Bond lengths [Å] and angles [°] for **La(S)**.

Selected bond distances (Å)			
La(1)-O(6)	2.390(3)	N(1)-C(3)	1.317(6)
La(1)-O(6)#1	2.390(3)	N(1)-C(2)	1.349(6)
La(1)-O(4)	2.418(3)	N(2)-C(1)	1.340(6)
La(1)-O(4)#1	2.418(3)	N(2)-C(2)	1.363(6)
La(1)-O(5)#2	2.580(3)	N(3)-C(3)	1.370(6)
La(1)-O(5)#3	2.580(3)	N(3)-C(1)	1.376(6)
La(1)-O(10)#4	2.623(3)	N(4)-C(2)	1.335(6)
La(1)-O(10)#5	2.623(3)	N(4)-C(7)	1.461(6)
La(2)-O(2)#6	2.541(4)	N(5)-C(3)	1.328(6)
La(2)-O(2)	2.541(4)	N(5)-C(4)	1.460(6)
La(2)-O(11)	2.571(4)	N(6)-C(11)	1.328(6)
La(2)-O(11)#6	2.571(4)	N(6)-C(12)	1.340(5)
La(2)-O(8)#7	2.593(3)	N(7)-C(10)	1.363(6)
La(2)-O(8)#8	2.593(3)	N(7)-C(11)	1.372(6)
La(2)-O(9)#7	2.600(4)	N(8)-C(10)	1.362(6)
La(2)-O(9)#8	2.600(4)	N(8)-C(12)	1.367(6)
La(2)-O(1)#6	2.715(3)	N(9)-C(11)	1.317(6)
La(2)-O(1)	2.715(3)	N(9)-C(16)	1.462(6)
O(1)-C(5)	1.254(7)	N(10)-C(12)	1.319(6)
O(2)-C(5)	1.248(6)	N(10)-C(13)	1.473(6)
O(3)-C(8)	1.244(6)	C(4)-C(6)	1.527(8)
O(4)-C(8)	1.267(6)	C(4)-C(5)	1.527(7)
O(5)-C(1)	1.251(6)	C(7)-C(9)	1.521(9)
O(6)-C(14)	1.274(5)	C(7)-C(8)	1.529(7)
O(7)-C(14)	1.232(6)	C(13)-C(14)	1.515(6)
O(8)-C(17)	1.257(6)	C(13)-C(15)	1.520(8)
O(9)-C(17)	1.256(6)	C(16)-C(18)	1.528(7)
O(10)-C(10)	1.237(6)	C(16)-C(17)	1.534(7)
Selected bond angle (°)			
O(6)-La(1)-O(6)#1	148.38(17)	O(11)-La(2)-O(1)	136.16(12)
O(6)-La(1)-O(4)	111.17(12)	O(8)#7-La(2)-O(1)	69.46(11)
O(6)#1-La(1)-O(4)	77.85(12)	O(8)#8-La(2)-O(1)	103.08(12)
O(6)-La(1)-O(4)#1	77.84(12)	O(9)#7-La(2)-O(1)	114.86(11)
O(6)#1-La(1)-O(4)#1	111.17(12)	O(9)#8-La(2)-O(1)	70.19(12)
O(4)-La(1)-O(4)#1	147.91(18)	O(1)#6-La(2)-O(1)	156.51(17)
O(6)-La(1)-O(5)#2	84.45(12)	C(5)-O(1)-La(2)	89.4(3)
O(6)#1-La(1)-O(5)#2	69.04(11)	C(5)-O(2)-La(2)	97.8(3)
O(4)-La(1)-O(5)#2	132.79(11)	C(8)-O(4)-La(1)	146.5(3)
O(4)#1-La(1)-O(5)#2	77.39(12)	C(1)-O(5)-La(1)#4	134.4(3)
O(6)-La(1)-O(5)#3	69.05(11)	C(14)-O(6)-La(1)	168.2(3)
O(6)#1-La(1)-O(5)#3	84.45(12)	C(17)-O(8)-La(2)#9	93.2(3)
O(4)-La(1)-O(5)#3	77.39(12)	C(17)-O(9)-La(2)#9	92.9(3)
O(4)#1-La(1)-O(5)#3	132.79(11)	C(10)-O(10)-La(1)#3	144.4(3)
O(5)#2-La(1)-O(5)#3	67.01(15)	C(3)-N(1)-C(2)	115.3(4)
O(6)-La(1)-O(10)#4	76.85(11)	C(1)-N(2)-C(2)	116.5(4)
O(6)#1-La(1)-O(10)#4	133.34(11)	C(3)-N(3)-C(1)	120.8(4)
O(4)-La(1)-O(10)#4	70.96(12)	C(2)-N(4)-C(7)	122.7(4)
O(4)#1-La(1)-O(10)#4	82.01(12)	C(3)-N(5)-C(4)	124.1(4)
O(5)#2-La(1)-O(10)#4	154.65(10)	C(11)-N(6)-C(12)	116.1(4)
O(5)#3-La(1)-O(10)#4	120.00(11)	C(10)-N(7)-C(11)	120.9(4)

O(6)-La(1)-O(10)#5	133.34(11)	C(10)-N(8)-C(12)	120.9(4)
O(6)#1-La(1)-O(10)#5	76.84(11)	C(11)-N(9)-C(16)	121.9(4)
O(4)-La(1)-O(10)#5	82.01(12)	C(12)-N(10)-C(13)	120.9(4)
O(4)#1-La(1)-O(10)#5	70.96(11)	O(5)-C(1)-N(2)	122.7(4)
O(5)#2-La(1)-O(10)#5	120.00(11)	O(5)-C(1)-N(3)	118.4(4)
O(5)#3-La(1)-O(10)#5	154.64(10)	N(2)-C(1)-N(3)	118.9(4)
O(10)#4-La(1)-O(10)#5	65.36(15)	N(4)-C(2)-N(1)	116.1(4)
O(2)#6-La(2)-O(2)	64.03(19)	N(4)-C(2)-N(2)	117.3(4)
O(2)#6-La(2)-O(11)	115.62(12)	N(1)-C(2)-N(2)	126.6(4)
O(2)-La(2)-O(11)	164.02(14)	N(1)-C(3)-N(5)	122.2(4)
O(2)#6-La(2)-O(11)#6	164.02(14)	N(1)-C(3)-N(3)	121.7(4)
O(2)-La(2)-O(11)#6	115.62(12)	N(5)-C(3)-N(3)	116.1(4)
O(11)-La(2)-O(11)#6	69.45(17)	N(5)-C(4)-C(6)	113.1(5)
O(2)#6-La(2)-O(8)#7	72.75(13)	N(5)-C(4)-C(5)	106.3(4)
O(2)-La(2)-O(8)#7	77.17(14)	C(6)-C(4)-C(5)	109.4(5)
O(11)-La(2)-O(8)#7	118.52(12)	O(2)-C(5)-O(1)	122.7(5)
O(11)#6-La(2)-O(8)#7	91.45(13)	O(2)-C(5)-C(4)	117.0(5)
O(2)#6-La(2)-O(8)#8	77.17(14)	O(1)-C(5)-C(4)	120.3(4)
O(2)-La(2)-O(8)#8	72.75(13)	N(4)-C(7)-C(9)	111.1(5)
O(11)-La(2)-O(8)#8	91.45(13)	N(4)-C(7)-C(8)	110.1(4)
O(11)#6-La(2)-O(8)#8	118.52(12)	C(9)-C(7)-C(8)	109.2(5)
O(8)#7-La(2)-O(8)#8	144.38(19)	O(3)-C(8)-O(4)	124.9(5)
O(2)#6-La(2)-O(9)#7	78.39(15)	O(3)-C(8)-C(7)	117.7(4)
O(2)-La(2)-O(9)#7	122.73(14)	O(4)-C(8)-C(7)	117.3(4)
O(11)-La(2)-O(9)#7	71.03(12)	O(10)-C(10)-N(8)	121.4(4)
O(11)#6-La(2)-O(9)#7	89.77(13)	O(10)-C(10)-N(7)	122.9(4)
O(8)#7-La(2)-O(9)#7	50.28(11)	N(8)-C(10)-N(7)	115.7(4)
O(8)#8-La(2)-O(9)#7	139.60(11)	N(9)-C(11)-N(6)	120.0(4)
O(2)#6-La(2)-O(9)#8	122.73(14)	N(9)-C(11)-N(7)	117.2(4)
O(2)-La(2)-O(9)#8	78.39(15)	N(6)-C(11)-N(7)	122.9(4)
O(11)-La(2)-O(9)#8	89.77(13)	N(10)-C(12)-N(6)	119.2(4)
O(11)#6-La(2)-O(9)#8	71.04(12)	N(10)-C(12)-N(8)	117.9(4)
O(8)#7-La(2)-O(9)#8	139.60(11)	N(6)-C(12)-N(8)	122.8(4)
O(8)#8-La(2)-O(9)#8	50.28(11)	N(10)-C(13)-C(14)	110.4(4)
O(9)#7-La(2)-O(9)#8	156.91(19)	N(10)-C(13)-C(15)	111.1(4)
O(2)#6-La(2)-O(1)#6	49.24(12)	C(14)-C(13)-C(15)	112.9(5)
O(2)-La(2)-O(1)#6	107.92(12)	O(7)-C(14)-O(6)	124.9(5)
O(11)-La(2)-O(1)#6	67.25(12)	O(7)-C(14)-C(13)	117.3(4)
O(11)#6-La(2)-O(1)#6	136.17(12)	O(6)-C(14)-C(13)	117.8(4)
O(8)#7-La(2)-O(1)#6	103.08(12)	N(9)-C(16)-C(18)	109.0(4)
O(8)#8-La(2)-O(1)#6	69.46(11)	N(9)-C(16)-C(17)	110.8(4)
O(9)#7-La(2)-O(1)#6	70.19(12)	C(18)-C(16)-C(17)	110.6(4)
O(9)#8-La(2)-O(1)#6	114.86(11)	O(9)-C(17)-O(8)	122.7(5)
O(2)#6-La(2)-O(1)	107.92(12)	O(9)-C(17)-C(16)	116.7(4)
O(2)-La(2)-O(1)	49.24(12)	O(8)-C(17)-C(16)	120.6(4)
O(11)#6-La(2)-O(1)	67.25(12)		

Symmetry operation: #1 -x+1,y,-z+1; #2 -x+1,y+1,-z+1; #3 x,y+1,z; #4 x,y-1,z; #5 -x+1,y-1,-z+1; #6 -x, y,-z; #7 -x+1/2,y-3/2,-z+1; #8 x-1/2,y-3/2,z-1; #9 x+1/2,y+3/2,z+1

Table S3. Bond lengths [Å] and angles [°] for **Ce(R)**.

Selected bond distances (Å)			
Ce(1)-O(6)	2.357(7)	N(1)-C(3)	1.312(13)
Ce(1)-O(6)#1	2.357(7)	N(1)-C(2)	1.346(12)
Ce(1)-O(4)	2.372(8)	N(2)-C(1)	1.325(14)
Ce(1)-O(4)#1	2.372(8)	N(2)-C(2)	1.365(13)
Ce(1)-O(5)#2	2.564(8)	N(3)-C(3)	1.360(13)
Ce(1)-O(5)#3	2.564(8)	N(3)-C(1)	1.366(13)
Ce(1)-O(10)#4	2.612(7)	N(4)-C(2)	1.322(13)
Ce(1)-O(10)#5	2.612(7)	N(4)-C(7)	1.460(13)
Ce(2)-O(2)#6	2.500(10)	N(5)-C(3)	1.327(13)
Ce(2)-O(2)	2.500(10)	N(5)-C(4)	1.449(13)
Ce(2)-O(11)#6	2.544(8)	N(6)-C(11)	1.326(13)
Ce(2)-O(11)	2.544(8)	N(6)-C(12)	1.338(12)
Ce(2)-O(9)#7	2.566(8)	N(7)-C(10)	1.344(13)
Ce(2)-O(9)#8	2.566(8)	N(7)-C(11)	1.361(13)
Ce(2)-O(8)#7	2.576(8)	N(8)-C(10)	1.359(13)
Ce(2)-O(8)#8	2.576(8)	N(8)-C(12)	1.371(13)
Ce(2)-O(1)#6	2.711(7)	N(9)-C(11)	1.318(13)
Ce(2)-O(1)	2.711(8)	N(9)-C(16)	1.454(13)
O(1)-C(5)	1.255(14)	N(10)-C(12)	1.301(13)
O(2)-C(5)	1.241(14)	N(10)-C(13)	1.463(13)
O(3)-C(8)	1.241(14)	C(4)-C(6)	1.51(2)
O(4)-C(8)	1.263(12)	C(4)-C(5)	1.536(15)
O(5)-C(1)	1.250(13)	C(7)-C(8)	1.523(15)
O(6)-C(14)	1.289(11)	C(7)-C(9)	1.54(2)
O(7)-C(14)	1.231(14)	C(13)-C(15)	1.491(19)
O(8)-C(17)	1.247(13)	C(13)-C(14)	1.511(15)
O(9)-C(17)	1.243(13)	C(16)-C(18)	1.534(16)
O(10)-C(10)	1.239(13)	C(16)-C(17)	1.541(16)
Selected bond angle (°)			
O(6)-Ce(1)-O(6)#1	148.5(4)	O(11)-Ce(2)-O(1)	135.3(3)
O(6)-Ce(1)-O(4)	111.4(3)	O(9)#7-Ce(2)-O(1)	70.2(3)
O(6)#1-Ce(1)-O(4)	78.0(3)	O(9)#8-Ce(2)-O(1)	114.8(3)
O(6)-Ce(1)-O(4)#1	78.0(3)	O(8)#7-Ce(2)-O(1)	103.2(3)
O(6)#1-Ce(1)-O(4)#1	111.4(3)	O(8)#8-Ce(2)-O(1)	69.8(3)
O(4)-Ce(1)-O(4)#1	146.4(4)	O(1)#6-Ce(2)-O(1)	158.0(3)
O(6)-Ce(1)-O(5)#2	69.2(2)	C(5)-O(1)-Ce(2)	87.8(6)
O(6)#1-Ce(1)-O(5)#2	84.4(3)	C(5)-O(2)-Ce(2)	98.0(8)
O(4)-Ce(1)-O(5)#2	78.1(3)	C(8)-O(4)-Ce(1)	147.0(8)
O(4)#1-Ce(1)-O(5)#2	133.6(2)	C(1)-O(5)-Ce(1)#5	134.4(7)
O(6)-Ce(1)-O(5)#3	84.4(3)	C(14)-O(6)-Ce(1)	168.8(7)
O(6)#1-Ce(1)-O(5)#3	69.2(2)	C(17)-O(8)-Ce(2)#9	92.5(7)
O(4)-Ce(1)-O(5)#3	133.6(3)	C(17)-O(9)-Ce(2)#9	93.1(7)
O(4)#1-Ce(1)-O(5)#3	78.1(3)	C(10)-O(10)-Ce(1)#2	144.3(7)
O(5)#2-Ce(1)-O(5)#3	67.1(4)	C(3)-N(1)-C(2)	115.6(9)
O(6)-Ce(1)-O(10)#4	133.4(2)	C(1)-N(2)-C(2)	116.4(9)
O(6)#1-Ce(1)-O(10)#4	76.7(2)	C(3)-N(3)-C(1)	120.5(9)
O(4)-Ce(1)-O(10)#4	80.9(3)	C(2)-N(4)-C(7)	122.4(9)
O(4)#1-Ce(1)-O(10)#4	70.8(3)	C(3)-N(5)-C(4)	124.1(10)
O(5)#2-Ce(1)-O(10)#4	154.2(2)	C(11)-N(6)-C(12)	116.3(9)
O(5)#3-Ce(1)-O(10)#4	120.3(2)	C(10)-N(7)-C(11)	121.2(9)

O(6)-Ce(1)-O(10)#5	76.7(2)	C(10)-N(8)-C(12)	121.0(9)
O(6)#1-Ce(1)-O(10)#5	133.4(2)	C(11)-N(9)-C(16)	122.5(9)
O(4)-Ce(1)-O(10)#5	70.8(3)	C(12)-N(10)-C(13)	121.6(8)
O(4)#1-Ce(1)-O(10)#5	80.9(3)	O(5)-C(1)-N(2)	122.2(10)
O(5)#2-Ce(1)-O(10)#5	120.3(2)	O(5)-C(1)-N(3)	118.1(10)
O(5)#3-Ce(1)-O(10)#5	154.2(2)	N(2)-C(1)-N(3)	119.7(10)
O(10)#4-Ce(1)-O(10)#5	65.1(3)	N(4)-C(2)-N(1)	117.3(9)
O(2)#6-Ce(2)-O(2)	64.1(4)	N(4)-C(2)-N(2)	116.8(9)
O(2)#6-Ce(2)-O(11)#6	163.8(3)	N(1)-C(2)-N(2)	125.8(9)
O(2)-Ce(2)-O(11)#6	115.7(3)	N(1)-C(3)-N(5)	121.7(10)
O(2)#6-Ce(2)-O(11)	115.7(3)	N(1)-C(3)-N(3)	121.7(9)
O(2)-Ce(2)-O(11)	163.8(3)	N(5)-C(3)-N(3)	116.6(10)
O(11)#6-Ce(2)-O(11)	69.4(4)	N(5)-C(4)-C(6)	113.1(11)
O(2)#6-Ce(2)-O(9)#7	122.9(3)	N(5)-C(4)-C(5)	106.7(9)
O(2)-Ce(2)-O(9)#7	79.3(3)	C(6)-C(4)-C(5)	109.4(11)
O(11)#6-Ce(2)-O(9)#7	71.3(3)	O(2)-C(5)-O(1)	123.6(11)
O(11)-Ce(2)-O(9)#7	88.5(3)	O(2)-C(5)-C(4)	117.5(11)
O(2)#6-Ce(2)-O(9)#8	79.3(3)	O(1)-C(5)-C(4)	118.9(10)
O(2)-Ce(2)-O(9)#8	122.9(3)	N(4)-C(7)-C(8)	110.4(9)
O(11)#6-Ce(2)-O(9)#8	88.5(3)	N(4)-C(7)-C(9)	111.6(11)
O(11)-Ce(2)-O(9)#8	71.3(3)	C(8)-C(7)-C(9)	108.8(10)
O(9)#7-Ce(2)-O(9)#8	155.7(4)	O(3)-C(8)-O(4)	124.6(10)
O(2)#6-Ce(2)-O(8)#7	76.8(3)	O(3)-C(8)-C(7)	118.4(9)
O(2)-Ce(2)-O(8)#7	73.1(3)	O(4)-C(8)-C(7)	117.0(9)
O(11)#6-Ce(2)-O(8)#7	119.1(3)	O(10)-C(10)-N(7)	124.1(10)
O(11)-Ce(2)-O(8)#7	90.9(3)	O(10)-C(10)-N(8)	119.9(9)
O(9)#7-Ce(2)-O(8)#7	50.5(3)	N(7)-C(10)-N(8)	116.0(9)
O(9)#8-Ce(2)-O(8)#7	140.0(3)	N(9)-C(11)-N(6)	119.6(9)
O(2)#6-Ce(2)-O(8)#8	73.1(3)	N(9)-C(11)-N(7)	117.5(9)
O(2)-Ce(2)-O(8)#8	76.8(3)	N(6)-C(11)-N(7)	122.9(9)
O(11)#6-Ce(2)-O(8)#8	90.9(3)	N(10)-C(12)-N(6)	118.9(9)
O(11)-Ce(2)-O(8)#8	119.1(3)	N(10)-C(12)-N(8)	119.1(9)
O(9)#7-Ce(2)-O(8)#8	140.0(3)	N(6)-C(12)-N(8)	122.0(9)
O(9)#8-Ce(2)-O(8)#8	50.5(3)	N(10)-C(13)-C(15)	111.4(11)
O(8)#7-Ce(2)-O(8)#8	144.3(4)	N(10)-C(13)-C(14)	110.5(9)
O(2)#6-Ce(2)-O(1)#6	49.7(3)	C(15)-C(13)-C(14)	112.7(10)
O(2)-Ce(2)-O(1)#6	108.8(3)	O(7)-C(14)-O(6)	124.9(10)
O(11)#6-Ce(2)-O(1)#6	135.3(3)	O(7)-C(14)-C(13)	117.1(9)
O(11)-Ce(2)-O(1)#6	66.6(3)	O(6)-C(14)-C(13)	118.0(9)
O(9)#7-Ce(2)-O(1)#6	114.8(3)	N(9)-C(16)-C(18)	109.5(10)
O(9)#8-Ce(2)-O(1)#6	70.2(3)	N(9)-C(16)-C(17)	111.1(9)
O(8)#7-Ce(2)-O(1)#6	69.8(3)	C(18)-C(16)-C(17)	110.1(10)
O(8)#8-Ce(2)-O(1)#6	103.2(3)	O(9)-C(17)-O(8)	123.3(11)
O(2)#6-Ce(2)-O(1)	108.8(3)	O(9)-C(17)-C(16)	117.4(9)
O(2)-Ce(2)-O(1)	49.7(3)	O(8)-C(17)-C(16)	119.3(10)
O(11)#6-Ce(2)-O(1)	66.6(3)		

Symmetry operation: #1 -x+1, y, -z+1; #2 x, y-1, z; #3 -x+1, y-1, -z+1; #4 -x+1, y+1, -z+1; #5 x, y+1, z; #6 -x, y, -z; #7 x-1/2, y+3/2, z-1; #8 -x+1/2, y+3/2, -z+1; #9 x+1/2, y-3/2, z+1

Table S4. Bond lengths [Å] and angles [°] for **Ce(S)**.

Selected bond distances (Å)			
Ce(1)-O(6)	2.369(6)	N(1)-C(3)	1.312(12)
Ce(1)-O(6)#1	2.369(6)	N(1)-C(2)	1.337(12)
Ce(1)-O(4)	2.384(7)	N(2)-C(1)	1.338(13)
Ce(1)-O(4)#1	2.384(7)	N(2)-C(2)	1.353(12)
Ce(1)-O(5)#2	2.571(7)	N(3)-C(3)	1.367(13)
Ce(1)-O(5)#3	2.571(7)	N(3)-C(1)	1.375(12)
Ce(1)-O(10)#4	2.617(7)	N(4)-C(2)	1.339(12)
Ce(1)-O(10)#5	2.617(7)	N(4)-C(7)	1.466(13)
Ce(2)-O(2)#6	2.517(9)	N(5)-C(3)	1.332(13)
Ce(2)-O(2)	2.517(9)	N(5)-C(4)	1.470(14)
Ce(2)-O(11)	2.553(8)	N(6)-C(11)	1.312(13)
Ce(2)-O(11)#6	2.553(8)	N(6)-C(12)	1.379(12)
Ce(2)-O(9)#7	2.571(8)	N(7)-C(10)	1.360(13)
Ce(2)-O(9)#8	2.571(8)	N(7)-C(11)	1.378(12)
Ce(2)-O(8)#7	2.574(8)	N(8)-C(12)	1.352(12)
Ce(2)-O(8)#8	2.574(8)	N(8)-C(10)	1.366(12)
Ce(2)-O(1)#6	2.698(8)	N(9)-C(11)	1.316(12)
Ce(2)-O(1)	2.698(8)	N(9)-C(16)	1.445(13)
O(1)-C(5)	1.256(14)	N(10)-C(12)	1.311(12)
O(2)-C(5)	1.259(13)	N(10)-C(13)	1.465(12)
O(3)-C(8)	1.251(13)	C(4)-C(5)	1.531(15)
O(4)-C(8)	1.273(12)	C(4)-C(6)	1.538(19)
O(5)-C(1)	1.242(12)	C(7)-C(8)	1.509(15)
O(6)-C(14)	1.264(12)	C(7)-C(9)	1.54(2)
O(7)-C(14)	1.238(14)	C(13)-C(15)	1.48(2)
O(8)-C(17)	1.278(13)	C(13)-C(14)	1.497(14)
O(9)-C(17)	1.241(13)	C(16)-C(17)	1.513(16)
O(10)-C(10)	1.220(12)	C(16)-C(18)	1.522(17)
Selected bond angle (°)			
O(6)-Ce(1)-O(6)#1	149.4(4)	O(11)#6-Ce(2)-O(1)	134.8(3)
O(6)-Ce(1)-O(4)	110.8(3)	O(9)#7-Ce(2)-O(1)	115.1(3)
O(6)#1-Ce(1)-O(4)	78.1(3)	O(9)#8-Ce(2)-O(1)	70.1(3)
O(6)-Ce(1)-O(4)#1	78.1(3)	O(8)#7-Ce(2)-O(1)	70.3(3)
O(6)#1-Ce(1)-O(4)#1	110.8(3)	O(8)#8-Ce(2)-O(1)	103.1(3)
O(4)-Ce(1)-O(4)#1	147.1(4)	O(1)#6-Ce(2)-O(1)	158.3(4)
O(6)-Ce(1)-O(5)#2	69.6(2)	C(5)-O(1)-Ce(2)	89.4(6)
O(6)#1-Ce(1)-O(5)#2	84.7(3)	C(5)-O(2)-Ce(2)	97.9(7)
O(4)-Ce(1)-O(5)#2	77.6(3)	C(8)-O(4)-Ce(1)	148.2(8)
O(4)#1-Ce(1)-O(5)#2	133.4(2)	C(1)-O(5)-Ce(1)#5	134.7(6)
O(6)-Ce(1)-O(5)#3	84.7(3)	C(14)-O(6)-Ce(1)	171.2(8)
O(6)#1-Ce(1)-O(5)#3	69.6(2)	C(17)-O(8)-Ce(2)#9	93.2(6)
O(4)-Ce(1)-O(5)#3	133.4(2)	C(17)-O(9)-Ce(2)#9	94.3(7)
O(4)#1-Ce(1)-O(5)#3	77.6(3)	C(10)-O(10)-Ce(1)#2	146.1(7)
O(5)#2-Ce(1)-O(5)#3	67.0(3)	C(3)-N(1)-C(2)	115.5(8)
O(6)-Ce(1)-O(10)#4	133.1(2)	C(1)-N(2)-C(2)	117.1(8)
O(6)#1-Ce(1)-O(10)#4	76.2(2)	C(3)-N(3)-C(1)	120.6(9)
O(4)-Ce(1)-O(10)#4	80.9(3)	C(2)-N(4)-C(7)	122.7(9)
O(4)#1-Ce(1)-O(10)#4	71.4(3)	C(3)-N(5)-C(4)	123.5(9)
O(5)#2-Ce(1)-O(10)#4	153.7(2)	C(11)-N(6)-C(12)	116.5(8)
O(5)#3-Ce(1)-O(10)#4	120.9(2)	C(10)-N(7)-C(11)	121.6(8)

O(6)-Ce(1)-O(10)#5	76.2(2)	C(12)-N(8)-C(10)	122.7(8)
O(6)#1-Ce(1)-O(10)#5	133.1(2)	C(11)-N(9)-C(16)	121.8(9)
O(4)-Ce(1)-O(10)#5	71.4(3)	C(12)-N(10)-C(13)	121.7(8)
O(4)#1-Ce(1)-O(10)#5	80.9(3)	O(5)-C(1)-N(2)	122.7(8)
O(5)#2-Ce(1)-O(10)#5	120.9(2)	O(5)-C(1)-N(3)	119.0(9)
O(5)#3-Ce(1)-O(10)#5	153.7(2)	N(2)-C(1)-N(3)	118.3(8)
O(10)#4-Ce(1)-O(10)#5	64.6(3)	N(1)-C(2)-N(4)	116.5(8)
O(2)#6-Ce(2)-O(2)	63.9(4)	N(1)-C(2)-N(2)	126.4(8)
O(2)#6-Ce(2)-O(11)	163.4(3)	N(4)-C(2)-N(2)	117.0(8)
O(2)-Ce(2)-O(11)	116.0(3)	N(1)-C(3)-N(5)	122.5(9)
O(2)#6-Ce(2)-O(11)#6	116.0(3)	N(1)-C(3)-N(3)	121.7(9)
O(2)-Ce(2)-O(11)#6	163.4(3)	N(5)-C(3)-N(3)	115.9(9)
O(11)-Ce(2)-O(11)#6	69.2(4)	N(5)-C(4)-C(5)	105.8(9)
O(2)#6-Ce(2)-O(9)#7	80.1(4)	N(5)-C(4)-C(6)	112.7(11)
O(2)-Ce(2)-O(9)#7	123.3(3)	C(5)-C(4)-C(6)	110.1(10)
O(11)-Ce(2)-O(9)#7	87.2(3)	O(1)-C(5)-O(2)	122.1(10)
O(11)#6-Ce(2)-O(9)#7	71.5(3)	O(1)-C(5)-C(4)	121.3(9)
O(2)#6-Ce(2)-O(9)#8	123.3(3)	O(2)-C(5)-C(4)	116.6(10)
O(2)-Ce(2)-O(9)#8	80.1(4)	N(4)-C(7)-C(8)	109.8(9)
O(11)-Ce(2)-O(9)#8	71.5(3)	N(4)-C(7)-C(9)	109.8(11)
O(11)#6-Ce(2)-O(9)#8	87.2(3)	C(8)-C(7)-C(9)	109.1(11)
O(9)#7-Ce(2)-O(9)#8	154.4(5)	O(3)-C(8)-O(4)	123.0(10)
O(2)#6-Ce(2)-O(8)#7	73.8(3)	O(3)-C(8)-C(7)	118.8(10)
O(2)-Ce(2)-O(8)#7	77.1(3)	O(4)-C(8)-C(7)	118.2(9)
O(11)-Ce(2)-O(8)#7	89.9(3)	O(10)-C(10)-N(7)	123.4(9)
O(11)#6-Ce(2)-O(8)#7	119.3(3)	O(10)-C(10)-N(8)	121.8(9)
O(9)#7-Ce(2)-O(8)#7	50.5(2)	N(7)-C(10)-N(8)	114.8(8)
O(9)#8-Ce(2)-O(8)#7	140.2(3)	N(6)-C(11)-N(9)	120.2(9)
O(2)#6-Ce(2)-O(8)#8	77.1(3)	N(6)-C(11)-N(7)	122.6(8)
O(2)-Ce(2)-O(8)#8	73.8(3)	N(9)-C(11)-N(7)	117.2(9)
O(11)-Ce(2)-O(8)#8	119.3(3)	N(10)-C(12)-N(8)	120.0(9)
O(11)#6-Ce(2)-O(8)#8	89.9(3)	N(10)-C(12)-N(6)	118.8(8)
O(9)#7-Ce(2)-O(8)#8	140.2(3)	N(8)-C(12)-N(6)	121.1(9)
O(9)#8-Ce(2)-O(8)#8	50.5(2)	N(10)-C(13)-C(15)	111.8(11)
O(8)#7-Ce(2)-O(8)#8	145.5(4)	N(10)-C(13)-C(14)	110.6(8)
O(2)#6-Ce(2)-O(1)#6	49.8(3)	C(15)-C(13)-C(14)	113.5(11)
O(2)-Ce(2)-O(1)#6	109.0(3)	O(7)-C(14)-O(6)	123.4(10)
O(11)-Ce(2)-O(1)#6	134.8(3)	O(7)-C(14)-C(13)	117.6(9)
O(11)#6-Ce(2)-O(1)#6	66.8(3)	O(6)-C(14)-C(13)	119.0(9)
O(9)#7-Ce(2)-O(1)#6	70.1(3)	N(9)-C(16)-C(17)	112.6(9)
O(9)#8-Ce(2)-O(1)#6	115.1(3)	N(9)-C(16)-C(18)	110.0(10)
O(8)#7-Ce(2)-O(1)#6	103.1(3)	C(17)-C(16)-C(18)	111.0(10)
O(8)#8-Ce(2)-O(1)#6	70.3(3)	O(9)-C(17)-O(8)	121.0(10)
O(2)#6-Ce(2)-O(1)	109.0(3)	O(9)-C(17)-C(16)	119.4(9)
O(2)-Ce(2)-O(1)	49.8(3)	O(8)-C(17)-C(16)	119.7(9)
O(11)-Ce(2)-O(1)	66.8(3)		

Symmetry operation: #1 -x+1, y, -z+1; #2 x, y+1, z; #3 -x+1, y+1, -z+1;#4 -x+1, y-1, -z+1; #5 x, y-1, z; #6 -x, y, -z; #7 -x+1/2, y-3/2, -z+1; #8 x-1/2, y-3/2, z-1; #9 x+1/2, y+3/2, z+1

Table S5. Bond lengths [Å] and angles [°] for **Pr(R)**.

Selected bond distances (Å)			
Pr(1)-O(6)	2.346(3)	N(1)-C(3)	1.319(6)
Pr(1)-O(6)#1	2.346(3)	N(1)-C(2)	1.348(6)
Pr(1)-O(4)#1	2.368(3)	N(2)-C(1)	1.338(6)
Pr(1)-O(4)	2.368(3)	N(2)-C(2)	1.358(6)
Pr(1)-O(5)#2	2.542(3)	N(3)-C(3)	1.368(6)
Pr(1)-O(5)#3	2.542(3)	N(3)-C(1)	1.378(6)
Pr(1)-O(10)#4	2.599(3)	N(4)-C(2)	1.332(6)
Pr(1)-O(10)#5	2.599(3)	N(4)-C(7)	1.467(6)
Pr(2)-O(2)#6	2.494(4)	N(5)-C(3)	1.318(6)
Pr(2)-O(2)	2.494(4)	N(5)-C(4)	1.455(6)
Pr(2)-O(11)#6	2.526(4)	N(6)-C(11)	1.326(6)
Pr(2)-O(11)	2.526(4)	N(6)-C(12)	1.338(6)
Pr(2)-O(9)#7	2.550(4)	N(7)-C(10)	1.359(6)
Pr(2)-O(9)#8	2.550(4)	N(7)-C(11)	1.369(6)
Pr(2)-O(8)#7	2.554(4)	N(8)-C(10)	1.358(6)
Pr(2)-O(8)#8	2.554(4)	N(8)-C(12)	1.364(6)
Pr(2)-O(1)	2.706(4)	N(9)-C(11)	1.316(6)
Pr(2)-O(1)#6	2.706(4)	N(9)-C(16)	1.457(6)
O(1)-C(5)	1.257(7)	N(10)-C(12)	1.321(6)
O(2)-C(5)	1.246(7)	N(10)-C(13)	1.469(6)
O(3)-C(8)	1.248(7)	C(4)-C(5)	1.526(7)
O(4)-C(8)	1.264(6)	C(4)-C(6)	1.529(9)
O(5)-C(1)	1.250(6)	C(7)-C(9)	1.522(9)
O(6)-C(14)	1.273(6)	C(7)-C(8)	1.522(7)
O(7)-C(14)	1.231(7)	C(13)-C(14)	1.507(6)
O(8)-C(17)	1.257(6)	C(13)-C(15)	1.512(8)
O(9)-C(17)	1.248(6)	C(16)-C(18)	1.525(7)
O(10)-C(10)	1.237(6)	C(16)-C(17)	1.537(7)
Selected bond angle (°)			
O(6)-Pr(1)-O(6)#1	148.48(17)	O(11)-Pr(2)-O(1)#6	66.45(12)
O(6)-Pr(1)-O(4)#1	78.20(12)	O(9)#7-Pr(2)-O(1)#6	114.91(12)
O(6)#1-Pr(1)-O(4)#1	111.16(12)	O(9)#8-Pr(2)-O(1)#6	70.13(12)
O(6)-Pr(1)-O(4)	111.16(12)	O(8)#7-Pr(2)-O(1)#6	69.37(12)
O(6)#1-Pr(1)-O(4)	78.20(12)	O(8)#8-Pr(2)-O(1)#6	103.69(12)
O(4)#1-Pr(1)-O(4)	146.52(18)	O(1)-Pr(2)-O(1)#6	158.18(17)
O(6)-Pr(1)-O(5)#2	84.33(12)	C(5)-O(1)-Pr(2)	88.0(3)
O(6)#1-Pr(1)-O(5)#2	69.28(11)	C(5)-O(2)-Pr(2)	98.3(3)
O(4)#1-Pr(1)-O(5)#2	77.85(12)	C(8)-O(4)-Pr(1)	146.8(3)
O(4)-Pr(1)-O(5)#2	133.66(12)	C(1)-O(5)-Pr(1)#5	135.0(3)
O(6)-Pr(1)-O(5)#3	69.28(12)	C(14)-O(6)-Pr(1)	169.1(3)
O(6)#1-Pr(1)-O(5)#3	84.33(12)	C(17)-O(8)-Pr(2)#9	92.4(3)
O(4)#1-Pr(1)-O(5)#3	133.66(12)	C(17)-O(9)-Pr(2)#9	92.8(3)
O(4)-Pr(1)-O(5)#3	77.85(12)	C(10)-O(10)-Pr(1)#3	144.4(3)
O(5)#2-Pr(1)-O(5)#3	67.15(16)	C(3)-N(1)-C(2)	115.3(4)
O(6)-Pr(1)-O(10)#4	133.36(11)	C(1)-N(2)-C(2)	116.5(4)
O(6)#1-Pr(1)-O(10)#4	76.77(11)	C(3)-N(3)-C(1)	120.9(4)
O(4)#1-Pr(1)-O(10)#4	70.54(12)	C(2)-N(4)-C(7)	122.3(4)
O(4)-Pr(1)-O(10)#4	81.24(12)	C(3)-N(5)-C(4)	124.6(4)
O(5)#2-Pr(1)-O(10)#4	120.23(11)	C(11)-N(6)-C(12)	115.9(4)
O(5)#3-Pr(1)-O(10)#4	154.25(11)	C(10)-N(7)-C(11)	121.0(4)

O(6)-Pr(1)-O(10)#5	76.77(11)	C(10)-N(8)-C(12)	120.9(4)
O(6)#1-Pr(1)-O(10)#5	133.36(11)	C(11)-N(9)-C(16)	122.0(4)
O(4)#1-Pr(1)-O(10)#5	81.24(12)	C(12)-N(10)-C(13)	120.9(4)
O(4)-Pr(1)-O(10)#5	70.54(12)	O(5)-C(1)-N(2)	122.9(4)
O(5)#2-Pr(1)-O(10)#5	154.25(11)	O(5)-C(1)-N(3)	118.2(4)
O(5)#3-Pr(1)-O(10)#5	120.23(11)	N(2)-C(1)-N(3)	118.9(4)
O(10)#4-Pr(1)-O(10)#5	65.16(15)	N(4)-C(2)-N(1)	116.3(4)
O(2)#6-Pr(2)-O(2)	64.26(19)	N(4)-C(2)-N(2)	116.8(4)
O(2)#6-Pr(2)-O(11)#6	163.02(14)	N(1)-C(2)-N(2)	126.8(4)
O(2)-Pr(2)-O(11)#6	115.67(13)	N(5)-C(3)-N(1)	122.2(5)
O(2)#6-Pr(2)-O(11)	115.67(13)	N(5)-C(3)-N(3)	116.3(4)
O(2)-Pr(2)-O(11)	163.02(14)	N(1)-C(3)-N(3)	121.4(4)
O(11)#6-Pr(2)-O(11)	69.75(18)	N(5)-C(4)-C(5)	106.7(4)
O(2)#6-Pr(2)-O(9)#7	123.42(14)	N(5)-C(4)-C(6)	113.1(5)
O(2)-Pr(2)-O(9)#7	79.23(15)	C(5)-C(4)-C(6)	109.0(5)
O(11)#6-Pr(2)-O(9)#7	71.52(13)	O(2)-C(5)-O(1)	122.9(5)
O(11)-Pr(2)-O(9)#7	87.96(13)	O(2)-C(5)-C(4)	117.5(5)
O(2)#6-Pr(2)-O(9)#8	79.23(15)	O(1)-C(5)-C(4)	119.5(5)
O(2)-Pr(2)-O(9)#8	123.42(14)	N(4)-C(7)-C(9)	111.3(5)
O(11)#6-Pr(2)-O(9)#8	87.97(13)	N(4)-C(7)-C(8)	109.5(4)
O(11)-Pr(2)-O(9)#8	71.52(13)	C(9)-C(7)-C(8)	108.7(5)
O(9)#7-Pr(2)-O(9)#8	155.2(2)	O(3)-C(8)-O(4)	124.2(5)
O(2)#6-Pr(2)-O(8)#7	76.84(14)	O(3)-C(8)-C(7)	117.8(5)
O(2)-Pr(2)-O(8)#7	73.17(14)	O(4)-C(8)-C(7)	117.9(5)
O(11)#6-Pr(2)-O(8)#7	119.92(12)	O(10)-C(10)-N(8)	121.1(4)
O(11)-Pr(2)-O(8)#7	90.12(13)	O(10)-C(10)-N(7)	123.1(4)
O(9)#7-Pr(2)-O(8)#7	51.07(12)	N(8)-C(10)-N(7)	115.8(4)
O(9)#8-Pr(2)-O(8)#7	139.43(12)	N(9)-C(11)-N(6)	120.0(4)
O(2)#6-Pr(2)-O(8)#8	73.18(14)	N(9)-C(11)-N(7)	117.2(4)
O(2)-Pr(2)-O(8)#8	76.84(14)	N(6)-C(11)-N(7)	122.8(4)
O(11)#6-Pr(2)-O(8)#8	90.12(13)	N(10)-C(12)-N(6)	119.0(4)
O(11)-Pr(2)-O(8)#8	119.92(12)	N(10)-C(12)-N(8)	117.9(4)
O(9)#7-Pr(2)-O(8)#8	139.43(12)	N(6)-C(12)-N(8)	123.0(4)
O(9)#8-Pr(2)-O(8)#8	51.07(12)	N(10)-C(13)-C(14)	110.6(4)
O(8)#7-Pr(2)-O(8)#8	144.45(19)	N(10)-C(13)-C(15)	110.9(5)
O(2)#6-Pr(2)-O(1)	108.93(12)	C(14)-C(13)-C(15)	112.6(5)
O(2)-Pr(2)-O(1)	49.84(12)	O(7)-C(14)-O(6)	124.9(5)
O(11)#6-Pr(2)-O(1)	66.45(12)	O(7)-C(14)-C(13)	117.1(4)
O(11)-Pr(2)-O(1)	135.24(12)	O(6)-C(14)-C(13)	118.0(4)
O(9)#7-Pr(2)-O(1)	70.13(12)	N(9)-C(16)-C(18)	109.2(4)
O(9)#8-Pr(2)-O(1)	114.91(12)	N(9)-C(16)-C(17)	110.8(4)
O(8)#7-Pr(2)-O(1)	103.69(12)	C(18)-C(16)-C(17)	110.3(4)
O(8)#8-Pr(2)-O(1)	69.37(12)	O(9)-C(17)-O(8)	122.9(5)
O(2)#6-Pr(2)-O(1)#6	49.84(12)	O(9)-C(17)-C(16)	117.0(4)
O(2)-Pr(2)-O(1)#6	108.93(12)	O(8)-C(17)-C(16)	120.2(4)
O(11)#6-Pr(2)-O(1)#6	135.24(12)		

Symmetry operation: #1 -x+1, y, -z+1; #2 -x+1, y-1, -z+1; #3 x, y-1, z; #4 -x+1, y+1, -z+1; #5 x, y+1, z; #6 -x, y, -z; #7 x-1/2, y+3/2, z-1; #8 -x+1/2, y+3/2, -z+1; #9 x+1/2, y-3/2, z+1

Table S6. Bond lengths [Å] and angles [°] for **Pr(S)**.

Selected bond distances (Å)			
Pr(1)-O(6)#1	2.350(5)	N(1)-C(3)	1.308(9)
Pr(1)-O(6)	2.350(5)	N(1)-C(2)	1.347(9)
Pr(1)-O(4)	2.378(5)	N(2)-C(1)	1.343(9)
Pr(1)-O(4)#1	2.378(5)	N(2)-C(2)	1.360(9)
Pr(1)-O(5)#2	2.554(5)	N(3)-C(3)	1.367(9)
Pr(1)-O(5)#3	2.554(5)	N(3)-C(1)	1.383(9)
Pr(1)-O(10)#4	2.602(5)	N(4)-C(2)	1.341(9)
Pr(1)-O(10)#5	2.602(5)	N(4)-C(7)	1.467(9)
Pr(2)-O(2)	2.516(6)	N(5)-C(3)	1.328(9)
Pr(2)-O(2)#6	2.516(6)	N(5)-C(4)	1.463(10)
Pr(2)-O(11)#6	2.529(6)	N(6)-C(11)	1.332(9)
Pr(2)-O(11)	2.529(6)	N(6)-C(12)	1.355(9)
Pr(2)-O(9)#7	2.555(6)	N(7)-C(11)	1.367(9)
Pr(2)-O(9)#8	2.555(6)	N(7)-C(10)	1.369(9)
Pr(2)-O(8)#7	2.561(6)	N(8)-C(10)	1.357(9)
Pr(2)-O(8)#8	2.561(6)	N(8)-C(12)	1.363(9)
Pr(2)-O(1)	2.699(5)	N(9)-C(11)	1.323(9)
Pr(2)-O(1)#6	2.699(5)	N(9)-C(16)	1.461(9)
O(1)-C(5)	1.261(10)	N(10)-C(12)	1.320(9)
O(2)-C(5)	1.246(10)	N(10)-C(13)	1.480(9)
O(3)-C(8)	1.252(9)	C(4)-C(5)	1.543(11)
O(4)-C(8)	1.256(9)	C(4)-C(6)	1.544(14)
O(5)-C(1)	1.244(9)	C(7)-C(9)	1.521(13)
O(6)-C(14)	1.277(8)	C(7)-C(8)	1.537(11)
O(7)-C(14)	1.225(10)	C(13)-C(15)	1.492(13)
O(8)-C(17)	1.271(9)	C(13)-C(14)	1.502(10)
O(9)-C(17)	1.252(10)	C(16)-C(17)	1.527(10)
O(10)-C(10)	1.237(9)	C(16)-C(18)	1.532(11)
Selected bond angle (°)			
O(6)#1-Pr(1)-O(6)	148.5(3)	O(11)-Pr(2)-O(1)#6	134.85(19)
O(6)#1-Pr(1)-O(4)	78.14(18)	O(9)#7-Pr(2)-O(1)#6	69.93(18)
O(6)-Pr(1)-O(4)	111.15(19)	O(9)#8-Pr(2)-O(1)#6	115.10(18)
O(6)#1-Pr(1)-O(4)#1	111.15(19)	O(8)#7-Pr(2)-O(1)#6	103.55(18)
O(6)-Pr(1)-O(4)#1	78.14(18)	O(8)#8-Pr(2)-O(1)#6	69.64(18)
O(4)-Pr(1)-O(4)#1	146.7(3)	O(1)-Pr(2)-O(1)#6	158.6(3)
O(6)#1-Pr(1)-O(5)#2	84.37(18)	C(5)-O(1)-Pr(2)	88.6(5)
O(6)-Pr(1)-O(5)#2	69.29(17)	C(5)-O(2)-Pr(2)	97.6(5)
O(4)-Pr(1)-O(5)#2	77.71(18)	C(8)-O(4)-Pr(1)	147.1(5)
O(4)#1-Pr(1)-O(5)#2	133.60(18)	C(1)-O(5)-Pr(1)#5	135.2(5)
O(6)#1-Pr(1)-O(5)#3	69.29(17)	C(14)-O(6)-Pr(1)	169.7(5)
O(6)-Pr(1)-O(5)#3	84.37(18)	C(17)-O(8)-Pr(2)#9	92.6(4)
O(4)-Pr(1)-O(5)#3	133.61(18)	C(17)-O(9)-Pr(2)#9	93.3(5)
O(4)#1-Pr(1)-O(5)#3	77.70(18)	C(10)-O(10)-Pr(1)#2	145.5(5)
O(5)#2-Pr(1)-O(5)#3	67.3(2)	C(3)-N(1)-C(2)	115.4(6)
O(6)#1-Pr(1)-O(10)#4	76.63(18)	C(1)-N(2)-C(2)	116.5(6)
O(6)-Pr(1)-O(10)#4	133.54(17)	C(3)-N(3)-C(1)	120.6(6)
O(4)-Pr(1)-O(10)#4	80.96(19)	C(2)-N(4)-C(7)	122.3(6)
O(4)#1-Pr(1)-O(10)#4	71.00(18)	C(3)-N(5)-C(4)	123.5(7)
O(5)#2-Pr(1)-O(10)#4	153.89(16)	C(11)-N(6)-C(12)	115.4(6)
O(5)#3-Pr(1)-O(10)#4	120.39(17)	C(11)-N(7)-C(10)	120.7(6)

O(6)#1-Pr(1)-O(10)#5	133.54(17)	C(10)-N(8)-C(12)	121.7(6)
O(6)-Pr(1)-O(10)#5	76.63(18)	C(11)-N(9)-C(16)	122.0(6)
O(4)-Pr(1)-O(10)#5	71.00(18)	C(12)-N(10)-C(13)	121.1(6)
O(4)#1-Pr(1)-O(10)#5	80.96(19)	O(5)-C(1)-N(2)	123.0(6)
O(5)#2-Pr(1)-O(10)#5	120.39(17)	O(5)-C(1)-N(3)	118.4(6)
O(5)#3-Pr(1)-O(10)#5	153.89(16)	N(2)-C(1)-N(3)	118.6(6)
O(10)#4-Pr(1)-O(10)#5	65.1(2)	N(4)-C(2)-N(1)	116.5(6)
O(2)-Pr(2)-O(2)#6	64.8(3)	N(4)-C(2)-N(2)	116.8(6)
O(2)-Pr(2)-O(11)#6	162.7(2)	N(1)-C(2)-N(2)	126.7(6)
O(2)#6-Pr(2)-O(11)#6	115.66(19)	N(1)-C(3)-N(5)	122.3(7)
O(2)-Pr(2)-O(11)	115.66(19)	N(1)-C(3)-N(3)	122.0(6)
O(2)#6-Pr(2)-O(11)	162.7(2)	N(5)-C(3)-N(3)	115.6(7)
O(11)#6-Pr(2)-O(11)	69.5(3)	N(5)-C(4)-C(5)	105.6(7)
O(2)-Pr(2)-O(9)#7	123.8(2)	N(5)-C(4)-C(6)	112.7(8)
O(2)#6-Pr(2)-O(9)#7	79.2(2)	C(5)-C(4)-C(6)	108.7(8)
O(11)#6-Pr(2)-O(9)#7	71.63(19)	O(2)-C(5)-O(1)	122.8(8)
O(11)-Pr(2)-O(9)#7	87.5(2)	O(2)-C(5)-C(4)	116.7(8)
O(2)-Pr(2)-O(9)#8	79.2(2)	O(1)-C(5)-C(4)	120.4(7)
O(2)#6-Pr(2)-O(9)#8	123.8(2)	N(4)-C(7)-C(9)	112.0(8)
O(11)#6-Pr(2)-O(9)#8	87.5(2)	N(4)-C(7)-C(8)	109.2(6)
O(11)-Pr(2)-O(9)#8	71.63(19)	C(9)-C(7)-C(8)	109.1(7)
O(9)#7-Pr(2)-O(9)#8	154.8(3)	O(3)-C(8)-O(4)	124.7(7)
O(2)-Pr(2)-O(8)#7	77.0(2)	O(3)-C(8)-C(7)	117.3(7)
O(2)#6-Pr(2)-O(8)#7	73.1(2)	O(4)-C(8)-C(7)	118.0(7)
O(11)#6-Pr(2)-O(8)#7	120.16(18)	O(10)-C(10)-N(8)	122.1(7)
O(11)-Pr(2)-O(8)#7	90.00(19)	O(10)-C(10)-N(7)	122.3(7)
O(9)#7-Pr(2)-O(8)#7	51.18(17)	N(8)-C(10)-N(7)	115.6(6)
O(9)#8-Pr(2)-O(8)#7	139.49(17)	N(9)-C(11)-N(6)	119.4(7)
O(2)-Pr(2)-O(8)#8	73.1(2)	N(9)-C(11)-N(7)	117.0(7)
O(2)#6-Pr(2)-O(8)#8	77.0(2)	N(6)-C(11)-N(7)	123.6(6)
O(11)#6-Pr(2)-O(8)#8	90.00(19)	N(10)-C(12)-N(6)	118.7(7)
O(11)-Pr(2)-O(8)#8	120.16(18)	N(10)-C(12)-N(8)	118.8(6)
O(9)#7-Pr(2)-O(8)#8	139.49(17)	N(6)-C(12)-N(8)	122.5(6)
O(9)#8-Pr(2)-O(8)#8	51.18(17)	N(10)-C(13)-C(15)	111.0(7)
O(8)#7-Pr(2)-O(8)#8	144.4(3)	N(10)-C(13)-C(14)	110.4(6)
O(2)-Pr(2)-O(1)	49.80(18)	C(15)-C(13)-C(14)	112.9(7)
O(2)#6-Pr(2)-O(1)	109.36(19)	O(7)-C(14)-O(6)	125.1(7)
O(11)#6-Pr(2)-O(1)	134.85(19)	O(7)-C(14)-C(13)	116.7(7)
O(11)-Pr(2)-O(1)	66.43(19)	O(6)-C(14)-C(13)	118.2(6)
O(9)#7-Pr(2)-O(1)	115.10(17)	N(9)-C(16)-C(17)	111.3(6)
O(9)#8-Pr(2)-O(1)	69.93(18)	N(9)-C(16)-C(18)	109.0(7)
O(8)#7-Pr(2)-O(1)	69.64(18)	C(17)-C(16)-C(18)	110.9(7)
O(8)#8-Pr(2)-O(1)	103.55(18)	O(9)-C(17)-O(8)	122.2(7)
O(2)-Pr(2)-O(1)#6	109.36(19)	O(9)-C(17)-C(16)	117.6(7)
O(2)#6-Pr(2)-O(1)#6	49.80(18)	O(8)-C(17)-C(16)	120.1(7)
O(11)#6-Pr(2)-O(1)#6	66.43(19)		

Symmetry operation: #1 -x+1, y, -z+1; #2 x, y+1, z; #3 -x+1, y+1, -z+1; #4 -x+1, y-1, -z+1; #5 x, y-1, z; #6 -x, y, -z; #7 -x+1/2, y-3/2, -z+1; #8 x-1/2, y-3/2, z-1;#9 x+1/2, y+3/2, z+1

Table S7. Hydrogen bond distances for **La(R)**.

Hydrogen bond distances (Å)			
Name	D–H···A	d(H···A)	d(D···A)
La(R)	O(11)-H(11A)...O(12)#4	1.92(3)	2.724(7)
	O(11)-H(11B)...O(15)#10	2.10(4)	2.878(6)
	O(12)-H(12)...O(13)#11	2.05(3)	2.823(7)
	O(13)-H(13A)...O(8)#5	2.18(3)	3.060(7)
	O(13)-H(13B)...O(2)#12	2.13(2)	2.933(6)
	O(14)-H(14A)...O(3)#13	2.59(9)	3.407(13)
	O(14)-H(14B)...O(1)#14	2.21(12)	2.848(9)
	O(14)-H(14B)...O(8)#5	2.44(7)	3.242(13)
	O(15)-H(15A)...O(1)#2	2.52(7)	2.948(6)
	O(15)-H(15A)...O(9)#15	2.08(5)	2.809(5)
	O(15)-H(15B)...O(3)	2.11(3)	2.919(6)
	N(3)-H(3N)...O(3)#4	2.05	2.860(6)
	N(3)-H(3N)...O(4)#4	2.45	3.230(6)
	N(4)-H(4N)...O(10)#4	2.31	3.174(5)
	N(5)-H(5N)...O(3)#4	2.20	2.986(6)
	N(7)-H(7N)...O(6)#2	2.65	3.377(6)
	N(7)-H(7N)...O(7)#2	1.95	2.684(6)
	N(8)-H(8N)...N(2)#2	2.03	2.871(5)
	N(9)-H(9N)...O(7)#2	2.60	3.159(7)
	N(9)-H(9N)...O(15)#3	2.09	2.822(6)
	N(10)-H(10N)...O(5)#2	2.02	2.894(5)

Symmetry operation: #1 -x+1, y, -z+1; #2 x, y-1, z; #3 -x+1, y-1, -z+1; #4 x, y+1, z; #5 -x+1, y+1, -z+1
#6 -x, y, -z; #7 x-1/2, y+3/2, z-1; #8 -x+1/2, y+3/2, -z+1; #9 x+1/2, y-3/2, z+1; #10 -x, y+1, -z
#11 x-1/2, y+1/2, z; #12 -x+1/2, y-1/2, -z; #13 x+1/2, y+1/2, z; #14 x+1/2, y-1/2, z; #15 x-1/2, y+1/2, z-1

Table S8. Hydrogen bond distances for **La(S)**.

Hydrogen bond distances (Å)			
Name	D–H···A	d(H···A)	d(D···A)
La(S)	O(11)-H(11A)...O(12)#4	2.25	2.723(7)
	O(11)-H(11B)...O(15)#10	2.07(4)	2.868(6)
	O(12)-H(12)...O(13)#11	2.05(3)	2.827(7)
	O(13)-H(13B)...O(2)#12	2.14(3)	2.927(6)
	O(13)-H(13A)...O(8)#5	2.18(3)	3.066(7)
	O(14)-H(14B)...O(1)#13	2.36(13)	2.858(8)
	O(14)-H(14A)...O(3)#14	2.53(4)	3.381(12)
	O(14)-H(14B)...O(1)#13	2.36(13)	2.858(8)
	O(14)-H(14B)...O(8)#5	2.37(4)	3.227(11)
	O(15)-H(15A)...O(3)	2.07(3)	2.920(6)
	O(15)-H(15B)...O(9)#15	2.19(6)	2.810(5)
	N(3)-H(3N)...O(3)#4	2.05	2.865(6)
	N(3)-H(3N)...O(4)#4	2.44	3.221(5)
	N(4)-H(4N)...O(10)#4	2.30	3.173(5)
	N(5)-H(5N)...O(3)#4	2.20	2.986(6)
	N(7)-H(7N)...O(6)#3	2.65	3.372(5)
	N(7)-H(7N)...O(7)#3	1.95	2.682(6)
	N(8)-H(8N)...N(2)#3	2.03	2.869(5)
	N(9)-H(9N)...O(7)#3	2.60	3.158(6)
	N(9)-H(9N)...O(15)#2	2.10	2.832(6)
	N(10)-H(10N)...O(5)#3	2.02	2.896(5)

Symmetry operation: #1 -x+1, y, -z+1; #2 -x+1, y+1, -z+1; #3 x, y+1, z; #4 x, y-1, z; #5 -x+1, y-1, -z+1
#6 -x, y, -z; #7 -x+1/2, y-3/2, -z+1; #8 x-1/2, y-3/2, z-1; #9 x+1/2, y+3/2, z+1; #10 -x, y-1, -z;
#11 x-1/2, y-1/2, z; #12 -x+1/2, y+1/2, -z; #13 x+1/2, y+1/2, z; #14 x+1/2, y-1/2, z; #15 x-1/2, y-1/2, z-1

Table S9. Hydrogen bond distances for **Ce(R)**.

Hydrogen bond distances (Å)			
Name	D–H···A	d(H···A)	d(D···A)
Ce(R)	O(11)-H(11B)...O(15)#10	2.06(5)	2.877(13)
	O(12)-H(12)...O(11)#2	2.32(6)	2.744(14)
	O(13)-H(13A)...O(8)#4	2.12(3)	3.021(14)
	O(13)-H(13B)...O(2)#11	2.11(3)	2.935(14)
	O(13)-H(13B)...O(12)#12	2.27(7)	2.814(14)
	O(14)-H(14A)...N(5)#12	2.56(10)	3.38(2)
	O(14)-H(14B)...O(1)#12	2.22(11)	2.830(18)
	O(14)-H(14B)...O(8)#4	2.38(5)	3.22(2)
	O(15)-H(15A)...O(9)#13	2.19(12)	2.806(12)
	O(15)-H(15B)...O(3)	2.11(7)	2.919(13)
	N(3)-H(3N)...O(3)#5	2.01	2.824(12)
	N(3)-H(3N)...O(4)#5	2.45	3.227(12)
	N(4)-H(4N)...O(10)#5	2.30	3.162(12)
	N(5)-H(5N)...O(3)#5	2.19	2.975(12)
	N(7)-H(7N)...O(7)#2	1.94	2.674(13)
	N(8)-H(8N)...N(2)#2	2.02	2.869(12)
	N(9)-H(9N)...O(7)#2	2.59	3.154(14)
	N(9)-H(9N)...O(15)#3	2.10	2.834(14)
	N(10)-H(10N)...O(5)#2	2.02	2.901(11)

Symmetry operation: #1 -x+1, y, -z+1; #2 x, y-1, z; #3 -x+1, y-1, -z+1; #4 -x+1, y+1, -z+1; #5 x, y+1, z
#6 -x, y, -z; #7 x-1/2, y+3/2, z-1; #8 -x+1/2, y+3/2, -z+1; #9 x+1/2, y-3/2, z+1; #10 -x, y+1, -z
#11 -x+1/2, y-1/2, -z; #12 x+1/2, y-1/2, z; #13 x-1/2, y+1/2, z-1

Table S10. Hydrogen bond distances for **Ce(S)**.

Hydrogen bond distances (Å)			
Name	D–H···A	d(H···A)	d(D···A)
Ce(S)	O(11)-H(11A)...O(12)#5	2.28	2.733(11)
	O(11)-H(11B)...O(15)#10	2.18(7)	2.895(9)
	O(12)-H(12)...O(13)#11	2.007(17)	2.828(10)
	O(13)-H(13A)...O(8)#4	2.235(11)	3.070(9)
	O(13)-H(13B)...O(2)#12	2.108(18)	2.930(9)
	O(14)-H(14A)...O(1)#13	2.03(3)	2.845(12)
	O(14)-H(14B)...O(8)#4	2.54(7)	3.221(14)
	O(15)-H(15A)...O(3)	2.01(4)	2.916(10)
	O(15)-H(15B)...O(9)#14	2.09(3)	2.820(8)
	N(3)-H(3N)...O(3)#5	2.03	2.848(9)
	N(3)-H(3N)...O(4)#5	2.46	3.229(8)
	N(4)-H(4N)...O(10)#5	2.30	3.172(8)
	N(5)-H(5N)...O(3)#5	2.22	2.997(9)
	N(7)-H(7N)...O(6)#2	2.65	3.372(8)
	N(7)-H(7N)...O(7)#2	1.93	2.672(9)
	N(8)-H(8N)...N(2)#2	2.02	2.865(8)
	N(9)-H(9N)...O(7)#2	2.60	3.163(10)
	N(9)-H(9N)...O(15)#3	2.11	2.842(9)
	N(10)-H(10N)...O(5)#2	2.01	2.884(7)
Symmetry operation: #1 -x+1, y, -z+1; #2 x, y+1, z; #3 -x+1, y+1, -z+1; #4 -x+1, y-1, -z+1; #5 x, y-1, z #6 -x, y, -z; #7 -x+1/2, y-3/2, -z+1; #8 x-1/2, y-3/2, z-1; #9 x+1/2, y+3/2, z+1; #10 -x, y-1, -z #11 x-1/2, y-1/2, z; #12 -x+1/2, y+1/2, -z; #13 x+1/2, y+1/2, z; #14 x-1/2, y-1/2, z-1			

Table S11. Hydrogen bond distances for **Pr(R)**.

Hydrogen bond distances (Å)			
Name	D–H···A	d(H···A)	d(D···A)
Pr(R)	O(11)-H(11A)...O(12)#5	1.94(4)	2.724(7)
	O(11)-H(11B)...O(15)#10	2.11(4)	2.894(6)
	O(12)-H(12)...O(13)#11	2.05(3)	2.818(6)
	O(13)-H(13A)...O(8)#4	2.17(2)	3.047(7)
	O(13)-H(13B)...O(2)#12	2.14(3)	2.921(6)
	O(14)-H(14A)...O(1)#13	2.15(9)	2.830(9)
	O(14)-H(14A)...N(5)#13	2.69(16)	3.391(11)
	O(14)-H(14B)...O(8)#4	2.33(3)	3.217(12)
	O(15)-H(15A)...O(9)#14	2.10(5)	2.808(6)
	O(15)-H(15B)...O(3)	2.09(3)	2.916(6)
	N(3)-H(3N)...O(3)#5	2.01	2.825(6)
	N(3)-H(3N)...O(4)#5	2.46	3.226(5)
	N(4)-H(4N)...O(10)#5	2.28	3.152(5)
	N(5)-H(5N)...O(3)#5	2.21	2.994(6)
	N(7)-H(7N)...O(6)#3	2.65	3.364(5)
	N(7)-H(7N)...O(7)#3	1.93	2.669(6)
	N(8)-H(8N)...N(2)#3	2.01	2.857(5)
	N(9)-H(9N)...O(7)#3	2.60	3.161(6)
	N(9)-H(9N)...O(15)#2	2.08	2.817(6)
	N(10)-H(10N)...O(5)#3	2.01	2.885(5)

Symmetry operation: #1 -x+1, y, -z+1; #2 -x+1, y-1, -z+1; #3 x, y-1, z; #4 -x+1, y+1, -z+1; #5 x, y+1, z
#6 -x, y, -z; #7 x-1/2, y+3/2, z-1; #8 -x+1/2, y+3/2, -z+1; #9 x+1/2, y-3/2, z+1; #10 -x, y+1, -z
#11 x-1/2, y+1/2, z; #12 -x+1/2, y-1/2, -z; #13 x+1/2, y-1/2, z; #14 x-1/2, y+1/2, z-1

Table S12. Hydrogen bond distances for **Pr(S)**.

Hydrogen bond distances (Å)			
Name	D–H···A	d(H···A)	d(D···A)
Pr(S)	O(11)-H(11A)...O(12)#5	1.94(4)	2.724(7)
	O(11)-H(11B)...O(15)#5	2.11(4)	2.894(6)
	O(12)-H(12)...O(13)#10	2.05(3)	2.818(6)
	O(13)-H(13B)...O(2)#11	2.17(2)	3.047(7)
	O(13)-H(13A)...O(8)#4	2.14(3)	2.921(6)
	O(14)-H(14A)...O(1)#12	2.15(9)	2.830(9)
	O(14)-H(14A)...N(5)#12	2.69(16)	3.391(11)
	O(14)-H(14B)...O(8)#4	2.33(3)	3.217(12)
	O(14)-H(14B)...N(6)#4	2.10(5)	2.808(6)
	O(15)-H(15A)...O(3)	2.09(3)	2.916(6)
	O(15)-H(15B)...O(9)#13	2.01	2.825(6)
	N(3)-H(3N)...O(3)#5	2.46	3.226(5)
	N(3)-H(3N)...O(4)#5	2.28	3.152(5)
	N(4)-H(4N)...O(10)#5	2.21	2.994(6)
	N(5)-H(5N)...O(3)#5	2.65	3.364(5)
	N(7)-H(7N)...O(6)#2	1.93	2.669(6)
	N(7)-H(7N)...O(7)#2	2.01	2.857(5)
	N(8)-H(8N)...N(2)#2	2.60	3.161(6)
	N(9)-H(9N)...O(7)#2	2.08	2.817(6)
	N(9)-H(9N)...O(15)#3	2.01	2.885(5)
	N(10)-H(10N)...O(5)#2	2.02	2.896(8)

Symmetry operation: #1 -x+1, y, -z+1; #2 x, y+1, z; #3 -x+1, y+1, -z+1; #4 -x+1, y-1, -z+1; #5 x, y-1, z #6 -x, y, -z; #7 -x+1/2, y-3/2, -z+1; #8 x-1/2, y-3/2, z-1; #9 x+1/2, y+3/2, z+1; #10 x-1/2, y-1/2, z
#11 -x+1/2, y+1/2, -z; #12 x+1/2, y+1/2, z; #13 x-1/2, y-1/2, z-1

Table S13. Bond-valence sum (BVS) calculations for **Ln(R)** and **Ln(S)** (Ln = La, Ce, and Pr).

	La(R)	La(S)	Ce(R)	Ce(S)	Pr(R)	Pr(S)
Ln (1)	3.40	3.39	3.48	3.38	3.46	3.46
Ln (2)	3.13	3.15	3.19	3.15	3.20	3.14

Table S14. SHG efficiencies of Ln-CPs composed of lanthanide cations and chiral organic ligands.

Name	Space group	Chiral template	SHG efficiency
$Ln_2((S,S)$-*TBA*$)_2((S,S)$-H*TBA*$)_2(H_2O)_2]\cdot 7H_2O$ [Ln = La, Ce, and Pr]	*C*2	1,3,5-triazin-2(1*H*)-one-4,6-bis(alanyl)	8 × α-SiO_2
$\{[Ln_2(HL)_2(NO_3)_4(H_2O)_4]\cdot NO_3\cdot Cl\cdot 7H_2O\}_n$[1] [Ln = Nd, Pr, Sm, Eu, and Tb]	$P2_1$	(*S*)-2-((4-([2,2′:6′,2″-terpyridin]-4′-yl) benzyl)amino)propanoic acid	0.28 × KDP
$[Ce_2((R$ or *S*$)$-CIA$)_2(H_2O)_5]\cdot 2H_2O$ [2]	*P*1	(*R* or *S*)-5-(1-carboxyethoxy) isophthalic acid	0.4 × urea
[Ce(L or D-tart)$(CH_2OHCH_2OH)(H_2O)$]Cl [3]	$P2_1$	L or D-tartaric acid	0.5 × urea
$\{[Gd_4$(R-ttpc$)_2$(R-Httpc$)_2(HCOO)_2(H_2O)_8]\cdot 4H_2O\}_n$[4]	$P2_1$	(3*R*,3′*R*,3″*R*)-1,1′,1″-(1,3,5-triazine-2,4,6-triyl)-tripiperidine-3-carboxylic acid	0.5 × urea
$[Ln_2(cpfa)_3]_n$[5] [Ln = Yb and Lu]	$P2_12_12_1$	(*R*)-4-(4-(1-carboxyethoxy)phenoxy)-3-fluorobenzoic acid	0.5 × urea

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