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Rational Design and Synthesis of a Series of 3D Lanthanide Metal-Organic Frameworks with Different Structures Driven by Reaction Conditions

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Figure S1. Powder X-ray diffraction patterns of the simulated sample **1**, and as-synthesized samples **1-8**, indicating the phase purity of the as-synthesized samples.

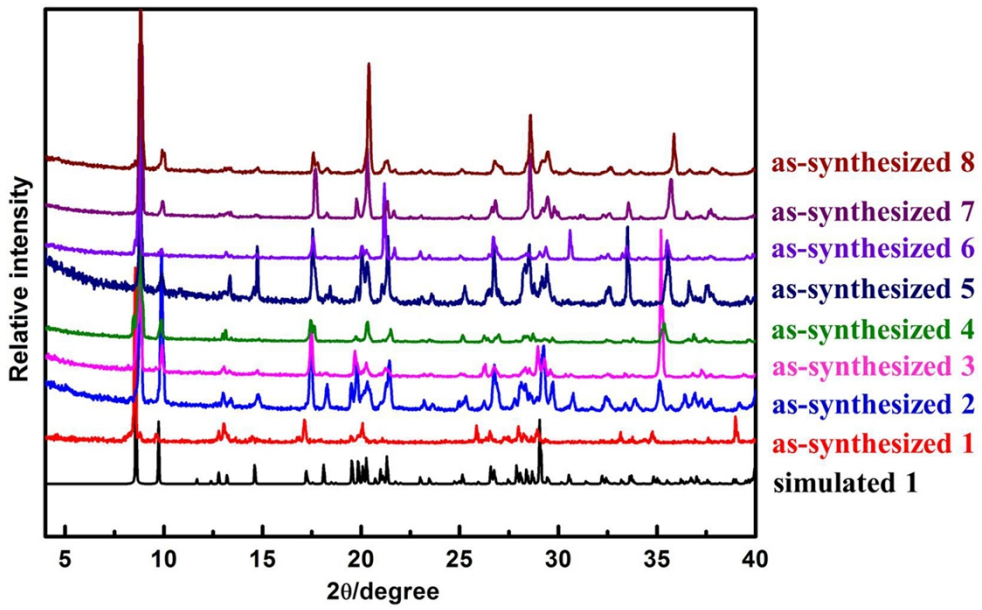

Figure S2. IR spectra for compounds **1-8** and H_2tdc ligand.

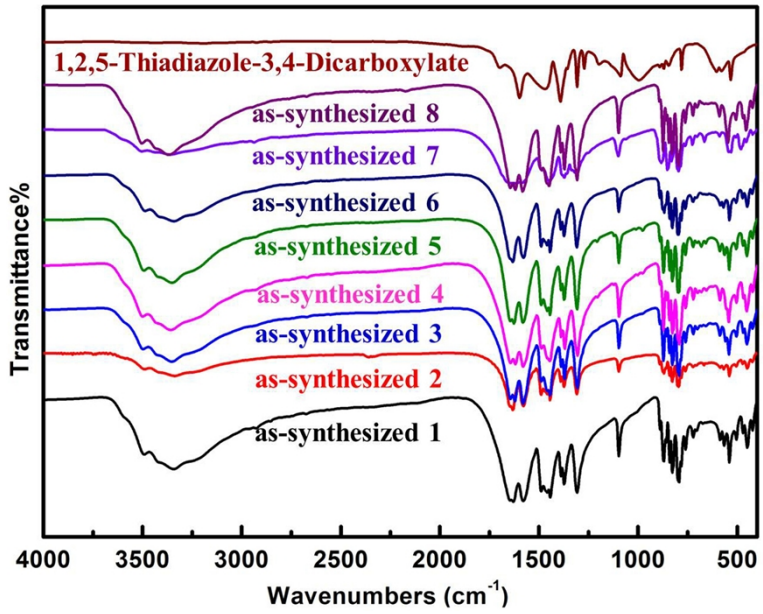

Figure S3. Powder X-ray diffraction patterns of the simulated sample **9**, and as-synthesized samples **9** and **10**, indicating the phase purity of the as-synthesized samples.

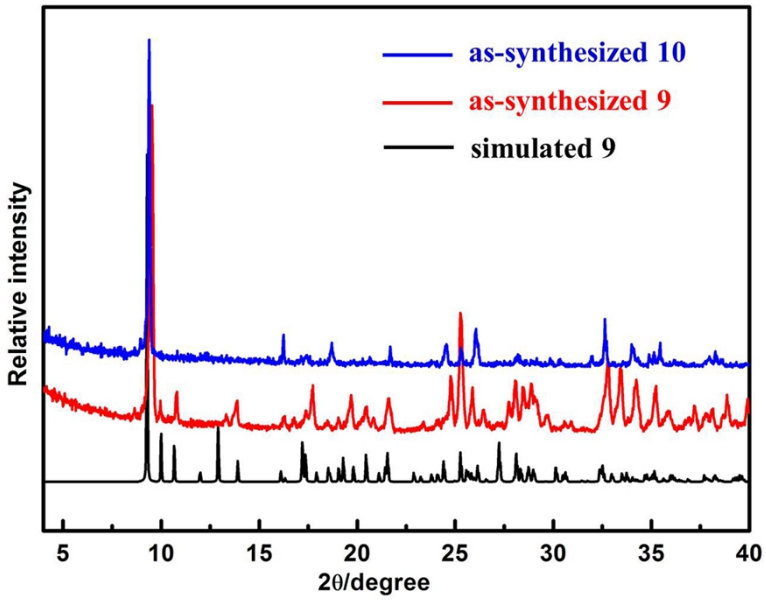

Figure S4. IR spectra for compounds **9** and **10**.

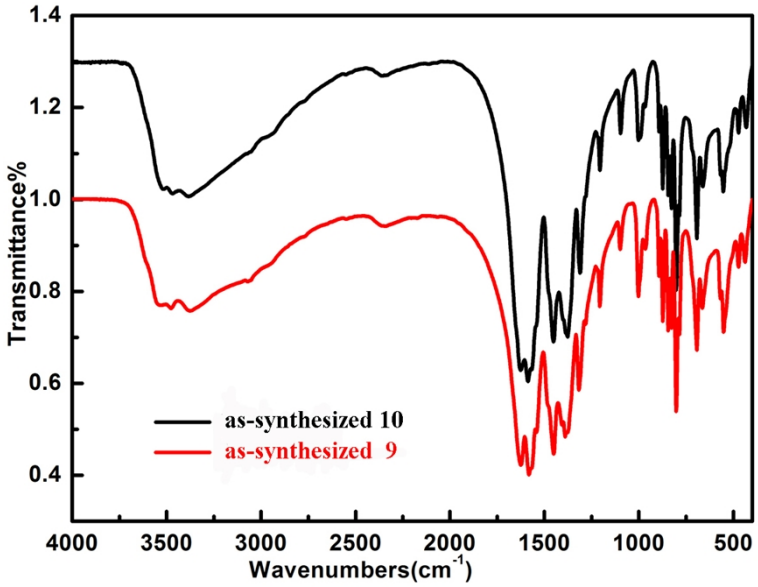

Figure S5. Powder X-ray diffraction patterns of the simulated sample **11**, and as-synthesized samples **11** and **12**, indicating the phase purity of the as-synthesized samples.

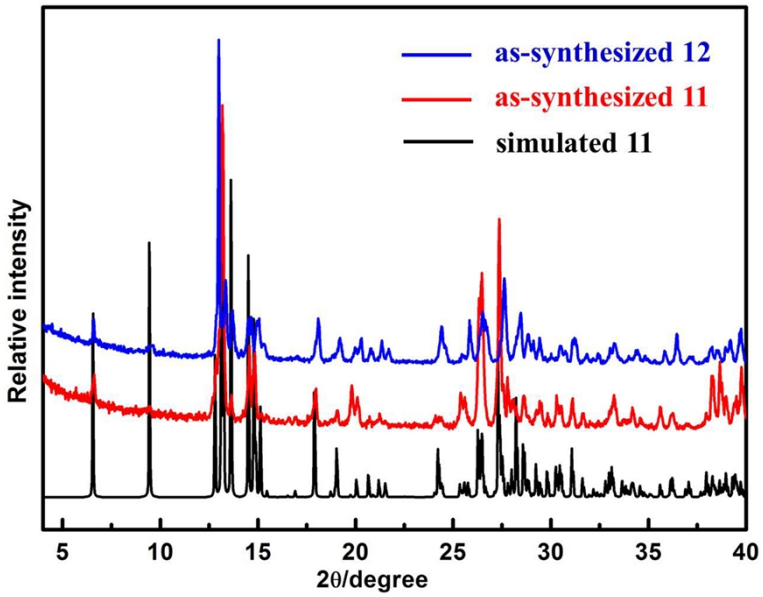

Figure S6. IR spectra for compounds **11** and **12**.

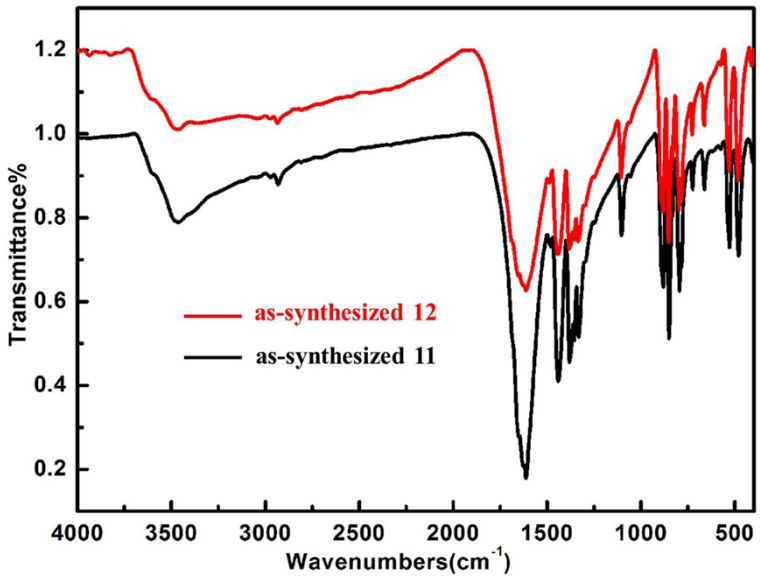

Figure S7. The coordination and geometry for La1 and K1 atoms in compound **1**.

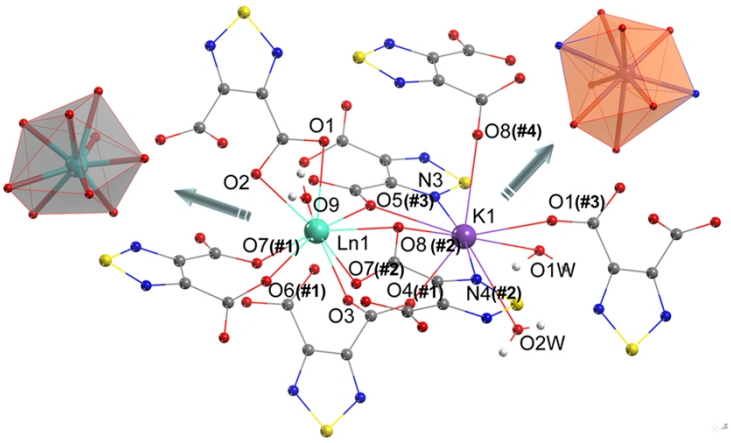

Figure S8. For compound **1**, 1D zigzag chains are linked by K atoms to form a 2D layer, showing the ring of thiadiazole parallel each other.

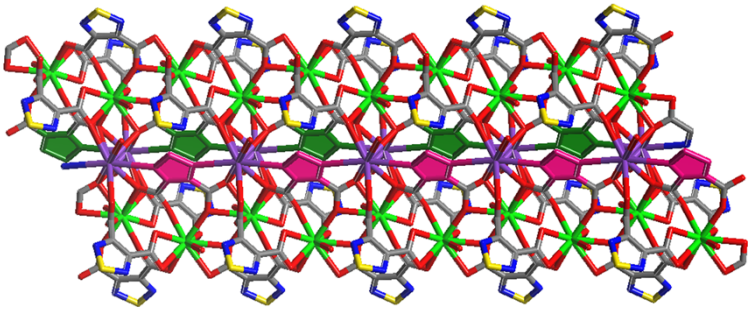

Figure S9. The coordination and geometry for La1 and K1 atoms in compound **9**.

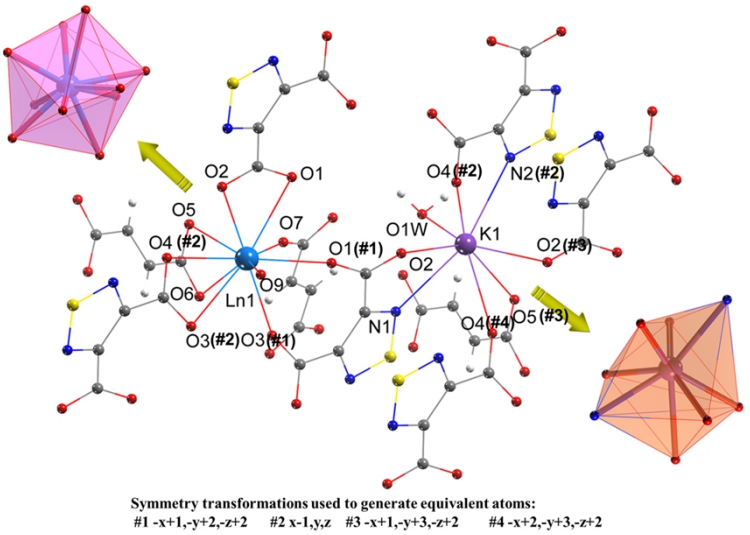

Figure S10. For compound **9**, 1D zigzag chains are linked via K atoms and Fac ligand to construct 2D layers, showing the thiadiazole ring parallel each other.

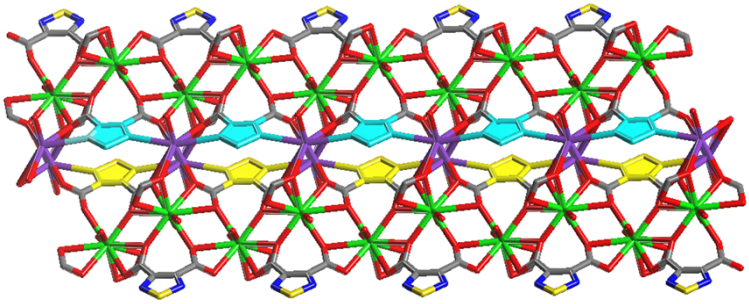

Figure S11. The coordination and geometry for La1 and La2 atoms in compound **11**.

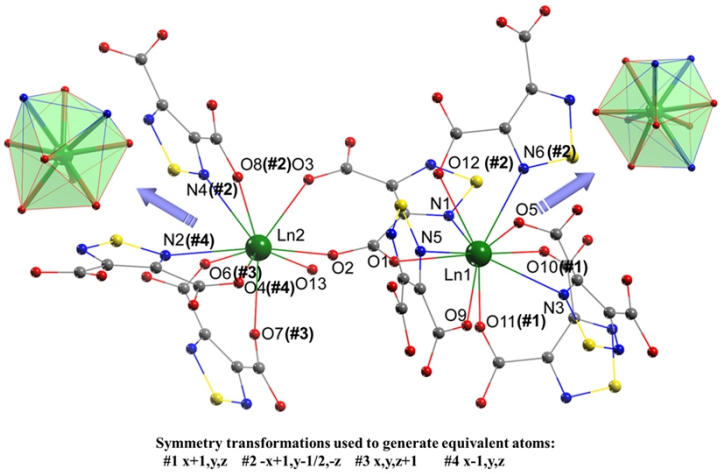

Figure S12. TGA curve for compounds **1-8**.

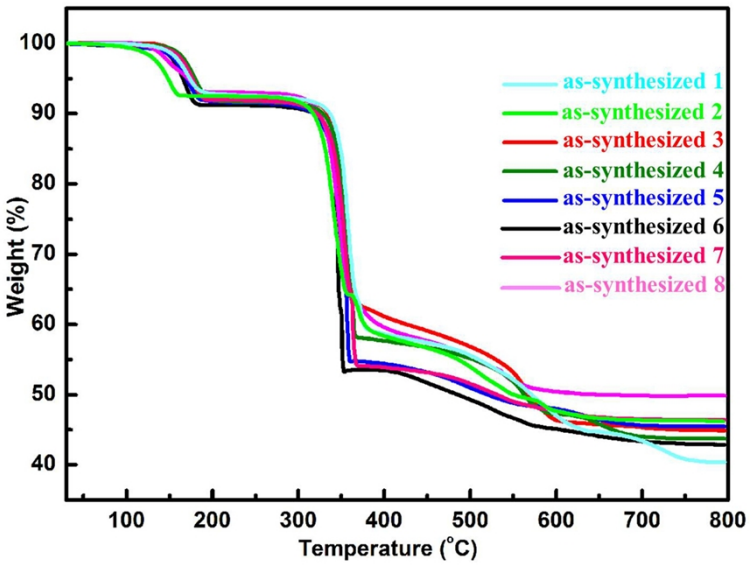

Figure S13. TGA curve for compounds **9** and **10**.

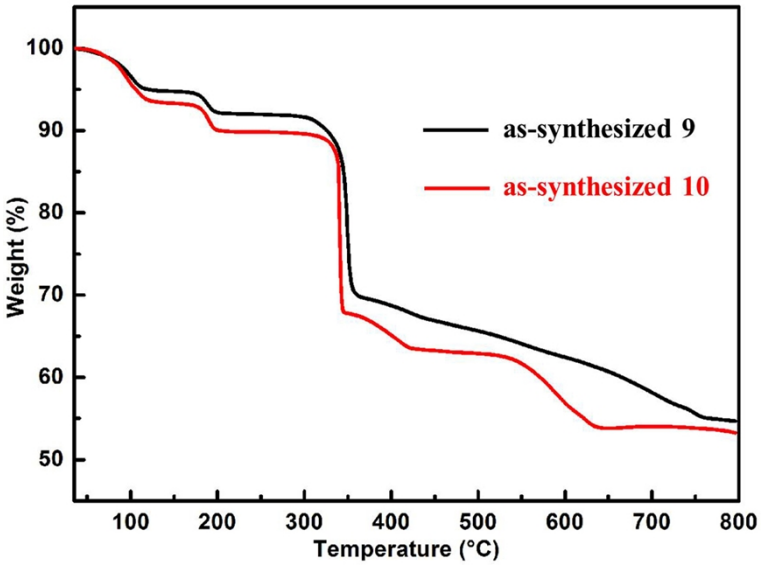

Figure S14. TGA curve for compounds **11** and **12**.

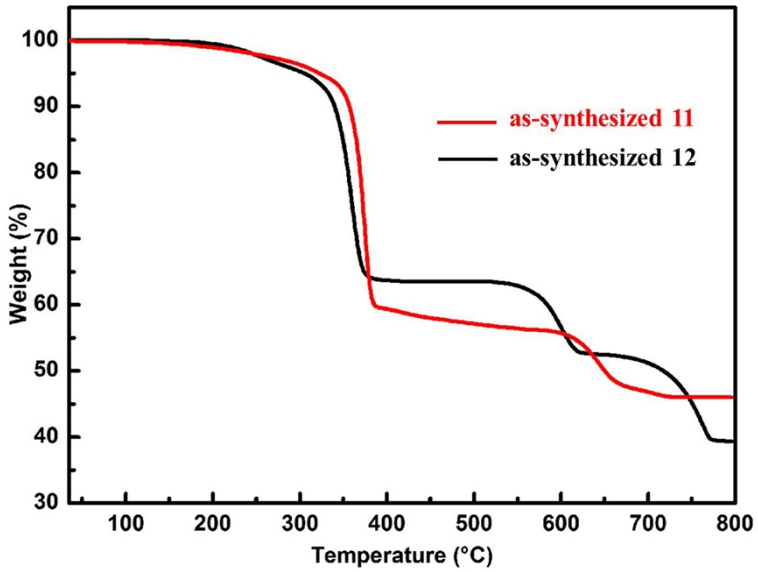

Figure S15. The excitation (upper right) and luminescent spectrum of H_2tdc ligand.

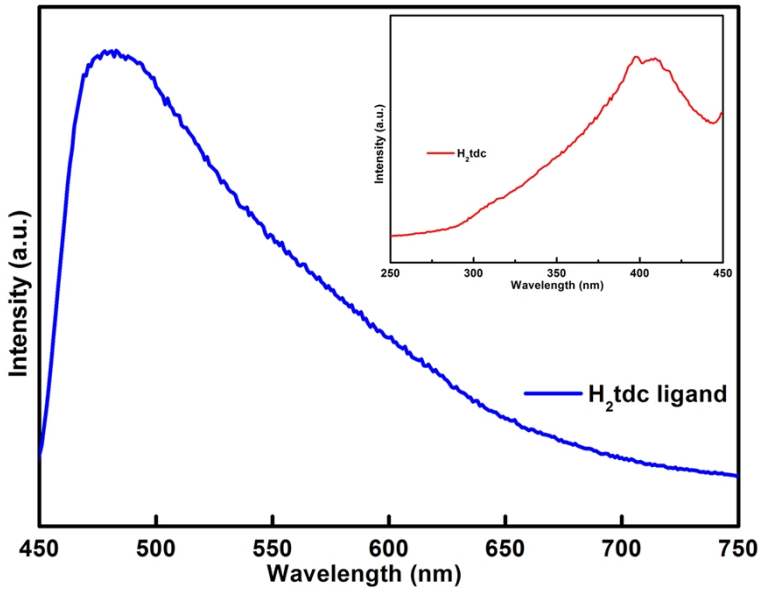

Table S1. Crystal data and structure refinement for compounds **1-12**.

Name	**1**	**2**	**3**
Empirical formula	$C_8H_5N_4O_{10.5}S_2LaK$	$C_8H_5N_4O_{10.5}S_2CeK$	$C_8H_5N_4O_{10.5}S_2PrK$
Formula weight	567.29	568.50	569.29
Temperature (K)	296(2)	296(2)	296(2)
Wave length (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	*C2/c*	*C2/c*	*C2/c*
a (Å)	18.175(3)	18.1751(6)	18.1372(13)
b (Å)	8.3358(13)	8.3432(3)	8.3620(6)
c (Å)	20.601(3)	20.5556(7)	20.4822(14)
α (deg)	90	90	90
β (deg)	91.868(2)	91.7010(10)	91.5060(10)
γ (deg)	90	90	90
Volume ($Å^3$)	3119.4(9)	3115.65(19)	3105.3(4)
Z, D_{calc} (Mg/m^3)	8, 2.416	8, 2.424	8, 2.435
Absorption coefficient (mm^{-1})	3.341	3.525	3.743
F (000)	2184	2192	2200
θ range (deg)	1.98 to 28.40	1.98 to 28.35	1.99 to 28.32
index range (deg)	-8<=h<=24,	-14<=h<=24,	-22<=h<=21,
	11<=k<=10,	10<=k<=10,	11<=k<=11,
	27<=l<=27	26<=l<=24	27<=l<=16
Reflections colected/	9457/3813	9447/3739	9395/3743
unique (Rint)	[R(int) = 0.0227]	[R(int) = 0.0160]	[R(int) = 0.0182]
Crystal size (mm^3)	0.24 × 0.21 × 0.19	0.24 × 0.23 × 0.19	0.21 × 0.17 × 0.14
Data/restraints/parameters	3813/7/255	3739/7/255	3743/7/255
Goodness-of-fit on F^2	1.035	1.067	1.063
R_1, wR_2 ($I>2\sigma(I)$)	0.0237, 0.0559	0.0196, 0.0501	0.0217, 0.0493
R_1, wR_2 (all data))	0.0309, 0.0601	0.0237, 0.0528	0.0267, 0.0519
largest difference in peak and hole (e $Å^{-3}$)	0.529, -0.580	0.549, -0.528	1.050, -0.393

$R_1=\sum||F_o|-|F_c||/\sum|F_o|$. $wR_2=[\sum[\,w\,(F_o^2-F_c^2)^2]\,/\,\sum[\,w\,(F_o^2)^2]]^{1/2}$

Name	Compound 4	Compound 5	Compound 6
Empirical formula	$C_8H_5N_4O_{10.5}S_2NdK$	$C_8H_5N_4O_{10.5}S_2SmK$	$C_8H_5N_4O_{10.5}S_2EuK$
Formula weight	572.62	578.73	580.34
Temperature (K)	293(2)	296(2)	296(2)
Wave length (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	*C2/c*	*C2/c*	*C2/c*
a (Å)	18.077(4)	18.0225(12)	18.018(7)
b (Å)	8.3675(17)	8.3808(6)	8.425(3)
c (Å)	20.380(4)	20.2445(14)	20.243(8)
α (deg)	90	90	90
β (deg)	91.14(3)	90.9410(10)	90.701(6)
γ (deg)	90	90	90
Volume ($Å^3$)	3082.1(11)	3057.4(4)	3073(2)
Z, D_{calc} (Mg/m^3)	8, 2.468	8, 2.515	8, 2.509
Absorption coefficient (mm^{-1})	3.979	4.456	4.693
F (000)	2208	2224	2232
θ range (deg)	3.36 to 27.47	2.01 to 28.38	2.01 to 28.27
index range (deg)	-23<=h<=23,	-22<=h<=23,	-19<=h<=23,
	10<=k<=10,	6<=k<=11,	11<=k<=10,
	26<=l<=26	-27<=l<=26	20<=l<=26
Reflections colected/	14640/3484	9194/3699	9244/3679
unique (Rint)	[R(int) = 0.0400]	[R(int) = 0.0216]	[R(int) = 0.0263]
Crystal size (mm^3)	0.23 × 0.23 × 0.20	0.24 × 0.21 × 0.19	0.24 × 0.19 × 0.17
Data/restraints/parameters	3484/7/255	3699/7/255	3679/9/255
Goodness-of-fit on F^2	1.042	1.166	1.038
R_1, wR_2 ($I>2\sigma(I)$)	0.0227, 0.0437	0.0280, 0.0664	0.0221, 0.0510
R_1, wR_2 (all data))	0.0309, 0.0464	0.0313, 0.0677	0.0256, 0.0528
largest difference in peak and hole (e $Å^{-3}$)	0.376, -0.676	1.132, -0.848	0.577, -0.746

$R_1=\sum||F_o|-|F_c||/\sum|F_o|$. $wR_2=[\sum[\ w\ (F_o^2-F_c^2)^2]\ /\ \sum[\ w\ (F_o^2)^2]]^{1/2}$

Name	Compound 7	Compound 8	Compound 9
Empirical formula	$C_8H_5N_4O_{10.5}S_2GdK$	$C_8H_5N_4O_{10.5}S_2TbK$	$C_{16}H_{10}N_4O_{21}S_2La_2K_2$
Formula weight	585.63	587.30	1014.42
Temperature (K)	296(2)	296(2)	296(2)
Wave length (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	*C2/c*	*C2/c*	*P*-1
a (Å)	17.9591(10)	17.9826(16)	8.2702(6)
b (Å)	8.3886(5)	8.4090(7)	10.3267(7)
c (Å)	20.1179(12)	20.1070(17)	10.9629(12)
α (deg)	90	90	102.7680(10)
β (deg)	90.6360(10)	90.5610(10)	109.2740(10)
γ (deg)	90	90	111.5240(10)
Volume ($Å^3$)	3030.6(3)	3040.3(5)	757.20(11)
Z, D_{calc} (Mg/m^3)	8, 2.468	8, 2.567	1, 2.225
Absorption coefficient (mm^{-1})	3.979	4.997	3.290
F (000)	2208	2240	486
θ range (deg)	3.36 to 27.47	2.27 to 28.21	2.14 to 28.48
index range (deg)	-23<=h<=23,	-23<=h<=18,	-11<=h<=4,
	10<=k<=10,	9<=k<=11,	-13<=k<=13,
	26<=l<=26	-26<=l<=26	-14<=l<=14
Reflections colected/	14640/3484	9152/3639	4801/3508
unique (Rint)	[R(int) = 0.0400]	[R(int) = 0.0252]	[R(int) = 0.0140]
Crystal size (mm^3)	0.23 × 0.23 × 0.20	0.27 × 0.24 × 0.23	0.26 × 0.24 × 0.20
Data/restraints/parameters	3484/7/255	3639/7/255	3508/11/232
Goodness-of-fit on F^2	1.042	1.035	1.071
R_1, wR_2 ($I>2\sigma(I)$)	0.0227, 0.0437	0.0205, 0.0457	0.0270, 0.0702
R_1, wR_2 (all data))	0.0309, 0.0464	0.0232, 0.0469	0.0311, 0.0725
largest difference in peak and hole (e $Å^{-3}$)	0.376, -0.676	0.532, -0.449	0.820, -0.577

$R_1=\sum||F_o|-|F_c||/\sum|F_o|$. $wR_2=[\sum[\ w\ (F_o^2-F_c^2)^2]\ /\ \sum[\ w\ (F_o^2)^2]]^{1/2}$

Name	Compound 10	Compound 11	Compound 12
Empirical formula	$C_{16}H_{10}N_4O_{21}S_2Ce_2K_2$	$C_{12}H_4N_6O_{14}S_3La_2$	$C_{12}H_4N_6O_{14}S_3Ce_2$
Formula weight	1016.84	830.21	832.63
Temperature (K)	293(2) K	296(2)	296(2) K
Wave length (Å)	0.71073	0.71073	0.71073 A
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	*P*-1	$P2_1$	$P2_1$
a (Å)	8.2470(12)	7.0404(3)	6.975(5)
b (Å)	10.2753(14)	13.0015(6)	12.901(8)
c (Å)	10.915(2)	13.7338(6)	13.551(9)
α (deg)	102.536(3)	90	90
β (deg)	109.193(3)	100.8810(6)	100.729(11)
γ (deg)	112.161(2)	90	90
Volume ($Å^3$)	744.9(2)	1234.53(9)	1198.0(14)
Z, D_{calc} (Mg/m^3)	1, 2.267	2, 2.233	2, 2.308
Absorption coefficient (mm^{-1})	3.533	3.744	4.092
F (000)	488	784	788
θ range (deg)	2.15 to 28.48	1.51 to 28.37	3.06 to 24.99
index range (deg)	-10<=h<=11,	-9<=h<=9,	-7<=h<=8,
	-13<=k<=12,	-17<=k<=15,	15<=k<=10,
	-7<=l<=14	-18<=l<=16	16<=l<=14
Reflections colected/	4747/3467	7808/4896	5916/3628
unique (Rint)	[R(int) = 0.0280]	[R(int) = 0.0186]	[R(int) = 0.0895]
Crystal size (mm^3)	0.26 × 0.25 × 0.21	0.24 × 0.21 × 0.17	0.24 × 0.21 × 0.17
Flack parameter		0.006(18)	-0.03(4)
Data/restraints/parameters	3467/11/223	4896/7/352	3628/7/361
Goodness-of-fit on F^2	1.054	1.102	1.007
R_1, wR_2 ($I>2\sigma(I)$)	0.0436, 0.0920	0.0279, 0.0908	0.0718, 0.1759
R_1, wR_2 (all data))	0.0521, 0.0976	0.0283, 0.0910	0.0766, 0.1796
largest difference in peak and hole (e $Å^{-3}$)	1.013, -1.570	2.360, -0.805	2.620, -2.946

$R_1=\sum||F_o|-|F_c||/\sum|F_o|$. $wR_2=[\sum[\ w\ (F_o^2-F_c^2)^2]\ /\ \sum[\ w\ (F_o^2)^2]]^{1/2}$

Table S2. Bond lengths [Å] and angles [º] for compounds **1-8**.

		1	
La(1)-O(3)#1	2.467(2)	La(1)-O(7)#1	2.4932(17)
La(1)-O(2)	2.5109(18)	La(1)-O(6)#1	2.5245(17)
La(1)-O(5)	2.5414(19)	La(1)-O(9)	2.545(2)
La(1)-O(8)#2	2.6307(18)	La(1)-O(1)	2.6647(18)
La(1)-O(7)#2	2.7718(18)	La(1)-O(6)	3.0159(19)
K(1)-O(1)#3	2.7044(19)	K(1)-O(5)	2.749(2)
K(1)-O(4)#1	2.750(2)	K(1)-O(8)#2	2.906(2)
K(1)-O(8)#4	2.9515(19)	K(1)-N(4)#2	2.956(2)
K(1)-N(3)	2.958(2)	K(1)-O(2W)#3	3.2218(14)
K(1)-O(5)#3	3.337(2)	K(1)-O(1W)#5	3.362(3)
O(3)#1-La(1)-O(7)#1	84.88(7)	O(3)#1-La(1)-O(2)	142.35(6)
O(7)#1-La(1)-O(2)	93.25(6)	O(3)#1-La(1)-O(6)#1	77.50(7)
O(7)#1-La(1)-O(6)#1	68.93(6)	O(2)-La(1)-O(6)#1	66.93(6)
O(3)#1-La(1)-O(5)	75.73(7)	O(7)#1-La(1)-O(5)	160.46(7)
O(2)-La(1)-O(5)	103.52(6)	O(6)#1-La(1)-O(5)	108.35(6)
O(3)#1-La(1)-O(9)	135.08(7)	O(7)#1-La(1)-O(9)	71.25(7)
O(2)-La(1)-O(9)	78.17(7)	O(6)#1-La(1)-O(9)	124.20(7)
O(5)-La(1)-O(9)	121.61(7)	O(3)#1-La(1)-O(8)#2	79.97(7)
O(7)#1-La(1)-O(8)#2	110.25(6)	O(2)-La(1)-O(8)#2	134.58(6)
O(6)#1-La(1)-O(8)#2	157.44(6)	O(5)-La(1)-O(8)#2	64.40(6)
O(9)-La(1)-O(8)#2	73.88(7)	O(3)#1-La(1)-O(1)	146.49(6)
O(7)#1-La(1)-O(1)	128.59(6)	O(2)-La(1)-O(1)	50.37(6)
O(6)#1-La(1)-O(1)	113.01(6)	O(5)-La(1)-O(1)	70.77(6)
O(9)-La(1)-O(1)	66.94(6)	O(8)#2-La(1)-O(1)	85.58(6)
O(3)#1-La(1)-O(7)#2	68.23(6)	O(7)#1-La(1)-O(7)#2	63.16(6)
O(2)-La(1)-O(7)#2	142.52(6)	O(6)#1-La(1)-O(7)#2	122.26(6)
O(5)-La(1)-O(7)#2	106.34(6)	O(9)-La(1)-O(7)#2	67.10(6)
O(8)#2-La(1)-O(7)#2	47.92(5)	O(1)-La(1)-O(7)#2	121.40(5)
O(3)#1-La(1)-O(6)	89.24(6)	O(7)#1-La(1)-O(6)	138.10(5)
O(2)-La(1)-O(6)	67.42(6)	O(6)#1-La(1)-O(6)	69.29(6)
O(5)-La(1)-O(6)	45.51(5)	O(9)-La(1)-O(6)	133.66(6)
O(8)#2-La(1)-O(6)	109.44(5)	O(1)-La(1)-O(6)	67.30(5)
O(7)#2-La(1)-O(6)	149.16(5)	O(1)#3-K(1)-O(5)	150.49(6)
O(1)#3-K(1)-O(4)#1	138.08(7)	O(5)-K(1)-O(4)#1	71.17(7)
O(1)#3-K(1)-O(8)#2	115.12(6)	O(5)-K(1)-O(8)#2	58.29(6)
O(4)#1-K(1)-O(8)#2	89.07(6)	O(1)#3-K(1)-O(8)#4	78.86(6)
O(5)-K(1)-O(8)#4	72.85(6)	O(4)#1-K(1)-O(8)#4	137.17(7)
O(8)#2-K(1)-O(8)#4	91.32(5)	O(1)#3-K(1)-N(4)#2	73.29(6)
O(5)-K(1)-N(4)#2	113.43(6)	O(4)#1-K(1)-N(4)#2	96.53(8)
O(8)#2-K(1)-N(4)#2	56.31(6)	O(8)#4-K(1)-N(4)#2	118.83(6)
O(1)#3-K(1)-N(3)	118.48(6)	O(5)-K(1)-N(3)	55.96(6)
O(4)#1-K(1)-N(3)	75.54(8)	O(8)#2-K(1)-N(3)	114.02(6)

O(8)#4-K(1)-N(3)	65.33(6)	N(4)#2-K(1)-N(3)	168.16(7)
O(1)#3-K(1)-O(2W)#3	71.70(5)	O(5)-K(1)-O(2W)#3	137.25(6)
O(4)#1-K(1)-O(2W)#3	66.39(6)	O(8)#2-K(1)-O(2W)#3	124.46(7)
O(8)#4-K(1)-O(2W)#3	140.69(5)	N(4)#2-K(1)-O(2W)#3	77.01(8)
N(3)-K(1)-O(2W)#3	106.98(8)	O(1)#3-K(1)-O(5)#3	58.80(5)
O(5)-K(1)-O(5)#3	96.04(5)	O(4)#1-K(1)-O(5)#3	154.22(7)
O(8)#2-K(1)-O(5)#3	65.33(5)	O(8)#4-K(1)-O(5)#3	51.57(5)
N(4)#2-K(1)-O(5)#3	67.42(6)	N(3)-K(1)-O(5)#3	116.50(6)
O(2W)#3-K(1)-O(5)#3	124.90(6)	O(1)#3-K(1)-O(1W)#5	65.95(7)
O(5)-K(1)-O(1W)#5	122.02(7)	O(4)#1-K(1)-O(1W)#5	88.77(7)
O(8)#2-K(1)-O(1W)#5	177.52(6)	O(8)#4-K(1)-O(1W)#5	91.09(6)
N(4)#2-K(1)-O(1W)#5	122.77(7)	N(3)-K(1)-O(1W)#5	66.57(7)
O(2W)#3-K(1)-O(1W)#5	53.42(7)	O(5)#3-K(1)-O(1W)#5	116.75(6)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y-1/2,-z+1 #2 x,y+1,#3 -x,-y,-z+1 #4 -x,-y-1,-z+1 #5 x-1/2,-y-1/2,z+1/2 #6 x,y-1,z #7 x+1/2,-y-1/2,z-1/2 #8 x,-y,z-1/2

2

Ce(1)-O(3)#1	2.4434(18)	Ce(1)-O(7)#1	2.4763(15)
Ce(1)-O(2)	2.4920(15)	Ce(1)-O(6)#1	2.5010(15)
Ce(1)-O(5)	2.5202(15)	Ce(1)-O(9)	2.5274(17)
Ce(1)-O(8)#2	2.6084(15)	Ce(1)-O(1)	2.6496(16)
Ce(1)-O(7)#2	2.7601(15)	K(1)-O(1)#3	2.7013(16)
K(1)-O(4)#1	2.7492(19)	K(1)-O(5)	2.7637(17)
K(1)-O(8)#2	2.8956(18)	K(1)-N(3)	2.9493(19)
K(1)-O(8)#4	2.9584(16)	K(1)-N(4)#2	2.966(2)
K(1)-O(2W)#3	3.2200(11)	K(1)-O(1W)#5	3.357(3)
K(1)-O(5)#3	3.3604(19)	O(3)#1-Ce(1)-O(7)#1	85.31(6)
O(3)#1-Ce(1)-O(2)	142.07(5)	O(7)#1-Ce(1)-O(2)	92.89(5)
O(3)#1-Ce(1)-O(6)#1	76.82(6)	O(7)#1-Ce(1)-O(6)#1	69.30(5)
O(2)-Ce(1)-O(6)#1	67.27(5)	O(3)#1-Ce(1)-O(5)	75.67(6)
O(7)#1-Ce(1)-O(5)	160.87(6)	O(2)-Ce(1)-O(5)	103.27(5)
O(6)#1-Ce(1)-O(5)	107.43(5)	O(3)#1-Ce(1)-O(9)	135.35(6)
O(7)#1-Ce(1)-O(9)	70.89(6)	O(2)-Ce(1)-O(9)	78.11(6)
O(6)#1-Ce(1)-O(9)	124.64(6)	O(5)-Ce(1)-O(9)	122.07(6)
O(3)#1-Ce(1)-O(8)#2	80.11(6)	O(7)#1-Ce(1)-O(8)#2	110.25(5)
O(2)-Ce(1)-O(8)#2	134.73(5)	O(6)#1-Ce(1)-O(8)#2	156.89(5)
O(5)-Ce(1)-O(8)#2	64.96(5)	O(9)-Ce(1)-O(8)#2	74.00(6)
O(3)#1-Ce(1)-O(1)	146.14(6)	O(7)#1-Ce(1)-O(1)	128.51(5)
O(2)-Ce(1)-O(1)	50.82(5)	O(6)#1-Ce(1)-O(1)	113.53(5)
O(5)-Ce(1)-O(1)	70.48(5)	O(9)-Ce(1)-O(1)	67.04(5)
O(8)#2-Ce(1)-O(1)	85.34(5)	O(3)#1-Ce(1)-O(7)#2	68.27(5)
O(7)#1-Ce(1)-O(7)#2	62.90(5)	O(2)-Ce(1)-O(7)#2	142.48(5)

O(6)#1-Ce(1)-O(7)#2	121.75(5)	O(5)-Ce(1)-O(7)#2	107.08(5)
O(9)-Ce(1)-O(7)#2	67.31(6)	O(8)#2-Ce(1)-O(7)#2	48.27(4)
O(1)-Ce(1)-O(7)#2	121.63(5)	O(1)#3-K(1)-O(4)#1	138.46(6)
O(1)#3-K(1)-O(5)	150.76(6)	O(4)#1-K(1)-O(5)	70.53(6)
O(1)#3-K(1)-O(8)#2	115.35(5)	O(4)#1-K(1)-O(8)#2	88.56(6)
O(5)-K(1)-O(8)#2	58.21(5)	O(1)#3-K(1)-N(3)	118.29(5)
O(4)#1-K(1)-N(3)	75.67(7)	O(5)-K(1)-N(3)	56.01(5)
O(8)#2-K(1)-N(3)	113.95(5)	O(1)#3-K(1)-O(8)#4	77.90(5)
O(4)#1-K(1)-O(8)#4	137.79(6)	O(5)-K(1)-O(8)#4	74.04(5)
O(8)#2-K(1)-O(8)#4	91.86(4)	N(3)-K(1)-O(8)#4	65.72(5)
O(1)#3-K(1)-N(4)#2	73.31(5)	O(4)#1-K(1)-N(4)#2	96.59(7)
O(5)-K(1)-N(4)#2	113.40(5)	O(8)#2-K(1)-N(4)#2	56.37(5)
N(3)-K(1)-N(4)#2	168.31(6)	O(8)#4-K(1)-N(4)#2	118.37(5)
O(1)#3-K(1)-O(2W)#3	72.20(4)	O(4)#1-K(1)-O(2W)#3	66.26(5)
O(5)-K(1)-O(2W)#3	136.49(5)	O(8)#2-K(1)-O(2W)#3	124.16(6)
N(3)-K(1)-O(2W)#3	106.94(7)	O(8)#4-K(1)-O(2W)#3	140.40(4)
N(4)#2-K(1)-O(2W)#3	77.09(7)	O(1)#3-K(1)-O(1W)#5	66.04(6)
O(4)#1-K(1)-O(1W)#5	88.89(6)	O(5)-K(1)-O(1W)#5	121.94(6)
O(8)#2-K(1)-O(1W)#5	177.16(6)	N(3)-K(1)-O(1W)#5	66.56(6)
O(8)#4-K(1)-O(1W)#5	90.87(5)	N(4)#2-K(1)-O(1W)#5	122.75(6)
O(2W)#3-K(1)-O(1W)#5	53.50(6)	O(1)#3-K(1)-O(5)#3	57.78(5)
O(4)#1-K(1)-O(5)#3	154.75(6)	O(5)-K(1)-O(5)#3	97.27(5)
O(8)#2-K(1)-O(5)#3	66.43(4)	N(3)-K(1)-O(5)#3	116.58(5)
O(8)#4-K(1)-O(5)#3	51.22(4)	N(4)#2-K(1)-O(5)#3	67.32(5)
O(2W)#3-K(1)-O(5)#3	124.45(5)	O(1W)#5-K(1)-O(5)#3	116.03(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y-1/2,-z+1 #2 x,y+1,z #3 -x,-y,-z+1 #4 -x,-y-1,-z+1 #5 x-1/2,-y-1/2,z+1/2 #6 x,y-1,z #7 x+1/2,-y-1/2,z-1/2 #8 x,-y,z-1/2

		3	
Pr(1)-O(3)#1	2.4287(19)	Pr(1)-O(7)#1	2.4653(17)
Pr(1)-O(2)	2.4789(17)	Pr(1)-O(6)#1	2.4800(18)
Pr(1)-O(5)	2.4995(18)	Pr(1)-O(9)	2.511(2)
Pr(1)-O(8)#2	2.5983(17)	Pr(1)-O(1)	2.6302(18)
Pr(1)-O(7)#2	2.7249(17)	K(1)-O(1)#3	2.6965(19)
K(1)-O(4)#1	2.743(2)	K(1)-O(5)	2.7808(19)
K(1)-O(8)#2	2.879(2)	K(1)-O(8)#4	2.9438(19)
K(1)-N(3)	2.944(2)	K(1)-N(4)#2	2.983(2)
K(1)-O(2W)	3.2076(13)	K(1)-O(1W)	3.349(3)
K(1)-O(5)#3	3.411(2)		
O(3)#1-Pr(1)-O(7)#1	85.51(6)	O(3)#1-Pr(1)-O(2)	141.48(6)
O(7)#1-Pr(1)-O(2)	93.24(6)	O(3)#1-Pr(1)-O(6)#1	76.10(6)
O(7)#1-Pr(1)-O(6)#1	69.38(6)	O(2)-Pr(1)-O(6)#1	67.59(6)
O(3)#1-Pr(1)-O(5)	75.16(7)	O(7)#1-Pr(1)-O(5)	160.65(6)

O(2)-Pr(1)-O(5)	102.32(6)	O(6)#1-Pr(1)-O(5)	105.90(6)
O(3)#1-Pr(1)-O(9)	135.76(7)	O(7)#1-Pr(1)-O(9)	70.77(7)
O(2)-Pr(1)-O(9)	78.43(7)	O(6)#1-Pr(1)-O(9)	124.89(7)
O(5)-Pr(1)-O(9)	123.33(7)	O(3)#1-Pr(1)-O(8)#2	80.33(6)
O(7)#1-Pr(1)-O(8)#2	110.60(6)	O(2)-Pr(1)-O(8)#2	134.69(6)
O(6)#1-Pr(1)-O(8)#2	156.37(6)	O(5)-Pr(1)-O(8)#2	65.85(6)
O(9)-Pr(1)-O(8)#2	74.35(7)	O(3)#1-Pr(1)-O(1)	145.56(6)
O(7)#1-Pr(1)-O(1)	128.88(6)	O(2)-Pr(1)-O(1)	51.33(6)
O(6)#1-Pr(1)-O(1)	114.38(6)	O(5)-Pr(1)-O(1)	70.42(6)
O(9)-Pr(1)-O(1)	67.12(6)	O(8)#2-Pr(1)-O(1)	84.60(6)
O(3)#1-Pr(1)-O(7)#2	68.35(6)	O(7)#1-Pr(1)-O(7)#2	62.71(6)
O(2)-Pr(1)-O(7)#2	143.08(6)	O(6)#1-Pr(1)-O(7)#2	121.17(6)
O(5)-Pr(1)-O(7)#2	108.12(5)	O(9)-Pr(1)-O(7)#2	67.63(6)
O(8)#2-Pr(1)-O(7)#2	48.85(5)	O(1)-Pr(1)-O(7)#2	121.63(5)
O(1)#3-K(1)-O(4)#1	138.91(7)	O(1)#3-K(1)-O(5)	151.12(6)
O(4)#1-K(1)-O(5)	69.67(7)	O(1)#3-K(1)-O(8)#2	114.92(6)
O(4)#1-K(1)-O(8)#2	89.07(6)	O(5)-K(1)-O(8)#2	58.62(5)
O(1)#3-K(1)-O(8)#4	77.06(5)	O(4)#1-K(1)-O(8)#4	138.01(7)
O(5)-K(1)-O(8)#4	75.17(6)	O(8)#2-K(1)-O(8)#4	91.78(5)
O(1)#3-K(1)-N(3)	117.97(6)	O(4)#1-K(1)-N(3)	75.55(8)
O(5)-K(1)-N(3)	55.99(6)	O(8)#2-K(1)-N(3)	114.20(6)
O(8)#4-K(1)-N(3)	65.93(6)	O(1)#3-K(1)-N(4)#2	73.11(6)
O(4)#1-K(1)-N(4)#2	97.23(8)	O(5)-K(1)-N(4)#2	113.69(6)
O(8)#2-K(1)-N(4)#2	56.40(5)	O(8)#4-K(1)-N(4)#2	117.81(6)
N(3)-K(1)-N(4)#2	168.80(7)	O(1)#3-K(1)-O(2W)	72.78(5)
O(4)#1-K(1)-O(2W)	66.13(5)	O(5)-K(1)-O(2W)	135.51(6)
O(8)#2-K(1)-O(2W)	124.33(7)	O(8)#4-K(1)-O(2W)	140.16(5)
N(3)-K(1)-O(2W)	106.76(8)	N(4)#2-K(1)-O(2W)	77.32(8)
O(1)#3-K(1)-O(1W)	66.17(7)	O(4)#1-K(1)-O(1W)	88.81(7)
O(5)-K(1)-O(1W)	121.60(6)	O(8)#2-K(1)-O(1W)	177.56(6)
O(8)#4-K(1)-O(1W)	90.60(6)	N(3)-K(1)-O(1W)	66.38(7)
N(4)#2-K(1)-O(1W)	122.72(7)	O(2W)-K(1)-O(1W)	53.58(7)
O(1)#3-K(1)-O(5)#3	56.53(5)	O(4)#1-K(1)-O(5)#3	155.64(6)
O(5)-K(1)-O(5)#3	98.91(5)	O(8)#2-K(1)-O(5)#3	66.87(5)
O(8)#4-K(1)-O(5)#3	51.09(5)	N(3)-K(1)-O(5)#3	116.75(6)
N(4)#2-K(1)-O(5)#3	66.93(6)	O(2W)-K(1)-O(5)#3	123.86(6)
O(1W)-K(1)-O(5)#3	115.16(6)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y-1/2,-z+1 #2 x,y+1,z #3 -x,-y,-z+1 #4 -x,-y-1,-z+1 #5 x,y-1,z #6 -x,y,-z+3/2

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Nd(1)-O(3)#1	2.415(2)	Nd(1)-O(7)#1	2.452(2)
Nd(1)-O(6)#1	2.456(2)	Nd(1)-O(2)	2.463(2)
Nd(1)-O(5)	2.475(2)	Nd(1)-O(9)	2.487(2)
Nd(1)-O(8)#2	2.580(2)	Nd(1)-O(1)	2.614(2)
Nd(1)-O(7)#2	2.692(2)	K(1)-O(1)#3	2.688(2)
K(1)-O(4)#1	2.747(3)	K(1)-O(5)	2.793(2)
K(1)-O(8)#2	2.861(2)	K(1)-N(3)	2.934(3)
K(1)-O(8)#4	2.940(2)	K(1)-N(4)#2	3.000(3)
K(1)-O(2W)	3.1862(15)	K(1)-O(1W)	3.328(3)
O(3)#1-Nd(1)-O(7)#1	85.64(8)	O(3)#1-Nd(1)-O(6)#1	75.16(8)
O(7)#1-Nd(1)-O(6)#1	69.44(7)	O(3)#1-Nd(1)-O(2)	140.95(7)
O(7)#1-Nd(1)-O(2)	93.55(7)	O(6)#1-Nd(1)-O(2)	68.17(7)
O(3)#1-Nd(1)-O(5)	74.80(8)	O(7)#1-Nd(1)-O(5)	160.44(7)
O(6)#1-Nd(1)-O(5)	104.26(7)	O(2)-Nd(1)-O(5)	101.26(7)
O(3)#1-Nd(1)-O(9)	136.19(7)	O(7)#1-Nd(1)-O(9)	70.91(8)
O(6)#1-Nd(1)-O(9)	125.51(8)	O(2)-Nd(1)-O(9)	78.70(8)
O(5)-Nd(1)-O(9)	124.31(8)	O(3)#1-Nd(1)-O(8)#2	80.57(7)
O(7)#1-Nd(1)-O(8)#2	111.03(6)	O(6)#1-Nd(1)-O(8)#2	155.65(7)
O(2)-Nd(1)-O(8)#2	134.55(7)	O(5)-Nd(1)-O(8)#2	66.76(7)
O(9)-Nd(1)-O(8)#2	74.57(8)	O(3)#1-Nd(1)-O(1)	145.10(7)
O(7)#1-Nd(1)-O(1)	129.21(7)	O(6)#1-Nd(1)-O(1)	115.20(7)
O(2)-Nd(1)-O(1)	51.62(7)	O(5)-Nd(1)-O(1)	70.35(7)
O(9)-Nd(1)-O(1)	67.10(7)	O(8)#2-Nd(1)-O(1)	84.01(7)
O(3)#1-Nd(1)-O(7)#2	68.46(7)	O(7)#1-Nd(1)-O(7)#2	62.77(8)
O(6)#1-Nd(1)-O(7)#2	120.71(7)	O(2)-Nd(1)-O(7)#2	143.68(7)
O(5)-Nd(1)-O(7)#2	109.06(7)	O(9)-Nd(1)-O(7)#2	67.95(7)
O(8)#2-Nd(1)-O(7)#2	49.26(6)	O(1)-Nd(1)-O(7)#2	121.61(6)
O(1)#3-K(1)-O(4)#1	139.38(7)	O(1)#3-K(1)-O(5)	151.30(7)
O(4)#1-K(1)-O(5)	68.99(7)	O(1)#3-K(1)-O(8)#2	114.44(7)
O(4)#1-K(1)-O(8)#2	89.54(7)	O(5)-K(1)-O(8)#2	58.95(6)
O(1)#3-K(1)-N(3)	117.67(7)	O(4)#1-K(1)-N(3)	75.54(8)
O(5)-K(1)-N(3)	56.01(6)	O(8)#2-K(1)-N(3)	114.39(7)
O(1)#3-K(1)-O(8)#4	76.14(6)	O(4)#1-K(1)-O(8)#4	138.34(8)
O(5)-K(1)-O(8)#4	76.22(7)	O(8)#2-K(1)-O(8)#4	91.70(6)
N(3)-K(1)-O(8)#4	66.14(7)	O(1)#3-K(1)-N(4)#2	72.90(7)
O(4)#1-K(1)-N(4)#2	97.88(8)	O(5)-K(1)-N(4)#2	113.84(7)
O(8)#2-K(1)-N(4)#2	56.35(6)	N(3)-K(1)-N(4)#2	169.21(7)
O(8)#4-K(1)-N(4)#2	117.11(7)	O(1)#3-K(1)-O(2W)	73.55(6)
O(4)#1-K(1)-O(2W)	65.83(6)	O(5)-K(1)-O(2W)	134.55(6)
O(8)#2-K(1)-O(2W)	124.29(8)	N(3)-K(1)-O(2W)	106.75(10)
O(8)#4-K(1)-O(2W)	140.13(6)	N(4)#2-K(1)-O(2W)	77.54(10)
O(1)#3-K(1)-O(1W)	66.51(8)	O(4)#1-K(1)-O(1W)	88.58(8)
O(5)-K(1)-O(1W)	121.26(8)	O(8)#2-K(1)-O(1W)	177.82(7)
N(3)-K(1)-O(1W)	66.17(8)	O(8)#4-K(1)-O(1W)	90.44(7)

N(4)#2-K(1)-O(1W)	122.85(8)	O(2W)-K(1)-O(1W)	53.82(8)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y-1/2,-z+1 #2 x,y+1,z #3 -x,-y,-z+1 #4 -x,-y-1,-z+1 #5 x,y-1,z #6 -x,y,-z+3/2

5

Sm(1)-O(3)#1	2.387(3)	Sm(1)-O(6)#1	2.420(3)
Sm(1)-O(7)#1	2.426(3)	Sm(1)-O(2)	2.437(3)
Sm(1)-O(5)	2.444(3)	Sm(1)-O(9)	2.456(3)
Sm(1)-O(8)#2	2.552(3)	Sm(1)-O(1)	2.588(3)
Sm(1)-O(7)#2	2.648(3)	K(1)-O(1)#3	2.685(3)
K(1)-O(4)#1	2.727(4)	K(1)-O(8)#2	2.832(3)
K(1)-O(5)	2.833(3)	K(1)-N(3)	2.921(4)
K(1)-O(8)#4	2.937(3)	K(1)-N(4)#2	3.026(4)
K(1)-O(2W)#3	3.166(2)	K(1)-O(1W)#5	3.299(5)
O(3)#1-Sm(1)-O(6)#1	74.46(11)	O(3)#1-Sm(1)-O(7)#1	86.49(11)
O(6)#1-Sm(1)-O(7)#1	69.43(10)	O(3)#1-Sm(1)-O(2)	140.39(11)
O(6)#1-Sm(1)-O(2)	68.64(11)	O(7)#1-Sm(1)-O(2)	93.56(10)
O(3)#1-Sm(1)-O(5)	74.46(11)	O(6)#1-Sm(1)-O(5)	102.24(11)
O(7)#1-Sm(1)-O(5)	160.78(11)	O(2)-Sm(1)-O(5)	99.46(11)
O(3)#1-Sm(1)-O(9)	136.83(12)	O(6)#1-Sm(1)-O(9)	125.69(12)
O(7)#1-Sm(1)-O(9)	70.57(11)	O(2)-Sm(1)-O(9)	78.88(12)
O(5)-Sm(1)-O(9)	125.74(12)	O(3)#1-Sm(1)-O(8)#2	80.42(11)
O(6)#1-Sm(1)-O(8)#2	154.78(10)	O(7)#1-Sm(1)-O(8)#2	111.71(9)
O(2)-Sm(1)-O(8)#2	134.60(10)	O(5)-Sm(1)-O(8)#2	68.19(10)
O(9)-Sm(1)-O(8)#2	75.32(12)	O(3)#1-Sm(1)-O(1)	144.32(11)
O(6)#1-Sm(1)-O(1)	116.13(11)	O(7)#1-Sm(1)-O(1)	129.12(10)
O(2)-Sm(1)-O(1)	52.03(10)	O(5)-Sm(1)-O(1)	70.03(11)
O(9)-Sm(1)-O(1)	67.07(11)	O(8)#2-Sm(1)-O(1)	83.44(10)
O(3)#1-Sm(1)-O(7)#2	68.39(10)	O(6)#1-Sm(1)-O(7)#2	119.69(10)
O(7)#1-Sm(1)-O(7)#2	62.65(11)	O(2)-Sm(1)-O(7)#2	144.40(10)
O(5)-Sm(1)-O(7)#2	110.99(10)	O(9)-Sm(1)-O(7)#2	68.62(11)
O(8)#2-Sm(1)-O(7)#2	50.16(9)	O(1)-Sm(1)-O(7)#2	121.95(10)
O(1)#3-K(1)-O(4)#1	140.22(11)	O(1)#3-K(1)-O(8)#2	114.17(10)
O(4)#1-K(1)-O(8)#2	89.59(10)	O(1)#3-K(1)-O(5)	151.52(11)
O(4)#1-K(1)-O(5)	67.88(11)	O(8)#2-K(1)-O(5)	59.29(9)
O(1)#3-K(1)-N(3)	117.22(11)	O(4)#1-K(1)-N(3)	75.44(13)
O(8)#2-K(1)-N(3)	114.60(10)	O(5)-K(1)-N(3)	56.05(10)
O(1)#3-K(1)-O(8)#4	74.82(9)	O(4)#1-K(1)-O(8)#4	138.81(12)
O(8)#2-K(1)-O(8)#4	91.74(9)	O(5)-K(1)-O(8)#4	77.66(9)
N(3)-K(1)-O(8)#4	66.69(10)	O(1)#3-K(1)-N(4)#2	72.67(10)
O(4)#1-K(1)-N(4)#2	98.70(13)	O(8)#2-K(1)-N(4)#2	56.37(9)
O(5)-K(1)-N(4)#2	114.12(10)	N(3)-K(1)-N(4)#2	169.77(11)
O(8)#4-K(1)-N(4)#2	116.00(10)	O(1)#3-K(1)-O(2W)#3	74.21(8)

O(4)#1-K(1)-O(2W)#3	66.02(9)	O(8)#2-K(1)-O(2W)#3	123.92(12)
O(5)-K(1)-O(2W)#3	133.68(9)	N(3)-K(1)-O(2W)#3	107.02(15)
O(8)#4-K(1)-O(2W)#3	140.04(8)	N(4)#2-K(1)-O(2W)#3	77.46(14)
O(1)#3-K(1)-O(1W)#5	66.62(11)	O(4)#1-K(1)-O(1W)#5	88.78(12)
O(8)#2-K(1)-O(1W)#5	178.03(11)	O(5)-K(1)-O(1W)#5	120.97(11)
N(3)-K(1)-O(1W)#5	66.01(11)	O(8)#4-K(1)-O(1W)#5	90.22(10)
N(4)#2-K(1)-O(1W)#5	122.84(11)	O(2W)#3-K(1)-O(1W)#5	54.32(13)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y-1/2,-z+1 #2 x,y+1,z #3 -x,-y,-z+1 #4 -x,-y-1,-z+1 #5 x-1/2,-y-1/2,z+1/2 #6 x,y-1,z #7 x+1/2,-y-1/2,z-1/2 #8 x,-y,z-1/2

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Eu(1)-O(3)#1	Eu(1)-O(3)#1	Eu(1)-O(6)#1	2.409(2)
Eu(1)-O(7)#1	Eu(1)-O(7)#1	Eu(1)-O(2)	2.432(2)
Eu(1)-O(5)	Eu(1)-O(5)	Eu(1)-O(9)	2.448(2)
Eu(1)-O(8)#2	Eu(1)-O(8)#2	Eu(1)-O(1)	2.597(2)
Eu(1)-O(7)#2	Eu(1)-O(7)#2	K(1)-O(1)#3	2.682(2)
K(1)-O(4)#1	K(1)-O(4)#1	K(1)-O(8)#2	2.833(2)
K(1)-O(5)	K(1)-O(5)	K(1)-N(3)	2.932(3)
K(1)-O(8)#4	K(1)-O(8)#4	K(1)-N(4)#2	3.059(3)
K(1)-O(2W)	K(1)-O(2W)	K(1)-O(1W)	3.294(3)
O(3)#1-Eu(1)-O(6)#1	73.99(7)	O(3)#1-Eu(1)-O(7)#1	86.52(7)
O(6)#1-Eu(1)-O(7)#1	69.63(7)	O(3)#1-Eu(1)-O(2)	140.19(7)
O(6)#1-Eu(1)-O(2)	69.02(7)	O(7)#1-Eu(1)-O(2)	93.95(7)
O(3)#1-Eu(1)-O(5)	74.46(7)	O(6)#1-Eu(1)-O(5)	100.58(7)
O(7)#1-Eu(1)-O(5)	160.56(7)	O(2)-Eu(1)-O(5)	98.09(7)
O(3)#1-Eu(1)-O(9)	136.93(7)	O(6)#1-Eu(1)-O(9)	126.28(7)
O(7)#1-Eu(1)-O(9)	70.73(7)	O(2)-Eu(1)-O(9)	79.18(8)
O(5)-Eu(1)-O(9)	126.52(7)	O(3)#1-Eu(1)-O(8)#2	80.45(7)
O(6)#1-Eu(1)-O(8)#2	154.29(6)	O(7)#1-Eu(1)-O(8)#2	111.98(7)
O(2)-Eu(1)-O(8)#2	134.42(6)	O(5)-Eu(1)-O(8)#2	69.35(7)
O(9)-Eu(1)-O(8)#2	75.38(7)	O(3)#1-Eu(1)-O(1)	144.03(7)
O(6)#1-Eu(1)-O(1)	116.47(7)	O(7)#1-Eu(1)-O(1)	129.39(6)
O(2)-Eu(1)-O(1)	52.05(6)	O(5)-Eu(1)-O(1)	69.84(7)
O(9)-Eu(1)-O(1)	67.12(7)	O(8)#2-Eu(1)-O(1)	83.14(6)
O(3)#1-Eu(1)-O(7)#2	68.39(6)	O(6)#1-Eu(1)-O(7)#2	119.66(7)
O(7)#1-Eu(1)-O(7)#2	62.80(7)	O(2)-Eu(1)-O(7)#2	144.91(6)
O(5)-Eu(1)-O(7)#2	112.07(6)	O(9)-Eu(1)-O(7)#2	68.72(7)
O(8)#2-Eu(1)-O(7)#2	50.27(6)	O(1)-Eu(1)-O(7)#2	121.89(6)
O(1)#3-K(1)-O(4)#1	140.34(8)	O(1)#3-K(1)-O(8)#2	113.87(7)
O(4)#1-K(1)-O(8)#2	89.99(7)	O(1)#3-K(1)-O(5)	151.78(7)
O(4)#1-K(1)-O(5)	67.46(7)	O(8)#2-K(1)-O(5)	59.63(6)
O(1)#3-K(1)-N(3)	117.04(7)	O(4)#1-K(1)-N(3)	75.45(8)
O(8)#2-K(1)-N(3)	114.76(6)	O(5)-K(1)-N(3)	56.00(6)
O(1)#3-K(1)-O(8)#4	74.35(6)	O(4)#1-K(1)-O(8)#4	138.93(7)

O(8)#2-K(1)-O(8)#4	91.90(6)	O(5)-K(1)-O(8)#4	78.37(6)
N(3)-K(1)-O(8)#4	66.61(6)	O(1)#3-K(1)-N(4)#2	72.48(6)
O(4)#1-K(1)-N(4)#2	99.21(8)	O(8)#2-K(1)-N(4)#2	56.24(6)
O(5)-K(1)-N(4)#2	114.28(6)	N(3)-K(1)-N(4)#2	170.02(7)
O(8)#4-K(1)-N(4)#2	115.66(6)	O(1)#3-K(1)-O(2W)	74.45(5)
O(4)#1-K(1)-O(2W)	65.91(6)	O(8)#2-K(1)-O(2W)	123.83(8)
O(5)-K(1)-O(2W)	133.17(6)	N(3)-K(1)-O(2W)	107.19(9)
O(8)#4-K(1)-O(2W)	139.82(6)	N(4)#2-K(1)-O(2W)	77.56(9)
O(1)#3-K(1)-O(1W)	66.91(7)	O(4)#1-K(1)-O(1W)	88.43(8)
O(8)#2-K(1)-O(1W)	178.11(7)	O(5)-K(1)-O(1W)	120.58(7)
N(3)-K(1)-O(1W)	65.82(7)	O(8)#4-K(1)-O(1W)	89.97(7)
N(4)#2-K(1)-O(1W)	123.02(7)	O(2W)-K(1)-O(1W)	54.49(8)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y-1/2,-z+1 #2 x,y+1,z #3 -x,-y,-z+1 #4 -x,-y-1,-z+1 #5 x,y-1,z #6 -x,y,-z+3/2

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Gd(1)-O(3)#1	2.372(2)	Gd(1)-O(6)#1	2.3855(18)
Gd(1)-O(7)#1	2.4056(17)	Gd(1)-O(5)	2.4115(18)
Gd(1)-O(2)	2.4152(18)	Gd(1)-O(9)	2.424(2)
Gd(1)-O(8)#2	2.5245(18)	Gd(1)-O(1)	2.5764(19)
Gd(1)-O(7)#2	2.6092(18)	K(1)-O(1)#3	2.6737(19)
K(1)-O(4)#1	2.719(2)	K(1)-O(8)#2	2.810(2)
K(1)-O(5)	2.872(2)	K(1)-N(3)	2.911(2)
K(1)-O(8)#4	2.942(2)	K(1)-N(4)#2	3.051(2)
K(1)-O(2W)	3.1420(13)	K(1)-O(1W)	3.272(3)
O(3)#1-Gd(1)-O(6)#1	73.61(7)	O(3)#1-Gd(1)-O(7)#1	86.73(7)
O(6)#1-Gd(1)-O(7)#1	69.55(6)	O(3)#1-Gd(1)-O(5)	74.33(7)
O(6)#1-Gd(1)-O(5)	99.64(7)	O(7)#1-Gd(1)-O(5)	160.41(7)
O(3)#1-Gd(1)-O(2)	139.87(6)	O(6)#1-Gd(1)-O(2)	69.17(6)
O(7)#1-Gd(1)-O(2)	93.88(6)	O(5)-Gd(1)-O(2)	97.37(6)
O(3)#1-Gd(1)-O(9)	137.31(7)	O(6)#1-Gd(1)-O(9)	126.37(7)
O(7)#1-Gd(1)-O(9)	70.75(7)	O(5)-Gd(1)-O(9)	127.13(7)
O(2)-Gd(1)-O(9)	79.18(7)	O(3)#1-Gd(1)-O(8)#2	80.45(7)
O(6)#1-Gd(1)-O(8)#2	153.89(6)	O(7)#1-Gd(1)-O(8)#2	112.46(6)
O(5)-Gd(1)-O(8)#2	69.89(6)	O(2)-Gd(1)-O(8)#2	134.44(6)
O(9)-Gd(1)-O(8)#2	75.81(7)	O(3)#1-Gd(1)-O(1)	143.68(7)
O(6)#1-Gd(1)-O(1)	116.83(6)	O(7)#1-Gd(1)-O(1)	129.53(6)
O(5)-Gd(1)-O(1)	69.68(6)	O(2)-Gd(1)-O(1)	52.31(6)
O(9)-Gd(1)-O(1)	67.13(7)	O(8)#2-Gd(1)-O(1)	82.82(6)
O(3)#1-Gd(1)-O(7)#2	68.44(6)	O(6)#1-Gd(1)-O(7)#2	119.39(6)
O(7)#1-Gd(1)-O(7)#2	62.95(7)	O(5)-Gd(1)-O(7)#2	112.80(6)
O(2)-Gd(1)-O(7)#2	145.20(6)	O(9)-Gd(1)-O(7)#2	69.04(7)
O(8)#2-Gd(1)-O(7)#2	50.61(5)	O(1)-Gd(1)-O(7)#2	121.93(6)
O(1)#3-K(1)-O(4)#1	140.83(7)	O(1)#3-K(1)-O(8)#2	113.81(6)

O(4)#1-K(1)-O(8)#2	90.18(7)	O(1)#3-K(1)-O(5)	151.73(7)
O(4)#1-K(1)-O(5)	66.96(7)	O(8)#2-K(1)-O(5)	59.71(5)
O(1)#3-K(1)-N(3)	116.81(6)	O(4)#1-K(1)-N(3)	75.12(8)
O(8)#2-K(1)-N(3)	114.74(6)	O(5)-K(1)-N(3)	55.98(6)
O(1)#3-K(1)-O(8)#4	73.68(6)	O(4)#1-K(1)-O(8)#4	138.88(7)
O(8)#2-K(1)-O(8)#4	91.91(5)	O(5)-K(1)-O(8)#4	78.93(6)
N(3)-K(1)-O(8)#4	66.82(6)	O(1)#3-K(1)-N(4)#2	72.59(6)
O(4)#1-K(1)-N(4)#2	99.72(8)	O(8)#2-K(1)-N(4)#2	56.24(6)
O(5)-K(1)-N(4)#2	114.30(6)	N(3)-K(1)-N(4)#2	170.08(7)
O(8)#4-K(1)-N(4)#2	115.30(6)	O(1)#3-K(1)-O(2W)	74.79(5)
O(4)#1-K(1)-O(2W)	66.07(6)	O(8)#2-K(1)-O(2W)	123.87(7)
O(5)-K(1)-O(2W)	132.86(6)	N(3)-K(1)-O(2W)	107.21(9)
O(8)#4-K(1)-O(2W)	139.65(5)	N(4)#2-K(1)-O(2W)	77.67(9)
O(1)#3-K(1)-O(1W)	66.77(7)	O(4)#1-K(1)-O(1W)	88.52(7)
O(8)#2-K(1)-O(1W)	178.37(7)	O(5)-K(1)-O(1W)	120.57(7)
N(3)-K(1)-O(1W)	65.86(7)	O(8)#4-K(1)-O(1W)	89.72(6)
N(4)#2-K(1)-O(1W)	123.04(7)	O(2W)-K(1)-O(1W)	54.63(8)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y-1/2,-z+1 #2 x,y+1,z #3 -x,-y,-z+1 #4 -x,-y-1,-z+1 #5 x,y-1,z #6 -x,y,-z+3/2

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Tb(1)-O(3)#1	2.3571(19)	Tb(1)-O(6)#1	2.3771(18)
Tb(1)-O(7)#1	2.3979(16)	Tb(1)-O(5)	2.4005(17)
Tb(1)-O(2)	2.4013(17)	Tb(1)-O(9)	2.4161(19)
Tb(1)-O(8)#2	2.5104(17)	Tb(1)-O(1)	2.580(2)
Tb(1)-O(7)#2	2.6105(17)	K(1)-O(1)#3	2.6719(18)
K(1)-O(4)#1	2.725(2)	K(1)-O(8)#2	2.8101(19)
K(1)-O(5)	2.8877(19)	K(1)-N(3)	2.909(2)
K(1)-O(8)#4	2.955(2)	K(1)-N(4)#2	3.065(2)
K(1)-O(2W)#3	3.1438(13)	K(1)-O(1W)#5	3.275(3)
O(3)#1-Tb(1)-O(6)#1	73.50(7)	O(3)#1-Tb(1)-O(7)#1	87.03(6)
O(6)#1-Tb(1)-O(7)#1	69.75(6)	O(3)#1-Tb(1)-O(5)	74.33(7)
O(6)#1-Tb(1)-O(5)	98.90(6)	O(7)#1-Tb(1)-O(5)	160.52(7)
O(3)#1-Tb(1)-O(2)	139.84(6)	O(6)#1-Tb(1)-O(2)	69.30(6)
O(7)#1-Tb(1)-O(2)	93.84(6)	O(5)-Tb(1)-O(2)	96.78(6)
O(3)#1-Tb(1)-O(9)	137.38(7)	O(6)#1-Tb(1)-O(9)	126.62(7)
O(7)#1-Tb(1)-O(9)	70.66(7)	O(5)-Tb(1)-O(9)	127.41(7)
O(2)-Tb(1)-O(9)	79.23(7)	O(3)#1-Tb(1)-O(8)#2	80.36(7)
O(6)#1-Tb(1)-O(8)#2	153.66(6)	O(7)#1-Tb(1)-O(8)#2	112.56(6)
O(5)-Tb(1)-O(8)#2	70.45(6)	O(2)-Tb(1)-O(8)#2	134.41(6)
O(9)-Tb(1)-O(8)#2	75.86(7)	O(3)#1-Tb(1)-O(1)	143.44(6)
O(6)#1-Tb(1)-O(1)	117.05(6)	O(7)#1-Tb(1)-O(1)	129.46(6)
O(5)-Tb(1)-O(1)	69.52(6)	O(2)-Tb(1)-O(1)	52.47(6)
O(9)-Tb(1)-O(1)	67.07(6)	O(8)#2-Tb(1)-O(1)	82.61(6)

O(3)#1-Tb(1)-O(7)#2	68.44(6)	O(6)#1-Tb(1)-O(7)#2	119.34(6)
O(7)#1-Tb(1)-O(7)#2	62.97(6)	O(5)-Tb(1)-O(7)#2	113.42(5)
O(2)-Tb(1)-O(7)#2	145.30(6)	O(9)-Tb(1)-O(7)#2	69.10(6)
O(8)#2-Tb(1)-O(7)#2	50.72(5)	O(1)-Tb(1)-O(7)#2	121.85(6)
O(1)#3-K(1)-O(4)#1	141.01(7)	O(1)#3-K(1)-O(8)#2	114.15(6)
O(4)#1-K(1)-O(8)#2	89.94(6)	O(1)#3-K(1)-O(5)	151.95(7)
O(4)#1-K(1)-O(5)	66.50(7)	O(8)#2-K(1)-O(5)	59.63(5)
O(1)#3-K(1)-N(3)	116.63(6)	O(4)#1-K(1)-N(3)	74.99(8)
O(8)#2-K(1)-N(3)	114.62(6)	O(5)-K(1)-N(3)	55.98(5)
O(1)#3-K(1)-O(8)#4	73.14(6)	O(4)#1-K(1)-O(8)#4	139.00(7)
O(8)#2-K(1)-O(8)#4	92.41(5)	O(5)-K(1)-O(8)#4	79.66(5)
N(3)-K(1)-O(8)#4	66.91(6)	O(1)#3-K(1)-N(4)#2	72.69(6)
O(4)#1-K(1)-N(4)#2	100.04(8)	O(8)#2-K(1)-N(4)#2	56.23(5)
O(5)-K(1)-N(4)#2	114.24(6)	N(3)-K(1)-N(4)#2	170.07(7)
O(8)#4-K(1)-N(4)#2	115.05(6)	O(1)#3-K(1)-O(2W)#3	74.83(5)
O(4)#1-K(1)-O(2W)#3	66.23(6)	O(8)#2-K(1)-O(2W)#3	123.71(7)
O(5)-K(1)-O(2W)#3	132.58(6)	N(3)-K(1)-O(2W)#3	107.32(9)
O(8)#4-K(1)-O(2W)#3	139.24(5)	N(4)#2-K(1)-O(2W)#3	77.77(8)
O(1)#3-K(1)-O(1W)#5	66.62(7)	O(4)#1-K(1)-O(1W)#5	88.51(7)
O(8)#2-K(1)-O(1W)#5	178.10(7)	O(5)-K(1)-O(1W)#5	120.60(6)
N(3)-K(1)-O(1W)#5	65.99(6)	O(8)#4-K(1)-O(1W)#5	89.47(6)
N(4)#2-K(1)-O(1W)#5	123.02(7)	O(2W)#3-K(1)-O(1W)#5	54.58(7)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y-1/2,-z+1 #2 x,y+1,z
#3 -x,-y,-z+1 #4 -x,-y-1,-z+1 #5 x-1/2,-y-1/2,z+1/2 #6 x,y-1,z #7 x+1/2,-y-1/2,z-1/2 #8 x,-y,z-1/2

Table S3. Bond lengths [Å] and angles [º] for compounds **9** and **10**.

		9	
La(1)-O(7)	2.412(3)	La(1)-O(3)#1	2.475(3)
La(1)-O(9)	2.527(3)	La(1)-O(6)	2.559(3)
La(1)-O(1)#1	2.586(3)	La(1)-O(2)	2.602(3)
La(1)-O(5)	2.619(3)	La(1)-O(4)#2	2.661(3)
La(1)-O(3)#2	2.850(3)	La(1)-O(1)	2.889(3)
K(1)-O(1W)	2.631(5)	K(1)-O(5)#3	2.675(3)
K(1)-O(2)#3	2.819(3)	K(1)-O(2)	2.852(3)
K(1)-O(4)#2	2.858(3)	K(1)-N(2)#2	2.950(3)
K(1)-N(1)	2.954(3)	K(1)-O(4)#4	3.127(3)
O(7)-La(1)-O(3)#1	90.41(10)	O(7)-La(1)-O(9)	142.50(12)
O(3)#1-La(1)-O(9)	79.50(10)	O(7)-La(1)-O(6)	75.71(11)
O(3)#1-La(1)-O(6)	73.47(9)	O(9)-La(1)-O(6)	133.22(10)
O(7)-La(1)-O(1)#1	69.13(11)	O(3)#1-La(1)-O(1)#1	69.40(9)
O(9)-La(1)-O(1)#1	73.52(10)	O(6)-La(1)-O(1)#1	127.67(9)

O(7)-La(1)-O(2)	109.86(10)	O(3)#1-La(1)-O(2)	156.89(10)
O(9)-La(1)-O(2)	77.63(10)	O(6)-La(1)-O(2)	121.23(9)
O(1)#1-La(1)-O(2)	106.77(9)	O(7)-La(1)-O(5)	71.22(11)
O(3)#1-La(1)-O(5)	123.32(9)	O(9)-La(1)-O(5)	143.34(10)
O(6)-La(1)-O(5)	50.33(9)	O(1)#1-La(1)-O(5)	138.36(10)
O(2)-La(1)-O(5)	75.36(9)	O(7)-La(1)-O(4)#2	140.04(11)
O(3)#1-La(1)-O(4)#2	109.09(8)	O(9)-La(1)-O(4)#2	76.74(10)
O(6)-La(1)-O(4)#2	77.05(10)	O(1)#1-La(1)-O(4)#2	149.98(10)
O(2)-La(1)-O(4)#2	62.23(8)	O(5)-La(1)-O(4)#2	68.92(10)
O(7)-La(1)-O(3)#2	138.51(9)	O(3)#1-La(1)-O(3)#2	62.26(10)
O(9)-La(1)-O(3)#2	66.57(9)	O(6)-La(1)-O(3)#2	67.16(9)
O(1)#1-La(1)-O(3)#2	121.07(9)	O(2)-La(1)-O(3)#2	104.93(8)
O(5)-La(1)-O(3)#2	97.14(9)	O(4)#2-La(1)-O(3)#2	46.91(8)
O(7)-La(1)-O(1)	78.69(10)	O(3)#1-La(1)-O(1)	132.52(8)
O(9)-La(1)-O(1)	81.94(9)	O(6)-La(1)-O(1)	143.48(9)
O(1)#1-La(1)-O(1)	63.50(10)	O(2)-La(1)-O(1)	46.64(8)
O(5)-La(1)-O(1)	96.77(9)	O(4)#2-La(1)-O(1)	108.48(8)
O(3)#2-La(1)-O(1)	142.80(8)	O(1W)-K(1)-O(5)#3	93.85(13)
O(1W)-K(1)-O(2)#3	152.50(13)	O(5)#3-K(1)-O(2)#3	70.96(9)
O(1W)-K(1)-O(2)	103.88(12)	O(5)#3-K(1)-O(2)	133.92(10)
O(2)#3-K(1)-O(2)	103.07(8)	O(1W)-K(1)-O(4)#2	107.30(13)
O(5)#3-K(1)-O(4)#2	153.42(9)	O(2)#3-K(1)-O(4)#2	83.12(8)
O(2)-K(1)-O(4)#2	56.89(8)	O(1W)-K(1)-N(2)#2	85.22(14)
O(5)#3-K(1)-N(2)#2	110.66(10)	O(2)#3-K(1)-N(2)#2	79.35(10)
O(2)-K(1)-N(2)#2	112.91(9)	O(4)#2-K(1)-N(2)#2	57.02(9)
O(1W)-K(1)-N(1)	82.14(13)	O(5)#3-K(1)-N(1)	86.19(10)
O(2)#3-K(1)-N(1)	118.23(10)	O(2)-K(1)-N(1)	55.55(9)
O(4)#2-K(1)-N(1)	112.01(9)	N(2)#2-K(1)-N(1)	159.60(10)
O(1W)-K(1)-O(4)#4	138.31(13)	O(5)#3-K(1)-O(4)#4	61.40(8)
O(2)#3-K(1)-O(4)#4	54.14(8)	O(2)-K(1)-O(4)#4	77.93(8)
O(4)#2-K(1)-O(4)#4	107.92(7)	N(2)#2-K(1)-O(4)#4	133.31(10)
N(1)-K(1)-O(4)#4	64.40(9)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z+2 #2 x-1,y,z #3 -x+1,-y+3,-z+2 #4 -x+2,-y+3,-z+2 #5 x+1,y,z #6 -x+1,-y+3,-z+3 #7 -x+1,-y+2,-z+3

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Ce(1)-O(7)	2.371(4)	Ce(1)-O(3)#1	2.447(4)
Ce(1)-O(9)	2.498(4)	Ce(1)-O(6)	2.525(4)
Ce(1)-O(2)	2.569(4)	Ce(1)-O(1)#1	2.572(4)
Ce(1)-O(5)	2.595(4)	Ce(1)-O(4)#2	2.642(4)
Ce(1)-O(3)#2	2.859(4)	Ce(1)-O(1)	2.884(4)
K(1)-O(1W)	2.599(7)	K(1)-O(5)#3	2.672(4)

K(1)-O(2)	2.831(4)	K(1)-O(4)#2	2.834(4)
K(1)-O(2)#3	2.843(5)	K(1)-N(1)	2.926(5)
K(1)-N(2)#2	2.940(5)	K(1)-O(4)#4	3.069(4)
O(7)-Ce(1)-O(3)#1	89.91(16)	O(7)-Ce(1)-O(9)	142.49(16)
O(3)#1-Ce(1)-O(9)	79.97(15)	O(7)-Ce(1)-O(6)	76.34(15)
O(3)#1-Ce(1)-O(6)	72.74(14)	O(9)-Ce(1)-O(6)	132.45(14)
O(7)-Ce(1)-O(2)	110.30(16)	O(3)#1-Ce(1)-O(2)	156.78(15)
O(9)-Ce(1)-O(2)	77.01(15)	O(6)-Ce(1)-O(2)	122.00(14)
O(7)-Ce(1)-O(1)#1	69.26(16)	O(3)#1-Ce(1)-O(1)#1	69.44(14)
O(9)-Ce(1)-O(1)#1	73.37(15)	O(6)-Ce(1)-O(1)#1	127.93(14)
O(2)-Ce(1)-O(1)#1	106.27(13)	O(7)-Ce(1)-O(5)	71.77(16)
O(3)#1-Ce(1)-O(5)	123.17(14)	O(9)-Ce(1)-O(5)	142.82(15)
O(6)-Ce(1)-O(5)	50.97(13)	O(2)-Ce(1)-O(5)	75.70(14)
O(1)#1-Ce(1)-O(5)	138.94(15)	O(7)-Ce(1)-O(4)#2	141.09(16)
O(3)#1-Ce(1)-O(4)#2	108.62(12)	O(9)-Ce(1)-O(4)#2	75.78(14)
O(6)-Ce(1)-O(4)#2	77.11(14)	O(2)-Ce(1)-O(4)#2	62.66(12)
O(1)#1-Ce(1)-O(4)#2	148.94(14)	O(5)-Ce(1)-O(4)#2	69.45(14)
O(7)-Ce(1)-O(3)#2	138.64(15)	O(3)#1-Ce(1)-O(3)#2	61.94(14)
O(9)-Ce(1)-O(3)#2	65.91(13)	O(6)-Ce(1)-O(3)#2	66.99(13)
O(2)-Ce(1)-O(3)#2	105.11(12)	O(1)#1-Ce(1)-O(3)#2	120.12(14)
O(5)-Ce(1)-O(3)#2	97.69(13)	O(4)#2-Ce(1)-O(3)#2	46.78(11)
O(7)-Ce(1)-O(1)	78.24(15)	O(3)#1-Ce(1)-O(1)	132.61(13)
O(9)-Ce(1)-O(1)	82.44(14)	O(6)-Ce(1)-O(1)	143.78(14)
O(2)-Ce(1)-O(1)	46.71(12)	O(1)#1-Ce(1)-O(1)	63.41(16)
O(5)-Ce(1)-O(1)	96.53(14)	O(4)#2-Ce(1)-O(1)	109.03(12)
O(3)#2-Ce(1)-O(1)	143.09(12)	O(1W)-K(1)-O(5)#3	93.43(19)
O(1W)-K(1)-O(2)	105.06(19)	O(5)#3-K(1)-O(2)	135.69(14)
O(1W)-K(1)-O(4)#2	108.04(19)	O(5)#3-K(1)-O(4)#2	151.43(14)
O(2)-K(1)-O(4)#2	57.16(11)	O(1W)-K(1)-O(2)#3	150.31(19)
O(5)#3-K(1)-O(2)#3	70.05(13)	O(2)-K(1)-O(2)#3	103.85(11)
O(4)#2-K(1)-O(2)#3	82.31(13)	O(1W)-K(1)-N(1)	83.31(19)
O(5)#3-K(1)-N(1)	87.87(15)	O(2)-K(1)-N(1)	55.81(14)
O(4)#2-K(1)-N(1)	112.64(14)	O(2)#3-K(1)-N(1)	119.14(15)
O(1W)-K(1)-N(2)#2	85.2(2)	O(5)#3-K(1)-N(2)#2	107.67(14)
O(2)-K(1)-N(2)#2	113.65(13)	O(4)#2-K(1)-N(2)#2	57.41(13)
O(2)#3-K(1)-N(2)#2	77.19(14)	N(1)-K(1)-N(2)#2	161.17(16)
O(1W)-K(1)-O(4)#4	139.34(19)	O(5)#3-K(1)-O(4)#4	62.16(13)
O(2)-K(1)-O(4)#4	78.46(12)	O(4)#2-K(1)-O(4)#4	107.40(11)
O(2)#3-K(1)-O(4)#4	54.41(12)	N(1)-K(1)-O(4)#4	65.00(14)
N(2)#2-K(1)-O(4)#4	131.45(14)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z+2 #2 x-1,y,z #3 -x+1,-y+3,-z+2 #4 -x+2,-y+3,-z+2 #5 x+1,y,z #6 -x+1,-y+3,-z+3 #7 -x+1,-y+2,-z+3

Table S4. Bond lengths [Å] and angles [º] for compounds **11** and **12**.

11			
La(1)-O(10)#1	2.497(5)	La(1)-O(5)	2.505(5)
La(1)-O(12)#2	2.516(5)	La(1)-O(11)#1	2.525(5)
La(1)-O(1)	2.534(5)	La(1)-O(9)	2.585(5)
La(1)-N(3)	2.734(6)	La(1)-N(5)	2.783(6)
La(1)-N(6)#2	2.823(6)	La(1)-N(1)	2.847(6)
La(2)-O(6)#3	2.426(5)	La(2)-O(7)#3	2.466(6)
La(2)-O(2)	2.483(5)	La(2)-O(3)	2.505(6)
La(2)-O(8)#2	2.515(6)	La(2)-O(13)	2.560(9)
La(2)-O(4)#4	2.581(6)	La(2)-N(2)#4	2.742(6)
La(2)-N(4)#2	2.788(7)	O(10)#1-La(1)-O(5)	76.96(18)
O(10)#1-La(1)-O(12)#2	69.54(18)	O(5)-La(1)-O(12)#2	88.00(19)
O(10)#1-La(1)-O(11)#1	68.39(17)	O(5)-La(1)-O(11)#1	120.06(18)
O(12)#2-La(1)-O(11)#1	120.61(18)	O(10)#1-La(1)-O(1)	138.43(18)
O(5)-La(1)-O(1)	134.43(18)	O(12)#2-La(1)-O(1)	83.29(19)
O(11)#1-La(1)-O(1)	102.55(18)	O(10)#1-La(1)-O(9)	147.91(18)
O(5)-La(1)-O(9)	73.89(16)	O(12)#2-La(1)-O(9)	121.92(17)
O(11)#1-La(1)-O(9)	116.12(16)	O(1)-La(1)-O(9)	73.37(16)
O(10)#1-La(1)-N(3)	81.5(2)	O(5)-La(1)-N(3)	59.40(18)
O(12)#2-La(1)-N(3)	140.8(2)	O(11)#1-La(1)-N(3)	68.09(19)
O(1)-La(1)-N(3)	134.61(19)	O(9)-La(1)-N(3)	72.36(19)
O(10)#1-La(1)-N(5)	127.94(18)	O(5)-La(1)-N(5)	117.68(18)
O(12)#2-La(1)-N(5)	150.25(19)	O(11)#1-La(1)-N(5)	61.21(17)
O(1)-La(1)-N(5)	68.14(19)	O(9)-La(1)-N(5)	58.61(17)
N(3)-La(1)-N(5)	68.91(19)	O(10)#1-La(1)-N(6)#2	119.07(17)
O(5)-La(1)-N(6)#2	71.53(17)	O(12)#2-La(1)-N(6)#2	58.78(17)
O(11)#1-La(1)-N(6)#2	168.23(17)	O(1)-La(1)-N(6)#2	65.75(18)
O(9)-La(1)-N(6)#2	63.14(17)	N(3)-La(1)-N(6)#2	120.59(19)
N(5)-La(1)-N(6)#2	112.83(17)	O(10)#1-La(1)-N(1)	81.45(18)
O(5)-La(1)-N(1)	150.46(19)	O(12)#2-La(1)-N(1)	65.5(2)
O(11)#1-La(1)-N(1)	68.5(2)	O(1)-La(1)-N(1)	58.38(16)
O(9)-La(1)-N(1)	130.50(16)	N(3)-La(1)-N(1)	136.5(2)
N(5)-La(1)-N(1)	91.50(19)	N(6)#2-La(1)-N(1)	102.64(19)
O(6)#3-La(2)-O(7)#3	71.50(19)	O(6)#3-La(2)-O(2)	153.3(2)
O(7)#3-La(2)-O(2)	109.3(2)	O(6)#3-La(2)-O(3)	92.4(2)
O(7)#3-La(2)-O(3)	140.5(2)	O(2)-La(2)-O(3)	69.90(19)
O(6)#3-La(2)-O(8)#2	74.2(2)	O(7)#3-La(2)-O(8)#2	130.1(2)
O(2)-La(2)-O(8)#2	117.5(2)	O(3)-La(2)-O(8)#2	75.0(2)
O(6)#3-La(2)-O(13)	81.1(3)	O(7)#3-La(2)-O(13)	70.8(3)
O(2)-La(2)-O(13)	74.5(3)	O(3)-La(2)-O(13)	71.2(3)
O(8)#2-La(2)-O(13)	136.8(3)	O(6)#3-La(2)-O(4)#4	88.5(2)
O(7)#3-La(2)-O(4)#4	69.2(2)	O(2)-La(2)-O(4)#4	117.14(18)

O(3)-La(2)-O(4)#4	148.3(2)	O(8)#2-La(2)-O(4)#4	74.80(19)
O(13)-La(2)-O(4)#4	139.9(3)	O(6)#3-La(2)-N(2)#4	135.8(2)
O(7)#3-La(2)-N(2)#4	69.78(18)	O(2)-La(2)-N(2)#4	62.84(18)
O(3)-La(2)-N(2)#4	131.40(18)	O(8)#2-La(2)-N(2)#4	117.43(18)
O(13)-La(2)-N(2)#4	105.0(3)	O(4)#4-La(2)-N(2)#4	58.33(17)
O(6)#3-La(2)-N(4)#2	132.3(2)	O(7)#3-La(2)-N(4)#2	132.2(2)
O(2)-La(2)-N(4)#2	68.0(2)	O(3)-La(2)-N(4)#2	85.5(2)
O(8)#2-La(2)-N(4)#2	59.16(17)	O(13)-La(2)-N(4)#2	140.8(3)
O(4)#4-La(2)-N(4)#2	70.9(2)	N(2)#4-La(2)-N(4)#2	67.4(2)

Symmetry transformations used to generate equivalent atoms: #1 x+1,y,z #2 -x+1,y-1/2,-z #3 x,y,z+1 #4 x-1,y,z #5 x,y,z-1 #6 -x+1,y+1/2,-z

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Ce(1)-O(10)#1	2.460(13)	Ce(1)-O(5)	2.476(12)
Ce(1)-O(12)#2	2.487(14)	Ce(1)-O(1)	2.487(13)
Ce(1)-O(11)#1	2.516(13)	Ce(1)-O(9)	2.565(13)
Ce(1)-N(3)	2.692(17)	Ce(1)-N(5)	2.772(16)
Ce(1)-N(6)#2	2.788(16)	Ce(1)-N(1)	2.792(17)
Ce(2)-O(6)#3	2.389(15)	Ce(2)-O(7)#3	2.435(15)
Ce(2)-O(2)	2.455(14)	Ce(2)-O(8)#2	2.488(14)
Ce(2)-O(3)	2.495(14)	Ce(2)-O(13)	2.51(2)
Ce(2)-O(4)#4	2.555(15)	Ce(2)-N(2)#4	2.715(15)
Ce(2)-N(4)#2	2.752(18)		
O(10)#1-Ce(1)-O(5)	75.8(4)	O(10)#1-Ce(1)-O(12)#2	69.4(5)
O(5)-Ce(1)-O(12)#2	87.0(5)	O(10)#1-Ce(1)-O(1)	139.8(5)
O(5)-Ce(1)-O(1)	133.3(4)	O(12)#2-Ce(1)-O(1)	83.5(5)
O(10)#1-Ce(1)-O(11)#1	68.9(5)	O(5)-Ce(1)-O(11)#1	120.0(4)
O(12)#2-Ce(1)-O(11)#1	121.0(5)	O(1)-Ce(1)-O(11)#1	103.8(4)
O(10)#1-Ce(1)-O(9)	147.2(5)	O(5)-Ce(1)-O(9)	74.5(4)
O(12)#2-Ce(1)-O(9)	122.1(5)	O(1)-Ce(1)-O(9)	72.5(4)
O(11)#1-Ce(1)-O(9)	115.6(4)	O(10)#1-Ce(1)-N(3)	81.4(5)
O(5)-Ce(1)-N(3)	59.8(5)	O(12)#2-Ce(1)-N(3)	140.5(5)
O(1)-Ce(1)-N(3)	134.3(5)	O(11)#1-Ce(1)-N(3)	68.0(5)
O(9)-Ce(1)-N(3)	71.8(5)	O(10)#1-Ce(1)-N(5)	128.5(5)
O(5)-Ce(1)-N(5)	118.9(5)	O(12)#2-Ce(1)-N(5)	150.1(5)
O(1)-Ce(1)-N(5)	67.9(5)	O(11)#1-Ce(1)-N(5)	61.2(4)
O(9)-Ce(1)-N(5)	58.5(5)	N(3)-Ce(1)-N(5)	69.4(5)
O(10)#1-Ce(1)-N(6)#2	118.9(5)	O(5)-Ce(1)-N(6)#2	70.4(4)
O(12)#2-Ce(1)-N(6)#2	59.7(5)	O(1)-Ce(1)-N(6)#2	65.4(4)
O(11)#1-Ce(1)-N(6)#2	169.3(4)	O(9)-Ce(1)-N(6)#2	62.4(5)
N(3)-Ce(1)-N(6)#2	119.0(5)	N(5)-Ce(1)-N(6)#2	112.3(5)
O(10)#1-Ce(1)-N(1)	81.9(4)	O(5)-Ce(1)-N(1)	148.6(5)

O(12)#2-Ce(1)-N(1)	64.5(6)	O(1)-Ce(1)-N(1)	59.4(4)
O(11)#1-Ce(1)-N(1)	70.0(5)	O(9)-Ce(1)-N(1)	130.8(4)
N(3)-Ce(1)-N(1)	138.0(6)	N(5)-Ce(1)-N(1)	92.3(6)
N(6)#2-Ce(1)-N(1)	102.9(6)	O(6)#3-Ce(2)-O(7)#3	72.6(5)
O(6)#3-Ce(2)-O(2)	153.2(5)	O(7)#3-Ce(2)-O(2)	107.7(5)
O(6)#3-Ce(2)-O(8)#2	72.6(5)	O(7)#3-Ce(2)-O(8)#2	130.1(5)
O(2)-Ce(2)-O(8)#2	119.4(5)	O(6)#3-Ce(2)-O(3)	92.2(5)
O(7)#3-Ce(2)-O(3)	139.9(5)	O(2)-Ce(2)-O(3)	70.2(5)
O(8)#2-Ce(2)-O(3)	75.5(4)	O(6)#3-Ce(2)-O(13)	79.8(6)
O(7)#3-Ce(2)-O(13)	70.3(8)	O(2)-Ce(2)-O(13)	75.4(6)
O(8)#2-Ce(2)-O(13)	134.9(7)	O(3)-Ce(2)-O(13)	70.6(7)
O(6)#3-Ce(2)-O(4)#4	87.4(5)	O(7)#3-Ce(2)-O(4)#4	69.6(5)
O(2)-Ce(2)-O(4)#4	118.2(4)	O(8)#2-Ce(2)-O(4)#4	74.3(5)
O(3)-Ce(2)-O(4)#4	148.4(5)	O(13)-Ce(2)-O(4)#4	139.9(7)
O(6)#3-Ce(2)-N(2)#4	135.8(5)	O(7)#3-Ce(2)-N(2)#4	69.1(5)
O(2)-Ce(2)-N(2)#4	62.7(4)	O(8)#2-Ce(2)-N(2)#4	118.5(4)
O(3)-Ce(2)-N(2)#4	131.6(5)	O(13)-Ce(2)-N(2)#4	106.3(6)
O(4)#4-Ce(2)-N(2)#4	59.3(4)	O(6)#3-Ce(2)-N(4)#2	132.2(5)
O(7)#3-Ce(2)-N(4)#2	132.4(5)	O(2)-Ce(2)-N(4)#2	68.2(5)
O(8)#2-Ce(2)-N(4)#2	60.6(5)	O(3)-Ce(2)-N(4)#2	85.4(5)
O(13)-Ce(2)-N(4)#2	141.5(6)	O(4)#4-Ce(2)-N(4)#2	71.9(5)
N(2)#4-Ce(2)-N(4)#2	67.7(5)		

Symmetry transformations used to generate equivalent atoms: #1 x-1,y,z #2 -x+1,y+1/2,-z+2 #3 x,y,z-1 #4 x+1,y,z #5 x,y,z+1 #6 -x+1,y-1/2,-z+