Supporting Information for

A Family of 3D Lanthanide Oxalatosuccinate with Rare Structures: 3D Host

Framework Incorporating 3D Alkali Metal Guest Lattice

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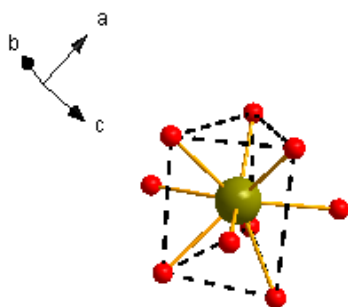
Hong-Yue Duan, Shi-Ping Yan, Dai-Zheng Liao

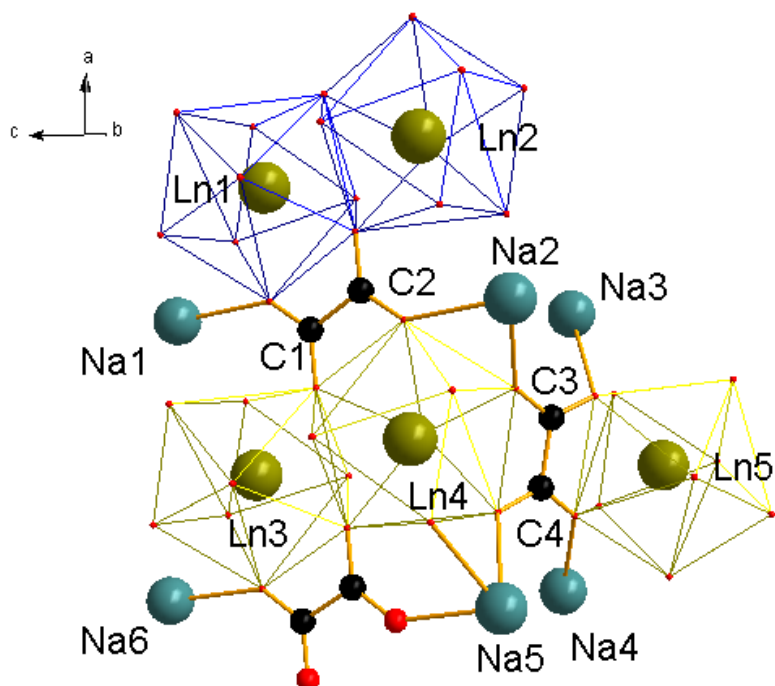Figure S1: Tricapped trigonal prisms of Ln^{3+}.

Figure S2: Dual-dual role of ox ligands. Key: polyhedra, LnO_9, brown circles, Ln ions; cyan circles, Na ions; black circles, C atoms; red circles, O atoms; H atoms, succinate and waters are omitted for clarity. The Na_1-Na_2 distance is 8.331 Å; The Na_2-Na_3 distance is 4.753 Å; The Na_2-Na_5 distance is 6.275 Å.
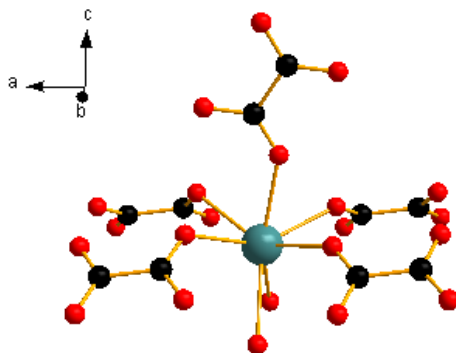
Figure S3: local environment of Na$^+$.
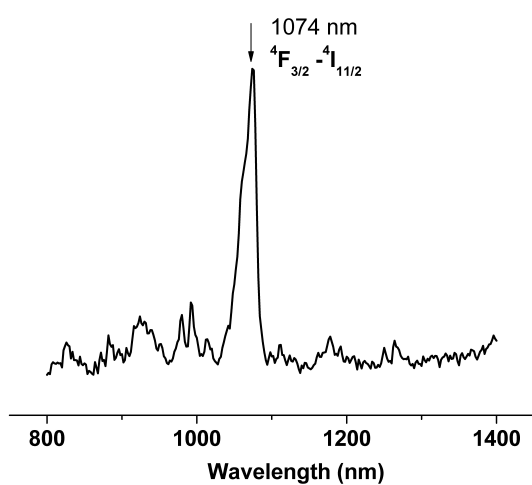
Figure S4: Room-temperature photoluminescence of **1**·Nd with excitation at 573 nm.

Explanation about problems in CIF files:

1. Restraints had been frequently used in producing CIF files. For example, there are no less than 162 restraints in CIF file of Tb complex. The thermal parameters of ligand atoms were restrain to be approximately isotropic.

2. The structure model of Nd complex is incomplete. 4 H atoms per formula unit are missing. It stems form the H atoms of disordered water were not determined.

Table S1: selected bond lengths (Å) and angles (°) data of complexes **1**.

Nd(1)-O(2)#1	2.459(4)	O(2)#1-Nd(1)-O(8)	75.38(14)
Nd(1)-O(7)#2	2.463(4)	O(7)#2-Nd(1)-O(8)	133.78(13)
Nd(1)-O(8)	2.465(4)	O(2)#1-Nd(1)-O(5)	141.13(13)
Nd(1)-O(5)	2.466(4)	O(7)#2-Nd(1)-O(5)	76.33(13)
Nd(1)-O(1)	2.484(4)	O(8)-Nd(1)-O(5)	77.80(13)
Nd(1)-O(3)	2.491(4)	O(2)#1-Nd(1)-O(1)	101.45(16)
Nd(1)-O(6)#3	2.493(4)	O(7)#2-Nd(1)-O(1)	72.73(15)
Nd(1)-O(4)#1	2.499(4)	O(8)-Nd(1)-O(1)	138.75(13)
Nd(1)-O(5)#2	2.603(4)	O(5)-Nd(1)-O(1)	81.05(14)
Na(1)-O(9)	2.201(15)	O(2)#1-Nd(1)-O(3)	70.15(15)
Na(1)-O(3)#4	2.369(5)	O(7)#2-Nd(1)-O(3)	73.70(14)
Na(1)-O(1)	2.374(5)	O(8)-Nd(1)-O(3)	142.46(13)
Na(1)-O(2)#5	2.418(5)	O(5)-Nd(1)-O(3)	139.57(13)
Na(1)-O(6)	2.466(5)	O(1)-Nd(1)-O(3)	64.57(13)
Na(1)-O(4)#1	2.502(5)	O(2)#1-Nd(1)-O(6)#3	67.08(13)
O(2)#1-Nd(1)-O(7)#2	141.91(14)	O(7)#2-Nd(1)-O(6)#3	88.41(13)
O(1)-Nd(1)-O(4)#1	69.07(14)	O(8)-Nd(1)-O(6)#3	85.93(13)
O(3)-Nd(1)-O(4)#1	104.61(14)	O(5)-Nd(1)-O(6)#3	138.00(13)
O(6)#3-Nd(1)-O(4)#1	131.01(12)	O(1)-Nd(1)-O(6)#3	131.59(13)
O(2)#1-Nd(1)-O(5)#2	119.48(14)	O(3)-Nd(1)-O(6)#3	67.44(12)
O(7)#2-Nd(1)-O(5)#2	67.44(12)	O(2)#1-Nd(1)-O(4)#1	65.05(13)
O(8)-Nd(1)-O(5)#2	69.21(12)	O(7)#2-Nd(1)-O(4)#1	137.70(13)
O(5)-Nd(1)-O(5)#2	75.00(14)	O(4)#1-Nd(1)-O(5)#2	138.07(12)
O(1)-Nd(1)-O(5)#2	137.18(14)	O(8)-Nd(1)-O(4)#1	72.74(14)
O(3)-Nd(1)-O(5)#2	116.18(13)	O(5)-Nd(1)-O(4)#1	80.44(13)
O(6)#3-Nd(1)-O(5)#2	63.02(12)		

Symmetry transformations used to generate equivalent atoms:

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

Table S2: selected bond lengths (Å) and angles (°) data of complexes **2**.

Eu(1)-O(7)#1	2.409(3)	O(7)#1-Eu(1)-O(3)	73.38(10)
Eu(1)-O(8)	2.419(3)	O(8)-Eu(1)-O(3)	143.23(10)
Eu(1)-O(2)#2	2.430(3)	O(2)#2-Eu(1)-O(3)	69.98(11)
Eu(1)-O(5)	2.435(3)	O(5)-Eu(1)-O(3)	138.48(10)
Eu(1)-O(1)	2.455(3)	O(1)-Eu(1)-O(3)	65.18(10)
Eu(1)-O(4)#2	2.459(3)	O(4)#2-Eu(1)-O(3)	104.45(11)
Eu(1)-O(6)#3	2.459(3)	O(6)#3-Eu(1)-O(3)	67.15(10)
Eu(1)-O(3)	2.470(3)	O(7)#1-Eu(1)-O(5)#1	67.66(10)
Eu(1)-O(5)#1	2.577(3)	O(8)-Eu(1)-O(5)#1	69.58(10)
Na(1)-O(9)	2.323(5)	O(2)#2-Eu(1)-O(5)#1	119.44(10)
Na(1)-O(3)#4	2.355(3)	O(5)-Eu(1)-O(5)#1	75.21(10)
Na(1)-O(1)	2.389(4)	O(1)-Eu(1)-O(5)#1	136.16(10)
Na(1)-O(2)#5	2.435(4)	O(4)#2-Eu(1)-O(5)#1	137.78(10)
Na(1)-O(6)	2.491(3)	O(6)#3-Eu(1)-O(5)#1	63.51(9)
Na(1)-O(4)#2	2.500(4)	O(3)-Eu(1)-O(5)#1	116.76(10)
Na(1)-O(10)	2.793(7)	O(7)#1-Eu(1)-C(1)#2	156.30(10)
O(7)#1-Eu(1)-O(8)	134.24(10)	O(8)-Eu(1)-C(1)#2	67.91(11)
O(7)#1-Eu(1)-O(2)#2	141.26(11)	O(2)#2-Eu(1)-C(1)#2	19.28(10)
O(8)-Eu(1)-O(2)#2	75.79(11)	O(5)-Eu(1)-C(1)#2	123.07(10)
O(7)#1-Eu(1)-O(5)	76.15(10)	O(1)-Eu(1)-C(1)#2	96.55(11)
O(8)-Eu(1)-O(5)	77.99(10)	O(4)#2-Eu(1)-C(1)#2	47.03(10)
O(2)#2-Eu(1)-O(5)	141.86(10)	O(6)#3-Eu(1)-C(1)#2	84.87(10)
O(7)#1-Eu(1)-O(1)	72.09(11)	O(3)-Eu(1)-C(1)#2	82.99(11)
O(8)-Eu(1)-O(1)	137.56(10)	O(5)#1-Eu(1)-C(1)#2	127.24(10)
O(2)#2-Eu(1)-O(1)	102.71(11)	O(7)#1-Eu(1)-C(2)#2	154.03(11)
O(5)-Eu(1)-O(1)	79.06(10)	O(8)-Eu(1)-C(2)#2	66.32(10)
O(7)#1-Eu(1)-O(4)#2	137.56(11)	O(2)#2-Eu(1)-C(2)#2	46.32(10)
O(8)-Eu(1)-O(4)#2	72.09(11)	O(5)-Eu(1)-C(2)#2	97.54(10)
O(2)#2-Eu(1)-O(4)#2	65.68(10)	O(1)-Eu(1)-C(2)#2	82.01(11)
O(5)-Eu(1)-O(4)#2	80.19(10)	O(4)#2-Eu(1)-C(2)#2	19.93(10)
O(1)-Eu(1)-O(4)#2	69.14(11)	O(6)#3-Eu(1)-C(2)#2	111.77(10)
O(7)#1-Eu(1)-O(6)#3	87.61(11)	O(3)-Eu(1)-C(2)#2	97.66(10)
O(8)-Eu(1)-O(6)#3	87.61(11)	O(5)#1-Eu(1)-C(2)#2	135.84(10)
O(2)#2-Eu(1)-O(6)#3	67.02(10)	C(1)#2-Eu(1)-C(2)#2	27.30(10)
O(5)-Eu(1)-O(6)#3	138.72(10)	O(4)#2-Eu(1)-O(6)#3	131.71(10)
O(1)-Eu(1)-O(6)#3	131.72(10)		

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

Table S3: selected bond lengths (Å) and angles (°) data of complexes **3**.

Gd(1)-O(7)#1	2.392(5)	O(5)-Gd(1)-O(4)#2	80.03(16)
Gd(1)-O(8)	2.400(5)	O(6)#3-Gd(1)-O(4)#2	131.82(16)
Gd(1)-O(2)#2	2.414(5)	O(1)-Gd(1)-O(4)#2	69.29(18)
Gd(1)-O(5)	2.415(5)	O(7)#1-Gd(1)-O(3)	73.20(17)
Gd(1)-O(6)#3	2.430(5)	O(8)-Gd(1)-O(3)	143.20(16)
Gd(1)-O(1)	2.438(5)	O(2)#2-Gd(1)-O(3)	70.00(18)
Gd(1)-O(4)#2	2.441(5)	O(5)-Gd(1)-O(3)	138.45(16)
Gd(1)-O(3)	2.453(5)	O(6)#3-Gd(1)-O(3)	67.06(16)
Gd(1)-O(5)#1	2.566(5)	O(1)-Gd(1)-O(3)	65.50(16)
Na(1)-O(10)	2.302(7)	O(4)#2-Gd(1)-O(3)	104.68(18)
Na(1)-O(9)	2.307(8)	O(7)#1-Gd(1)-O(5)#1	67.79(16)
Na(1)-O(3)#4	2.340(5)	O(8)-Gd(1)-O(5)#1	69.52(16)
Na(1)-O(1)	2.376(6)	O(2)#2-Gd(1)-O(5)#1	119.32(16)
Na(1)-O(2)#5	2.419(6)	O(5)-Gd(1)-O(5)#1	75.15(16)
Na(1)-O(6)	2.480(6)	O(6)#3-Gd(1)-O(5)#1	63.62(15)
Na(1)-O(4)#2	2.485(6)	O(1)-Gd(1)-O(5)#1	135.70(17)
O(7)#1-Gd(1)-O(8)	134.35(17)	O(4)#2-Gd(1)-O(5)#1	137.67(17)
O(7)#1-Gd(1)-O(2)#2	141.11(17)	O(3)-Gd(1)-O(5)#1	116.69(16)
O(8)-Gd(1)-O(2)#2	75.75(18)	O(8)-Gd(1)-O(1)	137.66(17)
O(7)#1-Gd(1)-O(5)	76.16(17)	O(2)#2-Gd(1)-O(1)	103.30(19)
O(8)-Gd(1)-O(5)	78.07(16)	O(5)-Gd(1)-O(1)	78.67(16)
O(2)#2-Gd(1)-O(5)	142.02(16)	O(6)#3-Gd(1)-O(1)	131.90(16)
O(7)#1-Gd(1)-O(6)#3	87.73(17)	O(7)#1-Gd(1)-O(4)#2	137.33(17)
O(8)-Gd(1)-O(6)#3	87.52(17)	O(8)-Gd(1)-O(4)#2	72.17(18)
O(2)#2-Gd(1)-O(6)#3	66.77(16)	O(2)#2-Gd(1)-O(4)#2	66.04(16)
O(5)-Gd(1)-O(6)#3	138.76(16)	O(7)#1-Gd(1)-O(1)	71.63(18)

Symmetry transformations used to generate equivalent atoms:

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

Table S4: selected bond lengths (Å) and angles (°) data of complexes **4**.

Tb(1)-O(7)#1	2.358(7)	O(8)-Tb(1)-O(6)#3	87.1(2)
Tb(1)-O(8)	2.393(7)	O(2)#2-Tb(1)-O(6)#3	66.7(2)
Tb(1)-O(2)#2	2.391(6)	O(5)-Tb(1)-O(6)#3	139.0(2)
Tb(1)-O(5)	2.393(6)	O(1)-Tb(1)-O(6)#3	132.4(2)
Tb(1)-O(1)	2.414(7)	O(4)#2-Tb(1)-O(6)#3	131.7(2)
Tb(1)-O(4)#2	2.425(7)	O(7)#1-Tb(1)-O(3)	72.9(2)
Tb(1)-O(6)#3	2.422(7)	O(8)-Tb(1)-O(3)	143.4(2)
Tb(1)-O(3)	2.441(6)	O(2)#2-Tb(1)-O(3)	70.1(2)
Tb(1)-O(5)#1	2.567(6)	O(5)-Tb(1)-O(3)	138.5(2)
O(7)#1-Tb(1)-O(8)	134.6(2)	O(1)-Tb(1)-O(3)	65.5(2)
O(7)#1-Tb(1)-O(2)#2	141.2(2)	O(4)#2-Tb(1)-O(3)	105.2(2)
O(8)-Tb(1)-O(2)#2	75.9(2)	O(6)#3-Tb(1)-O(3)	67.5(2)
O(7)#1-Tb(1)-O(5)	76.5(2)	O(7)#1-Tb(1)-O(5)#1	67.5(2)
O(8)-Tb(1)-O(5)	77.8(2)	O(8)-Tb(1)-O(5)#1	69.9(2)
O(2)#2-Tb(1)-O(5)	141.5(2)	O(2)#2-Tb(1)-O(5)#1	120.2(2)
O(7)#1-Tb(1)-O(1)	71.4(3)	O(5)-Tb(1)-O(5)#1	75.0(2)
O(8)-Tb(1)-O(1)	137.5(2)	O(1)-Tb(1)-O(5)#1	135.1(2)
O(2)#2-Tb(1)-O(1)	103.0(3)	O(4)#2-Tb(1)-O(5)#1	137.5(2)
O(5)-Tb(1)-O(1)	78.6(2)	O(6)#3-Tb(1)-O(5)#1	64.0(2)
O(7)#1-Tb(1)-O(4)#2	137.0(2)	O(3)-Tb(1)-O(5)#1	116.6(2)
O(8)-Tb(1)-O(4)#2	71.9(2)	O(1)-Tb(1)-O(4)#2	69.3(3)
O(2)#2-Tb(1)-O(4)#2	66.1(2)	O(7)#1-Tb(1)-O(6)#3	88.4(2)
O(5)-Tb(1)-O(4)#2	79.3(2)		

Symmetry transformations used to generate equivalent atoms:

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

Table S5: selected bond lengths (Å) and angles (°) data of complexes **5**.

Nd(1)-O(2)#1	2.402(3)	O(2)#3-Nd(1)-O(2)	172.32(11)
Nd(1)-O(2)#2	2.402(3)	O(2)#1-Nd(1)-C(1)#3	84.45(11)
Nd(1)-O(3)	2.473(3)	O(2)#2-Nd(1)-C(1)#3	102.22(11)
Nd(1)-O(3)#3	2.473(3)	O(3)-Nd(1)-C(1)#3	72.89(10)
Nd(1)-O(4)	2.507(3)	O(3)#3-Nd(1)-C(1)#3	88.12(10)
Nd(1)-O(4)#3	2.507(3)	O(4)-Nd(1)-C(1)#3	136.05(10)
Nd(1)-O(1)#3	2.525(3)	O(4)#3-Nd(1)-C(1)#3	66.12(11)
Nd(1)-O(1)	2.525(3)	O(1)#3-Nd(1)-C(1)#3	22.81(10)
O(2)#1-Nd(1)-O(2)#2	145.56(14)	O(1)-Nd(1)-C(1)#3	142.60(11)
O(2)#1-Nd(1)-O(3)	74.78(9)	O(2)#3-Nd(1)-C(1)#3	23.81(9)
O(2)#2-Nd(1)-O(3)	139.61(9)	O(2)-Nd(1)-C(1)#3	152.74(9)
O(2)#1-Nd(1)-O(3)#3	139.61(9)	O(2)#1-Nd(1)-C(1)	102.22(11)
O(2)#2-Nd(1)-O(3)#3	74.78(9)	O(2)#2-Nd(1)-C(1)	84.45(11)
O(3)-Nd(1)-O(3)#3	65.11(12)	O(3)-Nd(1)-C(1)	88.11(10)
O(2)#1-Nd(1)-O(4)	75.27(10)	O(3)#3-Nd(1)-C(1)	72.89(10)
O(2)#2-Nd(1)-O(4)	76.91(10)	O(4)-Nd(1)-C(1)	66.12(11)
O(3)-Nd(1)-O(4)	134.68(9)	O(4)#3-Nd(1)-C(1)	136.05(10)
O(3)#3-Nd(1)-O(4)	131.72(9)	O(1)#3-Nd(1)-C(1)	142.60(11)
O(2)#1-Nd(1)-O(4)#3	76.90(10)	O(1)-Nd(1)-C(1)	22.81(10)
O(2)#2-Nd(1)-O(4)#3	75.27(10)	O(2)#3-Nd(1)-C(1)	152.74(9)
O(3)-Nd(1)-O(4)#3	131.72(9)	O(2)-Nd(1)-C(1)	23.81(9)
O(3)#3-Nd(1)-O(4)#3	134.69(9)	O(3)-Nd(1)-O(1)	69.76(10)
O(4)-Nd(1)-O(4)#3	71.43(14)	O(3)#3-Nd(1)-O(1)	78.04(10)
O(2)#1-Nd(1)-O(1)#3	107.19(10)	O(4)-Nd(1)-O(1)	74.08(10)
O(2)#2-Nd(1)-O(1)#3	84.19(10)	O(4)#3-Nd(1)-O(1)	143.82(10)
O(3)-Nd(1)-O(1)#3	78.04(10)	O(2)#1-Nd(1)-O(1)	84.19(10)
O(3)#3-Nd(1)-O(1)#3	69.76(10)	O(2)#2-Nd(1)-O(1)	107.19(10)
O(4)-Nd(1)-O(1)#3	143.83(10)	O(1)#3-Nd(1)-O(1)	141.68(14)
O(4)#3-Nd(1)-O(1)#3	74.08(10)		

Symmetry transformations used to generate equivalent atoms:

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