Structures and properties of lanthanide metal-organic frameworks based on 1,2,3-triazole-containing tetracarboxylate ligand

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Fig. S1 Representation of the asymmetric unit of compound **1** showing ellipsoid at the 30% probability level. The hydrogen atoms and lattice water molecules are omitted for clarity.

Fig. S2 (a) The coordination modes of ligand (yellow: **C-IP**; grey: **N-IP**). (b) Six-connected binuclear unit and coordinated ligand. (c) The 3,6-connected **rtl** network of compound **1**.

Fig. S3 View of the hydrogen bonds of O(5)$^{\cdots}$H(20)-O(12) in compound **1**.

Fig. S4 Powder X-ray diffraction patterns of compound **1-4**.

Fig. S5 FT-IR spectra of compound **1-4** and H_4L.

Fig. S6 TGA curves for compound **1-4**.

Fig. S7 UV-vis absorption spectra of compound **1-4**.

Fig. S8 The solid state photoluminescence spectra of H_4L.

Fig. S9 The χ_M^{-1} vs T plots of compound **3** and **4**.

Fig. S10 Powder X-ray diffraction patterns of compound **3** dispersed in $Cu(NO_3)_2$ aqueous solution (0.01 mol/L).

Table S1 Selected bond distances (Å) and angles (°) for compound **1.**

Table S2 Selected bond distances (Å) and angles (°) for compound **2.**

Table S3 Selected bond distances (Å) and angles (°) for compound **3.**

Table S4 Selected bond distances (Å) and angles (°) for compound **4.**

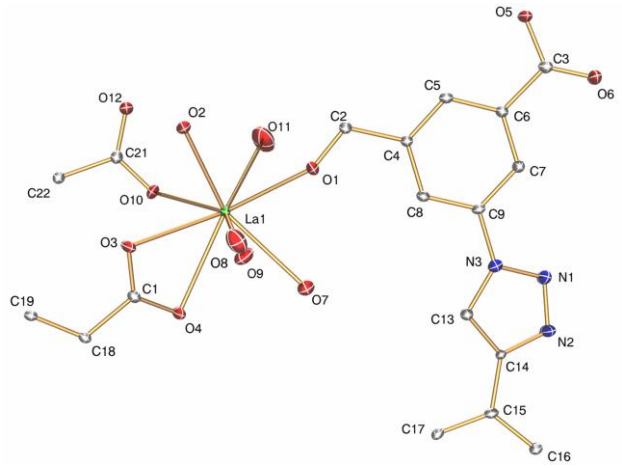

Fig. S1 Representation of the asymmetric unit of compound **1** showing ellipsoid at the 30% probability level. The hydrogen atoms and lattice water molecules are omitted for clarity.

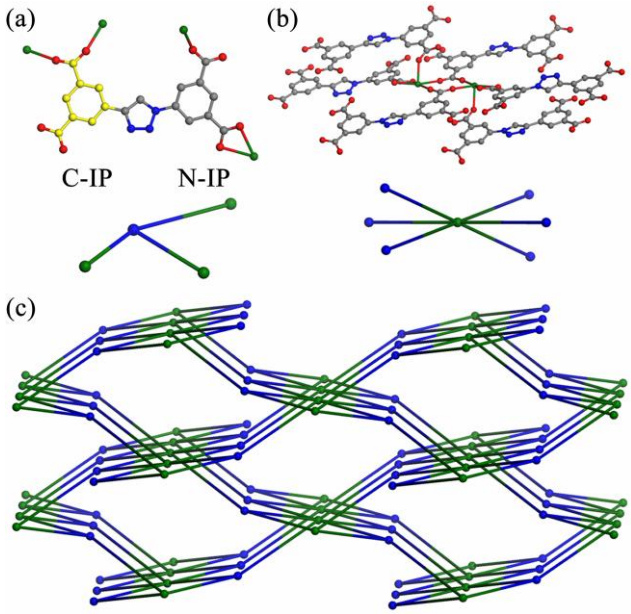

Fig. S2 (a) The coordination modes of ligand (yellow: **C-IP**; grey: **N-IP**). (b) Six-connected binuclear unit and coordinated ligand. (c) The 3,6-connected **rtl** network of compound **1**.

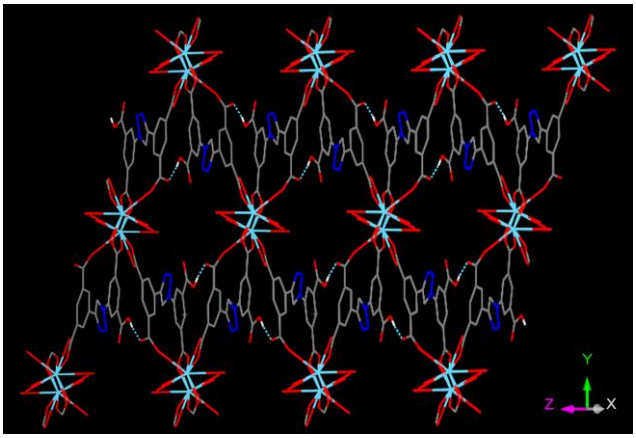

Fig. S3 View of the hydrogen bonds of O(5)···H(20)-O(12) in compound **1**.

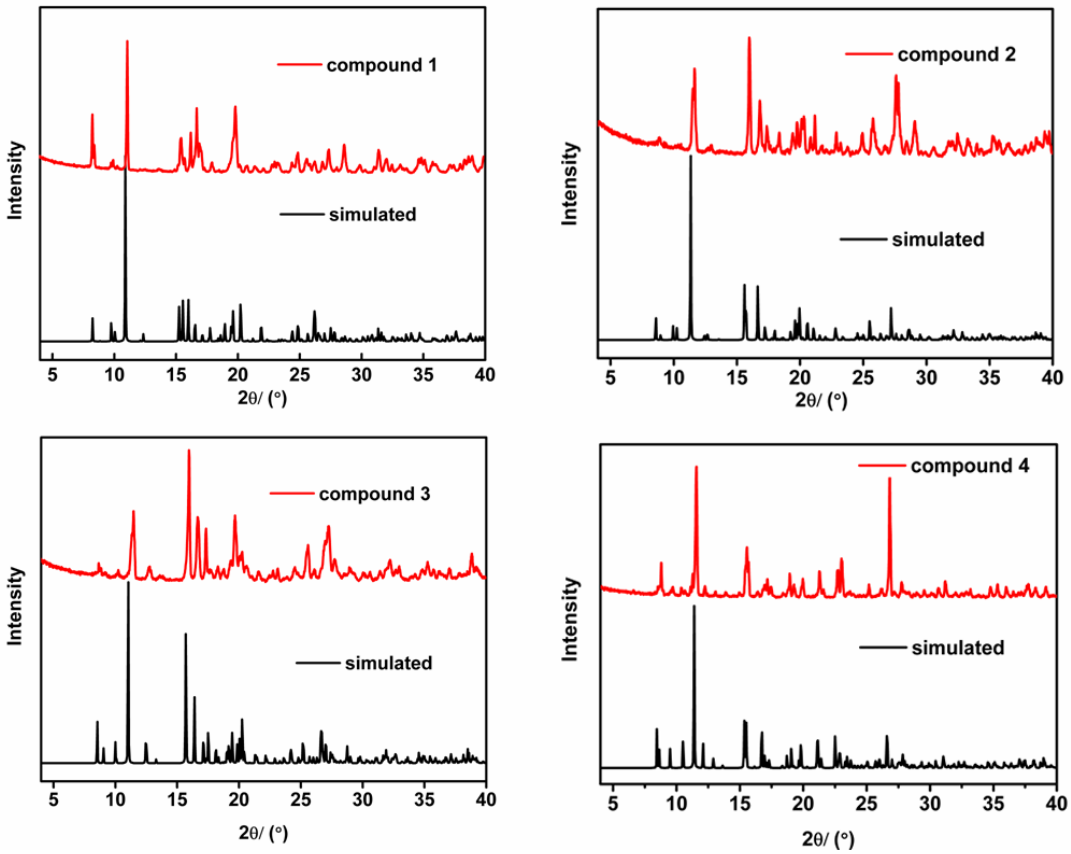

Fig. S4 Powder X-ray diffraction patterns of compound **1-4**.

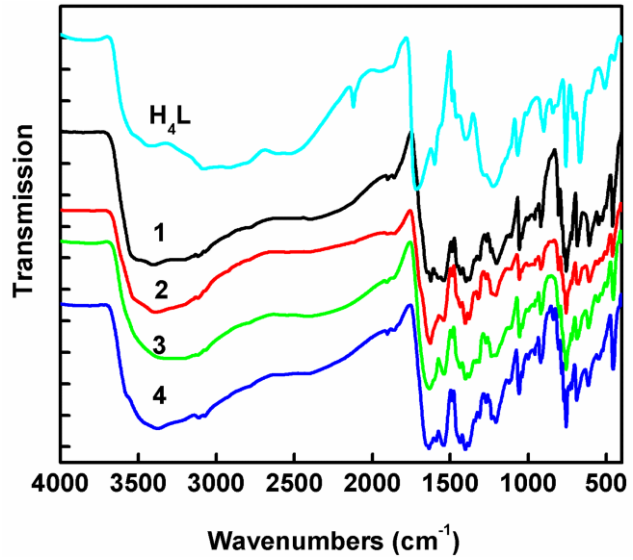

Fig. S5 FT-IR spectra of compound **1-4** and H_4L.

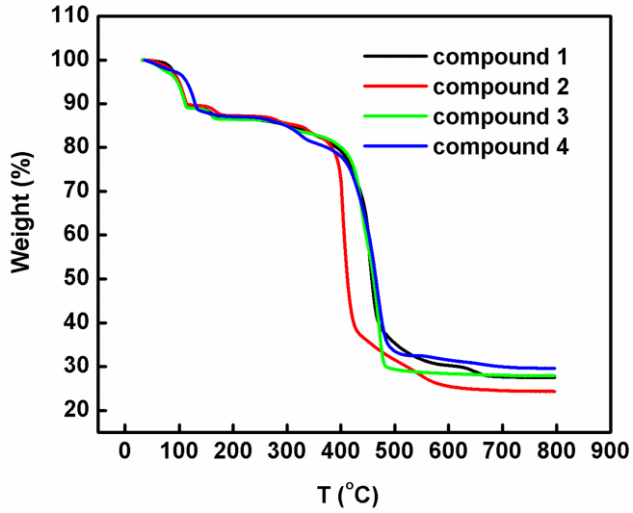

Fig. S6 TGA curves for compound **1-4**.

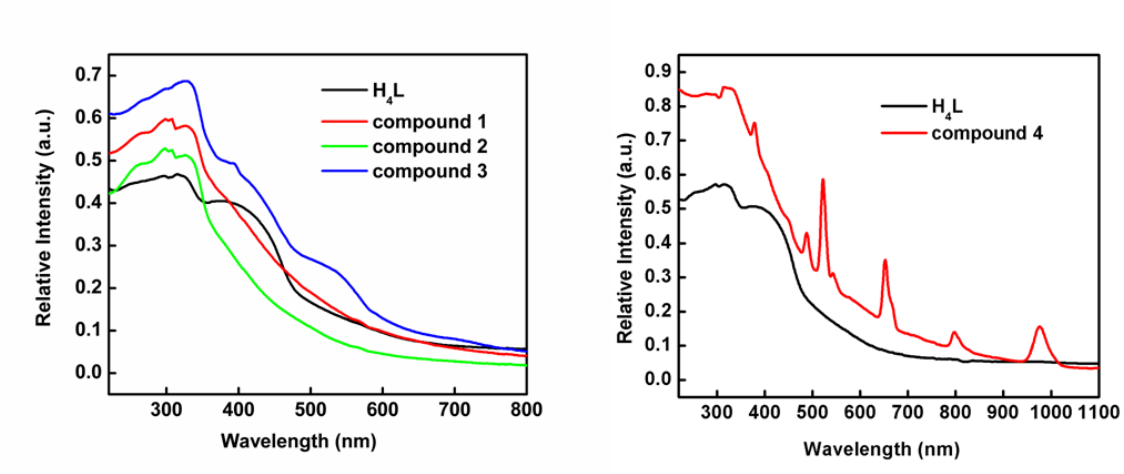

Fig. S7 UV-vis absorption spectra of compound **1-4**.

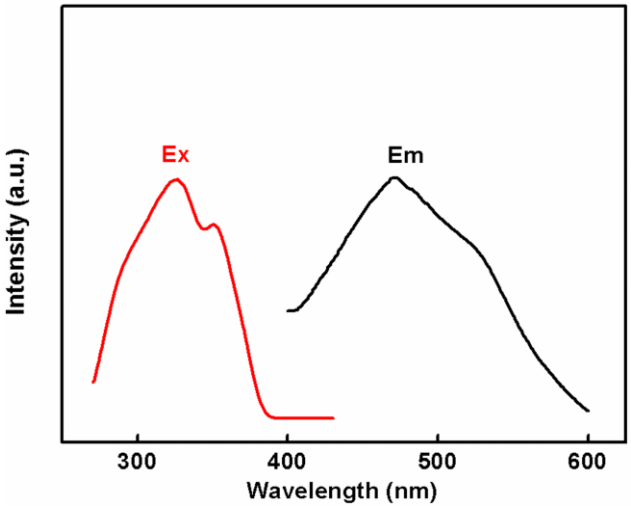

Fig. S8 The solid state photoluminescence spectra of H_4L.

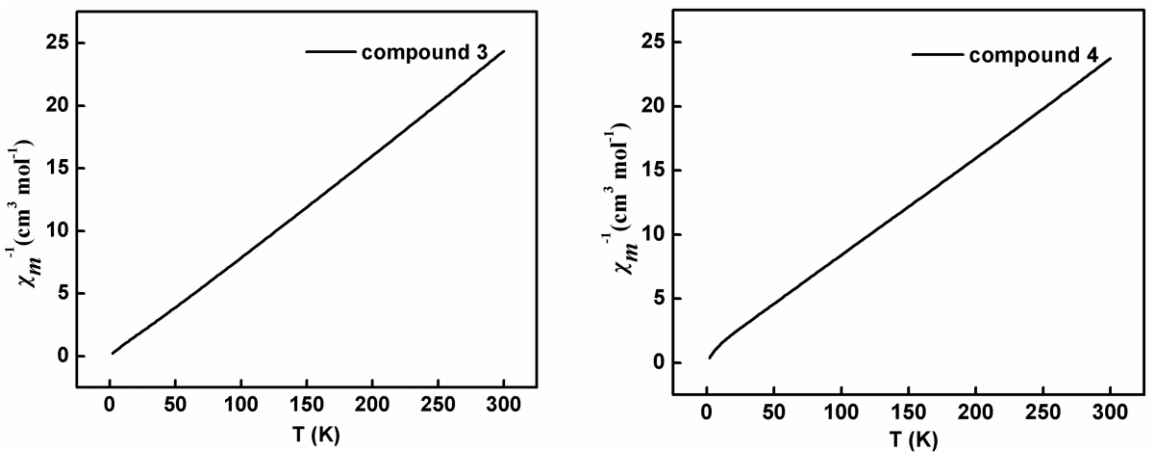

Fig. S9 The χ_M^{-1} vs T plots of compounds **3** and **4**.

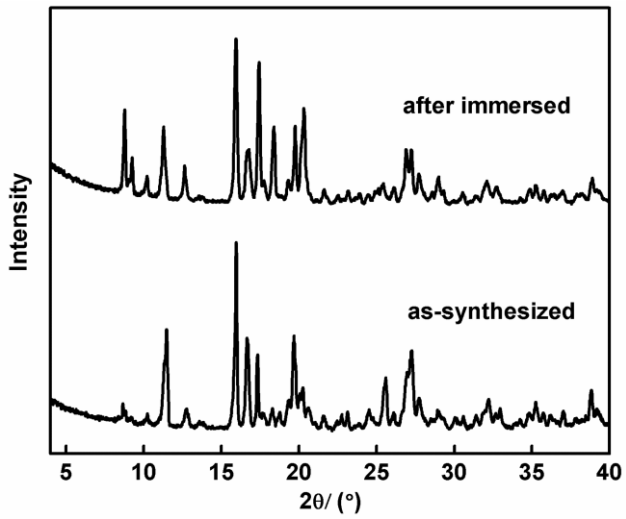

Fig. S10 Powder X-ray diffraction patterns of compound **3** dispersed in $Cu(NO_3)_2$ aqueous solution (0.01 mol/L).

Table S1 Selected bond distances (Å) and angles (°) for compound **1**

Bond distances/ Å

La(1)-O(2)	2.424(2)
La(1)-O(1)	2.478(3)
La(1)-O(10)	2.501(3)
La(1)-O(8)	2.542(3)
La(1)-O(3)	2.601(2)
La(1)-O(9)	2.601(3)
La(1)-O(11)	2.616(3)
La(1)-O(7)	2.666(3)
La(1)-O(4)	2.676(2)

Bond angles/ °

O(2)-La(1)-O(1)	81.29(9)
O(2)-La(1)-O(10)	80.15(9)
O(1)-La(1)-O(10)	138.81(9)
O(2)-La(1)-O(8)	82.72(11)
O(1)-La(1)-O(8)	71.42(10)
O(10)-La(1)-O(8)	140.91(9)
O(2)-La(1)-O(3)	76.11(8)
O(1)-La(1)-O(3)	136.79(10)
O(10)-La(1)-O(3)	72.32(9)
O(8)-La(1)-O(3)	69.55(9)
O(2)-La(1)-O(9)	141.55(10)
O(1)-La(1)-O(9)	109.94(10)
O(10)-La(1)-O(9)	67.26(9)
O(8)-La(1)-O(9)	135.64(10)
O(3)-La(1)-O(9)	110.69(9)
O(2)-La(1)-O(11)	80.69(13)
O(1)-La(1)-O(11)	68.70(12)
O(10)-La(1)-O(11)	72.20(11)
O(8)-La(1)-O(11)	138.57(12)
O(3)-La(1)-O(11)	140.24(10)
O(9)-La(1)-O(11)	70.58(13)
O(2)-La(1)-O(7)	147.57(9)
O(1)-La(1)-O(7)	70.52(8)
O(10)-La(1)-O(7)	131.95(8)

O(8)-La(1)-O(7)	73.49(10)
O(3)-La(1)-O(7)	114.12(8)
O(9)-La(1)-O(7)	66.26(9)
O(11)-La(1)-O(7)	102.79(11)
O(2)-La(1)-O(4)	125.54(8)
O(1)-La(1)-O(4)	136.07(8)
O(10)-La(1)-O(4)	83.90(8)
O(8)-La(1)-O(4)	78.01(9)
O(3)-La(1)-O(4)	49.44(7)
O(9)-La(1)-O(4)	72.08(9)
O(11)-La(1)-O(4)	141.15(12)
O(7)-La(1)-O(4)	71.02(8)

Hydrogen bonds /Å and °

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(20)...O(12)#7	0.87	1.70	2.556(3)	166.8

Symmetry transformations used to generate equivalent atoms:

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

Table S2 Selected bond distances (Å) and angles (°) for compound **2**

Bond distances/ Å

Eu(1)-O(11)#1	2.312(7)
Eu(1)-O(12)	2.365(7)
Eu(1)-O(1)	2.403(7)
Eu(1)-O(4)	2.440(7)
Eu(1)-O(13)	2.478(9)
Eu(1)-O(6)	2.520(7)
Eu(1)-O(7)	2.561(8)
Eu(1)-O(5)	2.600(8)
Eu(1)-O(2)	2.630(9)

Bond angles/ °

O(11)#1-Eu(1)-O(12)	137.8(3)
O(11)#1-Eu(1)-O(1)	86.5(3)
O(12)-Eu(1)-O(1)	82.1(3)
O(11)#1-Eu(1)-O(4)	138.4(2)
O(12)-Eu(1)-O(4)	75.8(3)
O(1)-Eu(1)-O(4)	73.2(3)
O(11)#1-Eu(1)-O(13)	91.1(3)
O(12)-Eu(1)-O(13)	70.0(3)
O(1)-Eu(1)-O(13)	134.8(3)
O(4)-Eu(1)-O(13)	129.0(3)
O(11)#1-Eu(1)-O(6)	70.9(3)
O(12)-Eu(1)-O(6)	144.8(3)
O(1)-Eu(1)-O(6)	80.2(3)
O(4)-Eu(1)-O(6)	70.1(2)
O(13)-Eu(1)-O(6)	140.8(3)
O(11)#1-Eu(1)-O(7)	141.9(3)
O(12)-Eu(1)-O(7)	74.7(3)
O(1)-Eu(1)-O(7)	123.6(2)
O(4)-Eu(1)-O(7)	51.6(2)
O(13)-Eu(1)-O(7)	83.1(3)
O(6)-Eu(1)-O(7)	90.3(3)
O(11)#1-Eu(1)-O(5)	74.6(3)
O(12)-Eu(1)-O(5)	127.8(3)
O(1)-Eu(1)-O(5)	149.5(3)

O(4)-Eu(1)-O(5)	105.6(3)
O(13)-Eu(1)-O(5)	70.5(3)
O(6)-Eu(1)-O(5)	71.2(3)
O(7)-Eu(1)-O(5)	68.0(3)
O(11)#1-Eu(1)-O(2)	69.1(3)
O(12)-Eu(1)-O(2)	68.8(3)
O(1)-Eu(1)-O(2)	70.2(3)
O(4)-Eu(1)-O(2)	131.6(3)
O(13)-Eu(1)-O(2)	66.8(3)
O(6)-Eu(1)-O(2)	130.9(3)
O(7)-Eu(1)-O(2)	138.7(3)
O(5)-Eu(1)-O(2)	122.1(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z+1

Hydrogen bonds /Å and °

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(8)-H(20)...O(10)#3	0.85	1.73	2.544(10)	158.8

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

Table S3 Selected bond distances (Å) and angles (°) for compound **3**

Bond distances/ Å

Tb(1)-O(2)	2.283(6)
Tb(1)-O(1)	2.312(6)
Tb(1)-O(7)	2.324(6)
Tb(1)-O(9)	2.396(7)
Tb(1)-O(6)	2.411(6)
Tb(1)-O(11)	2.417(11)
Tb(1)-O(10)	2.485(8)
Tb(1)-O(5)	2.501(6)

Bond angles/ °

O(2)-Tb(1)-O(1)	82.0(2)
O(2)-Tb(1)-O(7)	105.6(3)
O(1)-Tb(1)-O(7)	77.9(2)
O(2)-Tb(1)-O(9)	80.6(3)
O(1)-Tb(1)-O(9)	138.5(3)
O(7)-Tb(1)-O(9)	71.0(2)
O(2)-Tb(1)-O(6)	158.4(3)
O(1)-Tb(1)-O(6)	78.8(2)
O(7)-Tb(1)-O(6)	80.0(2)
O(9)-Tb(1)-O(6)	120.6(2)
O(2)-Tb(1)-O(11)	87.2(4)
O(1)-Tb(1)-O(11)	73.4(4)
O(7)-Tb(1)-O(11)	146.6(3)
O(9)-Tb(1)-O(11)	142.3(3)
O(6)-Tb(1)-O(11)	77.9(4)
O(2)-Tb(1)-O(10)	78.4(3)
O(1)-Tb(1)-O(10)	139.6(3)
O(7)-Tb(1)-O(10)	141.5(3)
O(9)-Tb(1)-O(10)	72.0(3)
O(6)-Tb(1)-O(10)	110.6(3)
O(11)-Tb(1)-O(10)	70.7(3)
O(2)-Tb(1)-O(5)	146.8(2)
O(1)-Tb(1)-O(5)	131.1(2)
O(7)-Tb(1)-O(5)	86.5(2)
O(9)-Tb(1)-O(5)	74.3(2)

O(6)-Tb(1)-O(5)	52.8(2)
O(11)-Tb(1)-O(5)	99.5(4)
O(10)-Tb(1)-O(5)	73.5(2)

Hydrogen bonds /Å and °

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(20)...O(8)#7	0.96	1.59	2.549(8)	177.1

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

Table S4 Selected bond distances (Å) and angles (°) for compound **4**

Bond distances/ Å

Er(1)-O(2)	2.255(4)
Er(1)-O(6)	2.299(4)
Er(1)-O(8)	2.299(4)
Er(1)-O(4)	2.355(4)
Er(1)-O(3)	2.375(5)
Er(1)-O(5)	2.401(4)
Er(1)-O(1)	2.402(4)
Er(1)-O(7)	2.423(4)

Bond angles/ °

O(2)-Er(1)-O(6)	103.47(14)
O(2)-Er(1)-O(8)	89.52(15)
O(6)-Er(1)-O(8)	141.71(15)
O(2)-Er(1)-O(4)	154.49(16)
O(6)-Er(1)-O(4)	74.21(15)
O(8)-Er(1)-O(4)	78.82(16)
O(2)-Er(1)-O(3)	85.30(17)
O(6)-Er(1)-O(3)	68.85(15)
O(8)-Er(1)-O(3)	149.05(15)
O(4)-Er(1)-O(3)	116.09(17)
O(2)-Er(1)-O(5)	74.11(13)
O(6)-Er(1)-O(5)	141.66(16)
O(8)-Er(1)-O(5)	76.40(15)
O(4)-Er(1)-O(5)	123.74(14)
O(3)-Er(1)-O(5)	72.83(15)
O(2)-Er(1)-O(1)	78.46(15)
O(6)-Er(1)-O(1)	75.19(14)
O(8)-Er(1)-O(1)	72.38(14)
O(4)-Er(1)-O(1)	76.41(15)
O(3)-Er(1)-O(1)	135.57(16)
O(5)-Er(1)-O(1)	138.18(14)
O(2)-Er(1)-O(7)	128.20(13)
O(6)-Er(1)-O(7)	116.51(13)
O(8)-Er(1)-O(7)	79.18(14)
O(4)-Er(1)-O(7)	72.12(14)

O(3)-Er(1)-O(7)	80.24(16)
O(5)-Er(1)-O(7)	54.09(13)
O(1)-Er(1)-O(7)	140.89(15)

Hydrogen bonds /Å and °

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(10)-H(20)...O(9)#5	0.86	1.73	2.562(6)	162.1

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