

## ACCESSORY PUBLICATION

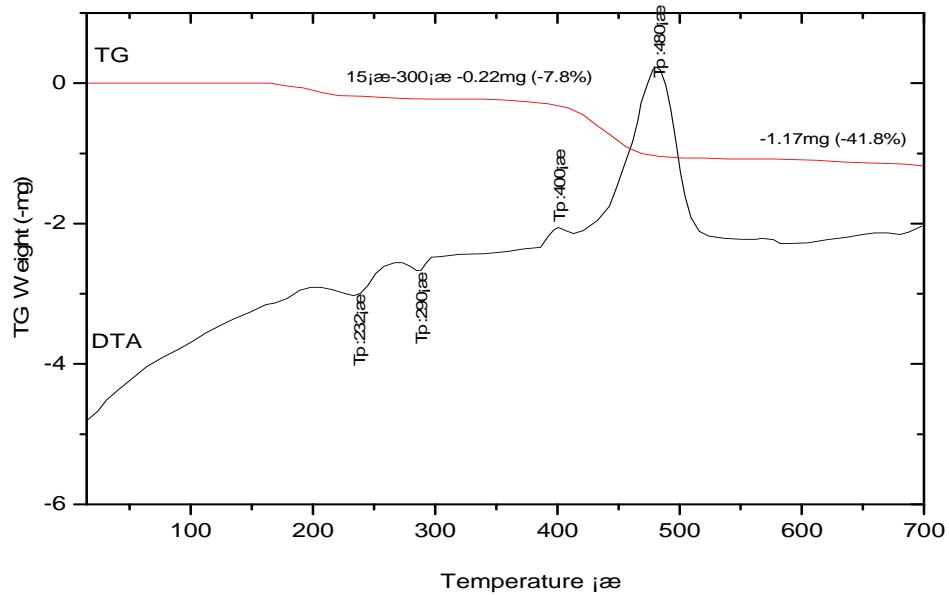
# A Series of 2D and 3D Novel Lanthanide Complexes Constructed from Squarate $C_4O_4^{2-}$ : Syntheses, Structures, Magnetic Properties and NIR Emission Properties

Li Wang<sup>A</sup>, Wen Gu<sup>A,B</sup>, Xiu-Jun Deng<sup>A</sup>, Ling-Fei Zeng<sup>A</sup>, Sheng-Yun Liao<sup>A</sup>, Ming Zhang<sup>A</sup>, Lin-Yan Yang<sup>A</sup>, Xin Liu\*<sup>A,B</sup>

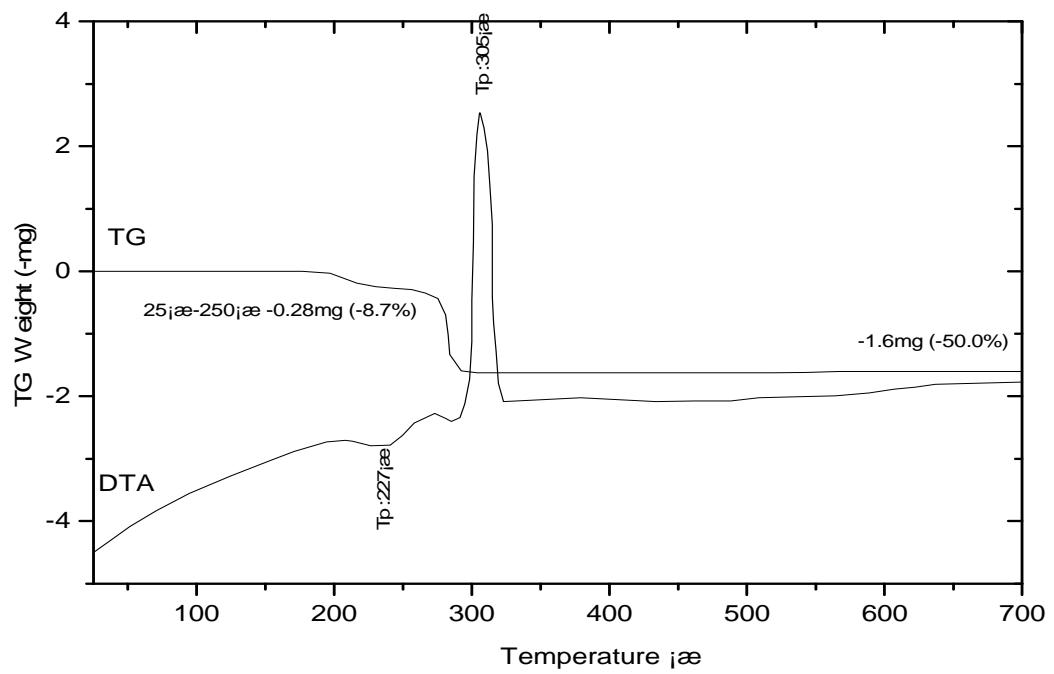
<sup>A</sup>Department of Chemistry, Nankai University

<sup>B</sup>Tianjin Key Laboratory of Metal and Molecule Based Material Chemistry, Tianjin, P.R. China

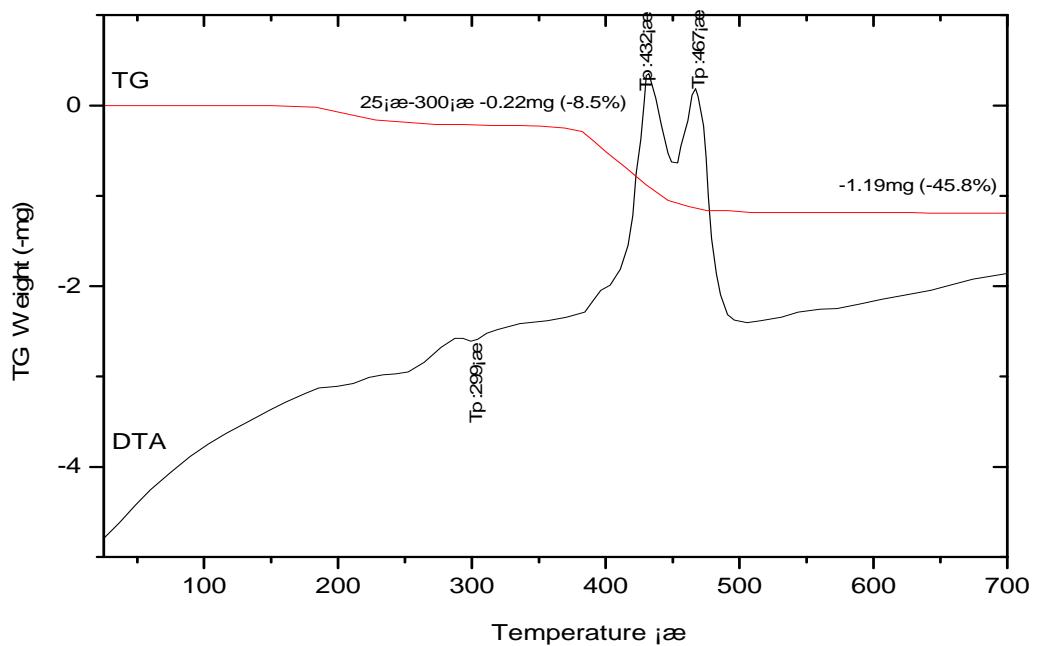
\*Corresponding author. Email: guwen68@nankai.edu.cn



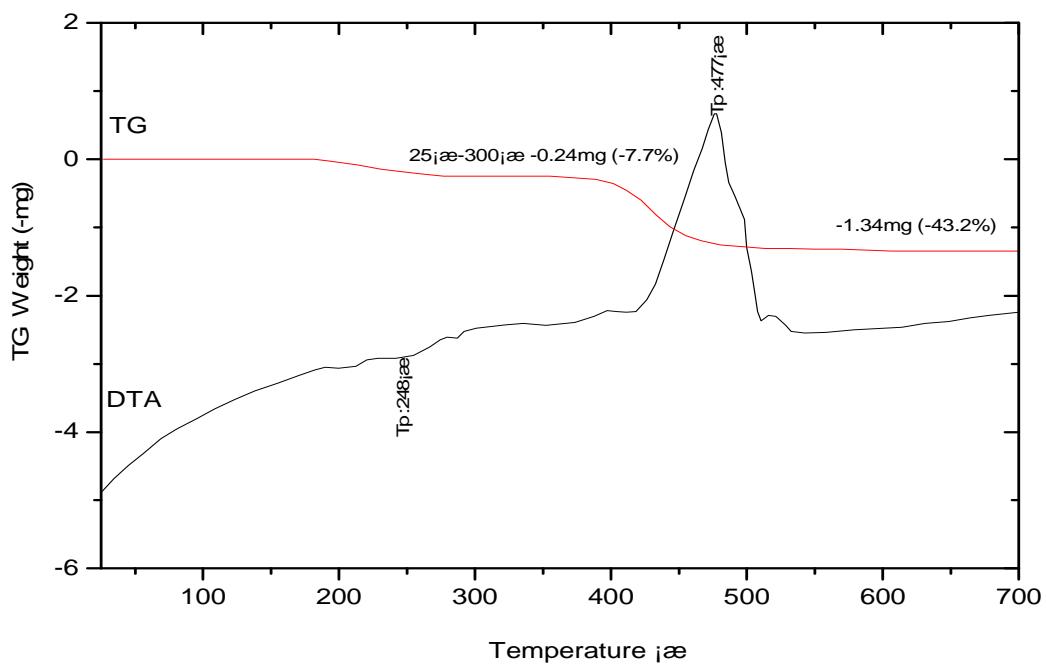
(1)



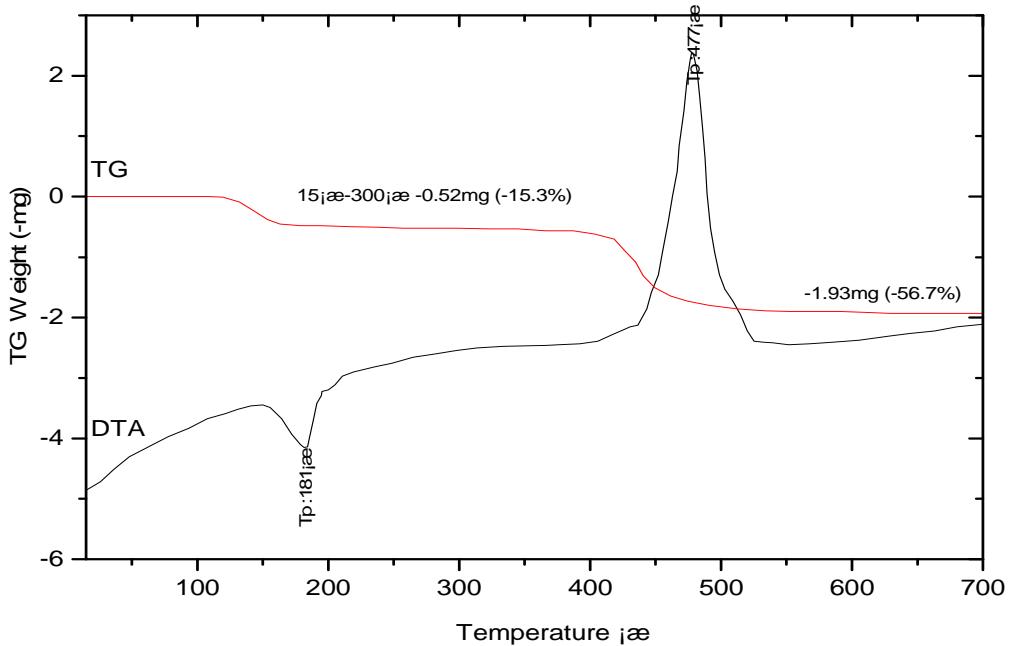
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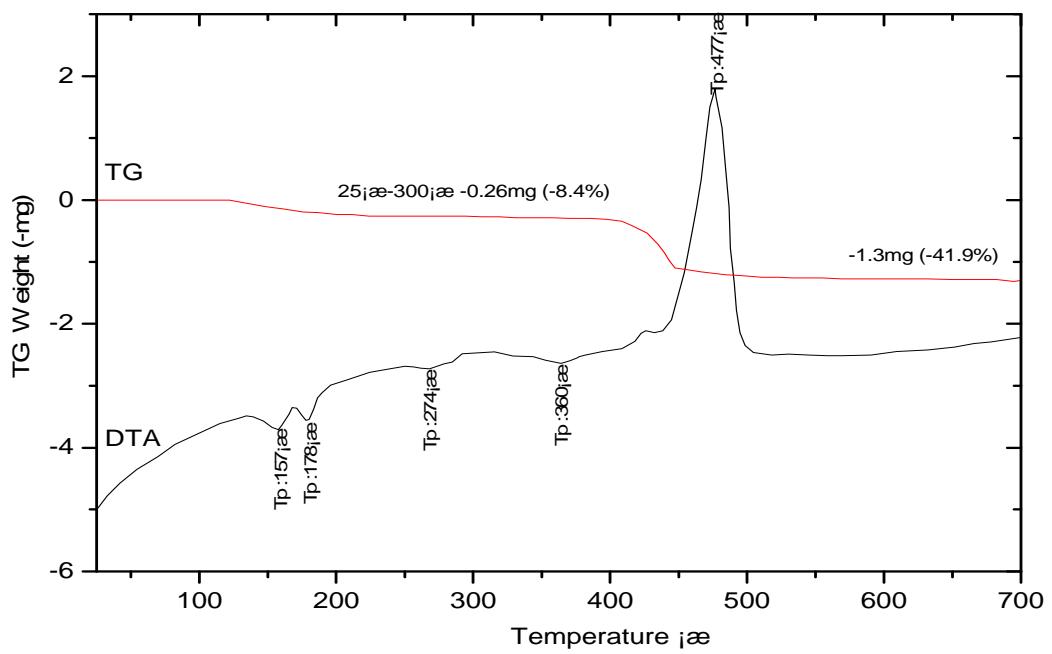
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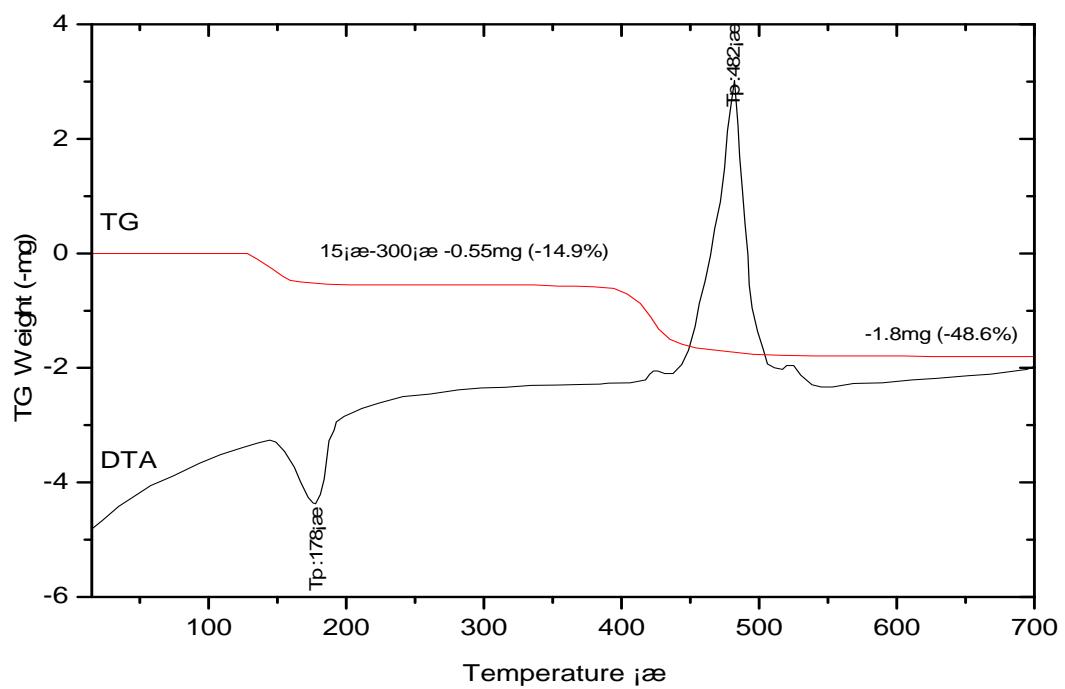
(4)



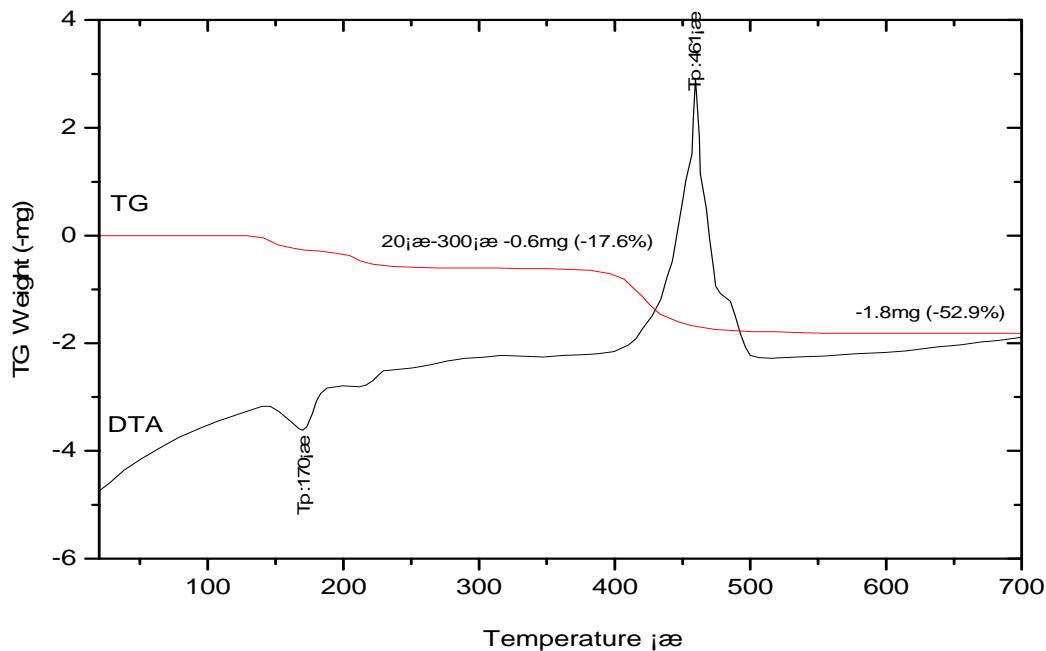
(5)



(6)



(7)



(8)

Fig.S1. Thermogravimetric analysis (TGA-DSC) on the crystalline sample 1-8.

Table3 Thermal decomposition of lanthanides(III) complexes (air atmosphere).

Complexes	M <sub>mol</sub>	□T <sub>1</sub> /°C	Mass loss/%		T <sub>2</sub> /°C	T <sub>3</sub> /°C	Residue/%	
			Calc.	Found			Calc.	Found
<b>1</b>	686.00	15-300	10.50	7.80	350	450	47.52	58.20
<b>2</b>	688.42	25-300	10.46	8.70	260	290	50.03	50.00
<b>3</b>	690.00	25-300	10.43	8.50	380	455	49.34	54.20
<b>4</b>	696.66	25-300	10.34	7.70	360	445	48.32	56.80
<b>5</b>	738.04	15-300	9.76	15.30	360	460	51.22	43.30
<b>6</b>	814.76	15-300	17.67	8.40	380	445	46.98	58.10
<b>7</b>	805.25	25-300	17.88	14.90	390	440	46.35	51.40
<b>8</b>	701.94	15-300	10.26	17.60	360	420	53.26	47.10

□T<sub>1</sub> Temperature range of dehydration process; T<sub>2</sub> Temperature of beginning of decomposition;  
T<sub>3</sub> Temperature of beginning of oxide formation

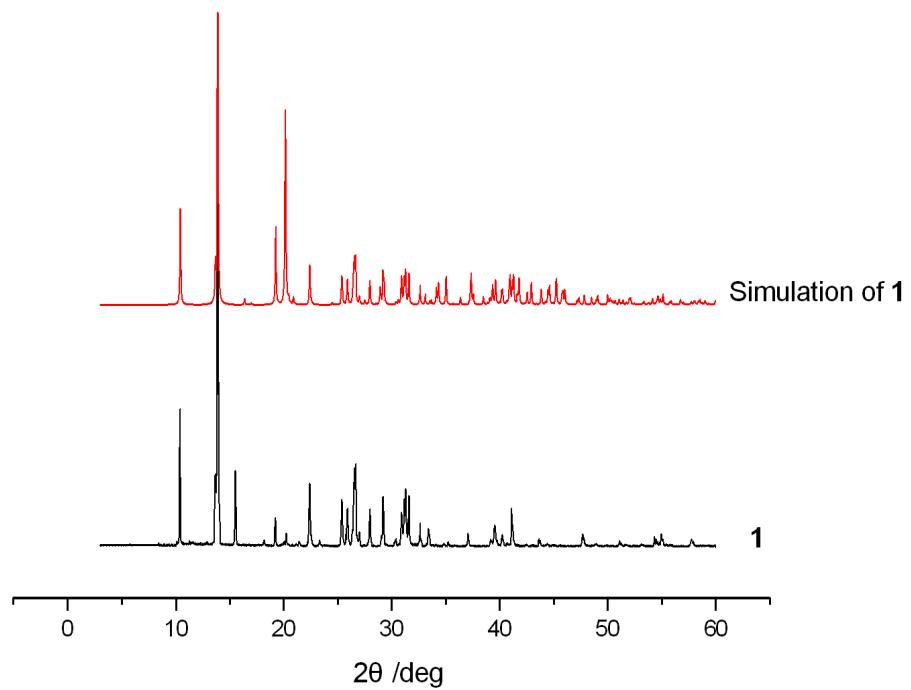


Fig.S2. XRD data of the complex **1** was collected on a Rigaku D\_max/3b diffractometer with Cu-KR radiation ( $\lambda = 1.5418 \text{ \AA}$ ) and the simulated XRD patterns generated on the basis of the single-crystal analyses.

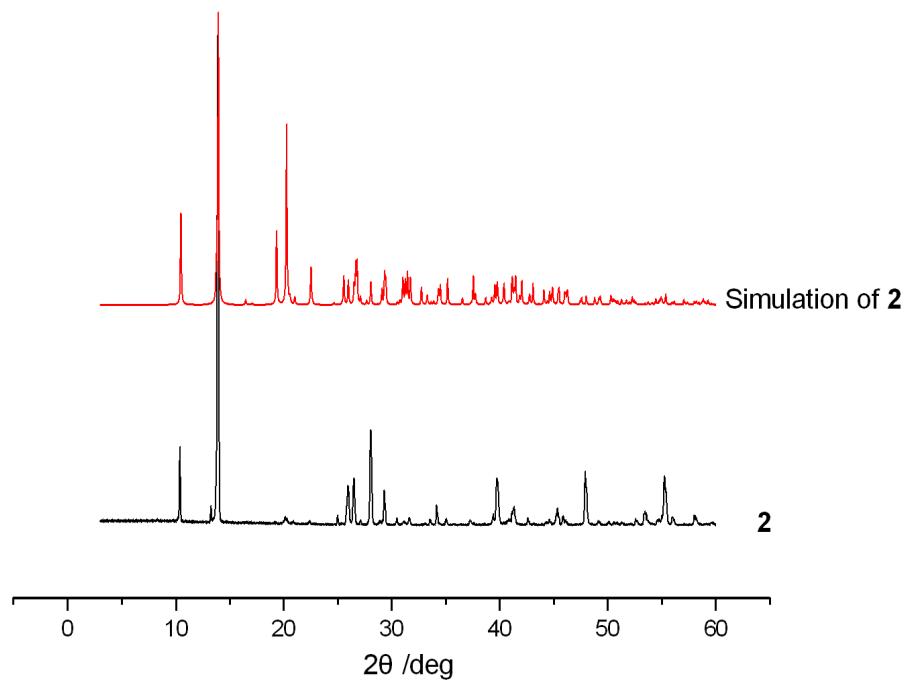


Fig.S3. XRD data of the complex **2** was collected on a Rigaku D\_max/3b diffractometer with Cu-KR radiation ( $\lambda = 1.5418 \text{ \AA}$ ) and the simulated XRD patterns generated on the basis of the single-crystal analyses.

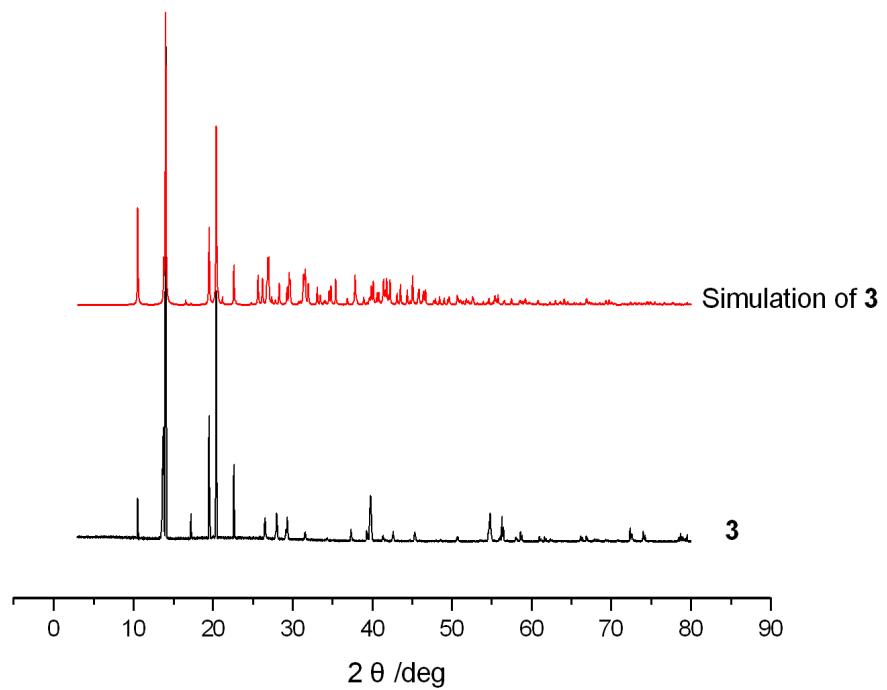


Fig.S4. XRD data of the complex **3** was collected on a Rigaku D\_max/3b diffractometer with Cu-KR radiation ( $\lambda = 1.5418 \text{ \AA}$ ) and the simulated XRD patterns generated on the basis of the single-crystal analyses.

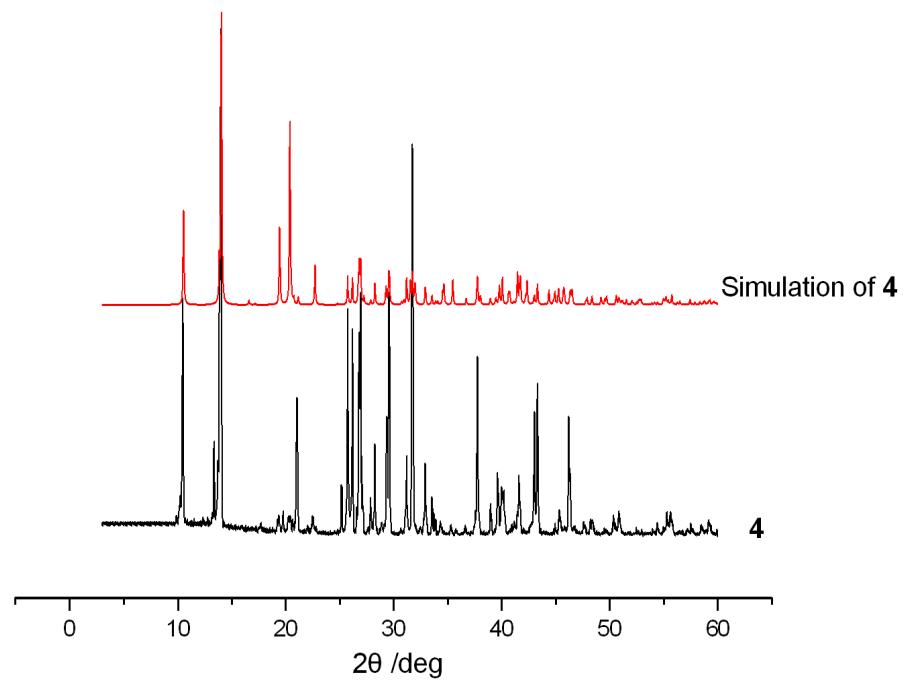


Fig.S5. XRD data of the complex **4** was collected on a Rigaku D\_max/3b diffractometer with Cu-KR radiation ( $\lambda = 1.5418 \text{ \AA}$ ) and the simulated XRD patterns generated on the basis of the single-crystal analyses.

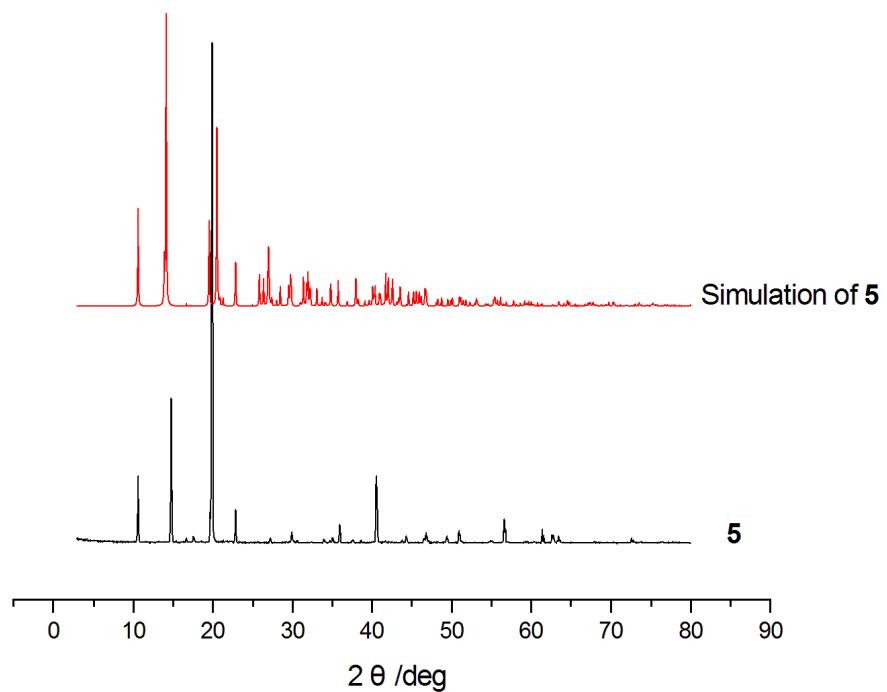


Fig.S6. XRD data of the complex **5** was collected on a Rigaku D\_max/3b diffractometer with Cu-KR radiation ( $\lambda = 1.5418 \text{ \AA}$ ) and the simulated XRD patterns generated on the basis of the single-crystal analyses.

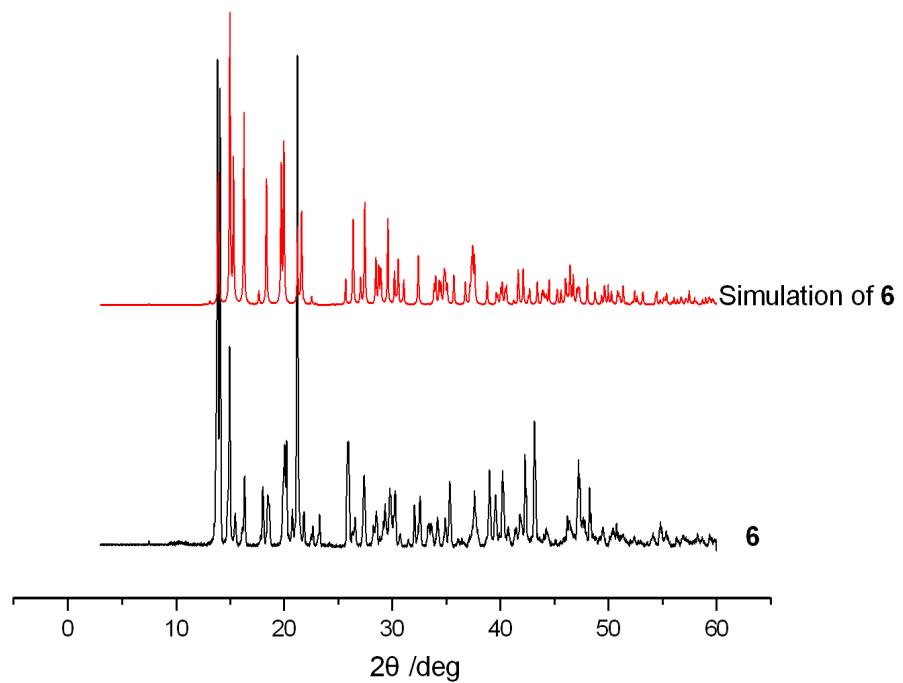


Fig.S7. XRD data of the complex **6** was collected on a Rigaku D\_max/3b diffractometer with Cu-KR radiation ( $\lambda = 1.5418 \text{ \AA}$ ) and the simulated XRD patterns generated on the basis of the single-crystal analyses.

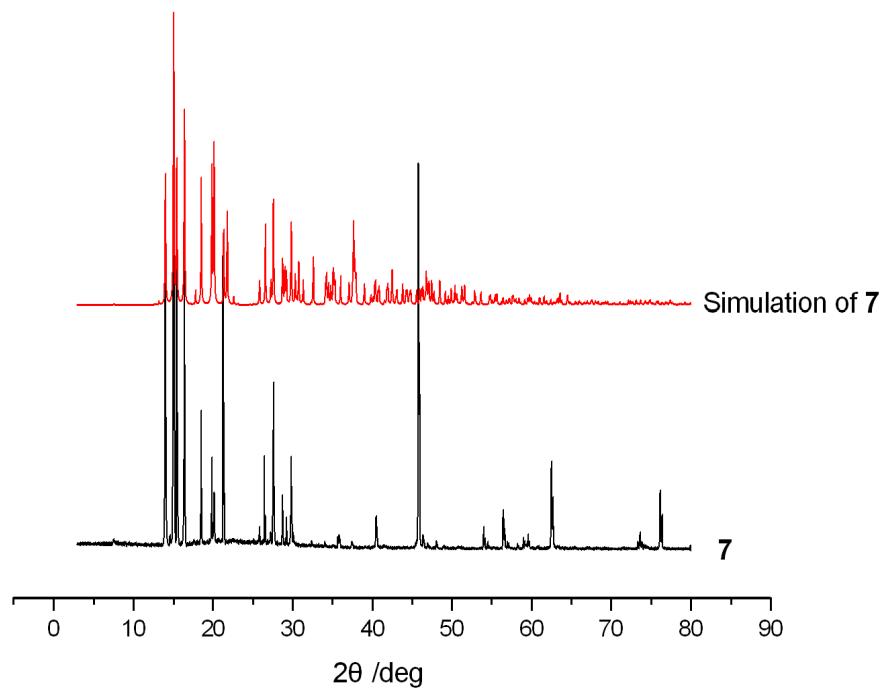


Fig.S8. XRD data of the complex **7** was collected on a Rigaku D\_max/3b diffractometer with Cu-KR radiation ( $\lambda = 1.5418 \text{ \AA}$ ) and the simulated XRD patterns generated on the basis of the single-crystal analyses.

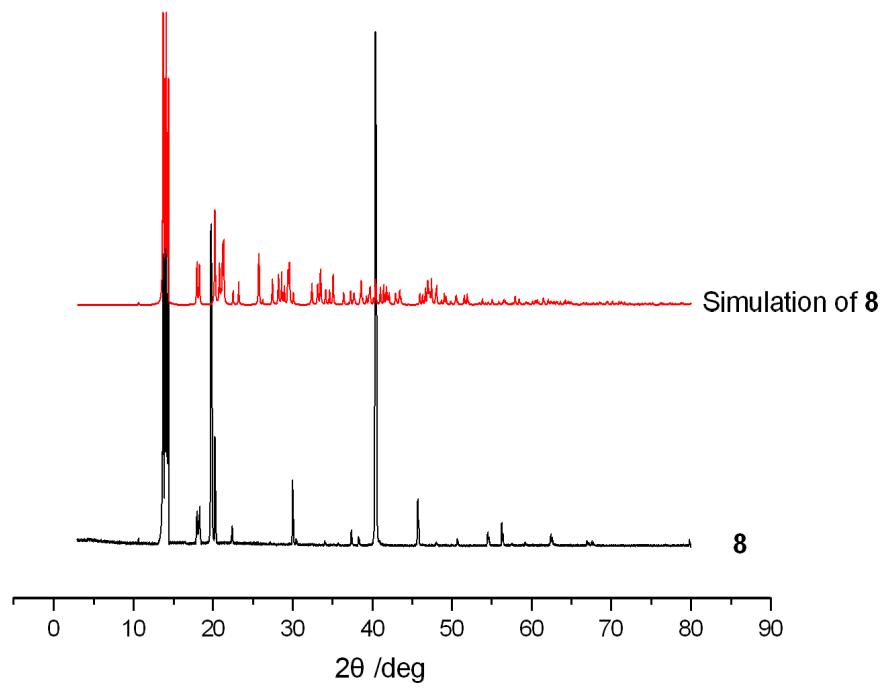
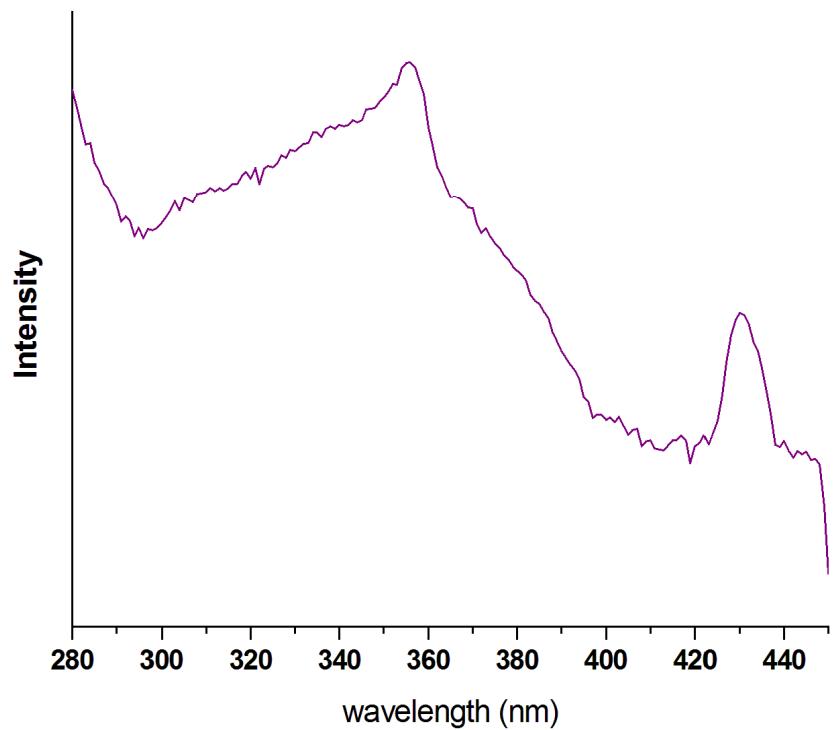
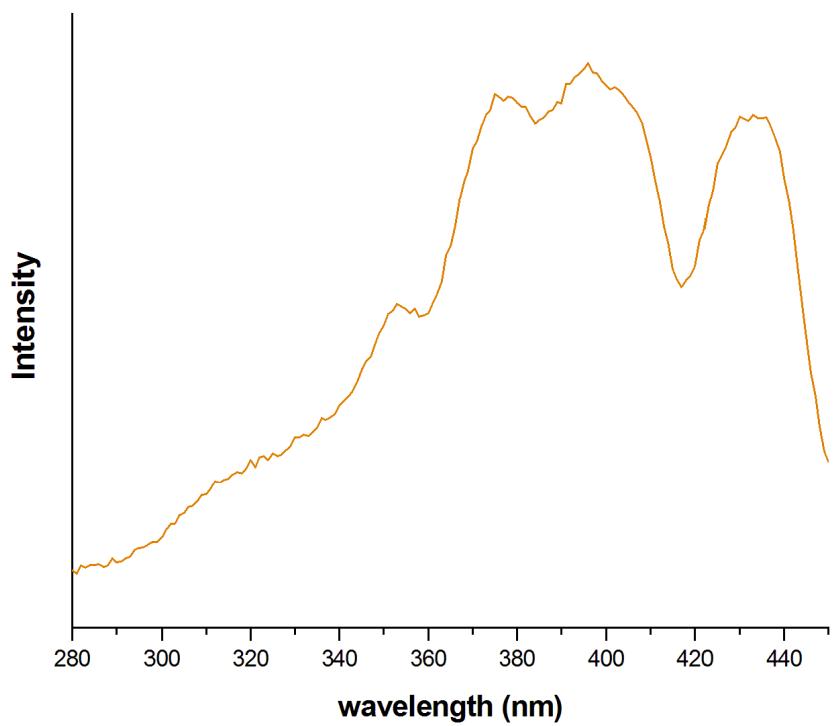


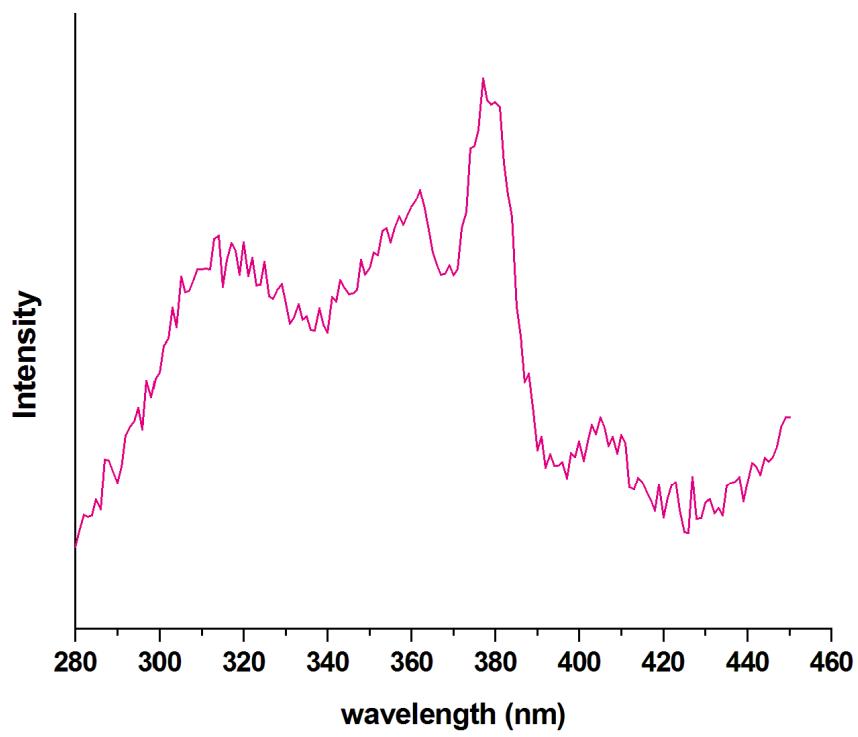
Fig.S9. (a) XRD data of the complex **8** was collected on a Rigaku D\_max/3b diffractometer with Cu-KR radiation ( $\lambda = 1.5418 \text{ \AA}$ ) and the simulated XRD patterns generated on the basis of the single-crystal analyses.



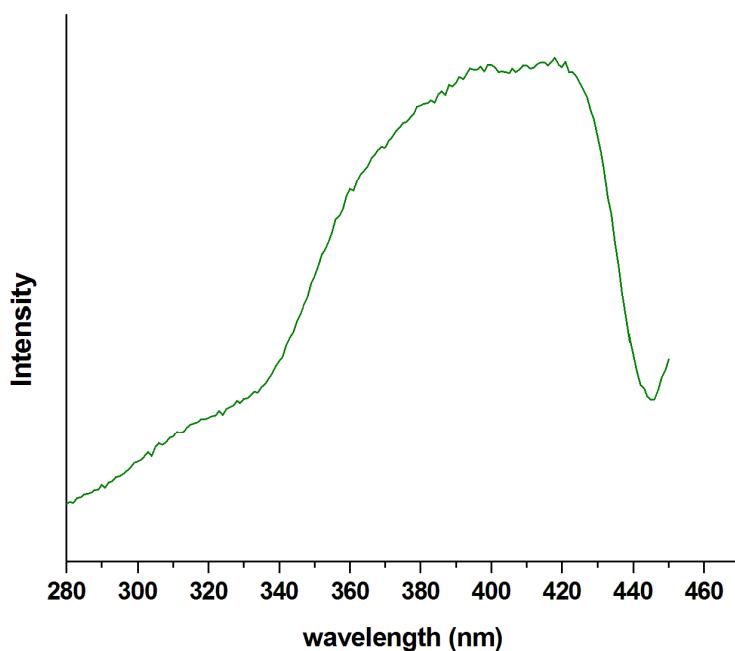
(a)



(b)



(c)



(d)

Fig.S10.(a) UV-vis absorption spectra of the Nd complex; (b) UV-vis absorption

spectra of the Ho complex; (c) UV-vis absorption spectra of the Er complex; (d) UV-vis absorption spectra of the Pr complex.

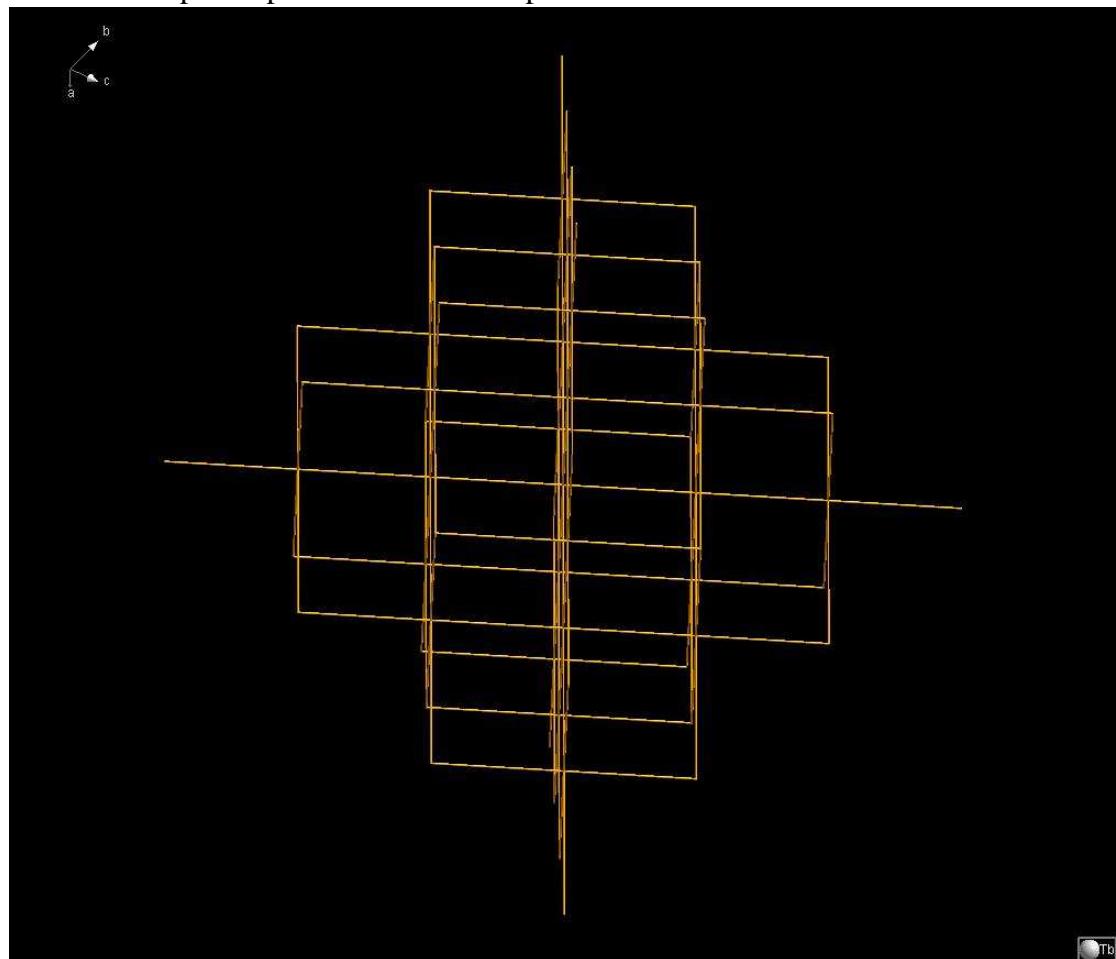


Fig.S11. The topology of **8**.

**Table S2.** Selected Bond Distances ( $\text{\AA}$ ) and Angles ( $^\circ$ ) for Complex **1-8**.

<b>La<sub>2</sub>(C<sub>4</sub>O<sub>4</sub>)<sub>3</sub>(H<sub>2</sub>O)<sub>4</sub> (1)</b>			
La(1)-O(2) <sup>#1</sup>	2.438(2)	La(1)-O(7)	2.501(3)
La(1)-O(5)	2.527(3)	La(1)-O(1)	2.530(2)
La(1)-O(6)	2.553(3)	La(1)-O(4) <sup>#2</sup>	2.574(3)
La(1)-O(8) <sup>#1</sup>	2.633(3)	La(1)-O(1) <sup>#2</sup>	2.691(3)
La(1)-O(7) <sup>#1</sup>	2.743(2)		
O(2) <sup>#1</sup> -La(1)-O(7)	86.88(8)	O(2) <sup>#1</sup> -La(1)-O(5)	140.06(9)
O(7)-La(1)-O(5)	85.07(9)	O(2) <sup>#1</sup> -La(1)-O(1)	138.93(8)
O(7)-La(1)-O(1)	78.93(8)	O(5)-La(1)-O(1)	77.20(8)
O(2) <sup>#1</sup> -La(1)-O(6)	71.76(9)	O(7)-La(1)-O(6)	68.06(8)
O(5)-La(1)-O(6)	68.94(9)	O(1)-La(1)-O(6)	133.87(9)
O(2) <sup>#1</sup> -La(1)-O(4) <sup>#2</sup>	76.51(8)	O(7)-La(1)-O(4) <sup>#2</sup>	141.55(8)
O(5)-La(1)-O(4) <sup>#2</sup>	85.99(8)	O(1)-La(1)-O(4) <sup>#2</sup>	134.75(8)
O(6)-La(1)-O(4) <sup>#2</sup>	73.81(8)	O(2) <sup>#1</sup> -La(1)-O(8) <sup>#1</sup>	70.28(9)

O(7)-La(1)-O(8) <sup>#1</sup>	128.31(8)	O(5)-La(1)-O(8) <sup>#1</sup>	140.81(9)
O(1)-La(1)-O(8) <sup>#1</sup>	88.81(8)	O(6)-La(1)-O(8) <sup>#1</sup>	136.96(9)
O(4) <sup>#2</sup> -La(1)-O(8) <sup>#1</sup>	78.28(8)	O(2) <sup>#1</sup> -La(1)-O(1) <sup>#2</sup>	131.51(8)
O(7)-La(1)-O(1) <sup>#2</sup>	139.95(8)	O(5)-La(1)-O(1) <sup>#2</sup>	71.86(9)
O(1)-La(1)-O(1) <sup>#2</sup>	64.52(9)	O(6)-La(1)-O(1) <sup>#2</sup>	127.81(8)
O(4) <sup>#2</sup> -La(1)-O(1) <sup>#2</sup>	70.37(8)	O(8) <sup>#1</sup> -La(1)-O(1) <sup>#2</sup>	69.08(8)
O(2) <sup>#1</sup> -La(1)-O(7) <sup>#1</sup>	67.29(8)	O(7)-La(1)-O(7) <sup>#1</sup>	59.34(10)
O(5)-La(1)-O(7) <sup>#1</sup>	136.50(8)	O(1)-La(1)-O(7) <sup>#1</sup>	72.35(8)
O(6)-La(1)-O(7) <sup>#1</sup>	113.10(8)	O(4) <sup>#2</sup> -La(1)-O(7) <sup>#1</sup>	137.37(8)
O(8) <sup>#1</sup> -La(1)-O(7) <sup>#1</sup>	69.06(8)	O(1) <sup>#2</sup> -La(1)-O(7) <sup>#1</sup>	119.01(8)
<b>Ce<sub>2</sub>(C<sub>4</sub>O<sub>4</sub>)<sub>3</sub>(H<sub>2</sub>O)<sub>4</sub> (2)</b>			
Ce(1)-O(4) <sup>#1</sup>	2.408(2)	Ce(1)-O(6) <sup>#2</sup>	2.466(2)
Ce(1)-O(1) <sup>#3</sup>	2.497(2)	Ce(1)-O(8)	2.505(3)
Ce(1)-O(7)	2.530(2)	Ce(1)-O(2)	2.543(2)
Ce(1)-O(5)	2.604(2)	Ce(1)-O(1)	2.685(2)
Ce(1)-O(6)	2.748(2)		
O(4) <sup>#1</sup> -Ce(1)-O(6) <sup>#2</sup>	87.74(8)	O(4) <sup>#1</sup> -Ce(1)-O(1) <sup>#3</sup>	138.67(8)
O(6) <sup>#2</sup> -Ce(1)-O(1) <sup>#3</sup>	78.59(8)	O(4) <sup>#1</sup> -Ce(1)-O(8)	140.29(8)
O(6) <sup>#2</sup> -Ce(1)-O(8)	84.47(8)	O(1) <sup>#3</sup> -Ce(1)-O(8)	77.39(8)
O(4) <sup>#1</sup> -Ce(1)-O(7)	71.66(9)	O(6) <sup>#2</sup> -Ce(1)-O(7)	68.44(8)
O(1) <sup>#3</sup> -Ce(1)-O(7)	134.51(8)	O(8)-Ce(1)-O(7)	69.25(8)
O(4) <sup>#1</sup> -Ce(1)-O(2)	76.15(8)	O(6) <sup>#2</sup> -Ce(1)-O(2)	142.05(8)
O(1) <sup>#3</sup> -Ce(1)-O(2)	134.73(8)	O(8)-Ce(1)-O(2)	86.54(8)
O(7)-Ce(1)-O(2)	73.88(8)	O(4) <sup>#1</sup> -Ce(1)-O(5)	70.27(8)
O(6) <sup>#2</sup> -Ce(1)-O(5)	128.58(8)	O(1) <sup>#3</sup> -Ce(1)-O(5)	88.23(8)
O(8)-Ce(1)-O(5)	140.74(8)	O(7)-Ce(1)-O(5)	136.89(8)
O(2)-Ce(1)-O(5)	78.04(8)	O(4) <sup>#1</sup> -Ce(1)-O(1)	131.56(8)
O(6) <sup>#2</sup> -Ce(1)-O(1)	139.02(8)	O(1) <sup>#3</sup> -Ce(1)-O(1)	64.18(9)
O(8)-Ce(1)-O(1)	71.73(8)	O(7)-Ce(1)-O(1)	127.93(8)
O(2)-Ce(1)-O(1)	70.63(7)	O(5)-Ce(1)-O(1)	69.12(8)
O(4) <sup>#1</sup> -Ce(1)-O(6)	67.03(8)	O(6) <sup>#2</sup> -Ce(1)-O(6)	59.32(9)
O(1) <sup>#3</sup> -Ce(1)-O(6)	72.49(7)	O(8)-Ce(1)-O(6)	136.34(8)
O(7)-Ce(1)-O(6)	112.61(8)	O(2)-Ce(1)-O(6)	136.94(7)
O(5)-Ce(1)-O(6)	69.28(7)	O(1)-Ce(1)-O(6)	119.39(7)
<b>Pr<sub>2</sub>(C<sub>4</sub>O<sub>4</sub>)<sub>3</sub>(H<sub>2</sub>O)<sub>4</sub> (3)</b>			
Pr(1)-O(1)	2.373(3)	Pr(1)-O(7)	2.421(3)
Pr(1)-O(4) <sup>#1</sup>	2.449(3)	Pr(1)-O(6)	2.469(3)
Pr(1)-O(3) <sup>#2</sup>	2.495(3)	Pr(1)-O(5)	2.502(3)
Pr(1)-O(8)	2.553(3)	Pr(1)-O(4) <sup>#2</sup>	2.667(3)
Pr(1)-O(7) <sup>#1</sup>	2.765(3)		
O(1)-Pr(1)-O(7)	87.20(9)	O(1)-Pr(1)-O(4) <sup>#1</sup>	138.38(10)
O(7)-Pr(1)-O(4) <sup>#1</sup>	79.20(9)	O(1)-Pr(1)-O(6)	139.90(11)
O(7)-Pr(1)-O(6)	84.84(10)	O(4) <sup>#1</sup> -Pr(1)-O(6)	78.13(10)
O(1)-Pr(1)-O(3) <sup>#2</sup>	76.64(9)	O(7)-Pr(1)-O(3) <sup>#2</sup>	142.29(10)

O(4) <sup>#1</sup> -Pr(1)-O(3) <sup>#2</sup>	134.11(9)	O(6)-Pr(1)-O(3) <sup>#2</sup>	86.14(10)
O(1)-Pr(1)-O(5)	71.55(11)	O(7)-Pr(1)-O(5)	68.88(10)
O(4) <sup>#1</sup> -Pr(1)-O(5)	135.37(11)	O(6)-Pr(1)-O(5)	68.91(11)
O(3) <sup>#2</sup> -Pr(1)-O(5)	73.69(10)	O(1)-Pr(1)-O(8)	70.57(9)
O(7)-Pr(1)-O(8)	127.93(9)	O(4) <sup>#1</sup> -Pr(1)-O(8)	87.27(9)
O(6)-Pr(1)-O(8)	140.99(10)	O(3) <sup>#2</sup> -Pr(1)-O(8)	78.46(9)
O(5)-Pr(1)-O(8)	137.01(11)	O(1)-Pr(1)-O(4) <sup>#2</sup>	132.45(9)
O(7)-Pr(1)-O(4) <sup>#2</sup>	138.66(9)	O(4) <sup>#1</sup> -Pr(1)-O(4) <sup>#2</sup>	63.38(10)
O(6)-Pr(1)-O(4) <sup>#2</sup>	71.39(10)	O(3) <sup>#2</sup> -Pr(1)-O(4) <sup>#2</sup>	70.76(8)
O(5)-Pr(1)-O(4) <sup>#2</sup>	127.55(10)	O(8)-Pr(1)-O(4) <sup>#2</sup>	69.72(9)
O(1)-Pr(1)-O(7) <sup>#1</sup>	66.78(10)	O(7)-Pr(1)-O(7) <sup>#1</sup>	59.09(10)
O(4) <sup>#1</sup> -Pr(1)-O(7) <sup>#1</sup>	72.52(9)	O(6)-Pr(1)-O(7) <sup>#1</sup>	136.66(9)
O(3) <sup>#2</sup> -Pr(1)-O(7) <sup>#1</sup>	137.01(9)	O(5)-Pr(1)-O(7) <sup>#1</sup>	112.86(10)
O(8)-Pr(1)-O(7) <sup>#1</sup>	68.87(8)	O(4) <sup>#2</sup> -Pr(1)-O(7) <sup>#1</sup>	119.50(9)

**Nd<sub>2</sub>(C<sub>4</sub>O<sub>4</sub>)<sub>3</sub>(H<sub>2</sub>O)<sub>4</sub> (4)**

Nd(1)-O(1)	2.380(3)	Nd(1)-O(5)	2.435(3)
Nd(1)-O(4) <sup>#1</sup>	2.463(3)	Nd(1)-O(8)	2.467(4)
Nd(1)-O(7)	2.498(3)	Nd(1)-O(3) <sup>#2</sup>	2.512(3)
Nd(1)-O(6) <sup>#1</sup>	2.570(3)	Nd(1)-O(4) <sup>#2</sup>	2.661(3)
Nd(1)-O(5) <sup>#1</sup>	2.729(3)		
O(1)-Nd(1)-O(5)	87.92(10)	O(1)-Nd(1)-O(4) <sup>#1</sup>	138.40(11)
O(5)-Nd(1)-O(4) <sup>#1</sup>	79.20(11)	O(1)-Nd(1)-O(8)	140.35(11)
O(5)-Nd(1)-O(8)	84.57(11)	O(4) <sup>#1</sup> -Nd(1)-O(8)	77.95(10)
O(1)-Nd(1)-O(7)	71.81(11)	O(5)-Nd(1)-O(7)	68.72(11)
O(4) <sup>#1</sup> -Nd(1)-O(7)	135.43(11)	O(8)-Nd(1)-O(7)	69.18(12)
O(1)-Nd(1)-O(3) <sup>#2</sup>	75.86(11)	O(5)-Nd(1)-O(3) <sup>#2</sup>	141.92(11)
O(4) <sup>#1</sup> -Nd(1)-O(3) <sup>#2</sup>	134.52(11)	O(8)-Nd(1)-O(3) <sup>#2</sup>	86.53(10)
O(7)-Nd(1)-O(3) <sup>#2</sup>	73.49(11)	O(1)-Nd(1)-O(6) <sup>#1</sup>	70.29(11)
O(5)-Nd(1)-O(6) <sup>#1</sup>	128.58(10)	O(4) <sup>#1</sup> -Nd(1)-O(6) <sup>#1</sup>	87.30(10)
O(8)-Nd(1)-O(6) <sup>#1</sup>	140.55(12)	O(7)-Nd(1)-O(6) <sup>#1</sup>	136.96(11)
O(3) <sup>#2</sup> -Nd(1)-O(6) <sup>#1</sup>	78.14(10)	O(1)-Nd(1)-O(4) <sup>#2</sup>	131.69(10)
O(5)-Nd(1)-O(4) <sup>#2</sup>	138.71(10)	O(4) <sup>#1</sup> -Nd(1)-O(4) <sup>#2</sup>	63.48(12)
O(8)-Nd(1)-O(4) <sup>#2</sup>	71.47(12)	O(7)-Nd(1)-O(4) <sup>#2</sup>	127.71(11)
O(3) <sup>#2</sup> -Nd(1)-O(4) <sup>#2</sup>	71.07(10)	O(6) <sup>#1</sup> -Nd(1)-O(4) <sup>#2</sup>	69.19(11)
O(1)-Nd(1)-O(5) <sup>#1</sup>	67.20(11)	O(5)-Nd(1)-O(5) <sup>#1</sup>	58.81(11)
O(4) <sup>#1</sup> -Nd(1)-O(5) <sup>#1</sup>	72.34(10)	O(8)-Nd(1)-O(5) <sup>#1</sup>	136.05(10)
O(7)-Nd(1)-O(5) <sup>#1</sup>	112.51(11)	O(3) <sup>#2</sup> -Nd(1)-O(5) <sup>#1</sup>	137.19(9)
O(6) <sup>#1</sup> -Nd(1)-O(5) <sup>#1</sup>	69.79(10)	O(4) <sup>#2</sup> -Nd(1)-O(5) <sup>#1</sup>	119.67(10)

**Ho<sub>2</sub>(C<sub>4</sub>O<sub>4</sub>)<sub>3</sub>(H<sub>2</sub>O)<sub>4</sub> (5)**

Ho(1)-O(3) <sup>#1</sup>	2.346(2)	Ho(1)-O(6) <sup>#2</sup>	2.396(3)
Ho(1)-O(2) <sup>#3</sup>	2.429(3)	Ho(1)-O(8)	2.434(3)
Ho(1)-O(1)	2.475(3)	Ho(1)-O(7)	2.479(3)
Ho(1)-O(5)	2.525(3)	Ho(1)-O(2)	2.654(2)
Ho(1)-O(6) <sup>#4</sup>	2.756(3)		

O(3) <sup>#1</sup> -Ho(1)-O(6) <sup>#2</sup>	88.19(8)	O(3) <sup>#1</sup> -Ho(1)-O(2) <sup>#3</sup>	137.77(8)
O(6) <sup>#2</sup> -Ho(1)-O(2) <sup>#3</sup>	79.25(8)	O(3) <sup>#1</sup> -Ho(1)-O(8)	140.49(9)
O(6) <sup>#2</sup> -Ho(1)-O(8)	84.33(9)	O(2) <sup>#3</sup> -Ho(1)-O(8)	78.54(8)
O(3) <sup>#1</sup> -Ho(1)-O(1)	76.12(8)	O(6) <sup>#2</sup> -Ho(1)-O(1)	142.30(8)
O(2) <sup>#3</sup> -Ho(1)-O(1)	134.21(8)	O(8)-Ho(1)-O(1)	86.53(8)
O(3) <sup>#1</sup> -Ho(1)-O(7)	71.61(9)	O(6) <sup>#2</sup> -Ho(1)-O(7)	68.87(9)
O(2) <sup>#3</sup> -Ho(1)-O(7)	136.29(9)	O(8)-Ho(1)-O(7)	69.50(9)
O(1)-Ho(1)-O(7)	73.66(9)	O(3) <sup>#1</sup> -Ho(1)-O(5)	70.61(9)
O(6) <sup>#2</sup> -Ho(1)-O(5)	128.49(8)	O(2) <sup>#3</sup> -Ho(1)-O(5)	86.14(8)
O(8)-Ho(1)-O(5)	140.40(9)	O(1)-Ho(1)-O(5)	78.44(8)
O(7)-Ho(1)-O(5)	137.20(9)	O(3) <sup>#1</sup> -Ho(1)-O(2)	131.95(8)
O(6) <sup>#2</sup> -Ho(1)-O(2)	138.15(8)	O(2) <sup>#3</sup> -Ho(1)-O(2)	63.17(9)
O(8)-Ho(1)-O(2)	71.31(9)	O(1)-Ho(1)-O(2)	71.05(8)
O(7)-Ho(1)-O(2)	127.93(8)	O(5)-Ho(1)-O(2)	69.18(9)
O(3) <sup>#1</sup> -Ho(1)-O(6) <sup>#4</sup>	66.84(8)	O(6) <sup>#2</sup> -Ho(1)-O(6) <sup>#4</sup>	58.72(10)
O(2) <sup>#3</sup> -Ho(1)-O(6) <sup>#4</sup>	72.25(8)	O(8)-Ho(1)-O(6) <sup>#4</sup>	136.03(8)
O(1)-Ho(1)-O(6) <sup>#4</sup>	137.19(8)	O(7)-Ho(1)-O(6) <sup>#4</sup>	111.98(8)
O(5)-Ho(1)-O(6) <sup>#4</sup>	69.78(8)	O(2)-Ho(1)-O(6) <sup>#4</sup>	119.98(8)

**Er<sub>2</sub>(C<sub>4</sub>O<sub>4</sub>)<sub>3</sub>(H<sub>2</sub>O)<sub>8</sub> (6)**

Er(1)-O(11)	2.367(4)	Er(1)-O(6) <sup>#1</sup>	2.369(5)
Er(1)-O(10)	2.381(4)	Er(1)-O(3) <sup>#2</sup>	2.407(4)
Er(1)-O(5)	2.418(4)	Er(1)-O(9)	2.425(4)
Er(1)-O(1)	2.451(4)	Er(1)-O(4) <sup>#3</sup>	2.456(4)
O(11)-Er(1)-O(6) <sup>#1</sup>	142.94(16)	O(11)-Er(1)-O(10)	80.57(14)
O(6) <sup>#1</sup> -Er(1)-O(10)	110.29(15)	O(11)-Er(1)-O(3) <sup>#2</sup>	75.38(14)
O(6) <sup>#1</sup> -Er(1)-O(3) <sup>#2</sup>	77.22(16)	O(10)-Er(1)-O(3) <sup>#2</sup>	145.37(15)
O(11)-Er(1)-O(5)	142.96(15)	O(6) <sup>#1</sup> -Er(1)-O(5)	71.88(16)
O(10)-Er(1)-O(5)	72.12(15)	O(3) <sup>#2</sup> -Er(1)-O(5)	139.26(15)
O(11)-Er(1)-O(9)	110.11(15)	O(6) <sup>#1</sup> -Er(1)-O(9)	85.22(16)
O(10)-Er(1)-O(9)	139.03(15)	O(3) <sup>#2</sup> -Er(1)-O(9)	73.72(15)
O(5)-Er(1)-O(9)	77.81(15)	O(11)-Er(1)-O(1)	74.82(14)
O(6) <sup>#1</sup> -Er(1)-O(1)	141.47(15)	O(10)-Er(1)-O(1)	76.41(14)
O(3) <sup>#2</sup> -Er(1)-O(1)	119.53(13)	O(5)-Er(1)-O(1)	74.79(14)
O(9)-Er(1)-O(1)	69.22(15)	O(11)-Er(1)-O(4) <sup>#3</sup>	75.21(14)
O(6) <sup>#1</sup> -Er(1)-O(4) <sup>#3</sup>	73.76(15)	O(10)-Er(1)-O(4) <sup>#3</sup>	75.49(14)
O(3) <sup>#2</sup> -Er(1)-O(4) <sup>#3</sup>	74.52(14)	O(5)-Er(1)-O(4) <sup>#3</sup>	119.62(14)
O(9)-Er(1)-O(4) <sup>#3</sup>	145.01(15)	O(1)-Er(1)-O(4) <sup>#3</sup>	141.61(13)

**Dy<sub>2</sub>(C<sub>4</sub>O<sub>4</sub>)<sub>3</sub>(H<sub>2</sub>O)<sub>8</sub> (7)**

Dy(1)-O(5)	2.320(4)	Dy(1)-O(9) <sup>#1</sup>	2.337(4)
Dy(1)-O(6)	2.337(4)	Dy(1)-O(8)	2.371(4)
Dy(1)-O(1)	2.383(4)	Dy(1)-O(7)	2.390(4)
Dy(1)-O(3) <sup>#2</sup>	2.422(4)	Dy(1)-O(2) <sup>#3</sup>	2.431(4)
O(5)-Dy(1)-O(9) <sup>#1</sup>	142.96(15)	O(5)-Dy(1)-O(6)	80.86(15)
O(9) <sup>#1</sup> -Dy(1)-O(6)	110.40(14)	O(5)-Dy(1)-O(8)	142.75(14)

O(9) <sup>#1</sup> -Dy(1)-O(8)	72.41(14)	O(6)-Dy(1)-O(8)	72.41(15)
O(5)-Dy(1)-O(1)	74.82(15)	O(9) <sup>#1</sup> -Dy(1)-O(1)	77.29(15)
O(6)-Dy(1)-O(1)	144.80(15)	O(8)-Dy(1)-O(1)	139.69(14)
O(5)-Dy(1)-O(7)	109.36(15)	O(9) <sup>#1</sup> -Dy(1)-O(7)	85.32(15)
O(6)-Dy(1)-O(7)	139.38(16)	O(8)-Dy(1)-O(7)	77.73(15)
O(1)-Dy(1)-O(7)	73.84(16)	O(5)-Dy(1)-O(3) <sup>#2</sup>	74.51(14)
O(9) <sup>#1</sup> -Dy(1)-O(3) <sup>#2</sup>	141.62(14)	O(6)-Dy(1)-O(3) <sup>#2</sup>	76.67(15)
O(8)-Dy(1)-O(3) <sup>#2</sup>	74.42(13)	O(1)-Dy(1)-O(3) <sup>#2</sup>	119.40(14)
O(7)-Dy(1)-O(3) <sup>#2</sup>	69.15(15)	O(5)-Dy(1)-O(2) <sup>#3</sup>	75.78(15)
O(9) <sup>#1</sup> -Dy(1)-O(2) <sup>#3</sup>	73.50(14)	O(6)-Dy(1)-O(2) <sup>#3</sup>	75.48(15)
O(8)-Dy(1)-O(2) <sup>#3</sup>	120.07(14)	O(1)-Dy(1)-O(2) <sup>#3</sup>	74.15(14)
O(7)-Dy(1)-O(2) <sup>#3</sup>	144.71(16)	O(3) <sup>#2</sup> -Dy(1)-O(2) <sup>#3</sup>	141.86(14)

### **Tb<sub>2</sub>(C<sub>4</sub>O<sub>4</sub>)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)(H<sub>2</sub>O)<sub>4</sub> (8)**

Tb(1)-O(2) <sup>#1</sup>	2.328(2)	Tb(1)-O(3) <sup>#2</sup>	2.374(2)
Tb(1)-O(4) <sup>#3</sup>	2.394(2)	Tb(1)-O(6) <sup>#4</sup>	2.406(2)
Tb(1)-O(8)	2.409(2)	Tb(1)-O(7)	2.411(2)
Tb(1)-O(5)	2.415(2)	Tb(1)-O(1)	2.436(2)
Tb(1)-O(2)	2.870(2)		
O(2) <sup>#1</sup> -Tb(1)-O(3) <sup>#2</sup>	78.09(8)	O(2) <sup>#1</sup> -Tb(1)-O(4) <sup>#3</sup>	90.11(8)
O(3) <sup>#2</sup> -Tb(1)-O(4) <sup>#3</sup>	128.43(7)	O(2) <sup>#1</sup> -Tb(1)-O(6) <sup>#4</sup>	71.79(8)
O(3) <sup>#2</sup> -Tb(1)-O(6) <sup>#4</sup>	143.63(8)	O(4) <sup>#3</sup> -Tb(1)-O(6) <sup>#4</sup>	72.26(7)
O(2) <sup>#1</sup> -Tb(1)-O(8)	77.86(8)	O(3) <sup>#2</sup> -Tb(1)-O(8)	81.26(8)
O(4) <sup>#3</sup> -Tb(1)-O(8)	145.22(7)	O(6) <sup>#4</sup> -Tb(1)-O(8)	72.98(7)
O(2) <sup>#1</sup> -Tb(1)-O(7)	138.50(8)	O(3) <sup>#2</sup> -Tb(1)-O(7)	72.71(8)
O(4) <sup>#3</sup> -Tb(1)-O(7)	131.22(8)	O(6) <sup>#4</sup> -Tb(1)-O(7)	119.02(8)
O(8)-Tb(1)-O(7)	69.18(8)	O(2) <sup>#1</sup> -Tb(1)-O(5)	138.86(7)
O(3) <sup>#2</sup> -Tb(1)-O(5)	141.41(7)	O(4) <sup>#3</sup> -Tb(1)-O(5)	73.15(8)
O(6) <sup>#4</sup> -Tb(1)-O(5)	67.38(8)	O(8)-Tb(1)-O(5)	94.66(8)
O(7)-Tb(1)-O(5)	70.06(8)	O(2) <sup>#1</sup> -Tb(1)-O(1)	129.23(8)
O(3) <sup>#2</sup> -Tb(1)-O(1)	75.39(8)	O(4) <sup>#3</sup> -Tb(1)-O(1)	74.37(7)
O(6) <sup>#4</sup> -Tb(1)-O(1)	140.31(8)	O(8)-Tb(1)-O(1)	137.65(7)
O(7)-Tb(1)-O(1)	70.34(8)	O(5)-Tb(1)-O(1)	82.88(8)
O(2) <sup>#1</sup> -Tb(1)-O(2)	60.28(8)	O(3) <sup>#2</sup> -Tb(1)-O(2)	66.94(7)
O(4) <sup>#3</sup> -Tb(1)-O(2)	63.76(7)	O(6) <sup>#4</sup> -Tb(1)-O(2)	112.44(7)
O(8)-Tb(1)-O(2)	130.99(8)	O(7)-Tb(1)-O(2)	128.52(7)
O(5)-Tb(1)-O(2)	133.41(7)	O(1)-Tb(1)-O(2)	69.63(7)

Symmetry transformations used to generate equivalent atoms:

- (1) #1 -x,-y+1,-z+1      #2 -x+1,-y+1,-z+1
- (2) #1 x+1,y,z      #2 -x+1,-y+1,-z+1      #3 -x,-y+1,-z+1
- (3) #1 -x+1,-y+1,-z+1      #2 x,y,z-1
- (4) #1 -x+2,-y+1,-z+1      #2 x+1,y,z
- (5) #1 x+1,y,z      #2 x,y,z-1      #3 -x,-y+1,-z+1      #4 -x+1,-y+1,-z+2
- (6) #1 -x,-y+1,-z+1      #2 x,y-1,z      #3 x,-y+3/2,z-1/2
- (7) #1 -x,-y+1,-z+1      #2 x,y+1,z      #3 x,-y+1/2,z-1/2

(8) #1 -x+2,-y+2,-z      #2 -x+5/2,y+1/2,-z+1/2      #3 x-1/2,-y+3/2,z-1/2      #4 -x+1,-y+2,-z