

# **A Family of 3D Lanthanide-Zinc Heterometal-Organic Frameworks from 4, 5-Imidazoledicarboxylate and Oxalate**

Zhi-Gang Gu, Hua-Cai Fang, Pei-Yi Yin, Long Tong, Yin Ying,

She-Jun Hu, Wei-Shan Li and Yue-Peng Cai\*<sup>†</sup>

*School of Chemistry and Environment, Key Laboratory of Electrochemical Technology on Energy Storage and Power Generation of Guangdong Higher Education Institutes, Engineering Research Center of Materials and Technology for Electrochemical Energy Storage (Ministry of Education), South China Normal University, Guangzhou, 510006, China*

## Content

**Table S1** Selected bond lengths and angles.

**Figure S1** The TG curves of compound **2** and **6**.

**Figure S2** The building block unit  $[\text{Zn}_{10}(\text{ImDC})_8]$  with *chair*-conformation in **6**.

**Figure S3** 3-connected Zn-containing layer with  $6^3$  topology in **6** along *a* axis.

**Figure S4** 3-D chain-layer MOF with the 1-D flat channels in **6** along the *b* axis.

**Figure S5** PXRD patterns of two compounds **4** (a) and **4'** (b) simulated from the X-ray single-crystal structure and as-synthesized/transformed samples.

**Figure S6** Solid-state emission spectra for compounds **3** (a), **4** (b) and **6** (c) in the solid state at room temperature.

**Figure S7** Photoluminescence decay curve for the emission at 620 nm of complex **4** and the corresponding single-exponential fit with  $\tau_1 = 0.232 \pm 0.007545$  ms.

**Figure S8** Solid-state emission spectrum for **4'** in the solid state at room temperature (excited at 395 nm).

**Figure S9** Photoluminescence decay curve for the emission at 620 nm of complex **4'** and the corresponding single-exponential fit with  $\tau_1 = 0.283 \pm 0.004673$  ms.

**Figure S10.** Powder X-ray diffraction (PXRD) patterns for compounds **3** (a) and **6** (b) based on the crystalline sample at different temperature: 30 °C; 200 °C; 250 °C; 300 °C; 345 °C and simulated from single crystal X-ray data.

**Table S1.** Selected Bond Distances (Å) and Angles (°) for complexes **1-4**, **4'** and **5-10**.\*

<b>1</b>			
La(1)-O(6)#1	2.473(5)	O(6)#1-La(1)-O(7)#1	71.47(16)
La(1)-O(7)#1	2.474(5)	O(6)#1-La(1)-O(11)	127.05(15)
La(1)-O(11)	2.491(4)	O(7)#1-La(1)-O(11)	152.62(14)
La(1)-O(1)#2	2.510(5)	O(6)#1-La(1)-O(1)#2	66.29(16)
La(1)-O(3)#2	2.511(4)	O(7)#1-La(1)-O(1)#2	108.97(16)
La(1)-O(9)	2.513(5)	O(11)-La(1)-O(1)#2	69.37(14)
La(1)-O(10)	2.547(4)	O(6)#1-La(1)-O(3)#2	105.08(16)
La(1)-O(3)	2.654(4)	O(7)#1-La(1)-O(3)#2	67.78(15)
La(1)-O(4)	2.807(5)	O(11)-La(1)-O(3)#2	86.55(13)
Zn(1)-N(2)#3	2.038(5)	O(1)#2-La(1)-O(3)#2	71.65(14)
Zn(1)-N(4)	2.073(6)	O(6)#1-La(1)-O(9)	74.73(17)
Zn(1)-N(1)	2.104(6)	O(7)#1-La(1)-O(9)	75.57(16)
Zn(1)-O(5)	2.180(5)	O(11)-La(1)-O(9)	125.66(14)
Zn(1)-O(4)	2.229(5)	O(1)#2-La(1)-O(9)	135.94(16)
Zn(1)-O(2)#3	2.313(5)	O(3)#2-La(1)-O(9)	140.83(15)
Zn(2)-O(2)#4	1.973(5)	O(6)#1-La(1)-O(10)	72.18(15)
Zn(2)-O(12)	2.011(4)	O(7)#1-La(1)-O(10)	132.28(14)
Zn(2)-N(3)	2.023(6)	O(11)-La(1)-O(10)	75.11(10)
Zn(2)-O(13)	2.076(4)	O(1)#2-La(1)-O(10)	82.94(13)
Zn(2)-O(8)	2.184(5)	O(3)#2-La(1)-O(10)	152.73(13)
N(1)-Zn(1)-O(5)	160.8(2)	O(9)-La(1)-O(10)	65.78(14)
N(2)#3-Zn(1)-O(4)	95.00(19)	O(6)#1-La(1)-O(3)	138.00(15)
N(4)-Zn(1)-O(4)	102.2(2)	O(7)#1-La(1)-O(3)	68.81(15)
N(1)-Zn(1)-O(4)	76.43(19)	O(11)-La(1)-O(3)	94.89(13)
O(5)-Zn(1)-O(4)	91.41(18)	O(1)#2-La(1)-O(3)	140.84(14)
N(2)#3-Zn(1)-O(2)#3	74.48(19)	O(3)#2-La(1)-O(3)	71.80(16)
N(4)-Zn(1)-O(2)#3	88.16(19)	O(9)-La(1)-O(3)	82.68(15)
N(1)-Zn(1)-O(2)#3	105.6(2)	O(10)-La(1)-O(3)	128.89(13)
O(5)-Zn(1)-O(2)#3	89.08(19)	O(6)#1-La(1)-O(4)	140.71(16)
O(4)-Zn(1)-O(2)#3	169.48(17)	O(7)#1-La(1)-O(4)	107.68(16)
O(2)#4-Zn(2)-O(12)	120.04(18)	O(11)-La(1)-O(4)	71.68(13)
O(2)#4-Zn(2)-N(3)	136.1(2)	O(1)#2-La(1)-O(4)	140.76(14)
O(12)-Zn(2)-N(3)	101.5(2)	O(3)#2-La(1)-O(4)	110.75(14)
O(2)#4-Zn(2)-O(13)	96.88(19)	O(9)-La(1)-O(4)	67.44(16)
O(12)-Zn(2)-O(13)	95.05(16)	O(10)-La(1)-O(4)	82.77(13)
N(3)-Zn(2)-O(13)	92.5(2)	O(3)-La(1)-O(4)	47.29(13)
O(2)#4-Zn(2)-O(8)	87.3(2)	N(2)#3-Zn(1)-N(4)	160.2(2)
O(12)-Zn(2)-O(8)	90.98(19)	N(2)#3-Zn(1)-N(1)	102.3(2)
N(3)-Zn(2)-O(8)	78.1(2)	N(4)-Zn(1)-N(1)	91.4(2)
O(13)-Zn(2)-O(8)	169.69(18)	N(2)#3-Zn(1)-O(5)	93.4(2)
N(4)-Zn(1)-O(5)	76.5(2)		

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**2**

Nd(1)-O(7)#1	2.411(3)	O(7)#1-Nd(1)-O(6)#1	72.61(11)
Nd(1)-O(6)#1	2.425(3)	O(7)#1-Nd(1)-O(1)#2	110.91(11)
Nd(1)-O(1)#2	2.458(3)	O(6)#1-Nd(1)-O(1)#2	66.48(10)
Nd(1)-O(9)	2.465(3)	O(7)#1-Nd(1)-O(9)	75.57(11)
Nd(1)-O(11)	2.470(2)	O(6)#1-Nd(1)-O(9)	75.96(11)
Nd(1)-O(3)#2	2.471(3)	O(1)#2-Nd(1)-O(9)	136.74(10)
Nd(1)-O(10)	2.495(2)	O(7)#1-Nd(1)-O(11)	151.72(9)
Nd(1)-O(3)	2.616(3)	O(6)#1-Nd(1)-O(11)	127.28(9)
Nd(1)-O(4)	2.801(3)	O(1)#2-Nd(1)-O(11)	68.78(9)
Zn(1)-N(2)#3	2.050(4)	O(9)-Nd(1)-O(11)	125.25(9)
Zn(1)-N(4)	2.083(4)	O(7)#1-Nd(1)-O(3)#2	68.85(10)
Zn(1)-N(1)	2.094(4)	O(6)#1-Nd(1)-O(3)#2	106.89(11)
Zn(1)-O(5)	2.164(3)	O(1)#2-Nd(1)-O(3)#2	73.04(10)
Zn(1)-O(4)	2.227(3)	O(9)-Nd(1)-O(3)#2	141.07(10)
Zn(1)-O(2)#3	2.312(3)	O(11)-Nd(1)-O(3)#2	84.84(9)
Zn(2)-O(2)#4	1.984(3)	O(7)#1-Nd(1)-O(10)	132.19(9)
Zn(2)-O(12)	2.016(3)	O(6)#1-Nd(1)-O(10)	71.76(10)
Zn(2)-N(3)	2.018(4)	O(1)#2-Nd(1)-O(10)	82.35(9)
Zn(2)-O(13)	2.081(3)	O(9)-Nd(1)-O(10)	65.65(9)
Zn(2)-O(8)	2.186(3)	O(11)-Nd(1)-O(10)	76.07(7)
N(4)-Zn(1)-O(4)	100.18(13)	O(3)#2-Nd(1)-O(10)	153.08(9)
N(1)-Zn(1)-O(4)	76.56(12)	O(7)#1-Nd(1)-O(3)	70.16(10)
O(5)-Zn(1)-O(4)	91.33(12)	O(6)#1-Nd(1)-O(3)	140.90(10)
N(2)#3-Zn(1)-O(2)#3	74.09(12)	O(1)#2-Nd(1)-O(3)	139.55(9)
N(4)-Zn(1)-O(2)#3	88.99(13)	O(9)-Nd(1)-O(3)	83.59(10)
N(1)-Zn(1)-O(2)#3	105.38(13)	O(11)-Nd(1)-O(3)	91.73(9)
O(5)-Zn(1)-O(2)#3	88.98(13)	O(3)#2-Nd(1)-O(3)	70.08(11)
O(4)-Zn(1)-O(2)#3	170.65(11)	O(10)-Nd(1)-O(3)	128.45(8)
O(2)#4-Zn(2)-O(12)	117.86(12)	O(7)#1-Nd(1)-O(4)	108.59(10)
O(2)#4-Zn(2)-N(3)	137.14(14)	O(6)#1-Nd(1)-O(4)	141.16(11)
O(12)-Zn(2)-N(3)	102.59(13)	O(1)#2-Nd(1)-O(4)	138.02(9)
O(2)#4-Zn(2)-O(13)	96.90(13)	O(9)-Nd(1)-O(4)	67.33(10)
O(12)-Zn(2)-O(13)	94.78(11)	O(11)-Nd(1)-O(4)	69.76(9)
N(3)-Zn(2)-O(13)	93.08(13)	O(3)#2-Nd(1)-O(4)	109.49(9)
O(2)#4-Zn(2)-O(8)	87.18(13)	O(10)-Nd(1)-O(4)	81.70(8)
O(12)-Zn(2)-O(8)	90.92(13)	O(3)-Nd(1)-O(4)	47.64(9)
N(3)-Zn(2)-O(8)	78.16(14)	N(2)#3-Zn(1)-N(4)	160.88(15)
O(13)-Zn(2)-O(8)	170.43(12)	N(2)#3-Zn(1)-N(1)	102.17(15)
N(4)-Zn(1)-O(5)	6.79(13)	N(4)-Zn(1)-N(1)	90.70(15)
N(1)-Zn(1)-O(5)	160.91(14)	N(2)#3-Zn(1)-O(5)	93.74(13)
N(2)#3-Zn(1)-O(4)	96.57(13)		

**3**

Sm(1)-O(7)#1	2.378(3)	O(7)#1-Sm(1)-O(6)#1	73.23(12)
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Sm(1)-O(6)#1	2.389(3)	O(7)#1-Sm(1)-O(1)#2	112.45(11)
Sm(1)-O(1)#2	2.433(3)	O(6)#1-Sm(1)-O(1)#2	66.74(11)
Sm(1)-O(9)	2.437(3)	O(7)#1-Sm(1)-O(9)	75.37(11)
Sm(1)-O(3)#2	2.443(3)	O(6)#1-Sm(1)-O(9)	76.73(12)
Sm(1)-O(11)	2.462(2)	O(1)#2-Sm(1)-O(9)	137.21(10)
Sm(1)-O(10)	2.467(2)	O(7)#1-Sm(1)-O(3)#2	69.46(11)
Sm(1)-O(3)	2.590(3)	O(6)#1-Sm(1)-O(3)#2	107.78(11)
Sm(1)-O(4)	2.813(3)	O(1)#2-Sm(1)-O(3)#2	74.00(10)
Zn(1)-N(2)#3	2.053(4)	O(9)-Sm(1)-O(3)#2	140.97(10)
Zn(1)-N(4)	2.088(4)	O(7)#1-Sm(1)-O(11)	151.34(9)
Zn(1)-N(1)	2.092(4)	O(6)#1-Sm(1)-O(11)	127.47(10)
Zn(1)-O(5)	2.158(3)	O(1)#2-Sm(1)-O(11)	68.27(9)
Zn(1)-O(4)	2.226(3)	O(9)-Sm(1)-O(11)	124.92(9)
Zn(1)-O(2)#3	2.301(3)	O(3)#2-Sm(1)-O(11)	84.06(9)
Zn(2)-O(2)#4	1.986(3)	O(7)#1-Sm(1)-O(10)	132.18(9)
Zn(2)-O(12)	2.015(3)	O(6)#1-Sm(1)-O(10)	71.82(11)
Zn(2)-N(3)	2.019(4)	O(1)#2-Sm(1)-O(10)	81.92(9)
Zn(2)-O(13)	2.081(3)	O(9)-Sm(1)-O(10)	65.65(9)
Zn(2)-O(8)	2.186(4)	O(3)#2-Sm(1)-O(10)	153.33(9)
O(5)-Zn(1)-O(4)	91.22(13)	O(11)-Sm(1)-O(10)	76.39(7)
N(2)#3-Zn(1)-O(2)#3	74.16(12)	O(7)#1-Sm(1)-O(3)	70.72(11)
N(4)-Zn(1)-O(2)#3	89.58(13)	O(6)#1-Sm(1)-O(3)	142.33(11)
N(1)-Zn(1)-O(2)#3	105.10(13)	O(1)#2-Sm(1)-O(3)	138.85(10)
O(5)-Zn(1)-O(2)#3	89.08(13)	O(9)-Sm(1)-O(3)	83.93(10)
O(4)-Zn(1)-O(2)#3	71.55(12)	O(3)#2-Sm(1)-O(3)	69.09(11)
O(2)#4-Zn(2)-O(12)	17.02(12)	O(11)-Sm(1)-O(3)	90.09(9)
O(2)#4-Zn(2)-N(3)	37.42(14)	O(10)-Sm(1)-O(3)	128.04(9)
O(12)-Zn(2)-N(3)	103.19(13)	O(7)#1-Sm(1)-O(4)	108.60(11)
O(2)#4-Zn(2)-O(13)	96.78(13)	O(6)#1-Sm(1)-O(4)	141.32(11)
O(12)-Zn(2)-O(13)	94.86(12)	O(1)#2-Sm(1)-O(4)	136.55(10)
N(3)-Zn(2)-O(13)	93.03(13)	O(9)-Sm(1)-O(4)	67.02(10)
O(2)#4-Zn(2)-O(8)	87.07(14)	O(3)#2-Sm(1)-O(4)	108.77(9)
O(12)-Zn(2)-O(8)	90.85(13)	O(11)-Sm(1)-O(4)	68.96(9)
N(3)-Zn(2)-O(8)	78.54(14)	O(10)-Sm(1)-O(4)	81.08(8)
O(13)-Zn(2)-O(8)	70.73(12)	O(3)-Sm(1)-O(4)	47.67(9)
N(4)-Zn(1)-O(5)	76.85(13)	N(2)#3-Zn(1)-N(4)	161.39(15)
N(1)-Zn(1)-O(5)	160.94(14)	N(2)#3-Zn(1)-N(1)	102.42(15)
N(2)#3-Zn(1)-O(4)	97.40(13)	N(4)-Zn(1)-N(1)	90.35(15)
N(4)-Zn(1)-O(4)	98.71(14)	N(2)#3-Zn(1)-O(5)	93.58(13)
N(1)-Zn(1)-O(4)	76.64(13)		
<b>4</b>			
Eu(1)-O(3)#1	2.376(3)	O(3)#1-Eu(1)-O(2)#1	73.21(11)
Eu(1)-O(2)#1	2.389(3)	O(3)#1-Eu(1)-O(11)	151.24(11)
Eu(1)-O(11)	2.431(3)	O(2)#1-Eu(1)-O(11)	128.07(11)

Eu(1)-O(7)#2	2.433(3)	O(3)#1-Eu(1)-O(7)#2	112.46(10)
Eu(1)-O(10)	2.437(3)	O(2)#1-Eu(1)-O(7)#2	66.76(10)
Eu(1)-O(6)#2	2.442(3)	O(11)-Eu(1)-O(7)#2	68.96(10)
Eu(1)-O(9)	2.472(3)	O(3)#1-Eu(1)-O(10)	75.41(10)
Eu(1)-O(6)	2.592(3)	O(2)#1-Eu(1)-O(10)	76.71(11)
Eu(1)-O(5)	2.813(3)	O(11)-Eu(1)-O(10)	124.41(11)
Zn(1)-N(4)#3	2.053(3)	O(7)#2-Eu(1)-O(10)	137.18(10)
Zn(1)-N(1)	2.089(4)	O(3)#1-Eu(1)-O(6)#2	69.43(10)
Zn(1)-N(3)	2.091(3)	O(2)#1-Eu(1)-O(6)#2	107.74(11)
Zn(1)-O(1)	2.158(3)	O(11)-Eu(1)-O(6)#2	84.27(11)
Zn(1)-O(5)	2.225(3)	O(7)#2-Eu(1)-O(6)#2	74.01(9)
Zn(1)-O(8)#3	2.299(3)	O(10)-Eu(1)-O(6)#2	141.00(10)
Zn(2)-O(8)#4	1.987(3)	O(3)#1-Eu(1)-O(9)	132.73(10)
Zn(2)-O(12)	1.999(4)	O(2)#1-Eu(1)-O(9)	72.06(11)
Zn(2)-N(2)	2.020(4)	O(11)-Eu(1)-O(9)	75.90(11)
Zn(2)-O(13)	2.073(4)	O(7)#2-Eu(1)-O(9)	81.47(10)
Zn(2)-O(4)	2.187(3)	O(10)-Eu(1)-O(9)	66.18(10)
N(4)#3-Zn(1)-O(8)#3	74.15(12)	O(6)#2-Eu(1)-O(9)	152.77(10)
N(1)-Zn(1)-O(8)#3	89.53(12)	O(3)#1-Eu(1)-O(6)	70.76(10)
N(3)-Zn(1)-O(8)#3	105.12(12)	O(2)#1-Eu(1)-O(6)	142.34(10)
O(1)-Zn(1)-O(8)#3	89.06(12)	O(11)-Eu(1)-O(6)	89.50(10)
O(5)-Zn(1)-O(8)#3	171.55(11)	O(7)#2-Eu(1)-O(6)	138.84(9)
O(8)#4-Zn(2)-O(12)	117.10(15)	O(10)-Eu(1)-O(6)	83.97(9)
O(8)#4-Zn(2)-N(2)	137.35(14)	O(6)#2-Eu(1)-O(6)	69.11(10)
O(12)-Zn(2)-N(2)	103.18(15)	O(9)-Eu(1)-O(6)	128.17(9)
O(8)#4-Zn(2)-O(13)	96.97(15)	O(3)#1-Eu(1)-O(5)	108.64(10)
O(12)-Zn(2)-O(13)	94.8(2)	O(2)#1-Eu(1)-O(5)	141.31(10)
N(2)-Zn(2)-O(13)	92.90(15)	O(11)-Eu(1)-O(5)	68.25(10)
O(8)#4-Zn(2)-O(4)	87.07(13)	O(7)#2-Eu(1)-O(5)	136.51(9)
O(12)-Zn(2)-O(4)	90.91(17)	O(10)-Eu(1)-O(5)	67.02(10)
N(2)-Zn(2)-O(4)	78.49(13)	O(6)#2-Eu(1)-O(5)	108.82(9)
O(13)-Zn(2)-O(4)	170.60(14)	O(9)-Eu(1)-O(5)	81.11(9)
N(1)-Zn(1)-O(1)	76.88(12)	O(6)-Eu(1)-O(5)	47.69(8)
N(3)-Zn(1)-O(1)	160.93(13)	N(4)#3-Zn(1)-N(1)	161.38(14)
N(4)#3-Zn(1)-O(5)	97.41(12)	N(4)#3-Zn(1)-N(3)	102.39(14)
N(1)-Zn(1)-O(5)	98.75(13)	N(1)-Zn(1)-N(3)	90.32(14)
N(3)-Zn(1)-O(5)	76.64(12)	N(4)#3-Zn(1)-O(1)	93.62(13)
O(1)-Zn(1)-O(5)	91.22(12)		
		<b>4'</b>	
Eu(1)-O(6)#4	2.3440(19)	O(6)#4-Eu(1)-O(3)	108.63(7)
Eu(1)-O(3)	2.3595(16)	O(6)#4-Eu(1)-O(12)	140.39(6)
Eu(1)-O(12)	2.3896(17)	O(3)-Eu(1)-O(12)	80.25(6)
Eu(1)-O(7)#4	2.4164(15)	O(6)#4-Eu(1)-O(7)#4	74.03(6)
Eu(1)-O(11)	2.448(2)	O(3)-Eu(1)-O(7)#4	75.91(5)

Eu(1)-O(9)	2.4794(17)	O(12)-Eu(1)-O(7)#4	143.77(6)
Eu(1)-O(1)	2.4803(16)	O(6)#4-Eu(1)-O(11)	74.86(8)
Eu(1)-O(10)#5	2.4926(16)	O(3)-Eu(1)-O(11)	148.26(6)
Zn(1)-N(4)#6	1.9909(18)	O(12)-Eu(1)-O(11)	78.64(7)
Zn(1)-N(2)#7	2.0106(18)	O(7)#4-Eu(1)-O(11)	133.02(7)
Zn(1)-N(1)	2.0667(18)	O(6)#4-Eu(1)-O(9)	95.74(6)
Zn(1)-O(2)	2.1749(16)	O(3)-Eu(1)-O(9)	133.36(5)
Zn(1)-O(4)#7	2.4368(16)	O(12)-Eu(1)-O(9)	105.61(6)
Zn(1)-O(8)#6	2.4857(19)	O(7)#4-Eu(1)-O(9)	73.47(6)
Zn(2)-N(3)	2.0064(18)	O(11)-Eu(1)-O(9)	75.60(7)
Zn(2)-O(4)	2.0126(17)	O(6)#4-Eu(1)-O(1)	70.09(5)
Zn(2)-O(13)	2.0530(16)	O(3)-Eu(1)-O(1)	73.52(5)
Zn(2)-O(14)	2.0624(17)	O(12)-Eu(1)-O(1)	76.23(6)
Zn(2)-O(5)	2.2035(16)	O(7)#4-Eu(1)-O(1)	121.17(6)
O(2)-Zn(1)-O(4)#7	167.00(5)	O(11)-Eu(1)-O(1)	78.59(7)
N(4)#6-Zn(1)-O(8)#6	71.78(7)	O(9)-Eu(1)-O(1)	153.12(5)
N(2)#7-Zn(1)-O(8)#6	82.18(7)	O(6)#4-Eu(1)-O(10)#5	148.75(5)
N(1)-Zn(1)-O(8)#6	169.23(7)	O(3)-Eu(1)-O(10)#5	74.37(6)
O(2)-Zn(1)-O(8)#6	95.76(7)	O(12)-Eu(1)-O(10)#5	70.68(5)
O(4)#7-Zn(1)-O(8)#6	97.12(7)	O(7)#4-Eu(1)-O(10)#5	76.82(5)
N(3)-Zn(2)-O(4)	130.24(7)	O(11)-Eu(1)-O(10)#5	119.54(7)
N(3)-Zn(2)-O(13)	106.83(7)	O(9)-Eu(1)-O(10)#5	65.00(5)
O(4)-Zn(2)-O(13)	120.02(6)	O(1)-Eu(1)-O(10)#5	136.94(5)
N(3)-Zn(2)-O(14)	96.85(7)	N(4)#6-Zn(1)-N(2)#7	146.17(8)
O(4)-Zn(2)-O(14)	93.37(7)	N(4)#6-Zn(1)-N(1)	100.06(7)
O(13)-Zn(2)-O(14)	97.02(7)	N(2)#7-Zn(1)-N(1)	107.93(7)
N(3)-Zn(2)-O(5)	78.30(6)	N(4)#6-Zn(1)-O(2)	98.13(7)
O(4)-Zn(2)-O(5)	90.30(6)	N(2)#7-Zn(1)-O(2)	105.77(7)
O(13)-Zn(2)-O(5)	83.91(6)	N(1)-Zn(1)-O(2)	78.16(7)
O(14)-Zn(2)-O(5)	175.11(6)	N(4)#6-Zn(1)-O(4)#6	87.59(7)
N(1)-Zn(1)-O(4)#7	89.38(6)	N(2)#7-Zn(1)-O(4)#7	74.35(6)
<b>5</b>			
Gd(1)-O(6)#4	2.3234(17)	O(6)#4-Gd(1)-O(3)	109.15(6)
Gd(1)-O(3)	2.3410(15)	O(6)#4-Gd(1)-O(12)	139.93(5)
Gd(1)-O(12)	2.3694(15)	O(3)-Gd(1)-O(12)	80.69(5)
Gd(1)-O(7)#4	2.4072(14)	O(6)#4-Gd(1)-O(7)#4	74.41(5)
Gd(1)-O(11)	2.428(2)	O(3)-Gd(1)-O(7)#4	75.84(5)
Gd(1)-O(9)	2.4649(16)	O(12)-Gd(1)-O(7)#4	144.08(5)
Gd(1)-O(1)	2.4682(14)	O(6)#4-Gd(1)-O(11)	74.86(7)
Gd(1)-O(10)#5	2.4793(15)	O(3)-Gd(1)-O(11)	148.34(6)
Zn(1)-N(4)#6	1.9942(17)	O(12)-Gd(1)-O(11)	77.83(6)
Zn(1)-N(2)#7	2.0070(16)	O(7)#4-Gd(1)-O(11)	133.27(6)
Zn(1)-N(1)	2.0591(17)	O(6)#4-Gd(1)-O(9)	95.25(6)
Zn(1)-O(2)	2.1703(15)	O(3)-Gd(1)-O(9)	133.49(5)

Zn(1)-O(4)#7	2.4365(15)	O(12)-Gd(1)-O(9)	105.52(6)
Zn(1)-O(8)#6	2.4877(17)	O(7)#4-Gd(1)-O(9)	73.49(5)
Zn(2)-N(3)	2.0045(17)	O(11)-Gd(1)-O(9)	75.22(6)
Zn(2)-O(4)	2.0097(15)	O(6)#4-Gd(1)-O(1)	70.11(5)
Zn(2)-O(13)	2.0425(15)	O(3)-Gd(1)-O(1)	73.78(5)
Zn(2)-O(14)	2.0629(16)	O(12)-Gd(1)-O(1)	76.22(5)
Zn(2)-O(5)	2.2012(14)	O(7)#4-Gd(1)-O(1)	121.32(5)
N(1)-Zn(1)-O(4)#7	89.29(6)	O(11)-Gd(1)-O(1)	78.68(6)
O(2)-Zn(1)-O(4)#7	166.94(5)	O(9)-Gd(1)-O(1)	152.72(5)
N(4)#6-Zn(1)-O(8)#6	71.62(6)	O(6)#4-Gd(1)-O(10)#5	148.85(5)
N(2)#7-Zn(1)-O(8)#6	82.40(6)	O(3)-Gd(1)-O(10)#5	74.46(5)
N(1)-Zn(1)-O(8)#6	169.02(6)	O(12)-Gd(1)-O(10)#5	70.92(5)
O(2)-Zn(1)-O(8)#6	95.48(6)	O(7)#4-Gd(1)-O(10)#5	76.77(5)
O(4)#7-Zn(1)-O(8)#6	97.46(6)	O(11)-Gd(1)-O(10)#5	118.92(6)
N(3)-Zn(2)-O(4)	130.32(7)	O(9)-Gd(1)-O(10)#5	65.09(5)
N(3)-Zn(2)-O(13)	106.84(7)	O(1)-Gd(1)-O(10)#5	137.17(5)
O(4)-Zn(2)-O(13)	120.05(6)	N(4)#6-Zn(1)-N(2)#7	146.09(7)
N(3)-Zn(2)-O(14)	96.64(6)	N(4)#6-Zn(1)-N(1)	100.16(7)
O(4)-Zn(2)-O(14)	93.38(7)	N(2)#7-Zn(1)-N(1)	107.86(6)
O(13)-Zn(2)-O(14)	96.85(7)	N(4)#6-Zn(1)-O(2)	98.20(6)
N(3)-Zn(2)-O(5)	78.62(6)	N(2)#7-Zn(1)-O(2)	105.79(6)
O(4)-Zn(2)-O(5)	90.54(6)	N(1)-Zn(1)-O(2)	78.20(6)
O(13)-Zn(2)-O(5)	83.64(6)	N(4)#6-Zn(1)-O(4)#7	87.57(6)
O(14)-Zn(2)-O(5)	175.14(6)	N(2)#7-Zn(1)-O(4)#7	74.31(6)
<b>6</b>			
Dy(1)-O(6)#4	2.2993(19)	O(6)#4-Dy(1)-O(12)	139.21(6)
Dy(1)-O(12)	2.3270(16)	O(6)#4-Dy(1)-O(3)	111.49(7)
Dy(1)-O(3)	2.3311(15)	O(12)-Dy(1)-O(3)	79.89(6)
Dy(1)-O(7)#4	2.3585(15)	O(6)#4-Dy(1)-O(7)#4	76.01(6)
Dy(1)-O(11)	2.401(2)	O(12)-Dy(1)-O(7)#4	143.54(5)
Dy(1)-O(9)	2.4610(16)	O(3)-Dy(1)-O(7)#4	76.32(5)
Dy(1)-O(1)	2.4612(15)	O(6)#4-Dy(1)-O(11)	73.75(7)
Dy(1)-O(10)#7	2.4750(15)	O(12)-Dy(1)-O(11)	77.61(7)
Zn(1)-N(4)#6	1.9946(17)	O(3)-Dy(1)-O(11)	148.22(6)
Zn(1)-N(2)#7	2.0048(17)	O(7)#4-Dy(1)-O(11)	133.54(6)
Zn(1)-N(1)	2.0732(17)	O(6)#4-Dy(1)-O(9)	93.69(6)
Zn(1)-O(2)	2.1706(15)	O(12)-Dy(1)-O(9)	105.97(6)
Zn(1)-O(4)#7	2.4376(15)	O(3)-Dy(1)-O(9)	133.91(5)
Zn(2)-N(3)	2.0097(18)	O(7)#4-Dy(1)-O(9)	73.20(6)
Zn(2)-O(4)	2.0237(16)	O(11)-Dy(1)-O(9)	74.45(6)
Zn(2)-O(13)	2.0288(16)	O(6)#4-Dy(1)-O(1)	69.88(5)
Zn(2)-O(14)	2.0700(16)	O(12)-Dy(1)-O(1)	76.76(5)
Zn(2)-O(5)	2.2219(15)	O(3)-Dy(1)-O(1)	73.97(5)
N(4)#6-Zn(1)-N(1)	99.88(7)	O(7)#4-Dy(1)-O(1)	121.37(5)



N(2)#7-Zn(1)-N(1)	108.55(7)	O(11)-Dy(1)-O(1)	79.21(6)
N(4)#6-Zn(1)-O(2)	99.08(7)	O(9)-Dy(1)-O(1)	152.09(5)
N(2)#7-Zn(1)-O(2)	105.35(7)	O(6)#4-Dy(1)-O(10)#5	149.54(5)
N(1)-Zn(1)-O(2)	77.67(6)	O(12)-Dy(1)-O(10)#5	70.59(5)
N(4)#6-Zn(1)-O(4)#7	86.83(6)	O(3)-Dy(1)-O(10)#5	74.06(5)
N(2)#7-Zn(1)-O(4)#7	75.03(6)	O(7)#4-Dy(1)-O(10)#5	76.51(5)
N(1)-Zn(1)-O(4)#7	89.11(6)	O(11)-Dy(1)-O(10)#5	118.10(7)
O(2)-Zn(1)-O(4)#7	166.24(5)	O(9)-Dy(1)-O(10)#5	65.82(5)
N(3)-Zn(2)-O(4)	131.12(7)	O(1)-Dy(1)-O(10)#5	137.44(5)
N(3)-Zn(2)-O(13)	106.49(7)	N(4)#6-Zn(1)-N(2)#7	145.68(8)
O(4)-Zn(2)-O(13)	119.47(6)	N(3)-Zn(2)-O(5)	77.71(6)
N(3)-Zn(2)-O(14)	97.36(7)	O(4)-Zn(2)-O(5)	90.83(6)
O(4)-Zn(2)-O(14)	93.36(7)	O(13)-Zn(2)-O(5)	83.95(6)
O(13)-Zn(2)-O(14)	96.45(7)	O(14)-Zn(2)-O(5)	174.93(6)
<b>7</b>			
Ho(1)-O(6)#4	2.2889(17)	O(6)#4-Ho(1)-O(3)	111.55(6)
Ho(1)-O(3)	2.3234(14)	O(6)#4-Ho(1)-O(12)	138.94(5)
Ho(1)-O(12)	2.3273(15)	O(3)-Ho(1)-O(12)	80.62(5)
Ho(1)-O(7)#4	2.3638(14)	O(6)#4-Ho(1)-O(7)#4	75.97(5)
Ho(1)-O(11)	2.3977(19)	O(3)-Ho(1)-O(7)#4	75.46(5)
Ho(1)-O(1)	2.4440(14)	O(12)-Ho(1)-O(7)#4	143.85(5)
Ho(1)-O(9)	2.4512(15)	O(6)#4-Ho(1)-O(11)	74.20(7)
Ho(1)-O(10)#5	2.4649(15)	O(3)-Ho(1)-O(11)	148.30(6)
Zn(1)-N(4)#6	1.9972(17)	O(12)-Ho(1)-O(11)	76.61(6)
Zn(1)-N(2)#7	2.0077(16)	O(7)#4-Ho(1)-O(11)	134.41(6)
Zn(1)-N(1)	2.0734(16)	O(6)#4-Ho(1)-O(1)	69.88(5)
Zn(1)-O(2)	2.1731(14)	O(3)-Ho(1)-O(1)	74.42(5)
Zn(1)-O(4)#7	2.4572(15)	O(12)-Ho(1)-O(1)	76.76(5)
Zn(2)-N(3)	2.0093(17)	O(7)#4-Ho(1)-O(1)	120.92(5)
Zn(2)-O(4)	2.0212(15)	O(11)-Ho(1)-O(1)	79.08(6)
Zn(2)-O(13)	2.0441(15)	O(6)#4-Ho(1)-O(9)	93.22(6)
Zn(2)-O(14)	2.0755(15)	O(3)-Ho(1)-O(9)	133.83(5)
Zn(2)-O(5)	2.2261(14)	O(12)-Ho(1)-O(9)	106.04(6)
N(4)#6-Zn(1)-O(4)#7	86.97(6)	O(7)#4-Ho(1)-O(9)	73.71(5)
N(2)#7-Zn(1)-O(4)#7	74.53(6)	O(11)-Ho(1)-O(9)	74.40(6)
N(1)-Zn(1)-O(4)#7	88.78(6)	O(1)-Ho(1)-O(9)	151.69(5)
O(2)-Zn(1)-O(4)#7	166.18(5)	O(6)#4-Ho(1)-O(10)#5	149.53(5)
N(3)-Zn(2)-O(4)	130.78(7)	O(3)-Ho(1)-O(10)#5	74.01(5)
N(3)-Zn(2)-O(13)	106.90(7)	O(12)-Ho(1)-O(10)#5	70.77(5)
O(4)-Zn(2)-O(13)	119.48(6)	O(7)#4-Ho(1)-O(10)#5	76.77(5)
N(3)-Zn(2)-O(14)	97.41(6)	O(11)-Ho(1)-O(10)#5	117.61(6)
O(4)-Zn(2)-O(14)	92.84(6)	O(1)-Ho(1)-O(10)#5	137.59(4)
O(13)-Zn(2)-O(14)	96.81(7)	O(9)-Ho(1)-O(10)#5	66.09(5)
N(3)-Zn(2)-O(5)	77.81(6)	N(4)#6-Zn(1)-N(2)#7	145.33(7)

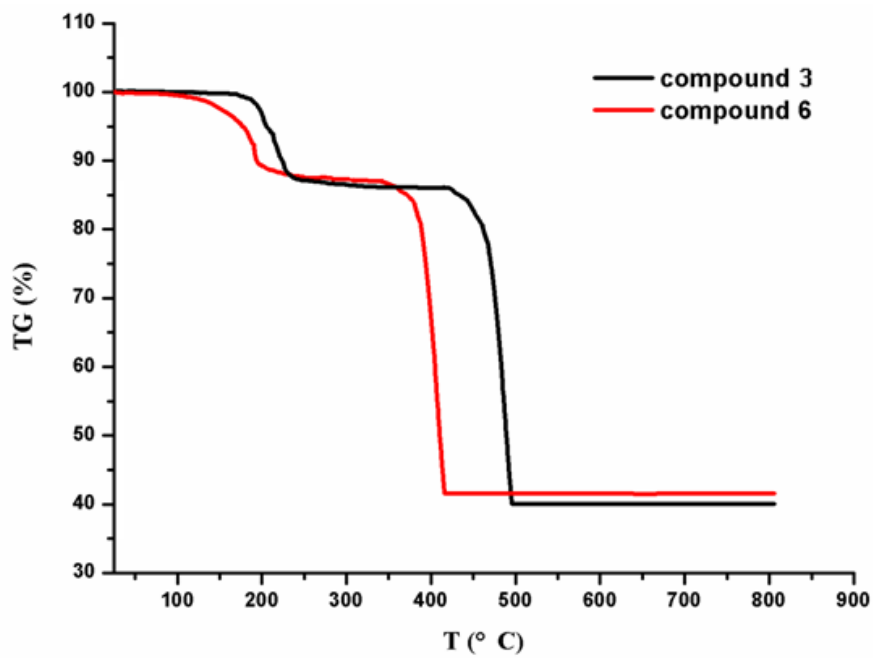
O(4)-Zn(2)-O(5)	91.27(6)	N(4)#6-Zn(1)-N(1)	100.17(7)
O(13)-Zn(2)-O(5)	83.52(6)	N(2)#7-Zn(1)-N(1)	108.31(6)
O(14)-Zn(2)-O(5)	175.06(6)	N(4)#6-Zn(1)-O(2)	98.85(6)
N(1)-Zn(1)-O(2)	77.90(6)	N(2)#7-Zn(1)-O(2)	106.01(6)
<b>8</b>			
Er(1)-O(6)#4	2.283(4)	O(6)#4-Er(1)-O(3)	112.01(16)
Er(1)-O(3)	2.304(3)	O(6)#4-Er(1)-O(12)	138.71(14)
Er(1)-O(12)	2.305(4)	O(3)-Er(1)-O(12)	80.26(14)
Er(1)-O(7)#4	2.346(4)	O(6)#4-Er(1)-O(7)#4	76.35(13)
Er(1)-O(11)	2.380(4)	O(3)-Er(1)-O(7)#4	75.96(12)
Er(1)-O(9)	2.444(3)	O(12)-Er(1)-O(7)#4	143.79(13)
Er(1)-O(1)	2.452(3)	O(6)#4-Er(1)-O(11)	74.8(2)
Er(1)-O(10)#5	2.457(3)	O(3)-Er(1)-O(11)	147.83(16)
Zn(1)-N(4)#6	2.003(4)	O(12)-Er(1)-O(11)	75.86(19)
Zn(1)-N(2)#7	2.003(4)	O(7)#4-Er(1)-O(11)	134.80(16)
Zn(1)-N(1)	2.073(4)	O(6)#4-Er(1)-O(9)	92.83(14)
Zn(1)-O(2)	2.166(3)	O(3)-Er(1)-O(9)	134.02(11)
Zn(1)-O(4)#7	2.451(3)	O(12)-Er(1)-O(9)	106.42(14)
Zn(2)-N(3)	2.009(4)	O(7)#4-Er(1)-O(9)	73.20(13)
Zn(2)-O(4)	2.026(3)	O(11)-Er(1)-O(9)	74.26(16)
Zn(2)-O(13)	2.032(4)	O(6)#4-Er(1)-O(1)	70.00(12)
Zn(2)-O(14)	2.080(4)	O(3)-Er(1)-O(1)	74.27(11)
Zn(2)-O(5)	2.227(3)	O(12)-Er(1)-O(1)	76.56(13)
N(3)-Zn(2)-O(13)	107.01(16)	O(7)#4-Er(1)-O(1)	121.35(12)
O(4)-Zn(2)-O(13)	118.76(15)	O(11)-Er(1)-O(1)	79.41(16)
N(3)-Zn(2)-O(14)	97.21(16)	O(9)-Er(1)-O(1)	151.65(11)
O(4)-Zn(2)-O(14)	93.47(16)	O(6)#4-Er(1)-O(10)#5	149.46(12)
O(13)-Zn(2)-O(14)	96.44(17)	O(3)-Er(1)-O(10)#5	74.08(11)
N(3)-Zn(2)-O(5)	78.08(15)	O(12)-Er(1)-O(10)#5	71.00(12)
O(4)-Zn(2)-O(5)	90.75(13)	O(7)#4-Er(1)-O(10)#5	76.42(12)
O(13)-Zn(2)-O(5)	83.72(14)	O(11)-Er(1)-O(10)#5	116.79(18)
O(14)-Zn(2)-O(5)	175.08(14)	O(9)-Er(1)-O(10)#5	66.14(11)
N(2)#7-Zn(1)-O(2)	105.87(15)	O(1)-Er(1)-O(10)#5	137.67(11)
N(1)-Zn(1)-O(2)	77.61(14)	N(4)#6-Zn(1)-N(2)#7	145.20(16)
N(4)#6-Zn(1)-O(4)#7	86.89(14)	N(4)#6-Zn(1)-N(1)	100.24(16)
N(2)#7-Zn(1)-O(4)#7	74.70(14)	N(2)#7-Zn(1)-N(1)	108.41(16)
N(1)-Zn(1)-O(4)#7	88.65(14)	N(4)#6-Zn(1)-O(2)	99.13(15)
O(2)-Zn(1)-O(4)#7	165.75(12)	N(3)-Zn(2)-O(4)	131.31(15)
<b>9</b>			
Yb(1)-O(6)#4	2.254(3)	O(6)#4-Yb(1)-O(12)	138.16(8)
Yb(1)-O(12)	2.280(2)	O(6)#4-Yb(1)-O(3)	112.75(9)
Yb(1)-O(3)	2.286(2)	O(12)-Yb(1)-O(3)	80.60(8)
Yb(1)-O(7)#4	2.312(2)	O(6)#4-Yb(1)-O(7)#4	76.84(8)
Yb(1)-O(11)	2.366(3)	O(12)-Yb(1)-O(7)#4	143.94(8)

Yb(1)-O(9)	2.418(2)	O(3)-Yb(1)-O(7)#4	75.52(7)
Yb(1)-O(1)	2.417(2)	O(6)#4-Yb(1)-O(11)	74.75(10)
Yb(1)-O(10)#5	2.438(2)	O(12)-Yb(1)-O(11)	75.06(9)
Zn(1)-N(4)#6	1.986(3)	O(3)-Yb(1)-O(11)	147.85(8)
Zn(1)-N(2)#7	1.999(2)	O(7)#4-Yb(1)-O(11)	135.41(8)
Zn(1)-N(1)	2.063(3)	O(6)#4-Yb(1)-O(9)	92.13(9)
Zn(1)-O(2)	2.179(2)	O(12)-Yb(1)-O(9)	106.37(8)
Zn(1)-O(4)#7	2.473(2)	O(3)-Yb(1)-O(9)	134.27(7)
Zn(2)-N(3)	2.004(3)	O(7)#4-Yb(1)-O(9)	73.73(8)
Zn(2)-O(4)	2.017(2)	O(11)-Yb(1)-O(9)	73.75(8)
Zn(2)-O(13)	2.042(2)	O(6)#4-Yb(1)-O(1)	69.65(8)
Zn(2)-O(14)	2.071(2)	O(12)-Yb(1)-O(1)	76.90(7)
Zn(2)-O(5)	2.228(2)	O(3)-Yb(1)-O(1)	74.76(7)
N(1)-Zn(1)-O(4)#7	88.30(9)	O(7)#4-Yb(1)-O(1)	120.94(8)
O(2)-Zn(1)-O(4)#7	165.78(7)	O(11)-Yb(1)-O(1)	79.46(8)
N(3)-Zn(2)-O(4)	130.61(10)	O(9)-Yb(1)-O(1)	150.88(7)
N(3)-Zn(2)-O(13)	107.26(10)	O(6)#4-Yb(1)-O(10)#5	150.26(7)
O(4)-Zn(2)-O(13)	119.31(8)	O(12)-Yb(1)-O(10)#5	70.45(7)
N(3)-Zn(2)-O(14)	98.16(10)	O(3)-Yb(1)-O(10)#5	74.04(8)
O(4)-Zn(2)-O(14)	92.30(10)	O(7)#4-Yb(1)-O(10)#5	77.19(7)
O(13)-Zn(2)-O(14)	96.55(10)	O(11)-Yb(1)-O(10)#5	115.76(9)
N(3)-Zn(2)-O(5)	77.27(9)	O(9)-Yb(1)-O(10)#5	66.74(7)
O(4)-Zn(2)-O(5)	91.77(9)	O(1)-Yb(1)-O(10)#5	137.71(7)
O(13)-Zn(2)-O(5)	83.62(8)	N(4)#6-Zn(1)-N(2)#7	144.73(11)
O(14)-Zn(2)-O(5)	175.22(8)	N(4)#6-Zn(1)-N(1)	99.90(10)
N(1)-Zn(1)-O(2)	78.02(9)	N(2)#7-Zn(1)-N(1)	108.91(10)
N(4)#6-Zn(1)-O(4)#7	86.53(9)	N(4)#6-Zn(1)-O(2)	99.49(9)
N(2)#7-Zn(1)-O(4)#7	74.70(9)	N(2)#7-Zn(1)-O(2)	105.93(9)
<b>10</b>			
Lu(1)-O(6)#4	2.229(5)	O(6)#4-Lu(1)-O(3)	113.3(2)
Lu(1)-O(3)	2.249(5)	O(6)#4-Lu(1)-O(12)	138.15(17)
Lu(1)-O(12)	2.272(5)	O(3)-Lu(1)-O(12)	80.43(19)
Lu(1)-O(7)#4	2.326(5)	O(6)#4-Lu(1)-O(7)#4	76.75(17)
Lu(1)-O(11)	2.348(6)	O(3)-Lu(1)-O(7)#4	75.43(16)
Lu(1)-O(9)	2.375(4)	O(12)-Lu(1)-O(7)#4	144.04(17)
Lu(1)-O(1)	2.390(4)	O(6)#4-Lu(1)-O(11)	74.9(2)
Lu(1)-O(10)#5	2.398(4)	O(3)-Lu(1)-O(11)	147.6(2)
Zn(1)-N(4)#6	1.970(5)	O(12)-Lu(1)-O(11)	74.6(2)
Zn(1)-N(2)#7	1.985(5)	O(7)#4-Lu(1)-O(11)	135.9(2)
Zn(1)-N(1)	2.059(5)	O(6)#4-Lu(1)-O(9)	91.27(18)
Zn(1)-O(2)	2.155(4)	O(3)-Lu(1)-O(9)	134.48(16)
Zn(1)-O(4)#7	2.453(5)	O(12)-Lu(1)-O(9)	106.84(19)
Zn(2)-O(4)	1.992(4)	O(7)#4-Lu(1)-O(9)	73.86(17)
Zn(2)-N(3)	1.994(5)	O(11)-Lu(1)-O(9)	73.69(19)

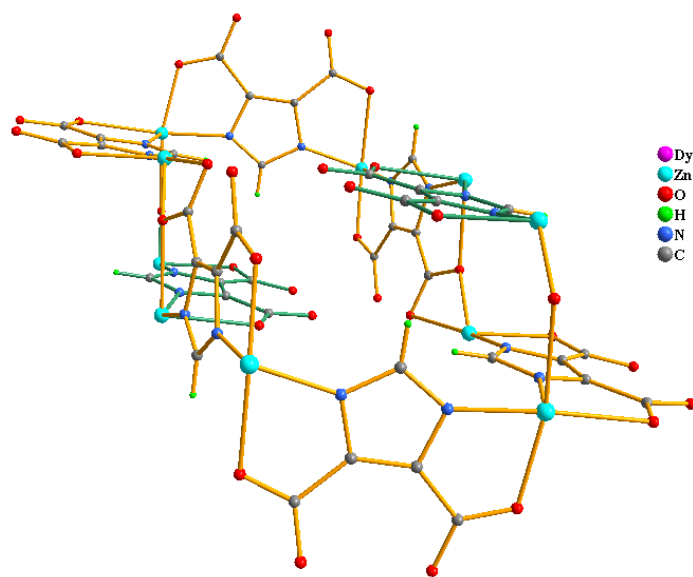
Zn(2)-O(13)	2.027(5)	O(6)#4-Lu(1)-O(1)	70.41(16)
Zn(2)-O(14)	2.057(5)	O(3)-Lu(1)-O(1)	75.12(15)
Zn(2)-O(5)	2.223(5)	O(12)-Lu(1)-O(1)	76.12(16)
N(1)-Zn(1)-O(4)#7	87.04(18)	O(7)#4-Lu(1)-O(1)	121.45(16)
O(2)-Zn(1)-O(4)#7	165.37(16)	O(11)-Lu(1)-O(1)	78.98(19)
O(4)-Zn(2)-N(3)	130.4(2)	O(9)-Lu(1)-O(1)	150.34(15)
O(4)-Zn(2)-O(13)	118.9(2)	O(6)#4-Lu(1)-O(10)#5	149.68(16)
N(3)-Zn(2)-O(13)	107.9(2)	O(3)-Lu(1)-O(10)#5	73.74(15)
O(4)-Zn(2)-O(14)	92.4(2)	O(12)-Lu(1)-O(10)#5	70.98(16)
N(3)-Zn(2)-O(14)	97.1(2)	O(7)#4-Lu(1)-O(10)#5	76.87(16)
O(13)-Zn(2)-O(14)	97.6(2)	O(11)-Lu(1)-O(10)#5	115.8(2)
O(4)-Zn(2)-O(5)	91.89(17)	O(9)-Lu(1)-O(10)#5	67.15(15)
N(3)-Zn(2)-O(5)	77.80(19)	O(1)-Lu(1)-O(10)#5	137.62(15)
O(13)-Zn(2)-O(5)	83.05(19)	N(4)#6-Zn(1)-N(2)#7	145.4(2)
O(14)-Zn(2)-O(5)	174.74(18)	N(4)#6-Zn(1)-N(1)	100.2(2)
N(1)-Zn(1)-O(2)	78.78(18)	N(2)#7-Zn(1)-N(1)	107.8(2)
N(4)#6-Zn(1)-O(4)#7	87.94(19)	N(4)#6-Zn(1)-O(2)	98.0(2)
N(2)#7-Zn(1)-O(4)#7	73.90(18)	N(2)#7-Zn(1)-O(2)	106.93(19)

\*Symmetry transformations used to generate equivalent atoms: 1#  $-x+2,y,-z+1/2$ ; #2  $-x+2,-y+1,-z+1$ ; #3  $-x+3/2,y+1/2,-z+1/2$ ; #4  $x,y+1,z$ ; #5  $-x+2,-y+1,-z$ ; #6  $x,-y+1/2,z+1/2$ ; #7  $-x+1,y+1/2,-z+1/2$ .

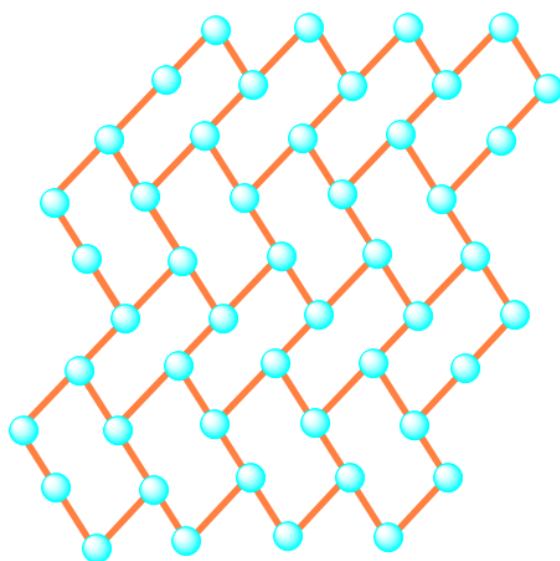
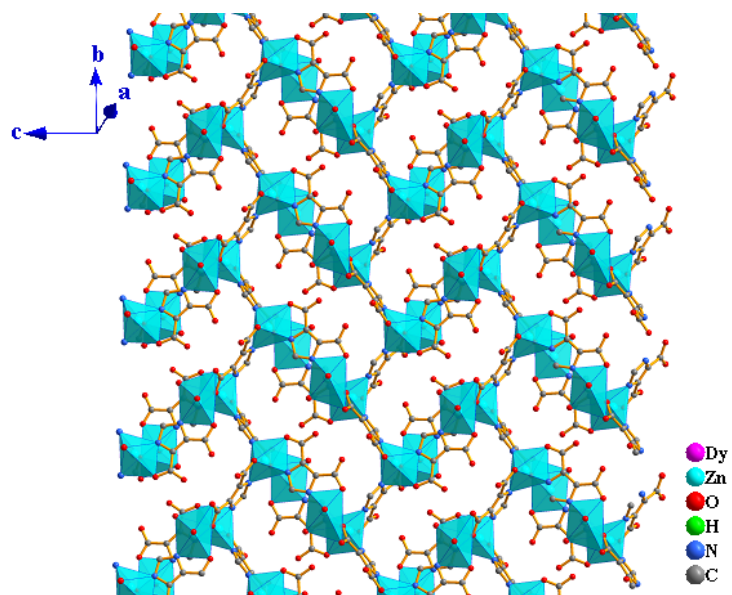
**Figure S1.** The TG curves of compounds **3** and **6**.



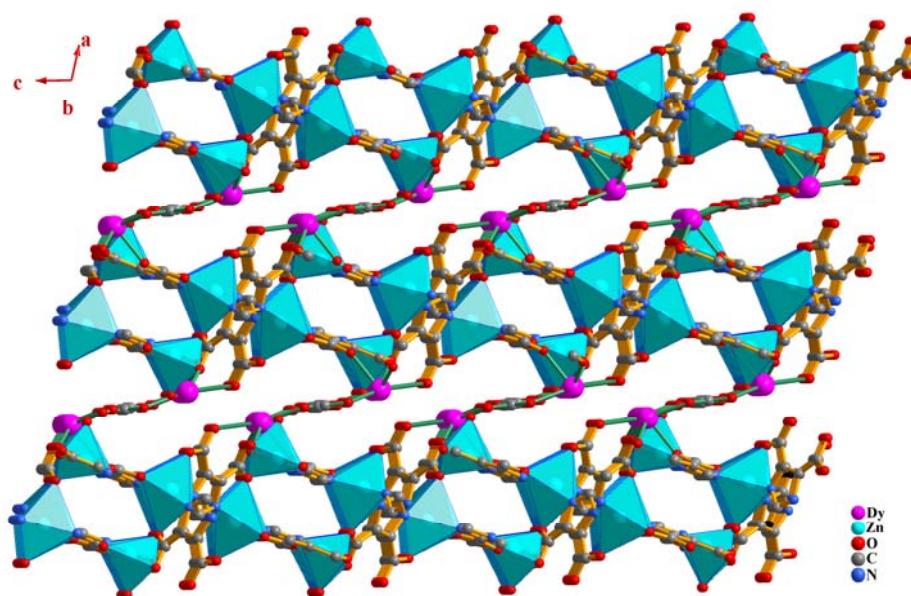
**Figure S2** The building block unit  $[\text{Zn}_{10}(\text{ImDC})_8]$  with chair-conformation. in **6**



**Figure S3** 3-connected Zn-containing layer with  $6^3$  topology in **6** along *a* axis.



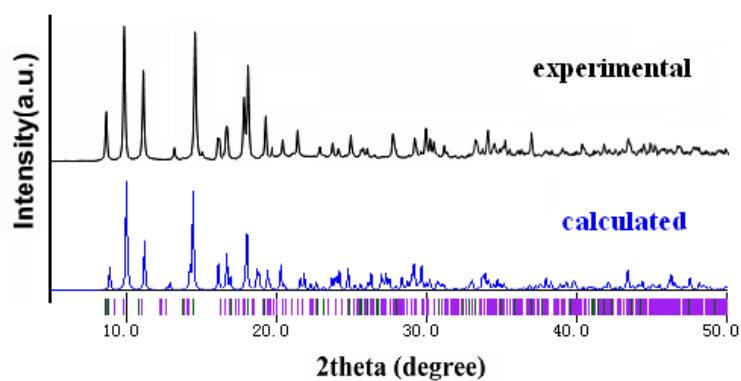
**Figure S4** 3-D chain-layer MOF with the 1-D flat channels in **6** along the *b* axis.



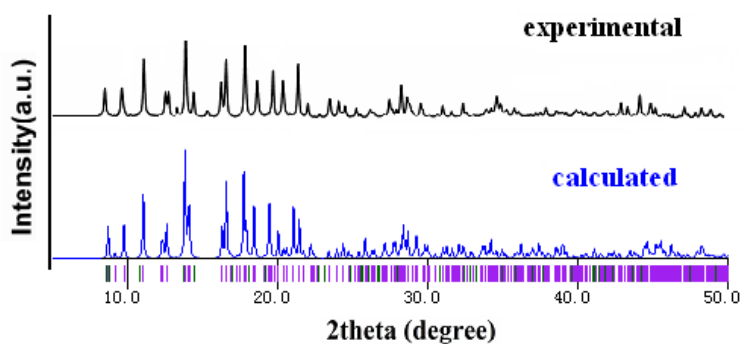


**Figure S5** PXRD patterns of two compounds **4** (a) and **4'**(b) simulated from the X-ray single-crystal structure and as-synthesized/transformed samples.

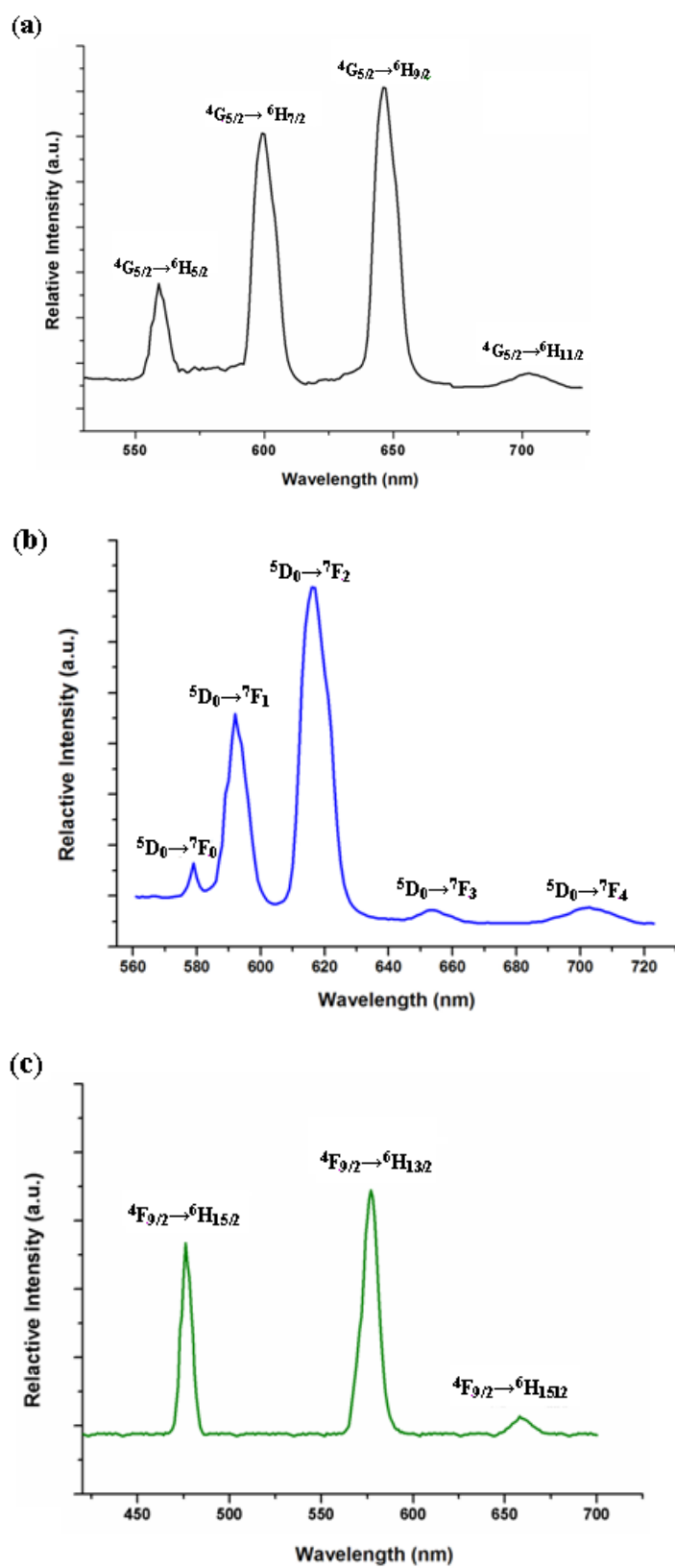
**(a) For compound 4**



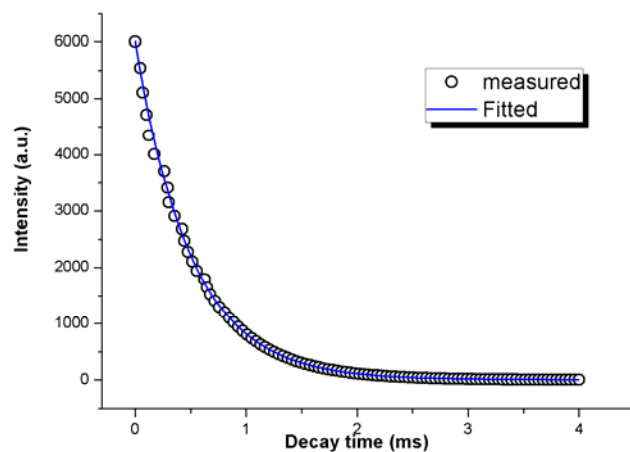
**(b) For compound 4'**



**Figure S6** Solid-state emission spectra for compounds **3** (a), **4** (b) and **6** (c) in the solid state at room temperature.

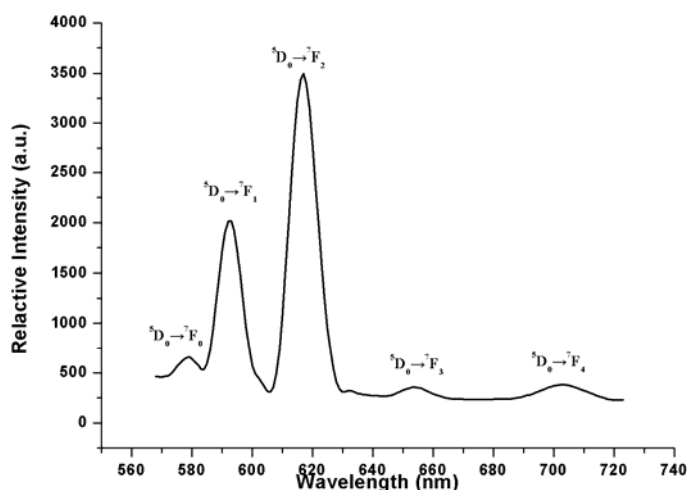


**Figure S7** Photoluminescence decay curve for the emission at 620 nm of complex **4** and the corresponding single-exponential fit with  $\tau_1 = 0.232 \pm 0.007545$  ms.



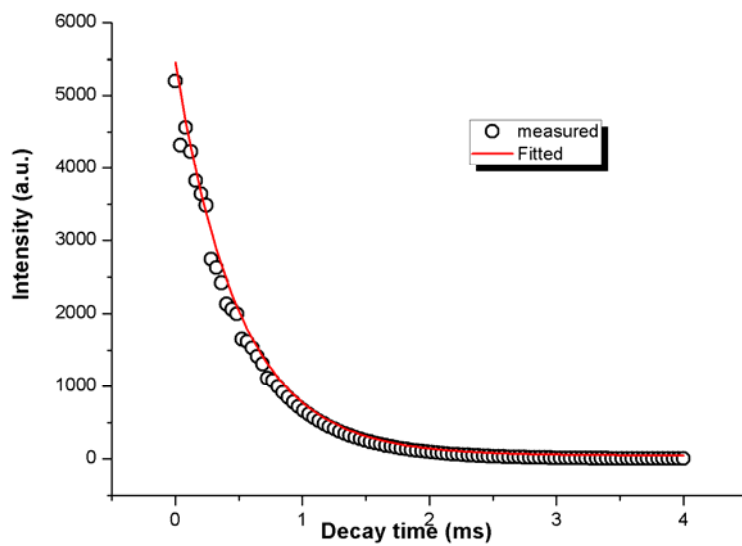
The photoluminescence decay curve of complex **4** was measured at room temperature. The decay curves are well fitted into a single-exponential function as  $I=I_0 \exp (-t/\tau)$ , indicating the existence of a single chemical environment of Ln(III) sites in the structure. The corresponding lifetime for complex **4** is about 0.232 ms (Figure S7).

**Figure S8** Solid-state emission spectrum for **4** at room temperature (excited at 395 nm).



From Figure S8, the emission spectra of complex **4'** was excited at 395nm, and its emission peaks show moderately strong bands at 578, 595, 618 nm and two weak bands peaked at 652 and 703 nm, corresponding to the electronic transition of  ${}^5D_0 \rightarrow {}^7F_0$ ,  ${}^5D_0 \rightarrow {}^7F_1$ ,  ${}^5D_0 \rightarrow {}^7F_2$ , and  ${}^5D_0 \rightarrow {}^7F_3$ ,  ${}^5D_0 \rightarrow {}^7F_4$ , respectively, which is similar to complex **4**. The photoluminescence decay curve of complex **4'** was measured at room temperature. The decay curves are well fitted into a single-exponential function as  $I=I_0 \exp(-t/\tau)$ , indicating the existence of a single chemical environment of Ln(III) sites in the structure. The corresponding lifetime for complex **4'** is about 0.283 ms (Figure S9). The most intense emission band at 618 nm suggests that it is an electric dipole transition and that the ligand is suitable for the sensibility of red luminescence for the Eu(III) ions.

**Figure S9** Photoluminescence decay curve for the emission at 620 nm of complex **4'** and the corresponding single-exponential fit with  $\tau_1 = 0.283 \pm 0.004673$  ms.



**Figure S10.** Powder X-ray diffraction (PXRD) patterns for compounds **3** (a) and **6** (b) based on the crystalline sample at different temperature: 30 °C; 200 °C; 250 °C; 300 °C; 345 °C; as well as simulated from single crystal X-ray data.

