Optical detection small biomolecule thiamines of micromolar level by highly luminescent lanthanide complexes with tridentate N-heterocyclic ligand

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Fig. S1 The IR spectra of the complex **5**. 2

Fig. S2 The PXRD pattern based on the X-ray single crystal diffraction of the complex **1** and the experimental samples of the complexes **1–8**, respectively. 2

Fig. S3 The TG curve for the complex **1**. 2

Fig. S4 Lattice parameters, volume of the crystal cell, Ln-O_{ave} (average value of O1, O2, O4, O5, O7 and O8), Ln-O10, Ln-N_{ave} (average value of N2 and N4) and Ln-N3 bonds lengths for the complexes **1–8** to show the decreasing trends as a function of the increasing atomic sequence number from lanthanum to terbium. 3

Table S1 Selected bond distances (Å) and angles (°) of the complexes **1-8**. 4

Table S2 Hydrogen bond lengths (Å) and angles (°) for the complexes **1-8** 13

Table S3 IR data for the complexes **1-8** 15

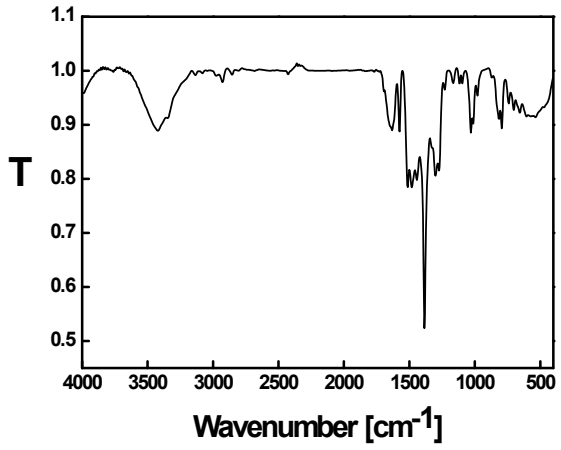

Fig. S1 The IR spectra of the complex **5.**

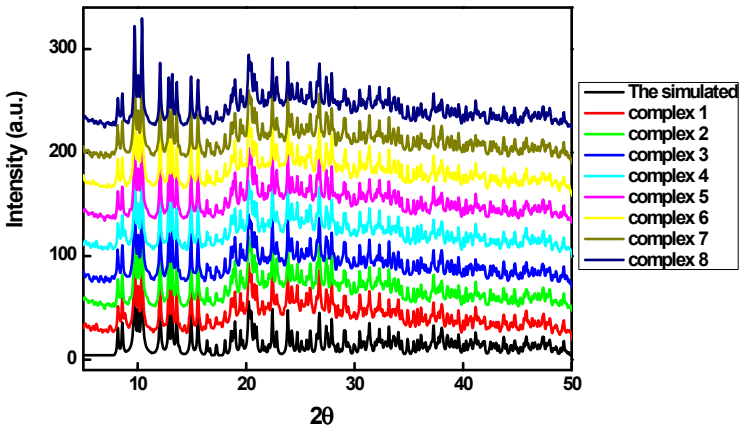

Fig. S2 The PXRD pattern based on the X-ray single crystal diffraction of the complex **1** and the experimental samples of the complexes **1–8**, respectively.

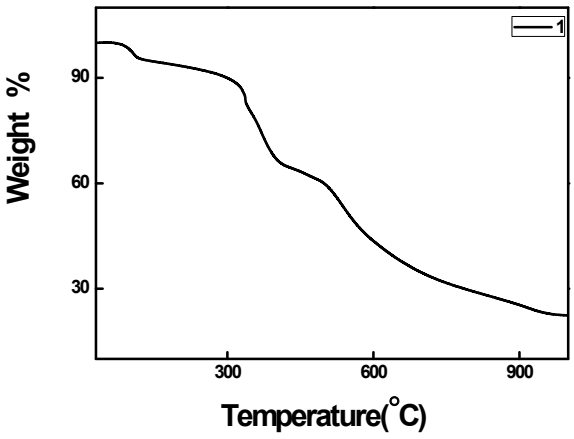

Fig. S3 The TG curve for the complex **1**.

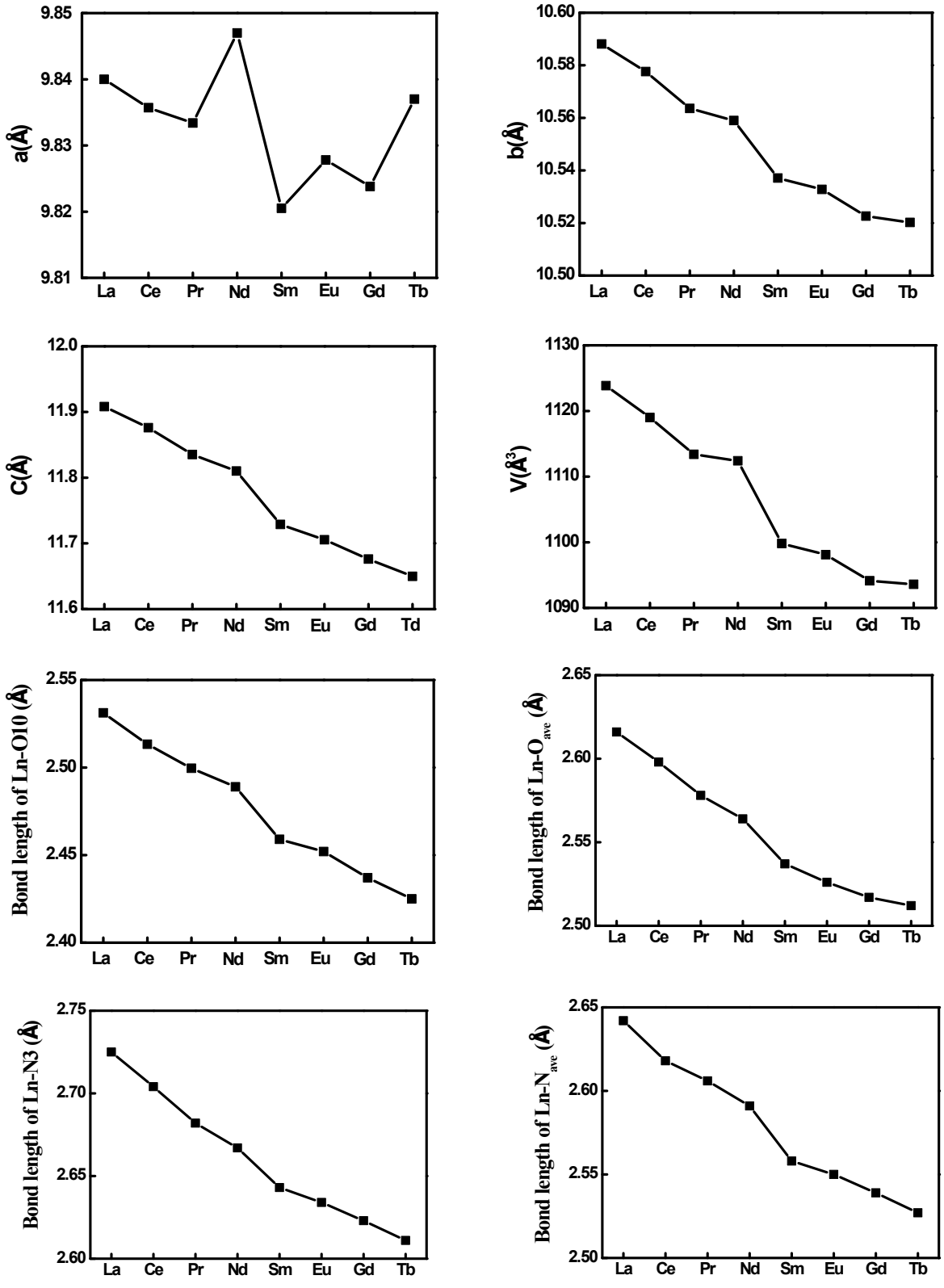

Fig. S4 Lattice parameters, volume of the crystal cell, Ln-O_{ave} (average value of O1, O2, O4, O5, O7 and O8), Ln-O10, Ln-N_{ave} (average value of N2 and N4) and Ln-N3 bonds lengths for the complexes **1–8** to show the decreasing trends as a function of the increasing atomic sequence number from lanthanum to terbium.

Table S1 Selected bond distances (Å) and angles (°) of the complexes **1-8**.

Complex **1**			
La(1)-O(10)	2.5312(18)	La(1)-O(2)	2.633(2)
La(1)-O(4)	2.558(2)	La(1)-N(4)	2.638(2)
La(1)-O(8)	2.592(2)	La(1)-N(2)	2.645(2)
La(1)-O(1)	2.600(2)	La(1)-O(5)	2.684(2)
La(1)-O(7)	2.628(2)	La(1)-N(3)	2.725(2)
O(10)-La(1)-O(4)	121.52(7)	O(4)-La(1)-O(5)	48.54(7)
O(10)-La(1)-O(8)	77.62(7)	O(8)-La(1)-O(5)	69.39(7)
O(4)-La(1)-O(8)	78.89(8)	O(1)-La(1)-O(5)	99.11(7)
O(10)-La(1)-O(1)	128.05(7)	O(7)-La(1)-O(5)	114.16(7)
O(4)-La(1)-O(1)	72.48(8)	O(2)-La(1)-O(5)	65.84(7)
O(8)-La(1)-O(1)	148.92(7)	N(4)-La(1)-O(5)	111.58(7)
O(10)-La(1)-O(7)	73.48(7)	N(2)-La(1)-O(5)	125.87(7)
O(4)-La(1)-O(7)	123.04(8)	O(10)-La(1)-N(3)	122.10(6)
O(8)-La(1)-O(7)	48.95(7)	O(4)-La(1)-N(3)	116.33(7)
O(1)-La(1)-O(7)	145.44(7)	O(8)-La(1)-N(3)	116.97(7)
O(10)-La(1)-O(2)	84.03(7)	O(1)-La(1)-N(3)	67.61(7)
O(4)-La(1)-O(2)	76.32(8)	O(7)-La(1)-N(3)	77.99(7)
O(8)-La(1)-O(2)	134.82(7)	O(2)-La(1)-N(3)	107.80(7)
O(1)-La(1)-O(2)	48.50(7)	N(4)-La(1)-N(3)	60.94(7)
O(7)-La(1)-O(2)	155.82(7)	N(2)-La(1)-N(3)	60.61(7)
O(10)-La(1)-N(4)	141.89(8)	O(5)-La(1)-N(3)	163.81(7)
O(4)-La(1)-N(4)	71.45(7)	C(4)-N(2)-La(1)	122.56(18)
O(8)-La(1)-N(4)	69.85(7)	N(1)-N(2)-La(1)	132.69(18)
O(1)-La(1)-N(4)	89.45(7)	C(5)-N(3)-La(1)	120.78(16)
O(7)-La(1)-N(4)	70.35(8)	C(9)-N(3)-La(1)	120.08(17)
O(2)-La(1)-N(4)	133.37(8)	C(10)-N(4)-La(1)	122.30(18)
O(10)-La(1)-N(2)	72.35(7)	N(5)-N(4)-La(1)	131.70(17)
O(4)-La(1)-N(2)	142.24(9)	N(6)-O(1)-La(1)	99.12(18)

O(8)-La(1)-N(2)	138.08(8)	N(6)-O(2)-La(1)	96.67(16)
O(1)-La(1)-N(2)	72.38(8)	N(7)-O(4)-La(1)	99.93(17)
O(7)-La(1)-N(2)	94.05(8)	N(7)-O(5)-La(1)	93.82(17)
O(2)-La(1)-N(2)	70.27(8)	N(8)-O(7)-La(1)	96.01(17)
N(4)-La(1)-N(2)	121.40(7)	N(8)-O(8)-La(1)	97.75(17)
O(10)-La(1)-O(5)	73.09(7)	C(14)-O(10)-La(1)	129.23(17)
Complex **2**			
Ce(1)-O(10)	2.5133(18)	Ce(1)-N(2)	2.612(2)
Ce(1)-O(4)	2.541(2)	Ce(1)-O(8)	2.619(2)
Ce(1)-O(2)	2.567(2)	Ce(1)-N(4)	2.623(2)
Ce(1)-O(7)	2.582(2)	Ce(1)-O(5)	2.670(2)
Ce(1)-O(1)	2.606(2)	Ce(1)-N(3)	2.704(2)
O(10)-Ce(1)-O(4)	121.29(7)	O(4)-Ce(1)-O(5)	48.92(7)
O(10)-Ce(1)-O(2)	77.54(7)	O(2)-Ce(1)-O(5)	68.84(7)
O(4)-Ce(1)-O(2)	78.44(8)	O(7)-Ce(1)-O(5)	99.46(7)
O(10)-Ce(1)-O(7)	128.00(6)	O(1)-Ce(1)-O(5)	113.95(7)
O(4)-Ce(1)-O(7)	72.67(8)	N(2)-Ce(1)-O(5)	111.41(7)
O(2)-Ce(1)-O(7)	148.79(7)	O(8)-Ce(1)-O(5)	65.66(7)
O(10)-Ce(1)-O(1)	73.70(7)	N(4)-Ce(1)-O(5)	125.34(7)
O(4)-Ce(1)-O(1)	122.87(8)	O(10)-Ce(1)-N(3)	122.28(6)
O(2)-Ce(1)-O(1)	49.37(6)	O(4)-Ce(1)-N(3)	116.39(7)
O(7)-Ce(1)-O(1)	145.33(7)	O(2)-Ce(1)-N(3)	117.14(6)
O(10)-Ce(1)-N(2)	141.90(7)	O(7)-Ce(1)-N(3)	67.77(7)
O(4)-Ce(1)-N(2)	71.04(7)	O(1)-Ce(1)-N(3)	77.72(6)
O(2)-Ce(1)-N(2)	69.77(7)	N(2)-Ce(1)-N(3)	61.21(7)
O(7)-Ce(1)-N(2)	89.59(7)	O(8)-Ce(1)-N(3)	108.34(6)
O(1)-Ce(1)-N(2)	70.35(7)	N(4)-Ce(1)-N(3)	61.11(7)
O(10)-Ce(1)-O(8)	83.66(6)	O(5)-Ce(1)-N(3)	164.32(7)
O(4)-Ce(1)-O(8)	76.43(8)	C(4)-N(2)-Ce(1)	122.63(17)

O(2)-Ce(1)-O(8)	134.12(6)	N(1)-N(2)-Ce(1)	131.88(16)
O(7)-Ce(1)-O(8)	48.83(6)	C(9)-N(3)-Ce(1)	120.52(16)
O(1)-Ce(1)-O(8)	155.73(7)	C(5)-N(3)-Ce(1)	120.42(16)
N(2)-Ce(1)-O(8)	133.55(7)	C(10)-N(4)-Ce(1)	122.59(17)
O(10)-Ce(1)-N(4)	72.16(7)	N(5)-N(4)-Ce(1)	132.52(18)
O(4)-Ce(1)-N(4)	142.37(8)	N(6)-O(1)-Ce(1)	95.76(16)
O(2)-Ce(1)-N(4)	138.26(7)	N(6)-O(2)-Ce(1)	97.73(15)
O(7)-Ce(1)-N(4)	72.46(8)	N(7)-O(4)-Ce(1)	99.97(17)
O(1)-Ce(1)-N(4)	94.15(7)	N(7)-O(5)-Ce(1)	93.79(16)
N(2)-Ce(1)-N(4)	122.19(7)	N(8)-O(7)-Ce(1)	98.87(16)
O(8)-Ce(1)-N(4)	70.19(7)	N(8)-O(8)-Ce(1)	96.63(15)
O(10)-Ce(1)-O(5)	72.49(7)	C(14)-O(10)-Ce(1)	129.25(17)
Complex **3**			
Pr(1)-O(10)	2.4996(19)	Pr(1)-O(8)	2.597(2)
Pr(1)-O(4)	2.513(2)	Pr(1)-N(2)	2.599(2)
Pr(1)-O(2)	2.550(2)	Pr(1)-N(4)	2.612(2)
Pr(1)-O(7)	2.558(2)	Pr(1)-O(5)	2.663(2)
Pr(1)-O(1)	2.587(2)	Pr(1)-N(3)	2.682(2)
O(10)-Pr(1)-O(4)	121.18(7)	O(4)-Pr(1)-O(5)	49.01(7)
O(10)-Pr(1)-O(2)	77.46(7)	O(2)-Pr(1)-O(5)	68.60(7)
O(4)-Pr(1)-O(2)	78.15(8)	O(7)-Pr(1)-O(5)	99.69(8)
O(10)-Pr(1)-O(7)	128.25(7)	O(1)-Pr(1)-O(5)	113.97(7)
O(4)-Pr(1)-O(7)	72.78(9)	O(8)-Pr(1)-O(5)	65.42(7)
O(2)-Pr(1)-O(7)	148.60(8)	N(2)-Pr(1)-O(5)	111.35(8)
O(10)-Pr(1)-O(1)	73.57(7)	N(4)-Pr(1)-O(5)	125.04(8)
O(4)-Pr(1)-O(1)	122.96(8)	O(10)-Pr(1)-N(3)	122.30(7)
O(2)-Pr(1)-O(1)	49.74(7)	O(4)-Pr(1)-N(3)	116.49(7)
O(7)-Pr(1)-O(1)	145.11(7)	O(2)-Pr(1)-N(3)	117.23(7)
O(10)-Pr(1)-O(8)	83.47(7)	O(7)-Pr(1)-N(3)	67.71(7)

O(4)-Pr(1)-O(8)	76.47(8)	O(1)-Pr(1)-N(3)	77.55(7)
O(2)-Pr(1)-O(8)	133.64(7)	O(8)-Pr(1)-N(3)	108.73(7)
O(7)-Pr(1)-O(8)	49.32(7)	N(2)-Pr(1)-N(3)	61.31(7)
O(1)-Pr(1)-O(8)	155.44(7)	N(4)-Pr(1)-N(3)	61.40(7)
O(10)-Pr(1)-N(2)	141.91(8)	O(5)-Pr(1)-N(3)	164.52(7)
O(4)-Pr(1)-N(2)	70.84(8)	C(10)-N(2)-Pr(1)	122.61(19)
O(2)-Pr(1)-N(2)	69.80(7)	N(1)-N(2)-Pr(1)	131.39(17)
O(7)-Pr(1)-N(2)	89.36(7)	C(5)-N(3)-Pr(1)	120.58(17)
O(1)-Pr(1)-N(2)	70.59(8)	C(9)-N(3)-Pr(1)	120.44(17)
O(8)-Pr(1)-N(2)	133.64(7)	C(4)-N(4)-Pr(1)	122.32(19)
O(10)-Pr(1)-N(4)	71.98(7)	N(5)-N(4)-Pr(1)	132.46(19)
O(4)-Pr(1)-N(4)	142.54(9)	N(6)-O(1)-Pr(1)	95.61(18)
O(2)-Pr(1)-N(4)	138.28(8)	N(6)-O(2)-Pr(1)	97.46(16)
O(7)-Pr(1)-N(4)	72.67(8)	N(7)-O(4)-Pr(1)	100.64(18)
O(1)-Pr(1)-N(4)	93.95(8)	N(7)-O(5)-Pr(1)	93.47(17)
O(8)-Pr(1)-N(4)	70.24(8)	N(8)-O(7)-Pr(1)	98.88(17)
N(2)-Pr(1)-N(4)	122.59(7)	N(8)-O(8)-Pr(1)	96.34(16)
O(10)-Pr(1)-O(5)	72.30(7)	C(14)-O(10)-Pr(1)	129.12(17)
Complex **4**			
Nd(1)-O(10)	2.489(2)	Nd(1)-O(8)	2.586(3)
Nd(1)-O(4)	2.501(3)	Nd(1)-N(2)	2.587(3)
Nd(1)-O(2)	2.534(3)	Nd(1)-N(4)	2.594(3)
Nd(1)-O(7)	2.537(3)	Nd(1)-O(5)	2.656(2)
Nd(1)-O(1)	2.569(3)	Nd(1)-N(3)	2.667(3)
O(10)-Nd(1)-O(4)	121.01(8)	O(4)-Nd(1)-O(5)	49.25(8)
O(10)-Nd(1)-O(2)	77.18(8)	O(2)-Nd(1)-O(5)	68.35(8)
O(4)-Nd(1)-O(2)	78.22(9)	O(7)-Nd(1)-O(5)	99.78(9)
O(10)-Nd(1)-O(7)	128.52(8)	O(1)-Nd(1)-O(5)	114.09(8)
O(4)-Nd(1)-O(7)	72.46(10)	O(8)-Nd(1)-O(5)	65.12(8)

O(2)-Nd(1)-O(7)	148.40(9)	N(2)-Nd(1)-O(5)	111.10(9)
O(10)-Nd(1)-O(1)	73.61(8)	N(4)-Nd(1)-O(5)	124.70(9)
O(4)-Nd(1)-O(1)	123.34(9)	O(10)-Nd(1)-N(3)	122.41(8)
O(2)-Nd(1)-O(1)	50.17(8)	O(4)-Nd(1)-N(3)	116.55(8)
O(7)-Nd(1)-O(1)	144.92(8)	O(2)-Nd(1)-N(3)	117.45(8)
O(10)-Nd(1)-O(8)	83.27(8)	O(7)-Nd(1)-N(3)	67.79(9)
O(4)-Nd(1)-O(8)	76.23(9)	O(1)-Nd(1)-N(3)	77.29(8)
O(2)-Nd(1)-O(8)	133.10(8)	O(8)-Nd(1)-N(3)	109.08(8)
O(7)-Nd(1)-O(8)	49.72(8)	N(2)-Nd(1)-N(3)	61.72(8)
O(1)-Nd(1)-O(8)	155.24(8)	N(4)-Nd(1)-N(3)	61.58(9)
O(10)-Nd(1)-N(2)	142.06(9)	O(5)-Nd(1)-N(3)	164.83(8)
O(4)-Nd(1)-N(2)	70.45(9)	C(4)-N(2)-Nd(1)	122.5(2)
O(2)-Nd(1)-N(2)	69.93(9)	N(1)-N(2)-Nd(1)	131.8(2)
O(7)-Nd(1)-N(2)	89.05(9)	C(9)-N(3)-Nd(1)	120.7(2)
O(1)-Nd(1)-N(2)	70.99(9)	C(5)-N(3)-Nd(1)	120.5(2)
O(8)-Nd(1)-N(2)	133.48(9)	C(10)-N(4)-Nd(1)	122.4(2)
O(10)-Nd(1)-N(4)	71.94(9)	N(5)-N(4)-Nd(1)	132.4(2)
O(4)-Nd(1)-N(4)	142.44(10)	N(6)-O(1)-Nd(1)	95.6(2)
O(2)-Nd(1)-N(4)	138.19(9)	N(6)-O(2)-Nd(1)	97.1(2)
O(7)-Nd(1)-N(4)	73.02(9)	N(7)-O(4)-Nd(1)	100.4(2)
O(1)-Nd(1)-N(4)	93.69(9)	N(7)-O(5)-Nd(1)	93.04(19)
O(8)-Nd(1)-N(4)	70.36(9)	N(8)-O(7)-Nd(1)	98.9(2)
N(2)-Nd(1)-N(4)	123.20(9)	N(8)-O(8)-Nd(1)	95.98(19)
O(10)-Nd(1)-O(5)	71.88(8)	C(14)-O(10)-Nd(1)	129.4(2)
Complex **5**			
Sm(1)-O(10)	2.4590(19)	Sm(1)-O(4)	2.473(2)
Sm(1)-O(7)	2.504(2)	Sm(1)-O(2)	2.505(2)
Sm(1)-O(1)	2.539(2)	Sm(1)-N(2)	2.554(2)
Sm(1)-O(8)	2.558(2)	Sm(1)-N(4)	2.562(2)

Sm(1)-N(3)	2.643(2)	Sm(1)-O(5)	2.645(2)
O(10)-Sm(1)-O(4)	120.53(7)	O(10)-Sm(1)-O(7)	128.82(7)
O(4)-Sm(1)-O(7)	72.64(9)	O(10)-Sm(1)-O(2)	76.71(7)
O(4)-Sm(1)-O(2)	77.88(8)	O(7)-Sm(1)-O(2)	148.31(8)
O(10)-Sm(1)-O(1)	73.49(7)	O(4)-Sm(1)-O(1)	123.48(8)
O(7)-Sm(1)-O(1)	144.76(7)	O(2)-Sm(1)-O(1)	50.69(7)
O(10)-Sm(1)-N(2)	141.72(8)	O(4)-Sm(1)-N(2)	70.22(8)
O(7)-Sm(1)-N(2)	89.17(8)	O(2)-Sm(1)-N(2)	69.84(7)
O(1)-Sm(1)-N(2)	71.13(8)	O(10)-Sm(1)-O(8)	83.02(7)
O(4)-Sm(1)-O(8)	76.22(8)	O(7)-Sm(1)-O(8)	50.24(7)
O(2)-Sm(1)-O(8)	132.31(7)	O(1)-Sm(1)-O(8)	154.87(7)
N(2)-Sm(1)-O(8)	133.78(8)	O(10)-Sm(1)-N(4)	72.00(8)
O(4)-Sm(1)-N(4)	142.50(9)	O(7)-Sm(1)-N(4)	73.15(8)
O(2)-Sm(1)-N(4)	138.24(8)	O(1)-Sm(1)-N(4)	93.58(8)
N(2)-Sm(1)-N(4)	124.01(8)	O(8)-Sm(1)-N(4)	70.30(8)
O(10)-Sm(1)-N(3)	122.61(7)	O(4)-Sm(1)-N(3)	116.84(7)
O(7)-Sm(1)-N(3)	67.92(7)	O(2)-Sm(1)-N(3)	117.68(7)
O(1)-Sm(1)-N(3)	76.98(7)	N(2)-Sm(1)-N(3)	62.12(7)
O(8)-Sm(1)-N(3)	109.67(7)	N(4)-Sm(1)-N(3)	61.98(7)
O(10)-Sm(1)-O(5)	71.28(7)	O(4)-Sm(1)-O(5)	49.38(7)
O(7)-Sm(1)-O(5)	100.10(8)	O(2)-Sm(1)-O(5)	67.84(7)
O(1)-Sm(1)-O(5)	114.01(7)	N(2)-Sm(1)-O(5)	110.86(8)
O(8)-Sm(1)-O(5)	64.84(8)	N(4)-Sm(1)-O(5)	124.21(8)
N(3)-Sm(1)-O(5)	165.31(8)	C(4)-N(2)-Sm(1)	122.39(19)
N(1)-N(2)-Sm(1)	131.75(18)	C(9)-N(3)-Sm(1)	120.66(18)
C(5)-N(3)-Sm(1)	120.43(18)	C(10)-N(4)-Sm(1)	122.49(19)
N(5)-N(4)-Sm(1)	132.64(19)	N(6)-O(1)-Sm(1)	95.14(17)
N(6)-O(2)-Sm(1)	96.96(16)	N(7)-O(4)-Sm(1)	100.74(18)
N(7)-O(5)-Sm(1)	92.55(18)	N(8)-O(7)-Sm(1)	98.71(17)

N(8)-O(8)-Sm(1)	95.53(16)	C(14)-O(10)-Sm(1)	129.47(18)
Complex **6**			
Eu(1)-O(10)	2.452(2)	Eu(1)-O(8)	2.545(2)
Eu(1)-O(4)	2.458(3)	Eu(1)-N(2)	2.544(3)
Eu(1)-O(7)	2.487(3)	Eu(1)-N(4)	2.555(3)
Eu(1)-O(2)	2.492(2)	Eu(1)-N(3)	2.634(3)
Eu(1)-O(1)	2.525(2)	Eu(1)-O(5)	2.649(2)
O(10)-Eu(1)-O(4)	120.34(8)	O(4)-Eu(1)-N(3)	116.81(8)
O(10)-Eu(1)-O(7)	129.05(8)	O(7)-Eu(1)-N(3)	67.82(8)
O(4)-Eu(1)-O(7)	72.43(9)	O(2)-Eu(1)-N(3)	117.79(8)
O(10)-Eu(1)-O(2)	76.52(8)	O(1)-Eu(1)-N(3)	76.98(8)
O(4)-Eu(1)-O(2)	78.01(9)	O(8)-Eu(1)-N(3)	109.89(8)
O(7)-Eu(1)-O(2)	148.20(8)	N(2)-Eu(1)-N(3)	62.38(8)
O(10)-Eu(1)-O(1)	73.40(8)	N(4)-Eu(1)-N(3)	62.26(8)
O(4)-Eu(1)-O(1)	123.85(9)	O(10)-Eu(1)-O(5)	70.79(8)
O(7)-Eu(1)-O(1)	144.66(8)	O(4)-Eu(1)-O(5)	49.68(8)
O(2)-Eu(1)-O(1)	50.90(8)	O(7)-Eu(1)-O(5)	100.28(8)
O(10)-Eu(1)-O(8)	82.82(8)	O(2)-Eu(1)-O(5)	67.78(8)
O(4)-Eu(1)-O(8)	76.02(9)	O(1)-Eu(1)-O(5)	113.99(8)
O(7)-Eu(1)-O(8)	50.62(8)	O(8)-Eu(1)-O(5)	64.55(8)
O(2)-Eu(1)-O(8)	131.98(8)	N(2)-Eu(1)-O(5)	110.85(8)
O(1)-Eu(1)-O(8)	154.58(8)	N(4)-Eu(1)-O(5)	123.76(9)
O(10)-Eu(1)-N(2)	141.72(9)	N(3)-Eu(1)-O(5)	165.55(8)
O(4)-Eu(1)-N(2)	70.06(9)	C(4)-N(2)-Eu(1)	122.3(2)
O(7)-Eu(1)-N(2)	89.00(9)	N(1)-N(2)-Eu(1)	132.0(2)
O(2)-Eu(1)-N(2)	69.81(8)	C(9)-N(3)-Eu(1)	120.4(2)
O(1)-Eu(1)-N(2)	71.45(9)	C(5)-N(3)-Eu(1)	120.4(2)
O(8)-Eu(1)-N(2)	133.79(9)	C(10)-N(4)-Eu(1)	122.3(2)
O(10)-Eu(1)-N(4)	71.85(8)	N(5)-N(4)-Eu(1)	132.6(2)

O(4)-Eu(1)-N(4)	142.48(10)	N(6)-O(1)-Eu(1)	95.58(19)
O(7)-Eu(1)-N(4)	73.52(9)	N(6)-O(2)-Eu(1)	97.60(18)
O(2)-Eu(1)-N(4)	138.01(9)	N(7)-O(4)-Eu(1)	101.4(2)
O(1)-Eu(1)-N(4)	93.28(9)	N(7)-O(5)-Eu(1)	92.14(19)
O(8)-Eu(1)-N(4)	70.41(9)	N(8)-O(7)-Eu(1)	98.9(2)
N(2)-Eu(1)-N(4)	124.54(9)	N(8)-O(8)-Eu(1)	95.49(18)
O(10)-Eu(1)-N(3)	122.83(8)	C(14)-O(10)-Eu(1)	129.53(19)
Complex **7**			
Gd(1)-O(10)	2.437(2)	Gd(1)-O(8)	2.534(2)
Gd(1)-O(4)	2.446(2)	Gd(1)-N(2)	2.538(2)
Gd(1)-O(7)	2.473(2)	Gd(1)-N(4)	2.540(3)
Gd(1)-O(2)	2.484(2)	Gd(1)-N(3)	2.623(2)
Gd(1)-O(1)	2.508(2)	Gd(1)-O(5)	2.654(2)
O(10)-Gd(1)-O(4)	120.18(7)	O(4)-Gd(1)-N(3)	116.84(8)
O(10)-Gd(1)-O(7)	128.96(7)	O(7)-Gd(1)-N(3)	67.81(8)
O(4)-Gd(1)-O(7)	72.49(9)	O(2)-Gd(1)-N(3)	118.09(7)
O(10)-Gd(1)-O(2)	76.36(7)	O(1)-Gd(1)-N(3)	76.85(7)
O(4)-Gd(1)-O(2)	77.88(8)	O(8)-Gd(1)-N(3)	110.04(7)
O(7)-Gd(1)-O(2)	148.24(8)	N(2)-Gd(1)-N(3)	62.36(8)
O(10)-Gd(1)-O(1)	73.57(7)	N(4)-Gd(1)-N(3)	62.42(8)
O(4)-Gd(1)-O(1)	123.93(8)	O(10)-Gd(1)-O(5)	70.53(7)
O(7)-Gd(1)-O(1)	144.52(7)	O(4)-Gd(1)-O(5)	49.77(8)
O(2)-Gd(1)-O(1)	51.25(7)	O(7)-Gd(1)-O(5)	100.45(8)
O(10)-Gd(1)-O(8)	82.61(7)	O(2)-Gd(1)-O(5)	67.38(7)
O(4)-Gd(1)-O(8)	76.00(8)	O(1)-Gd(1)-O(5)	113.98(7)
O(7)-Gd(1)-O(8)	50.75(7)	O(8)-Gd(1)-O(5)	64.53(7)
O(2)-Gd(1)-O(8)	131.54(7)	N(2)-Gd(1)-O(5)	110.88(8)
O(1)-Gd(1)-O(8)	154.52(8)	N(4)-Gd(1)-O(5)	123.60(8)
O(10)-Gd(1)-N(2)	141.88(8)	N(3)-Gd(1)-O(5)	165.69(7)

O(4)-Gd(1)-N(2)	70.04(8)	C(4)-N(2)-Gd(1)	122.5(2)
O(7)-Gd(1)-N(2)	88.95(8)	N(1)-N(2)-Gd(1)	131.62(18)
O(2)-Gd(1)-N(2)	70.12(8)	C(9)-N(3)-Gd(1)	120.82(19)
O(1)-Gd(1)-N(2)	71.50(8)	C(5)-N(3)-Gd(1)	120.57(19)
O(8)-Gd(1)-N(2)	133.80(8)	C(10)-N(4)-Gd(1)	122.4(2)
O(10)-Gd(1)-N(4)	71.79(8)	N(5)-N(4)-Gd(1)	132.52(19)
O(4)-Gd(1)-N(4)	142.47(9)	N(6)-O(1)-Gd(1)	95.35(18)
O(7)-Gd(1)-N(4)	73.51(8)	N(6)-O(2)-Gd(1)	96.78(17)
O(2)-Gd(1)-N(4)	138.03(8)	N(7)-O(4)-Gd(1)	101.41(19)
O(1)-Gd(1)-N(4)	93.23(8)	N(7)-O(5)-Gd(1)	91.62(18)
O(8)-Gd(1)-N(4)	70.38(8)	N(8)-O(7)-Gd(1)	98.57(17)
N(2)-Gd(1)-N(4)	124.68(8)	N(8)-O(8)-Gd(1)	94.95(17)
O(10)-Gd(1)-N(3)	122.95(7)	C(14)-O(10)-Gd(1)	129.33(18)
Complex **8**			
Tb(1)-O(10)	2.425(2)	Tb(1)-N(4)	2.524(3)
Tb(1)-O(5)	2.437(2)	Tb(1)-O(2)	2.526(2)
Tb(1)-O(1)	2.465(2)	Tb(1)-N(2)	2.529(3)
Tb(1)-O(8)	2.471(2)	Tb(1)-N(3)	2.611(3)
Tb(1)-O(7)	2.503(2)	Tb(1)-O(4)	2.668(2)
O(10)-Tb(1)-O(5)	119.85(8)	O(5)-Tb(1)-N(3)	117.29(8)
O(10)-Tb(1)-O(1)	129.18(7)	O(1)-Tb(1)-N(3)	68.01(8)
O(5)-Tb(1)-O(1)	72.64(9)	O(8)-Tb(1)-N(3)	118.22(7)
O(10)-Tb(1)-O(8)	76.17(7)	O(7)-Tb(1)-N(3)	76.63(8)
O(5)-Tb(1)-O(8)	77.52(8)	N(4)-Tb(1)-N(3)	62.69(8)
O(1)-Tb(1)-O(8)	148.06(8)	O(2)-Tb(1)-N(3)	110.57(7)
O(10)-Tb(1)-O(7)	73.52(7)	N(2)-Tb(1)-N(3)	62.42(8)
O(5)-Tb(1)-O(7)	123.85(8)	O(10)-Tb(1)-O(4)	70.34(7)
O(1)-Tb(1)-O(7)	144.48(8)	O(5)-Tb(1)-O(4)	49.62(8)
O(8)-Tb(1)-O(7)	51.50(7)	O(1)-Tb(1)-O(4)	100.68(8)

O(10)-Tb(1)-N(4)	141.76(8)	O(8)-Tb(1)-O(4)	66.91(7)
O(5)-Tb(1)-N(4)	69.91(8)	O(7)-Tb(1)-O(4)	113.76(8)
O(1)-Tb(1)-N(4)	88.89(8)	N(4)-Tb(1)-O(4)	110.55(8)
O(8)-Tb(1)-N(4)	70.09(8)	O(2)-Tb(1)-O(4)	64.38(8)
O(7)-Tb(1)-N(4)	71.62(8)	N(2)-Tb(1)-O(4)	123.63(8)
O(10)-Tb(1)-O(2)	82.39(7)	N(3)-Tb(1)-O(4)	166.10(8)
O(5)-Tb(1)-O(2)	75.95(8)	N(6)-O(1)-Tb(1)	98.18(18)
O(1)-Tb(1)-O(2)	51.20(7)	N(6)-O(2)-Tb(1)	94.90(17)
O(8)-Tb(1)-O(2)	130.92(7)	N(7)-O(4)-Tb(1)	91.26(19)
O(7)-Tb(1)-O(2)	154.32(8)	N(7)-O(5)-Tb(1)	102.29(19)
N(4)-Tb(1)-O(2)	133.94(8)	N(8)-O(7)-Tb(1)	94.91(18)
O(10)-Tb(1)-N(2)	71.85(8)	N(8)-O(8)-Tb(1)	96.58(17)
O(5)-Tb(1)-N(2)	142.62(9)	C(15)-O(10)-Tb(1)	129.52(19)
O(1)-Tb(1)-N(2)	73.66(8)	C(4)-N(2)-Tb(1)	122.8(2)
O(8)-Tb(1)-N(2)	138.09(8)	N(1)-N(2)-Tb(1)	132.4(2)
O(7)-Tb(1)-N(2)	93.20(8)	C(9)-N(3)-Tb(1)	120.64(19)
N(4)-Tb(1)-N(2)	125.03(8)	C(5)-N(3)-Tb(1)	121.0(2)
O(2)-Tb(1)-N(2)	70.54(8)	C(10)-N(4)-Tb(1)	122.7(2)
O(10)-Tb(1)-N(3)	122.84(7)	N(5)-N(4)-Tb(1)	131.7(2)

Table S2 Hydrogen bond lengths (Å) and angles (°) for the complexes **1**-**8**

D–H···A	d(D–H)/Å	d(H···A)/Å	d(D···A)/Å	∠D–H···A/°
Complex **1**				
N(1)-H(1)...O(5)#1	0.86	2.31	3.136(3)	161.4
O(10)-H(10)...O(2)#1	0.93	1.86	2.752(3)	159.0
C(1)-H(1C)...O(6)#1	0.84	2.50	3.265(6)	151.0
N(5)-H(5)...O(8)#2	0.86	2.45	3.167(3)	141.8
Complex **2**				
N(5)-H(5)...O(5)#1	0.86	2.29	3.125(3)	162.3

O(10)-H(10)...O(8)#1	0.93	1.88	2.762(3)	158.3
N(1)-H(1)...O(2)#2	0.86	2.49	3.194(3)	140.2
C(1)-H(1C)...O(2)#2	0.94	2.57	3.362(4)	142.4
Complex **3**				
N(5)-H(5)...O(5)#1	0.86	2.28	3.113(3)	163.0
O(10)-H(10)...O(8)#1	0.93	1.89	2.771(3)	158.0
Complex **4**				
N(5)-H(5)...O(5)#1	0.86	2.28	3.109(4)	163.0
O(10)-H(10)...O(8)#1	0.93	1.90	2.781(3)	157.1
C(1)-H(1C)...O(2)#2	0.95	2.48	3.349(5)	151.8
Complex **5**				
N(5)-H(5)...O(5)#1	0.86	2.25	3.092(4)	164.6
O(10)-H(10)...O(8)#1	0.93	1.92	2.793(3)	156.1
C(13)-H(13B)...O(6)#1	0.99	2.34	3.235(6)	149.0
Complex **6**				
N(5)-H(5)...O(5)#1	0.86	2.24	3.076(4)	164.0
O(10)-H(10)...O(8)#1	0.93	1.93	2.800(3)	155.4
C(13)-H(13D)...O(6)#1	0.98	2.32	3.225(6)	152.7
Complex **7**				
N(5)-H(5)...O(5)#1	0.86	2.23	3.063(4)	164.3
O(10)-H(10)...O(8)#1	0.93	1.94	2.812(3)	155.0
C(13)-H(13C)...O(6)#1	0.91	2.38	3.222(6)	155.1
Complex **8**				
O(10)-H(10)...O(2)#1	0.93	1.96	2.827(3)	154.6
N(1)-H(1)...O(4)#1	0.86	2.22	3.056(4)	164.8

*Symmetry transformation used to generate equivalent atoms: complex **1**: #1 -x+1,-y,-z; #2 -x+1,-y,-z+1; complex **2**: #1 -x,-y,-z ; #2 -x,-y,-z+1; complex **3**: #1 -x+1,-y+2,-z+1; complex **4**: #1 -x+1,-y+1,-z+1; #2 -x+1,-y+1,-z; complex **5**: #1 2-x, 1-y,1-z; complex **6**: #1 -x,-y,-z; complex **7**: #1 -x+1,-y+1,-z+2; complex **8**: #1 -x+2,-y+1,-z+1.

Table S3 IR data for the complexes **1-8**

Complex	IR data (KBr, cm^{-1})
1	3446, 3250, 3074, 3045, 2928, 2849, 1638, 1605, 1509, 1457, 1446
2	3414, 3347, 3074, 3049, 2934, 2865, 1635, 1599, 1588, 1492, 1459
3	3451, 3335, 3093, 3082, 2995, 2961, 1638, 1589, 1559, 1497, 1462
4	3414, 3336, 3121, 3082, 2984, 2925, 1638, 1577, 1522, 1483, 1444
5	3422, 3347, 3090, 3080, 2929, 2854, 1638, 1570, 1510, 1471, 1442
6	3446, 3387, 3133, 3045, 2967, 2928, 1638, 1580, 1521, 1482, 1436
7	3421, 3353, 3137, 3089, 2971, 2932, 1635, 1576, 1517, 1478, 1439
8	3430, 3336, 3103, 3067, 2958, 2902, 1637, 1585, 1532, 1480, 1446