Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Lanthanide CPs: the Guest-Tunable Drastic Changes of Luminescent Quantum Yields, and Two Photon Luminescence

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Table S1. Selective bond lengths and angles for **1**, **2**, **3a**, **3b**, **3c** and **4**.

1

Tb(1)-O(4)	2.2264(19)	Tb(1)-O(3)	2.3463(19)
Tb(1)-O(2)	2.285(2)	Tb(1)-N(4)	2.612(3)
Tb(1)-O(6)	2.3276(19)	Tb(1)-O(5)	2.877(2)
Tb(1)-O(1)	2.3309(19)	Tb(1)-Tb(1)#1	3.9802(3)
Tb(1)-O(5)#1	2.343(2)		
O(4)-Tb(1)-O(2)	111.29(8)	O(5)#1-Tb(1)-O(3)	140.11(7)
O(2)-Tb(1)-O(6)	146.56(7)	O(4)-Tb(1)-N(4)	73.08(8)
O(4)-Tb(1)-O(1)	91.73(8)	O(2)-Tb(1)-N(4)	146.82(8)
O(2)-Tb(1)-O(1)	96.08(7)	O(6)-Tb(1)-N(4)	74.50(8)
O(6)-Tb(1)-O(1)	135.29(7)	O(1)-Tb(1)-N(4)	73.72(8)
O(4)-Tb(1)-O(5)#1	82.49(7)	O(5)#1-Tb(1)-N(4)	137.97(8)
O(2)-Tb(1)-O(5)#1	82.01(8)	O(3)-Tb(1)-N(4)	73.88(8)
O(6)-Tb(1)-O(5)#1	73.84(7)	O(4)-Tb(1)-O(5)	161.82(7)
O(1)-Tb(1)-O(5)#1	129.05(7)	O(2)-Tb(1)-O(5)	70.24(7)
O(4)-Tb(1)-O(3)	75.95(7)	O(6)-Tb(1)-O(5)	48.34(6)
O(2)-Tb(1)-O(3)	89.38(7)	O(1)-Tb(1)-O(5)	73.20(7)
O(6)-Tb(1)-O(3)	73.32(7)	O(5)#1-Tb(1)-O(5)	81.14(7)
O(1)-Tb(1)-O(3)	73.89(7)	O(3)-Tb(1)-O(5)	107.99(6)
N(4)-Tb(1)-O(5)	116.19(8)		

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

2

Tb(1)-O(5)	2.269(3)	Tb(1)-O(2)	2.358(3)
Tb(1)-O(1)	2.300(3)	Tb(1)-O(6)	2.362(3)
Tb(1)-O(3)	2.328(3)	Tb(1)-O(8)	2.486(3)
Tb(1)-O(4)	2.341(3)		
O(5)-Tb(1)-O(1)	83.39(10)	O(2)-Tb(1)-O(6)	76.73(9)
O(5)-Tb(1)-O(3)	132.25(10)	O(5)-Tb(1)-O(8)	70.19(9)
O(1)-Tb(1)-O(3)	77.33(9)	O(1)-Tb(1)-O(8)	138.09(9)
O(5)-Tb(1)-O(4)	89.63(9)	O(3)-Tb(1)-O(8)	144.20(9)
O(1)-Tb(1)-O(4)	77.67(9)	O(4)-Tb(1)-O(8)	70.44(10)
O(3)-Tb(1)-O(4)	127.00(10)	O(2)-Tb(1)-O(8)	75.63(9)
O(5)-Tb(1)-O(2)	145.80(9)	O(6)-Tb(1)-O(8)	76.85(9)
O(1)-Tb(1)-O(2)	124.94(10)	O(5)-Tb(1)-O(7)	70.84(9)
O(3)-Tb(1)-O(2)	77.57(10)	O(1)-Tb(1)-O(7)	73.54(10)
O(4)-Tb(1)-O(2)	79.86(9)	O(3)-Tb(1)-O(7)	61.93(9)
O(5)-Tb(1)-O(6)	94.23(9)	O(4)-Tb(1)-O(7)	146.66(9)
O(1)-Tb(1)-O(6)	138.81(10)	O(2)-Tb(1)-O(7)	130.97(9)
O(3)-Tb(1)-O(6)	74.23(9)	O(6)-Tb(1)-O(7)	66.99(9)
O(4)-Tb(1)-O(6)	143.52(10)	O(8)-Tb(1)-O(7)	123.48(10)

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

3a

Tb(1)-O(12)	2.257(3)	Tb(1)-O(1)	2.361(3)
Tb(1)-O(7)	2.301(3)	Tb(1)-O(9)	2.362(3)
Tb(1)-O(5)	2.331(3)	Tb(1)-O(3)	2.395(3)
Tb(1)-O(2)#1	2.352(3)	Tb(1)-O(1)#1	2.868(4)
O(12)-Tb(1)-O(7)	112.23(11)	O(1)-Tb(1)-O(9)	137.31(11)
O(12)-Tb(1)-O(5)	98.47(11)	O(12)-Tb(1)-O(3)	76.12(12)
O(7)-Tb(1)-O(5)	133.85(11)	O(7)-Tb(1)-O(3)	147.31(11)
O(12)-Tb(1)-O(2)#1	148.61(11)	O(5)-Tb(1)-O(3)	71.54(11)
O(7)-Tb(1)-O(2)#1	84.99(12)	O(2)#1-Tb(1)-O(3)	75.87(12)
O(5)-Tb(1)-O(2)#1	85.82(11)	O(1)-Tb(1)-O(3)	138.33(11)
O(12)-Tb(1)-O(1)	82.70(12)	O(9)-Tb(1)-O(3)	76.52(11)
O(7)-Tb(1)-O(1)	74.11(11)	O(12)-Tb(1)-O(1)#1	160.77(11)
O(5)-Tb(1)-O(1)	76.74(11)	O(7)-Tb(1)-O(1)#1	70.14(10)
O(2)#1-Tb(1)-O(1)	128.24(12)	O(5)-Tb(1)-O(1)#1	70.02(10)
O(12)-Tb(1)-O(9)	85.37(11)	O(2)#1-Tb(1)-O(1)#1	48.59(10)
O(7)-Tb(1)-O(9)	72.93(11)	O(1)-Tb(1)-O(1)#1	79.69(12)
O(5)-Tb(1)-O(9)	145.75(11)	O(9)-Tb(1)-O(1)#1	112.94(10)
O(2)#1-Tb(1)-O(9)	74.58(11)	O(3)-Tb(1)-O(1)#1	112.74(11)

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

3b

Gd(1)-O(1)	2.261(5)	Gd(1)-O(2)#2	2.370(5)
Gd(1)-O(5)	2.314(5)	Gd(1)-O(3)	2.376(5)
Gd(1)-O(6)#1	2.341(5)	Gd(1)-O(7)	2.402(5)
Gd(1)-O(4)#1	2.359(5)	Gd(1)-O(3)#1	2.833(5)
O(1)-Gd(1)-O(5)	111.02(18)	O(2)#2-Gd(1)-O(3)	137.61(17)
O(1)-Gd(1)-O(6)#1	98.73(17)	O(1)-Gd(1)-O(7)	76.48(18)
O(5)-Gd(1)-O(6)#1	134.80(17)	O(5)-Gd(1)-O(7)	147.20(18)
O(5)-Gd(1)-O(4)#1	85.96(18)	O(6)#1-Gd(1)-O(7)	71.21(17)
O(6)#1-Gd(1)-O(4)#1	85.95(17)	O(2)#2-Gd(1)-O(7)	76.62(17)
O(1)-Gd(1)-O(2)#2	85.26(17)	O(3)-Gd(1)-O(7)	138.28(17)
O(5)-Gd(1)-O(2)#2	72.43(17)	O(1)-Gd(1)-O(3)#1	161.05(16)
O(6)#1-Gd(1)-O(2)#2	145.54(18)	O(5)-Gd(1)-O(3)#1	71.20(16)
O(4)#1-Gd(1)-O(2)#2	74.03(17)	O(6)#1-Gd(1)-O(3)#1	70.09(15)
O(1)-Gd(1)-O(3)	82.95(17)	O(4)#1-Gd(1)-O(3)#1	49.02(15)
O(5)-Gd(1)-O(3)	74.24(17)	O(2)#2-Gd(1)-O(3)#1	112.74(15)
O(6)#1-Gd(1)-O(3)	76.67(17)	O(3)-Gd(1)-O(3)#1	79.62(16)
O(4)#1-Gd(1)-O(3)	128.60(17)	O(7)-Gd(1)-O(3)#1	112.36(16)

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

3c

Eu(1)-O(1)	2.280(4)	Eu(1)-O(2)#2	2.385(4)
Eu(1)-O(5)	2.327(5)	Eu(1)-O(3)	2.393(4)
Eu(1)-O(6)#1	2.348(5)	Eu(1)-O(7)	2.416(4)
Eu(1)-O(4)#1	2.384(4)	Eu(1)-O(3)#1	2.811(5)
O(1)-Eu(1)-O(5)	110.87(15)	O(2)#2-Eu(1)-O(3)	138.00(15)
O(1)-Eu(1)-O(6)#1	98.26(16)	O(1)-Eu(1)-O(7)	76.48(16)
O(5)-Eu(1)-O(6)#1	135.16(16)	O(5)-Eu(1)-O(7)	147.18(16)
O(1)-Eu(1)-O(4)#1	147.75(16)	O(6)#1-Eu(1)-O(7)	71.16(16)
O(5)-Eu(1)-O(4)#1	86.15(16)	O(4)#1-Eu(1)-O(7)	75.02(17)
O(6)#1-Eu(1)-O(4)#1	86.55(16)	O(2)#2-Eu(1)-O(7)	76.38(15)
O(1)-Eu(1)-O(2)#2	85.32(15)	O(3)-Eu(1)-O(7)	138.24(16)
O(5)-Eu(1)-O(2)#2	72.58(15)	O(1)-Eu(1)-O(3)#1	161.16(14)
O(6)#1-Eu(1)-O(2)#2	145.39(15)	O(5)-Eu(1)-O(3)#1	71.33(14)
O(4)#1-Eu(1)-O(2)#2	73.61(15)	O(6)#1-Eu(1)-O(3)#1	70.58(14)
O(1)-Eu(1)-O(3)	83.06(16)	O(4)#1-Eu(1)-O(3)#1	49.23(14)
O(5)-Eu(1)-O(3)	74.29(16)	O(2)#2-Eu(1)-O(3)#1	112.60(14)
O(6)#1-Eu(1)-O(3)	76.38(15)	O(3)-Eu(1)-O(3)#1	79.60(15)
O(4)#1-Eu(1)-O(3)	128.80(16)	O(7)-Eu(1)-O(3)#1	112.32(15)

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

4

Tb(1)-O(3)	2.249(6)	Tb(1)-O(4)#2	2.348(6)
Tb(1)-O(5)	2.291(7)	Tb(1)-O(1)#1	2.382(7)
Tb(1)-O(6)#1	2.316(7)	Tb(1)-O(7)	2.391(7)
Tb(1)-O(2)	2.346(7)	Tb(1)-O(1)	2.779(7)
O(3)-Tb(1)-O(5)	111.8(2)	O(4)#2-Tb(1)-O(1)#1	133.6(2)
O(3)-Tb(1)-O(6)#1	96.6(2)	O(3)-Tb(1)-O(7)	77.2(2)
O(5)-Tb(1)-O(6)#1	135.1(2)	O(5)-Tb(1)-O(7)	147.3(2)
O(3)-Tb(1)-O(2)	148.8(2)	O(6)#1-Tb(1)-O(7)	70.7(2)
O(5)-Tb(1)-O(2)	84.2(2)	O(2)-Tb(1)-O(7)	75.7(2)
O(6)#1-Tb(1)-O(2)	88.9(2)	O(4)#2-Tb(1)-O(7)	78.6(2)
O(3)-Tb(1)-O(4)#2	84.4(2)	O(1)#1-Tb(1)-O(7)	139.7(2)
O(5)-Tb(1)-O(4)#2	71.5(2)	O(3)-Tb(1)-O(1)	159.9(2)
O(6)#1-Tb(1)-O(4)#2	148.2(2)	O(5)-Tb(1)-O(1)	70.7(2)
O(2)-Tb(1)-O(4)#2	75.4(2)	O(6)#1-Tb(1)-O(1)	71.3(2)
O(3)-Tb(1)-O(1)#1	82.4(2)	O(2)-Tb(1)-O(1)	49.6(2)
O(5)-Tb(1)-O(1)#1	72.7(2)	O(4)#2-Tb(1)-O(1)	114.6(2)
O(6)#1-Tb(1)-O(1)#1	77.7(2)	O(1)#1-Tb(1)-O(1)	79.4(2)
O(2)-Tb(1)-O(1)#1	128.7(2)	O(7)-Tb(1)-O(1)	112.0(2)

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

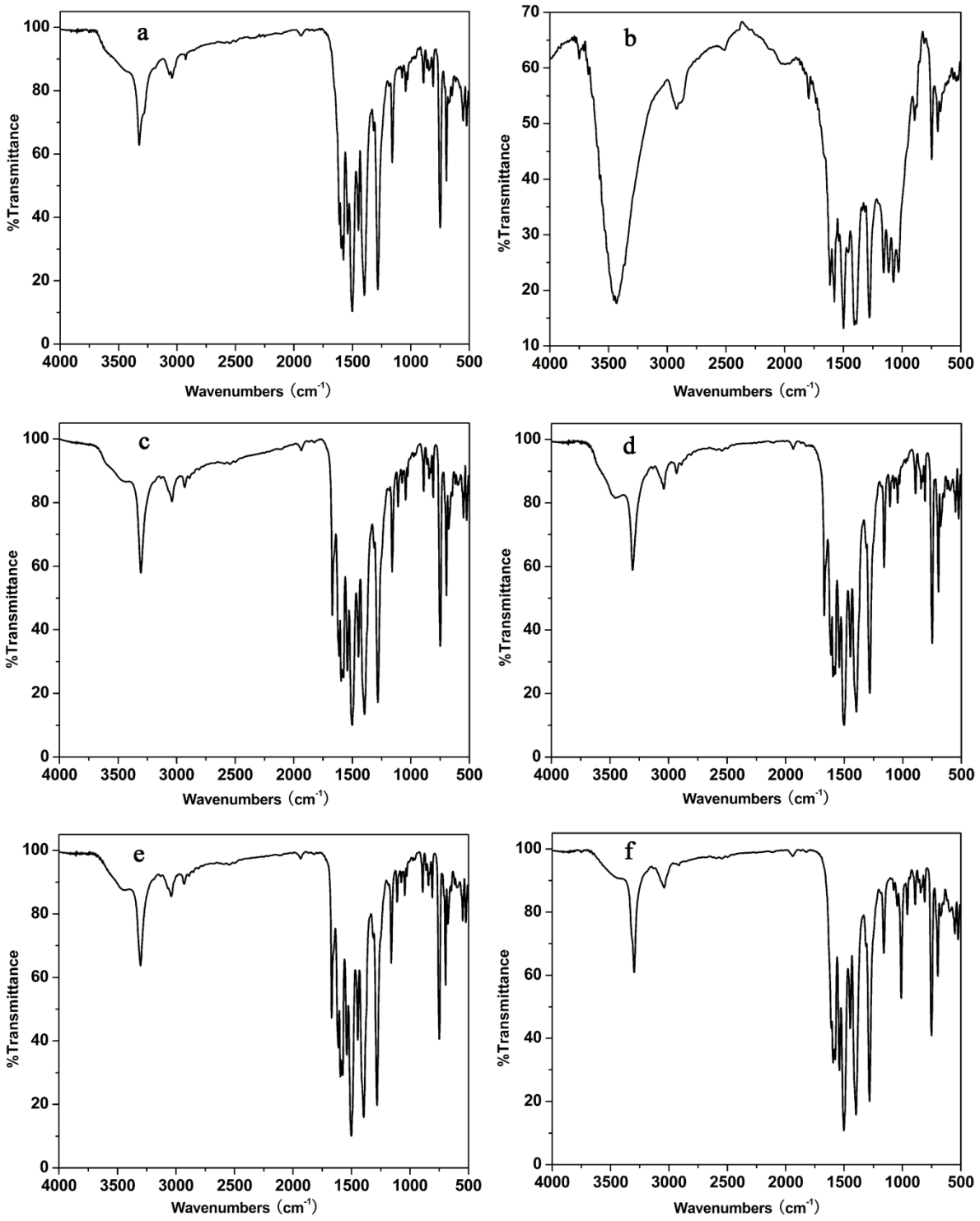

Figure S1. FT-IR spectra a-f corresponding to complexes **1**, **2**, **3a**, **3b**, **3c** and **4**, respectively.

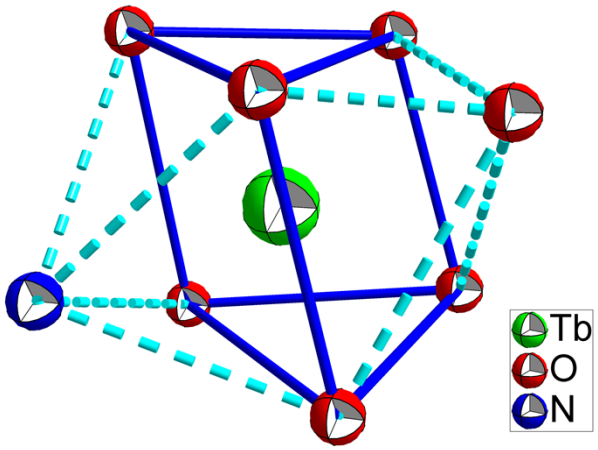

Figure S2. Arrangement of the one nitrogen and seven oxygen around Tb^{3+} in **1**.

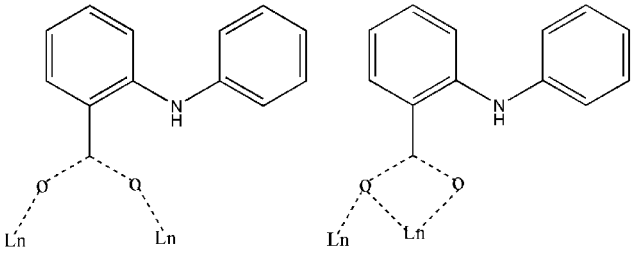

Figure S3. Coordination mode of ligands in **1**.

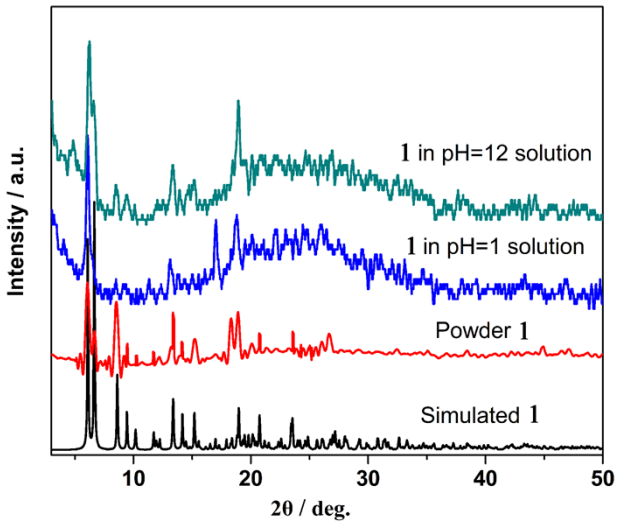

Figure S4. PXRD patterns of simulated **1**, as synthesized **1**, powder **1** in pH = 1 and pH = 12 water solution.

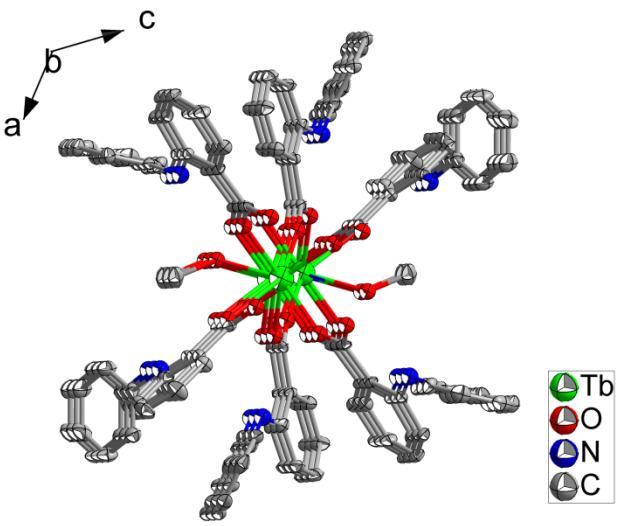

Figure S5. Octupolar-like structure of **2** along the *ob* direction.

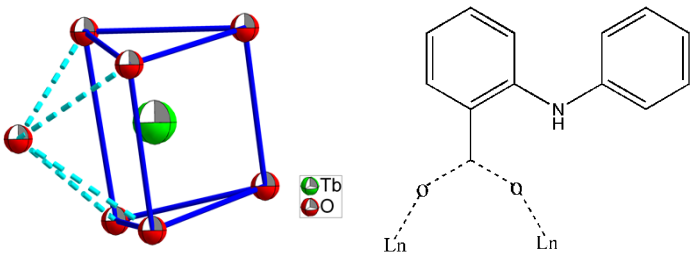

Figure S6. Arrangement of the seven oxygen around Tb^{3+} (left, a) and coordination mode of ligands in **2** (right, b).

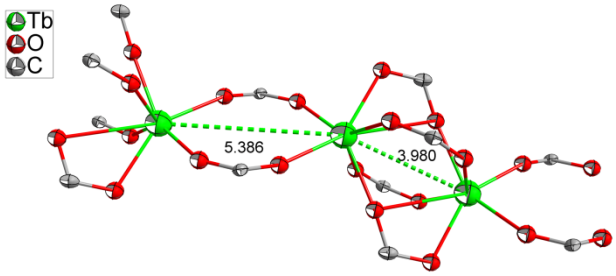

Figure S7. Short and long Tb···Tb distances in **2**.

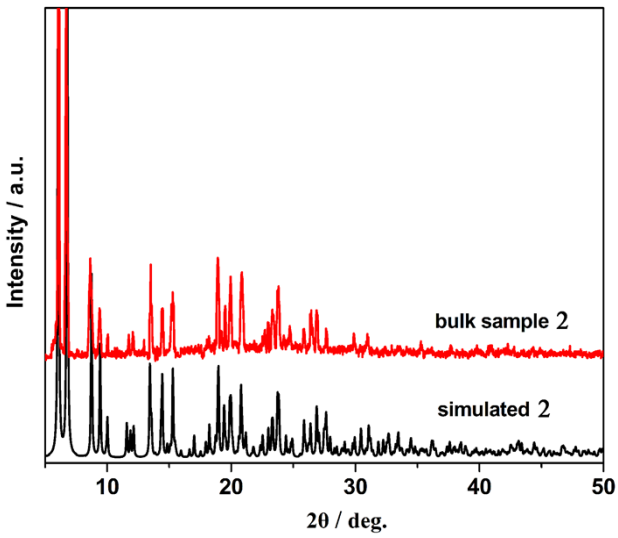

Figure S8. PXRD patterns of simulated **2** and as synthesized **2**.

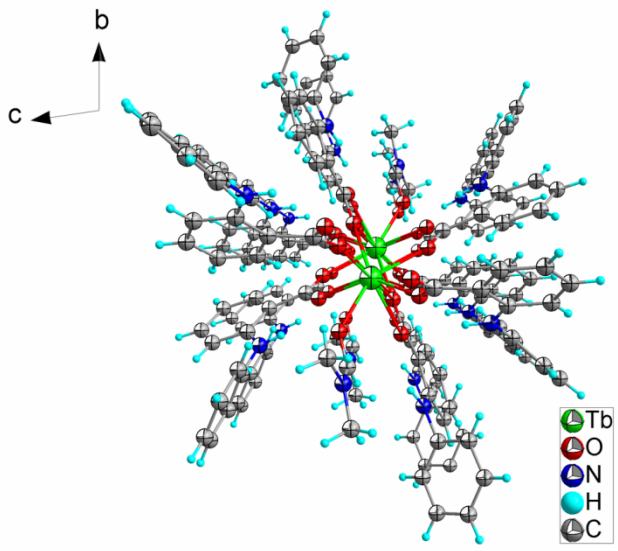

Figure S9. 1D structure of **3a** in *oa* direction.

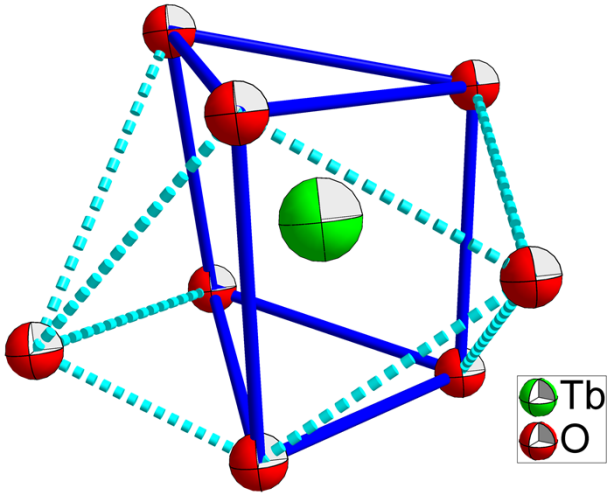

Figure S10. Arrangement of the seven oxygen around Tb^{3+} in **3a**.

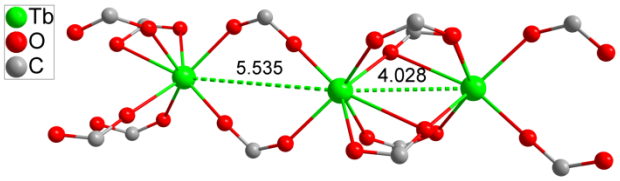

Figure S11. Short and long Tb···Tb distances in **3a**.

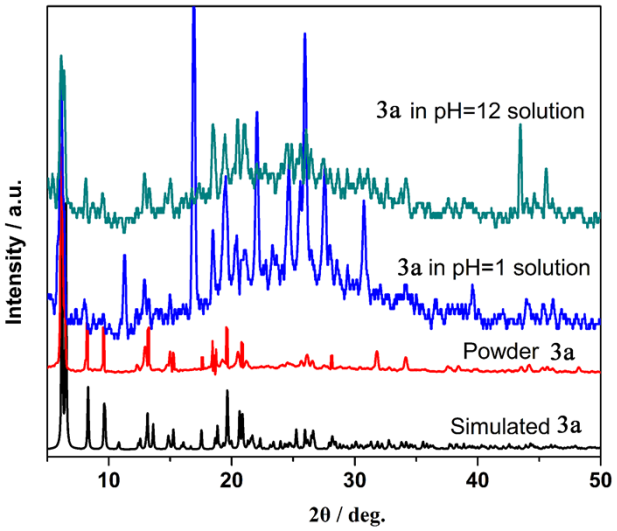

Figure S12. PXRD patterns of simulated **3a**, as synthesized **3a**, powder **3a** in pH = 1 and pH = 12 water solution.

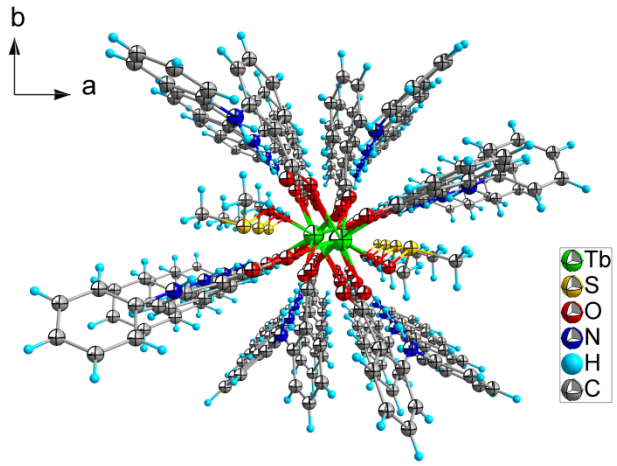

Figure S13. 1D structure of **4** along the *oc* direction.

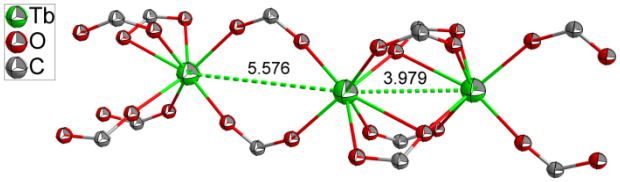

Figure S14. Short and long Tb···Tb distances in **4**.

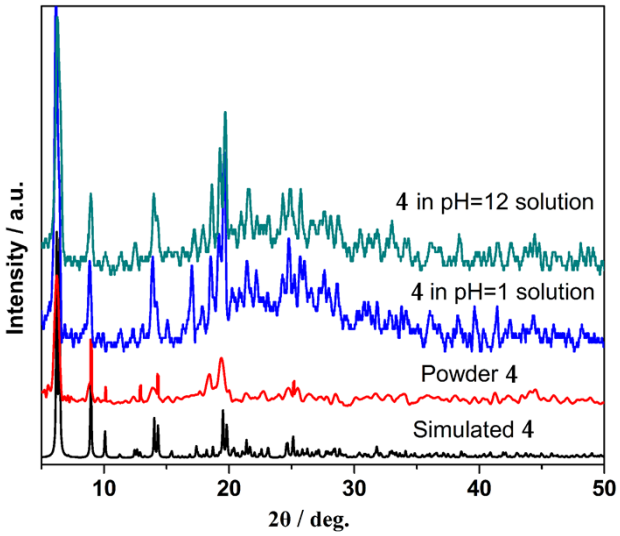

Figure S15. PXRD patterns of simulated **4**, as synthesized **4**, powder **4** in pH = 1 and pH = 12 water solution.

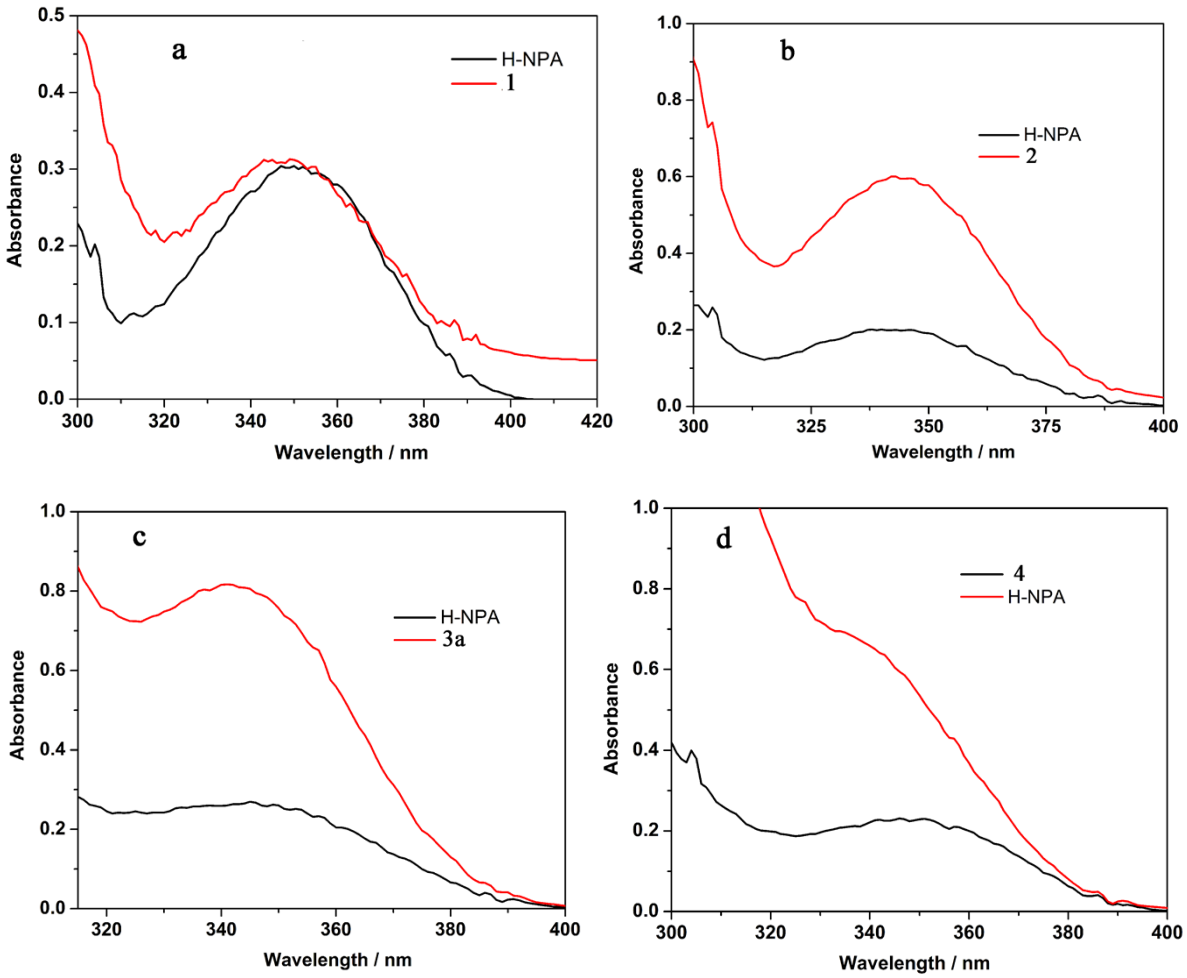

Figure S16. Diffuse-reflectance UV−visible spectra of a, b, c and d, which corresponding to complexes **1**, **2**, **3a** and **4**.

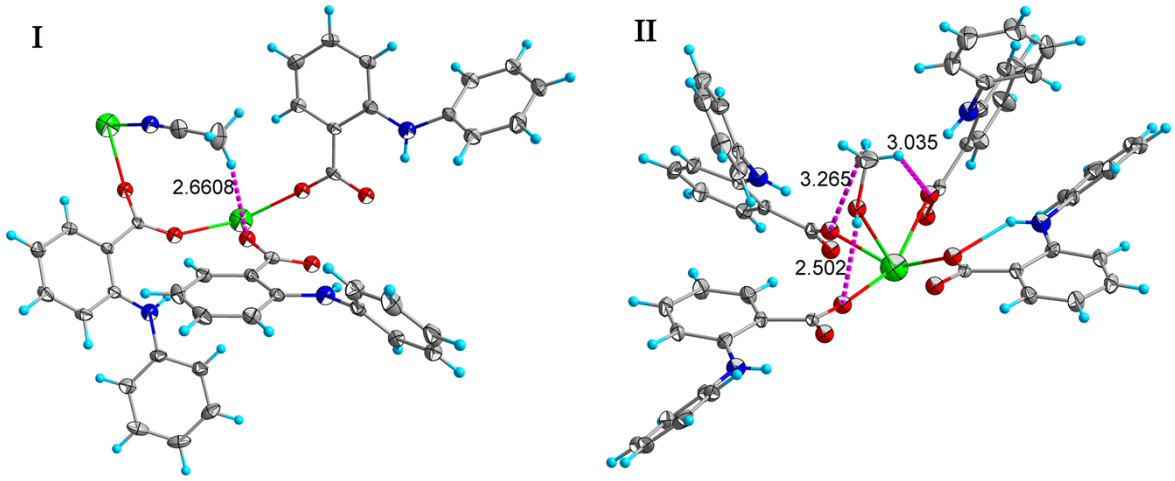

Figure S17. Hydrogen bonds of oscillators in coordination solvents for **1**(I) and **2**(II).