

# **Lanthanide coordination frameworks: Crystal structure, down- and up-conversion luminescence and white light emission**

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## **Supporting Information**

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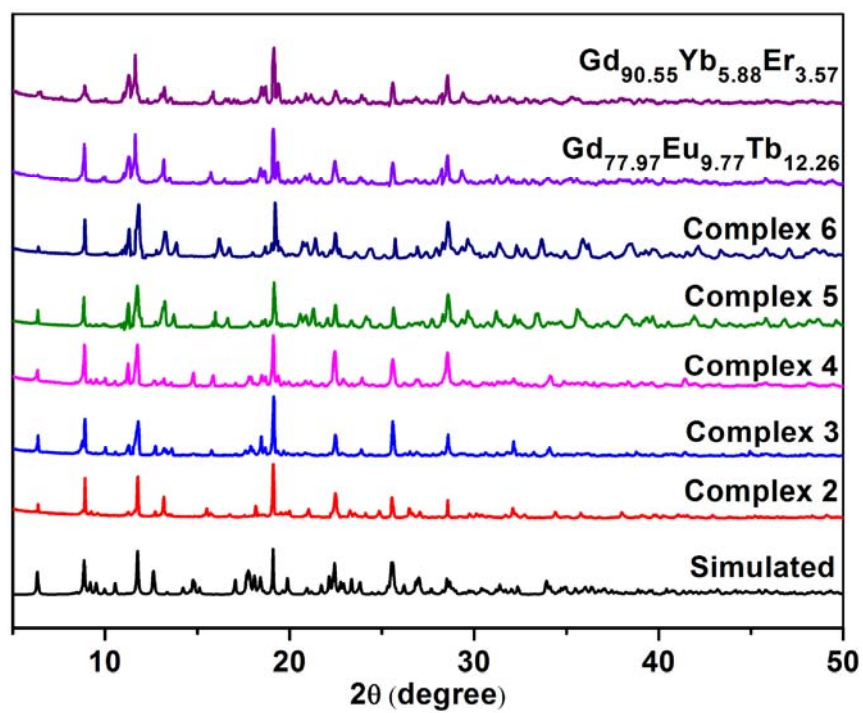


Figure S1. The PXRD patterns for complexes 2-6 and the doped complexes.

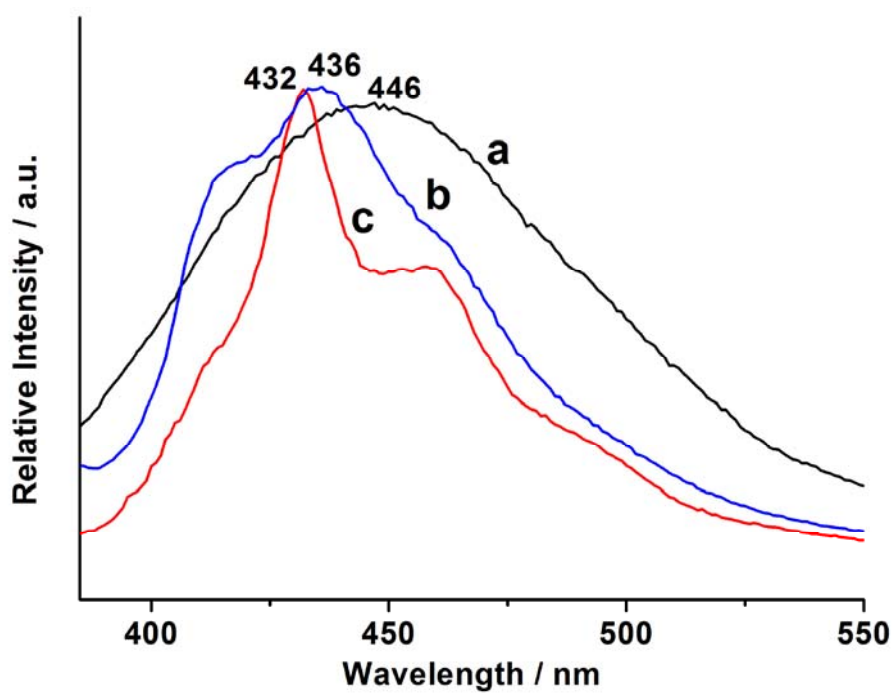
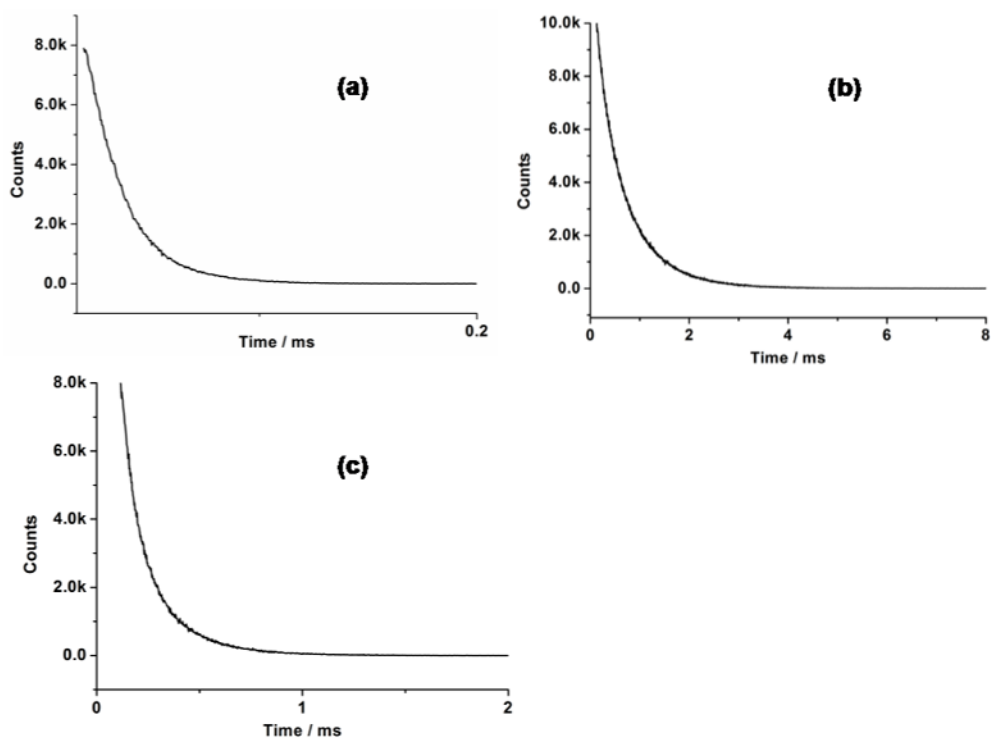
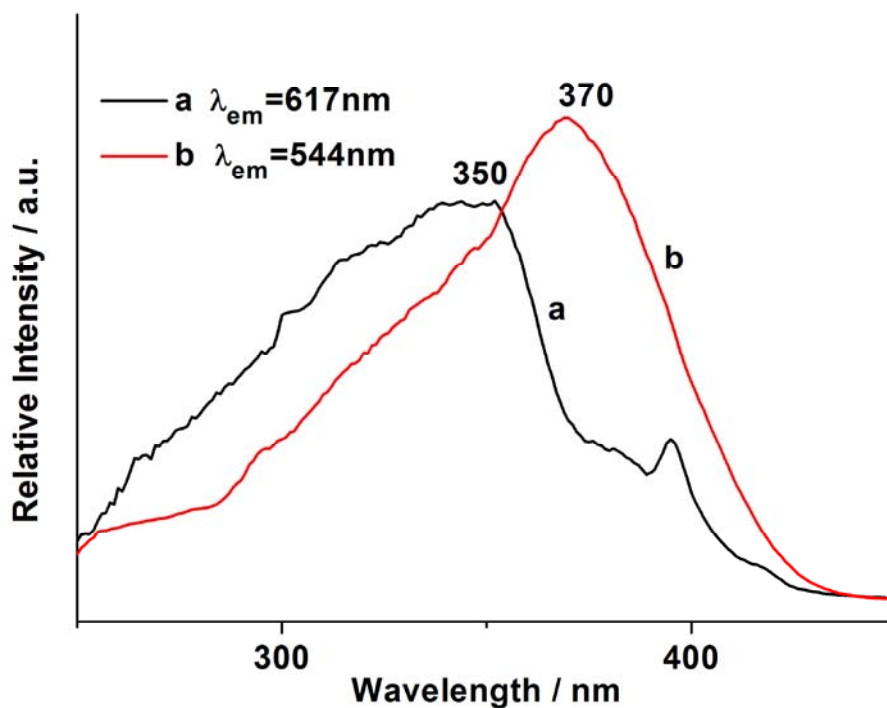


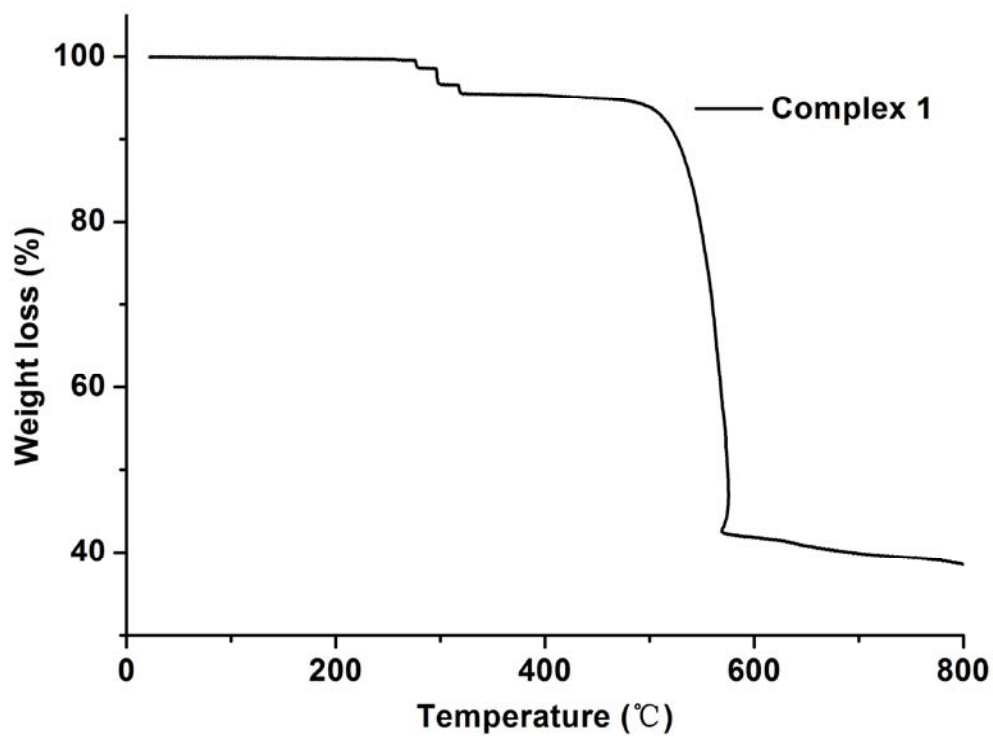
Figure S2. Emission spectra of H<sub>2</sub>N-BDS (a), phen (b) and ox (c).



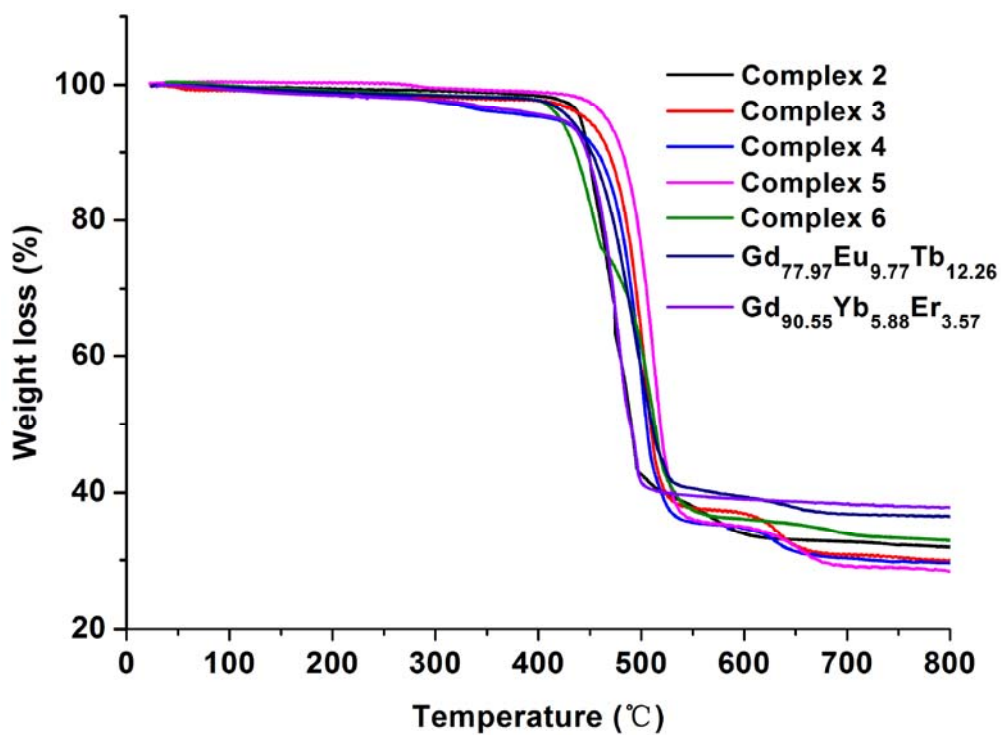
**Figure S3.** Decay profile of the complexes **1** (a), **2**(b) and **4**(c).



**Figure S4.** Excitation spectra of complexes **2** (a) and **4** (b) in the solid state at room temperature.



(a)



(b)

Figure S5. The TGA curves of complex 1 (a), complexes 2 - 6 and the doped complexes (b).

**Table S1.** Selected bond lengths [Å] and angles [°] for complexes **1- 6**

| <b>1</b>            |            |                     |            |
|---------------------|------------|---------------------|------------|
| Sm(1)-O(3)          | 2.394(3)   | Sm(1)-O(4)#3        | 2.399(3)   |
| Sm(1)-O(7)#2        | 2.399(3)   | Sm(1)-O(1)          | 2.426(3)   |
| Sm(1)-O(6)          | 2.422(3)   | Sm(1)-O(2)#1        | 2.437(3)   |
| Sm(1)-N(1)          | 2.572(3)   | Sm(1)-N(2)          | 2.580(4)   |
| O(3)-Sm(1)-O(7)#2   | 142.37(10) | O(3)-Sm(1)-O(4)#3   | 80.47(10)  |
| O(7)#2-Sm(1)-O(4)#3 | 79.50(10)  | O(3)-Sm(1)-O(6)     | 140.50(10) |
| O(7)#2-Sm(1)-O(6)   | 67.13(10)  | O(4)#3-Sm(1)-O(6)   | 138.92(10) |
| O(3)-Sm(1)-O(1)     | 119.11(11) | O(7)#2-Sm(1)-O(1)   | 85.73(10)  |
| O(4)#3-Sm(1)-O(1)   | 75.16(10)  | O(6)-Sm(1)-O(1)     | 79.01(11)  |
| O(3)-Sm(1)-O(2)#1   | 76.26(10)  | O(7)#2-Sm(1)-O(2)#1 | 141.34(10) |
| O(4)#3-Sm(1)-O(2)#1 | 115.75(11) | O(6)-Sm(1)-O(2)#1   | 81.06(10)  |
| O(1)-Sm(1)-O(2)#1   | 66.45(9)   | O(3)-Sm(1)-N(1)     | 73.31(11)  |
| O(7)#2-Sm(1)-N(1)   | 73.40(11)  | O(4)#3-Sm(1)-N(1)   | 84.72(11)  |
| O(6)-Sm(1)-N(1)     | 106.75(12) | O(1)-Sm(1)-N(1)     | 153.35(11) |
| O(2)#1-Sm(1)-N(1)   | 139.58(11) | O(3)-Sm(1)-N(2)     | 74.01(11)  |
| O(7)#2-Sm(1)-N(2)   | 105.71(11) | O(4)#3-Sm(1)-N(2)   | 143.60(11) |
| O(6)-Sm(1)-N(2)     | 71.45(11)  | O(1)-Sm(1)-N(2)     | 140.35(11) |
| O(2)#1-Sm(1)-N(2)   | 83.04(11)  | N(1)-Sm(1)-N(2)     | 63.48(12)  |
| <b>2</b>            |            |                     |            |
| Eu(1)-O(7)#1        | 2.345(5)   | Eu(1)-O(2)          | 2.349(5)   |
| Eu(1)-O(4)          | 2.351(6)   | Eu(1)-O(8)          | 2.396(5)   |
| Eu(1)-N(1)          | 2.557(6)   | Eu(1)-N(4)          | 2.562(6)   |
| Eu(1)-N(3)          | 2.575(6)   | Eu(1)-N(2)          | 2.583(7)   |
| O(7)#1-Eu(1)-O(2)   | 87.53(19)  | O(7)#1-Eu(1)-O(4)   | 75.7(2)    |
| O(2)-Eu(1)-O(4)     | 140.81(19) | O(7)#1-Eu(1)-O(8)   | 68.45(17)  |
| O(2)-Eu(1)-O(8)     | 78.6(2)    | O(4)-Eu(1)-O(8)     | 124.7(2)   |
| O(7)#1-Eu(1)-N(1)   | 88.7(2)    | O(2)-Eu(1)-N(1)     | 71.5(2)    |
| O(4)-Eu(1)-N(1)     | 72.9(2)    | O(8)-Eu(1)-N(1)     | 143.0(2)   |
| O(7)#1-Eu(1)-N(4)   | 104.8(2)   | O(2)-Eu(1)-N(4)     | 141.8(2)   |
| O(4)-Eu(1)-N(4)     | 77.3(2)    | O(8)-Eu(1)-N(4)     | 73.0(2)    |
| N(1)-Eu(1)-N(4)     | 143.0(2)   | O(7)#1-Eu(1)-N(3)   | 138.53(19) |
| O(2)-Eu(1)-N(3)     | 82.18(19)  | O(4)-Eu(1)-N(3)     | 132.9(2)   |
| O(8)-Eu(1)-N(3)     | 70.15(19)  | N(1)-Eu(1)-N(3)     | 124.8(2)   |
| N(4)-Eu(1)-N(3)     | 64.5(2)    | O(7)#1-Eu(1)-N(2)   | 146.7(2)   |
| O(2)-Eu(1)-N(2)     | 100.0(2)   | O(4)-Eu(1)-N(2)     | 78.3(2)    |
| O(8)-Eu(1)-N(2)     | 144.8(2)   | N(1)-Eu(1)-N(2)     | 63.8(2)    |
| N(4)-Eu(1)-N(2)     | 89.3(2)    | N(3)-Eu(1)-N(2)     | 74.8(2)    |
| <b>3</b>            |            |                     |            |
| Gd(1)-O(2)#2        | 2.327(5)   | Gd(1)-O(3)          | 2.332(5)   |
| Gd(1)-O(6)          | 2.343(5)   | Gd(1)-O(1)          | 2.389(5)   |

|                   |            |                   |            |
|-------------------|------------|-------------------|------------|
| Gd(1)-N(1)        | 2.532(6)   | Gd(1)-N(2)        | 2.550(7)   |
| Gd(1)-N(4)        | 2.558(7)   | Gd(1)-N(3)        | 2.579(7)   |
| O(2)#2-Gd(1)-O(3) | 87.66(19)  | O(2)#2-Gd(1)-O(6) | 75.5(2)    |
| O(3)-Gd(1)-O(6)   | 141.3(2)   | O(2)#2-Gd(1)-O(1) | 68.89(18)  |
| O(3)-Gd(1)-O(1)   | 78.52(18)  | O(6)-Gd(1)-O(1)   | 124.51(19) |
| O(2)#2-Gd(1)-N(1) | 105.1(2)   | O(3)-Gd(1)-N(1)   | 141.3(2)   |
| O(6)-Gd(1)-N(1)   | 77.4(2)    | O(1)-Gd(1)-N(1)   | 72.7(2)    |
| O(2)#2-Gd(1)-N(2) | 138.66(19) | O(3)-Gd(1)-N(2)   | 81.4(2)    |
| O(6)-Gd(1)-N(2)   | 133.2(2)   | O(1)-Gd(1)-N(2)   | 69.88(19)  |
| N(1)-Gd(1)-N(2)   | 64.7(2)    | O(2)#2-Gd(1)-N(4) | 88.8(2)    |
| O(3)-Gd(1)-N(4)   | 71.7(2)    | O(6)-Gd(1)-N(4)   | 73.3(2)    |
| O(1)-Gd(1)-N(4)   | 143.4(2)   | N(1)-Gd(1)-N(4)   | 143.1(2)   |
| N(2)-Gd(1)-N(4)   | 124.3(2)   | O(2)#2-Gd(1)-N(3) | 146.3(2)   |
| O(3)-Gd(1)-N(3)   | 100.1(2)   | O(6)-Gd(1)-N(3)   | 78.3(2)    |
| O(1)-Gd(1)-N(3)   | 144.7(2)   | N(1)-Gd(1)-N(3)   | 89.2(2)    |
| N(2)-Gd(1)-N(3)   | 75.0(2)    | N(4)-Gd(1)-N(3)   | 63.5(2)    |

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|-------------------|----------|-------------------|----------|
| Tb(1)-O(7)#1      | 2.312(6) | Tb(1)-O(2)        | 2.324(6) |
| Tb(1)-O(4)        | 2.329(6) | Tb(1)-O(8)        | 2.378(6) |
| Tb(1)-N(4)        | 2.530(7) | Tb(1)-N(1)        | 2.537(7) |
| Tb(1)-N(2)        | 2.561(8) | Tb(1)-N(3)        | 2.562(7) |
| O(7)#1-Tb(1)-O(2) | 87.6(2)  | O(7)#1-Tb(1)-O(4) | 75.7(2)  |
| O(2)-Tb(1)-O(4)   | 141.2(2) | O(7)#1-Tb(1)-O(8) | 69.4(2)  |
| O(2)-Tb(1)-O(8)   | 78.5(2)  | O(4)-Tb(1)-O(8)   | 125.0(2) |
| O(7)#1-Tb(1)-N(4) | 105.3(2) | O(2)-Tb(1)-N(4)   | 141.2(2) |
| O(4)-Tb(1)-N(4)   | 77.5(2)  | O(8)-Tb(1)-N(4)   | 72.6(2)  |
| O(7)#1-Tb(1)-N(1) | 88.1(2)  | O(2)-Tb(1)-N(1)   | 71.7(2)  |
| O(4)-Tb(1)-N(1)   | 73.0(2)  | O(8)-Tb(1)-N(1)   | 143.3(2) |
| N(4)-Tb(1)-N(1)   | 143.3(2) | O(7)#1-Tb(1)-N(2) | 146.0(2) |
| O(2)-Tb(1)-N(2)   | 100.3(2) | O(4)-Tb(1)-N(2)   | 77.8(2)  |
| O(8)-Tb(1)-N(2)   | 144.5(2) | N(4)-Tb(1)-N(2)   | 89.1(3)  |
| N(1)-Tb(1)-N(2)   | 63.8(3)  | O(7)#1-Tb(1)-N(3) | 139.2(2) |
| O(2)-Tb(1)-N(3)   | 81.0(2)  | O(4)-Tb(1)-N(3)   | 133.4(2) |
| O(8)-Tb(1)-N(3)   | 70.0(2)  | N(4)-Tb(1)-N(3)   | 65.2(2)  |
| N(1)-Tb(1)-N(3)   | 124.0(2) | N(2)-Tb(1)-N(3)   | 74.8(2)  |

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|              |           |            |           |
|--------------|-----------|------------|-----------|
| Er(1)-O(7)#1 | 2.275(8)  | Er(1)-O(4) | 2.289(8)  |
| Er(1)-O(2)   | 2.297(7)  | Er(1)-O(8) | 2.346(8)  |
| Er(1)-N(4)   | 2.496(8)  | Er(1)-N(1) | 2.497(10) |
| Er(1)-N(3)   | 2.510(11) | Er(1)-N(2) | 2.516(10) |

|                   |          |                   |          |
|-------------------|----------|-------------------|----------|
| O(7)#1-Er(1)-O(4) | 74.9(3)  | O(7)#1-Er(1)-O(2) | 87.6(3)  |
| O(4)-Er(1)-O(2)   | 141.5(3) | O(7)#1-Er(1)-O(8) | 69.9(3)  |
| O(4)-Er(1)-O(8)   | 124.5(3) | O(2)-Er(1)-O(8)   | 78.3(2)  |
| O(7)#1-Er(1)-N(4) | 105.6(3) | O(4)-Er(1)-N(4)   | 76.4(3)  |
| O(2)-Er(1)-N(4)   | 142.0(3) | O(8)-Er(1)-N(4)   | 73.6(3)  |
| O(7)#1-Er(1)-N(1) | 86.5(3)  | O(4)-Er(1)-N(1)   | 73.7(3)  |
| O(2)-Er(1)-N(1)   | 71.2(3)  | O(8)-Er(1)-N(1)   | 142.0(3) |
| N(4)-Er(1)-N(1)   | 143.4(3) | O(7)#1-Er(1)-N(3) | 139.4(3) |
| O(4)-Er(1)-N(3)   | 134.4(3) | O(2)-Er(1)-N(3)   | 80.0(3)  |
| O(8)-Er(1)-N(3)   | 69.7(3)  | N(4)-Er(1)-N(3)   | 66.7(3)  |
| N(1)-Er(1)-N(3)   | 124.3(3) | O(7)#1-Er(1)-N(2) | 146.9(3) |
| O(4)-Er(1)-N(2)   | 78.9(3)  | O(2)-Er(1)-N(2)   | 100.9(3) |
| O(8)-Er(1)-N(2)   | 143.1(3) | N(4)-Er(1)-N(2)   | 87.3(3)  |
| N(1)-Er(1)-N(2)   | 66.7(4)  | N(3)-Er(1)-N(2)   | 73.8(4)  |

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|                   |            |                   |            |
|-------------------|------------|-------------------|------------|
| Yb(1)-O(2)        | 2.261(3)   | Yb(1)-O(7)#1      | 2.274(3)   |
| Yb(1)-O(4)        | 2.275(4)   | Yb(1)-O(8)        | 2.332(3)   |
| Yb(1)-N(4)        | 2.466(4)   | Yb(1)-N(1)        | 2.486(4)   |
| Yb(1)-N(3)        | 2.490(4)   | Yb(1)-N(2)        | 2.504(5)   |
|                   |            |                   |            |
| O(2)-Yb(1)-O(7)#1 | 87.73(13)  | O(2)-Yb(1)-O(4)   | 141.51(14) |
| O(7)#1-Yb(1)-O(4) | 75.62(13)  | O(2)-Yb(1)-O(8)   | 78.63(13)  |
| O(7)#1-Yb(1)-O(8) | 70.23(11)  | O(4)-Yb(1)-O(8)   | 125.11(13) |
| O(2)-Yb(1)-N(4)   | 141.78(13) | O(7)#1-Yb(1)-N(4) | 105.74(13) |
| O(4)-Yb(1)-N(4)   | 76.66(14)  | O(8)-Yb(1)-N(4)   | 73.04(13)  |
| O(2)-Yb(1)-N(1)   | 71.33(13)  | O(7)#1-Yb(1)-N(1) | 86.19(14)  |
| O(4)-Yb(1)-N(1)   | 73.11(14)  | O(8)-Yb(1)-N(1)   | 142.38(14) |
| N(4)-Yb(1)-N(1)   | 143.48(14) | O(2)-Yb(1)-N(3)   | 79.89(13)  |
| O(7)#1-Yb(1)-N(3) | 139.96(12) | O(4)-Yb(1)-N(3)   | 133.82(14) |
| O(8)-Yb(1)-N(3)   | 70.04(12)  | N(4)-Yb(1)-N(3)   | 66.71(13)  |
| N(1)-Yb(1)-N(3)   | 124.18(14) | O(2)-Yb(1)-N(2)   | 100.15(14) |
| O(7)#1-Yb(1)-N(2) | 145.87(14) | O(4)-Yb(1)-N(2)   | 77.88(15)  |
| O(8)-Yb(1)-N(2)   | 143.79(14) | N(4)-Yb(1)-N(2)   | 88.46(15)  |
| N(1)-Yb(1)-N(2)   | 65.65(16)  | N(3)-Yb(1)-N(2)   | 74.11(15)  |

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Symmetry transformations used to generate equivalent atoms: For **1** : #1 -x,-y,-z+1; #2: -x,-y+1,-z+1; #3: -x+1,-y,-z+1; For **2 -6**, #1: -x, -y, 1-z; #2: 1-x, -y, -z.