

Supporting Information

Multifunctional Luminescence properties of Co-doped Lanthanide Metal Organic Frameworks

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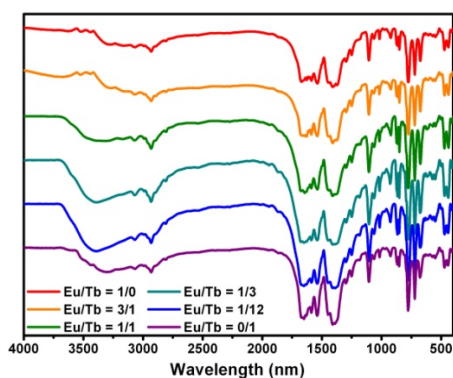


Figure S1. IR spectra of compound 1-6.

Table S1. Selected bond lengths (Å) for compound 1-6.

| | Eu:Tb=3/1 | Eu:Tb=1/1 | Eu:Tb=1/3 | Eu:Tb=1/12 | Eu:Tb=0/1 |
|--------------|-----------|-----------|-----------|------------|-----------|
| M(1)-O(1)#1 | 2.348(5) | 2.335(5) | 2.339(4) | 2.320(4) | 2.318(5) |
| M(1)-O(10)#2 | 2.366(4) | 2.360(4) | 2.365(5) | 2.352(4) | 2.341(5) |
| M(1)-O(9)#3 | 2.383(4) | 2.380(4) | 2.375(4) | 2.372(4) | 2.363(5) |
| M(1)-O(2) | 2.418(4) | 2.414(5) | 2.409(5) | 2.399(4) | 2.388(5) |
| M(1)-O(26) | 2.435(5) | 2.426(5) | 2.427(5) | 2.417(5) | 2.398(6) |
| M(1)-O(24) | 2.472(5) | 2.462(5) | 2.459(5) | 2.448(4) | 2.437(5) |
| M(1)-O(25) | 2.467(6) | 2.466(6) | 2.474(6) | 2.453(5) | 2.470(6) |
| M(1)-O(23) | 2.479(5) | 2.472(5) | 2.474(5) | 2.466(5) | 2.460(6) |
| M(1)-O(1) | 2.827(5) | 2.831(5) | 2.836(5) | 2.847(5) | 2.816(6) |
| | | | | | |
| M(2)-O(17) | 2.295(4) | 2.288(4) | 2.292(5) | 2.281(4) | 2.274(5) |
| M(2)-O(3) | 2.320(5) | 2.315(5) | 2.327(5) | 2.297(5) | 2.297(5) |
| M(2)-O(4)#4 | 2.331(4) | 2.322(4) | 2.324(5) | 2.315(4) | 2.304(5) |
| M(2)-O(27) | 2.344(6) | 2.335(6) | 2.346(6) | 2.338(5) | 2.328(7) |
| M(2)-O(28) | 2.473(5) | 2.464(5) | 2.468(5) | 2.453(5) | 2.457(6) |
| M(2)-O(8) | 2.483(5) | 2.471(4) | 2.473(5) | 2.470(4) | 2.457(5) |
| M(2)-O(29) | 2.477(5) | 2.468(5) | 2.482(5) | 2.463(5) | 2.460(6) |
| M(2)-O(7) | 2.502(5) | 2.503(4) | 2.500(4) | 2.489(4) | 2.487(5) |
| | | | | | |
| M(3)-O(21)#1 | 2.306(4) | 2.300(4) | 2.296(5) | 2.286(4) | 2.286(6) |
| M(3)-O(13) | 2.342(5) | 2.339(4) | 2.338(5) | 2.327(4) | 2.317(5) |
| M(3)-O(14)#5 | 2.404(4) | 2.397(4) | 2.399(4) | 2.381(4) | 2.374(5) |
| M(3)-O(22)#6 | 2.408(5) | 2.396(5) | 2.402(4) | 2.387(4) | 2.379(5) |
| M(3)-O(30) | 2.418(5) | 2.407(5) | 2.410(6) | 2.407(5) | 2.393(6) |
| M(3)-O(5) | 2.455(5) | 2.449(5) | 2.452(5) | 2.438(5) | 2.429(6) |
| M(3)-O(6) | 2.468(5) | 2.460(4) | 2.456(5) | 2.450(4) | 2.452(6) |
| M(3)-O(31) | 2.469(6) | 2.459(5) | 2.471(5) | 2.441(5) | 2.442(6) |

| | | | | | |
|--------------|----------|----------|----------|----------|----------|
| M(4)-O(19) | 2.321(5) | 2.309(5) | 2.309(5) | 2.295(4) | 2.286(6) |
| M(4)-O(20)#7 | 2.319(5) | 2.315(4) | 2.313(5) | 2.308(4) | 2.301(5) |
| M(4)-O(12)#2 | 2.327(5) | 2.321(5) | 2.323(5) | 2.311(4) | 2.303(6) |
| M(4)-O(33) | 2.445(5) | 2.437(5) | 2.439(5) | 2.429(5) | 2.425(6) |
| M(4)-O(15)#8 | 2.453(4) | 2.448(4) | 2.451(5) | 2.438(4) | 2.431(5) |
| M(4)-O(32) | 2.456(7) | 2.450(7) | 2.450(6) | 2.432(6) | 2.444(7) |
| M(4)-O(34) | 2.462(5) | 2.461(5) | 2.465(5) | 2.449(4) | 2.455(6) |
| M(4)-O(16)#8 | 2.486(5) | 2.476(4) | 2.478(4) | 2.472(4) | 2.459(6) |

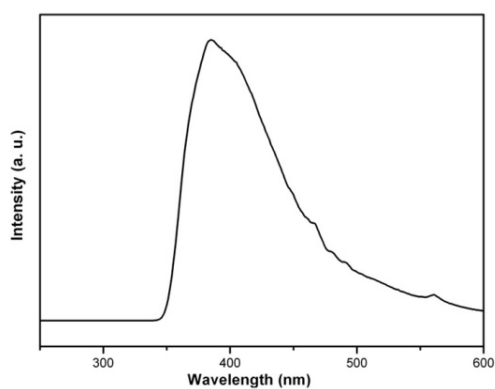


Figure S2. The emission spectra of Ligand H₃bpt.

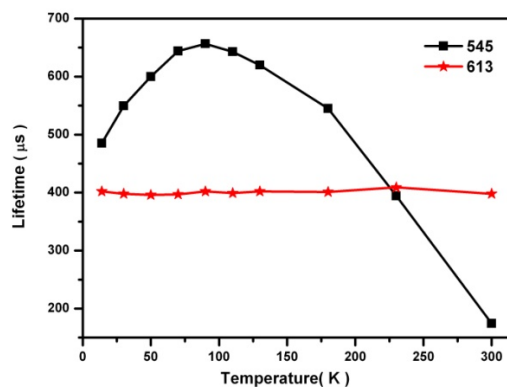


Figure S3. Temperature dependence of the ⁵D₄ and ⁵D₀ lifetime (14–300 K) for compound 3. The decay curves are monitored at 545 and 613 nm, respectively, excited at 355 nm.

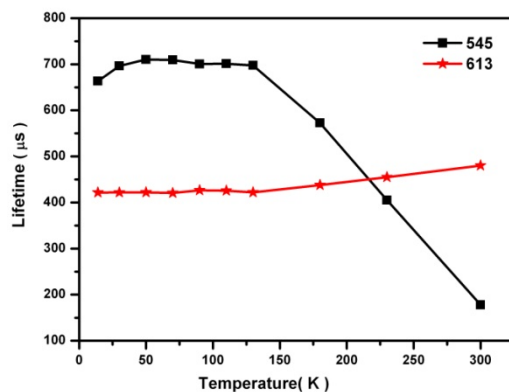


Figure S4. Temperature dependence of the 5D_4 and 5D_0 lifetime (14–300 K) for compound 4. The decay curves are monitored at 545 and 613nm, respectively, excited at 355nm.

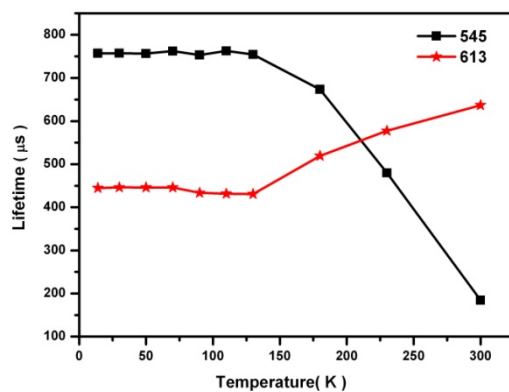


Figure S5. Temperature dependence of the 5D_4 and 5D_0 lifetime (14–300 K) for compound 5. The decay curves are monitored at 545 and 613nm, respectively, excited at 355nm.

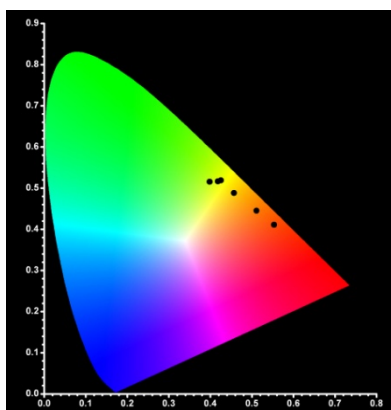


Figure S6. The CIE chromaticity coordinates diagram for compound 6 monitored under 320 nm.

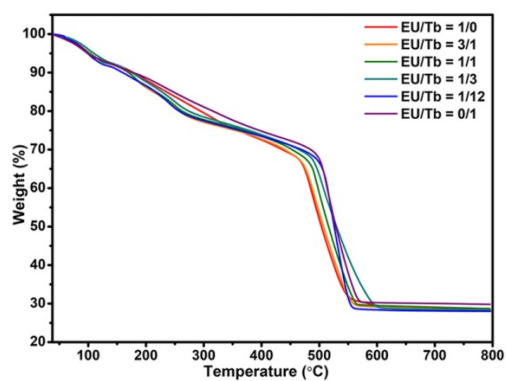


Figure S7. The TG curves for compounds 1-6.

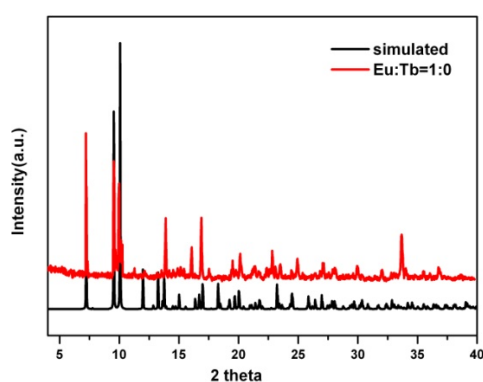


Figure S8. Powder X-ray diffraction patterns of simulated 1-Eu, and as-synthesized compound 1.

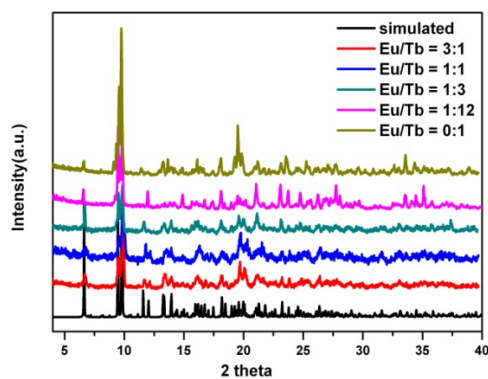


Figure S9. Powder X-ray diffraction patterns of simulated 2-Tb, and as-synthesized compound 2-6.

Table S2. The Quantum Yield of the compounds 1-6.

| Compounds | Eu/Tb = 1/0 | Eu/Tb = 3/1 | Eu/Tb = 1/1 | Eu/Tb = 1/3 | Eu/Tb = 1/12 | Eu/Tb = 0/1 |
|---------------|-------------|-------------|-------------|-------------|--------------|-------------|
| Quantum Yield | 27.38% | 56.75% | 54.94% | 31.81% | 47.32% | 28.11% |

Table S3. The chemical composition of the compounds 3-6 by ICP.

| Compounds | The mole ratio (Eu/Tb) Measured | Molecular formula |
|--------------|---------------------------------|--|
| Eu/Tb = 3/1 | 20.25/6.79 | C ₈₁ H ₉₉ N ₇ O ₄₂ TbEu ₃ |
| Eu/Tb = 1/1 | 12.42/13.16 | C ₈₁ H ₉₉ N ₇ O ₄₂ Tb ₂ Eu ₂ |
| Eu/Tb = 1/3 | 5.98/20.31 | C ₈₁ H ₉₉ N ₇ O ₄₂ Tb ₃ Eu |
| Eu/Tb = 1/12 | 2.06/24.69 | C ₈₁ H ₉₉ N ₇ O ₄₂ Tb _{3.69} Eu _{0.31} |

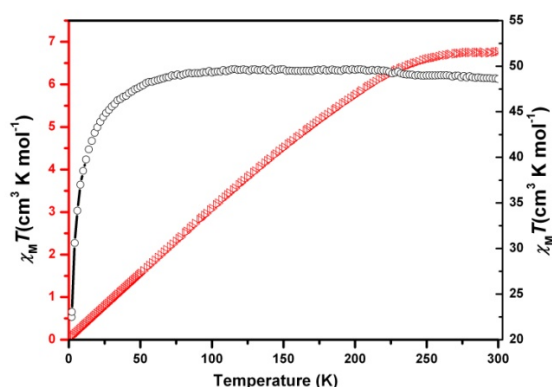


Figure S10. Temperature dependence of the $\chi_M T$ product at 1000 Oe for compound 1 (red) and 2 (black).

Table S3. Bond lengths (Å) for compounds 1-6.

Eu/Tb=1/0

| | | | |
|---------------------|------------|---------------------|------------|
| Eu(1)-O(3)#1 | 2.369(3) | Eu(1)-O(10) | 2.469(5) |
| Eu(1)-O(1)#2 | 2.372(3) | Eu(1)-O(5) | 2.483(3) |
| Eu(1)-O(2)#3 | 2.402(3) | Eu(1)-O(6) | 2.494(3) |
| Eu(1)-O(9) | 2.439(5) | Eu(1)-O(3)#4 | 2.727(3) |
| Eu(1)-O(4)#4 | 2.445(3) | | |
| | | | |
| O(9)-Eu(1)-O(4)#4 | 146.03(16) | O(1)#2-Eu(1)-O(5) | 75.49(12) |
| O(3)#1-Eu(1)-O(10) | 149.69(15) | O(2)#3-Eu(1)-O(5) | 146.80(12) |
| O(1)#2-Eu(1)-O(10) | 135.62(16) | O(9)-Eu(1)-O(5) | 95.06(16) |
| O(2)#3-Eu(1)-O(10) | 74.29(14) | O(4)#4-Eu(1)-O(6) | 126.86(11) |
| O(9)-Eu(1)-O(4)#4 | 146.03(16) | O(10)-Eu(1)-O(6) | 109.29(16) |
| O(9)-Eu(1)-O(10) | 73.8(2) | O(5)-Eu(1)-O(6) | 52.28(11) |
| O(4)#4-Eu(1)-O(10) | 72.89(19) | O(3)#1-Eu(1)-O(3)#4 | 75.52(10) |
| O(3)#1-Eu(1)-O(5) | 131.22(10) | O(1)#2-Eu(1)-O(3)#4 | 67.78(10) |
| O(2)#3-Eu(1)-O(4)#4 | 90.71(12) | O(6)-Eu(1)-O(3)#4 | 137.97(12) |
| O(9)-Eu(1)-O(10) | 72.89(2) | O(3)#1-Eu(1)-O(1)#2 | 74.27(11) |
| O(4)#4-Eu(1)-O(10) | 72.89(19) | O(3)#1-Eu(1)-O(2)#3 | 79.75(11) |
| O(3)#1-Eu(1)-O(5) | 131.22(10) | O(1)#2-Eu(1)-O(2)#3 | 132.57(10) |
| O(1)#2-Eu(1)-O(5) | 75.49(12) | O(3)#1-Eu(1)-O(9) | 84.27(15) |

| | | | |
|---------------------|------------|---------------------|------------|
| O(2)#3-Eu(1)-O(5) | 146.80(12) | O(1)#2-Eu(1)-O(9) | 139.57(16) |
| O(4)#4-Eu(1)-O(5) | 81.26(11) | O(2)#3-Eu(1)-O(9) | 73.97(15) |
| O(4)#4-Eu(1)-O(3)#4 | 49.83(9) | O(3)#1-Eu(1)-O(4)#4 | 123.36(10) |
| O(5)-Eu(1)-O(3)#4 | 125.04(11) | O(1)#2-Eu(1)-O(4)#4 | 72.43(12) |
| O(10)-Eu(1)-O(5) | 72.55(14) | O(9)-Eu(1)-O(6) | 71.32(15) |
| O(3)#1-Eu(1)-O(6) | 82.21(11) | O(2)#3-Eu(1)-O(3)#4 | 67.67(10) |
| O(1)#2-Eu(1)-O(6) | 72.09(12) | O(9)-Eu(1)-O(3)#4 | 139.04(14) |
| O(2)#3-Eu(1)-O(6) | 142.14(12) | O(4)#4-Eu(1)-O(3)#4 | 49.83(9) |

Eu/Tb=3/1

| | | | |
|---------------------|------------|--------------------|------------|
| Eu(1)-O(1)#1 | 2.348(5) | Eu(3)-O(21)#1 | 2.306(4) |
| Eu(1)-O(10)#2 | 2.366(4) | Eu(3)-O(13) | 2.342(5) |
| Eu(1)-O(9)#3 | 2.383(4) | Eu(3)-O(14)#5 | 2.404(4) |
| Eu(1)-O(2) | 2.418(4) | Eu(3)-O(22)#6 | 2.408(5) |
| Eu(1)-O(26) | 2.435(5) | Eu(3)-O(30) | 2.418(5) |
| Eu(1)-O(24) | 2.472(5) | Eu(3)-O(5) | 2.455(5) |
| Eu(1)-O(25) | 2.467(6) | Eu(3)-O(6) | 2.468(5) |
| Eu(1)-O(23) | 2.479(5) | Eu(3)-O(31) | 2.469(6) |
| Eu(1)-O(1) | 2.827(5) | Eu(4)-O(20)#7 | 2.319(5) |
| Eu(2)-O(17) | 2.295(4) | Eu(4)-O(19) | 2.321(5) |
| Eu(2)-O(3) | 2.320(5) | Eu(4)-O(12)#2 | 2.327(5) |
| Eu(2)-O(4)#4 | 2.331(4) | Eu(4)-O(33) | 2.445(5) |
| Eu(2)-O(27) | 2.344(6) | Eu(4)-O(15)#8 | 2.453(4) |
| Eu(2)-O(28) | 2.473(5) | Eu(4)-O(32) | 2.456(7) |
| Eu(2)-O(29) | 2.477(5) | Eu(4)-O(34) | 2.462(5) |
| Eu(2)-O(8) | 2.483(5) | Eu(4)-O(16)#8 | 2.486(5) |
| Eu(2)-O(7) | 2.502(5) | | |
| | | | |
| O(23)-Eu(1)-O(1) | 124.20(17) | O(25)-Eu(1)-O(1) | 105.24(18) |
| C(60)-Eu(1)-O(1) | 138.12(17) | O(17)-Eu(2)-O(29) | 80.40(19) |
| O(26)-Eu(1)-O(25) | 75.6(2) | O(3)-Eu(2)-O(29) | 141.43(19) |
| O(24)-Eu(1)-O(25) | 106.0(2) | O(4)#4-Eu(2)-O(29) | 74.53(19) |
| O(1)#1-Eu(1)-O(23) | 133.35(17) | O(27)-Eu(2)-O(29) | 71.5(2) |
| O(10)#2-Eu(1)-O(23) | 76.60(19) | O(28)-Eu(2)-O(29) | 68.47(19) |
| O(2)-Eu(1)-O(1) | 48.67(14) | O(17)-Eu(2)-O(8) | 130.02(17) |
| O(26)-Eu(1)-O(1) | 137.85(16) | O(3)-Eu(2)-O(8) | 71.66(18) |
| O(9)#3-Eu(1)-O(26) | 72.13(17) | O(4)#4-Eu(2)-O(8) | 75.42(17) |
| O(2)-Eu(1)-O(26) | 143.0(2) | O(27)-Eu(2)-O(8) | 79.8(2) |
| O(1)#1-Eu(1)-O(24) | 84.89(17) | O(28)-Eu(2)-O(8) | 133.62(17) |
| O(10)#2-Eu(1)-O(24) | 74.42(18) | O(29)-Eu(2)-O(8) | 140.43(17) |
| O(9)#3-Eu(1)-O(24) | 140.59(16) | O(17)-Eu(2)-O(7) | 78.06(17) |
| O(2)-Eu(1)-O(24) | 129.39(16) | O(4)#4-Eu(2)-O(28) | 100.93(18) |
| O(26)-Eu(1)-O(24) | 70.14(18) | O(27)-Eu(2)-O(28) | 76.8(2) |

| | | | |
|-----------------------|------------|-----------------------|------------|
| O(9)#3-Eu(1)-O(23) | 144.69(19) | O(3)-Eu(2)-O(7) | 75.65(18) |
| O(2)-Eu(1)-O(23) | 81.50(18) | O(4)#4-Eu(2)-O(7) | 125.59(17) |
| O(26)-Eu(1)-O(23) | 96.2(2) | O(27)-Eu(2)-O(7) | 74.1(2) |
| O(24)-Eu(1)-O(23) | 52.06(17) | O(28)-Eu(2)-O(7) | 140.52(18) |
| O(25)-Eu(1)-O(23) | 70.1(2) | O(29)-Eu(2)-O(7) | 136.96(17) |
| O(1)#1-Eu(1)-O(1) | 77.80(15) | O(8)-Eu(2)-O(7) | 52.64(14) |
| O(10)#2-Eu(1)-O(1) | 69.42(15) | O(17)-Eu(2)-O(3) | 90.51(19) |
| O(9)#3-Eu(1)-O(1) | 67.78(15) | O(17)-Eu(2)-O(4)#4 | 154.0(2) |
| O(24)-Eu(1)-O(1) | 142.79(17) | O(3)-Eu(2)-O(4)#4 | 104.84(18) |
| O(17)-Eu(2)-O(27) | 95.5(2) | O(20)#7-Eu(4)-O(19) | 105.80(17) |
| O(3)-Eu(2)-O(27) | 147.0(2) | O(20)#7-Eu(4)-O(12)#2 | 152.80(18) |
| O(4)#4-Eu(2)-O(27) | 83.0(2) | O(19)-Eu(4)-O(12)#2 | 84.88(19) |
| O(17)-Eu(2)-O(28) | 78.77(17) | O(20)#7-Eu(4)-O(33) | 80.36(18) |
| O(3)-Eu(2)-O(28) | 73.0(2) | O(19)-Eu(4)-O(33) | 140.24(2) |
| O(22)#6-Eu(3)-O(30) | 73.01(2) | O(12)#2-Eu(4)-O(33) | 75.86(18) |
| O(21)#1-Eu(3)-O(5) | 86.17(18) | O(20)#7-Eu(4)-O(15)#8 | 126.03(18) |
| O(13)-Eu(3)-O(5) | 78.28(19) | O(19)-Eu(4)-O(15)#8 | 80.06(18) |
| O(14)#5-Eu(3)-O(5) | 145.93(18) | O(12)#2-Eu(4)-O(15)#8 | 79.94(17) |
| O(22)#6-Eu(3)-O(5) | 133.39(17) | O(33)-Eu(4)-O(15)#8 | 128.60(18) |
| O(30)-Eu(3)-O(5) | 104.2(2) | O(20)#7-Eu(4)-O(32) | 77.0(2) |
| O(21)#1-Eu(3)-O(6) | 133.05(16) | O(19)-Eu(4)-O(32) | 147.0(2) |
| O(13)-Eu(3)-O(6) | 75.65(17) | O(12)#2-Eu(4)-O(32) | 107.8(2) |
| O(14)#5-Eu(3)-O(6) | 149.03(16) | O(33)-Eu(4)-O(32) | 72.5(2) |
| O(21)#1-Eu(3)-O(13) | 75.06(18) | O(15)#8-Eu(4)-O(32) | 72.7(2) |
| O(21)#1-Eu(3)-O(14)#5 | 77.69(16) | O(20)#7-Eu(4)-O(34) | 76.43(18) |
| O(13)-Eu(3)-O(14)#5 | 124.63(16) | O(19)-Eu(4)-O(34) | 72.45(17) |
| O(21)#1-Eu(3)-O(22)#6 | 121.85(17) | O(12)#2-Eu(4)-O(34) | 83.45(18) |
| O(13)-Eu(3)-O(22)#6 | 75.09(18) | O(33)-Eu(4)-O(34) | 71.07(18) |
| O(14)#5-Eu(3)-O(22)#6 | 80.08(17) | O(15)#8-Eu(4)-O(34) | 148.95(19) |
| O(21)#1-Eu(3)-O(30) | 147.23(2) | O(32)-Eu(4)-O(34) | 137.86(18) |
| O(22)#6-Eu(3)-O(6) | 84.09(17) | O(20)#7-Eu(4)-O(16)#8 | 76.69(17) |
| O(30)-Eu(3)-O(6) | 73.27(18) | O(19)-Eu(4)-O(16)#8 | 74.39(18) |
| O(5)-Eu(3)-O(6) | 52.34(17) | O(12)#2-Eu(4)-O(16)#8 | 130.52(15) |
| O(21)#1-Eu(3)-O(31) | 80.93(19) | O(33)-Eu(4)-O(16)#8 | 143.25(18) |
| O(13)-Eu(3)-O(31) | 142.00(19) | O(15)#8-Eu(4)-O(16)#8 | 52.79(15) |
| O(14)#5-Eu(3)-O(31) | 76.85(18) | O(32)-Eu(4)-O(16)#8 | 74.4(2) |
| O(22)#6-Eu(3)-O(31) | 142.87(19) | O(34)-Eu(4)-O(16)#8 | 128.98(15) |
| O(30)-Eu(3)-O(31) | 73.6(2) | O(6)-Eu(3)-O(31) | 101.32(19) |
| O(5)-Eu(3)-O(31) | 71.04(19) | | |

Eu:Tb=1/1

| | | | |
|---------------|----------|--------------|----------|
| Tb(1)-O(1)#1 | 2.335(5) | Tb(2)-O(3) | 2.315(5) |
| Tb(1)-O(10)#2 | 2.360(4) | Tb(2)-O(4)#4 | 2.322(4) |

| | | | |
|----------------------|------------|-----------------------|------------|
| Tb(1)-O(9)#3 | 2.380(4) | Tb(2)-O(27) | 2.335(6) |
| Tb(1)-O(2) | 2.414(5) | Tb(2)-O(28) | 2.464(5) |
| Tb(1)-O(26) | 2.426(5) | Tb(2)-O(8) | 2.471(4) |
| Tb(1)-O(24) | 2.462(5) | Tb(2)-O(29) | 2.468(5) |
| Tb(1)-O(25) | 2.466(6) | Tb(2)-O(7) | 2.503(4) |
| Tb(1)-O(23) | 2.472(5) | Tb(3)-O(21)#1 | 2.300(4) |
| Tb(1)-O(1) | 2.831(5) | Tb(3)-O(13) | 2.339(4) |
| Tb(2)-O(17) | 2.288(4) | Tb(3)-O(22)#5 | 2.396(5) |
| Tb(3)-O(14)#6 | 2.397(4) | Tb(4)-O(12)#2 | 2.321(5) |
| Tb(3)-O(30) | 2.407(5) | Tb(4)-O(33) | 2.437(5) |
| Tb(3)-O(5) | 2.449(5) | Tb(4)-O(15)#8 | 2.448(4) |
| Tb(3)-O(6) | 2.460(4) | Tb(4)-O(32) | 2.450(7) |
| Tb(3)-O(31) | 2.459(5) | Tb(4)-O(34) | 2.461(5) |
| Tb(4)-O(19) | 2.309(5) | Tb(4)-O(16)#8 | 2.476(4) |
| Tb(4)-O(20)#7 | 2.315(4) | | |
| | | | |
| O(1)#1-Tb(1)-O(10)#2 | 74.73(16) | O(4)#4-Tb(2)-O(27) | 82.7(2) |
| O(1)#1-Tb(1)-O(9)#3 | 79.46(16) | O(17)-Tb(2)-O(28) | 78.75(16) |
| O(10)#2-Tb(1)-O(9)#3 | 133.33(15) | O(3)-Tb(2)-O(28) | 72.85(19) |
| O(1)#1-Tb(1)-O(2) | 125.25(16) | O(4)#4-Tb(2)-O(28) | 85.61(17) |
| O(10)#2-Tb(1)-O(2) | 76.33(17) | O(27)-Tb(2)-O(28) | 139.7(2) |
| O(9)#3-Tb(1)-O(2) | 88.28(17) | O(17)-Tb(2)-O(8) | 129.94(16) |
| O(1)#1-Tb(1)-O(26) | 82.6(2) | O(3)-Tb(2)-O(8) | 71.57(18) |
| O(10)#2-Tb(1)-O(26) | 139.3(2) | O(4)#4-Tb(2)-O(8) | 75.47(16) |
| O(9)#3-Tb(1)-O(26) | 72.41(17) | O(27)-Tb(2)-O(8) | 80.1(2) |
| O(1)#1-Tb(1)-O(1) | 77.58(16) | O(28)-Tb(2)-O(8) | 133.43(16) |
| O(10)#2-Tb(1)-O(1) | 69.15(15) | O(13)-Tb(3)-O(31) | 142.16(19) |
| O(9)#3-Tb(1)-O(1) | 67.70(14) | O(22)#5-Tb(3)-O(31) | 142.54(19) |
| O(2)-Tb(1)-O(1) | 48.81(14) | O(14)#6-Tb(3)-O(31) | 76.55(17) |
| O(26)-Tb(1)-O(1) | 137.92(15) | O(30)-Tb(3)-O(31) | 73.4(2) |
| O(24)-Tb(1)-O(1) | 142.50(16) | O(5)-Tb(3)-O(31) | 71.07(19) |
| O(25)-Tb(1)-O(1) | 105.55(18) | O(6)-Tb(3)-O(31) | 101.28(18) |
| O(23)-Tb(1)-O(1) | 124.09(17) | O(21)#1-Tb(3)-O(13) | 75.45(18) |
| O(17)-Tb(2)-O(29) | 80.36(19) | O(21)#1-Tb(3)-O(22)#5 | 121.92(17) |
| O(3)-Tb(2)-O(29) | 141.07(19) | O(13)-Tb(3)-O(22)#5 | 75.23(18) |
| O(4)#4-Tb(2)-O(29) | 74.70(18) | O(21)#1-Tb(3)-O(14)#6 | 77.38(16) |
| O(27)-Tb(2)-O(29) | 71.5(2) | O(13)-Tb(3)-O(14)#6 | 124.90(15) |
| O(28)-Tb(2)-O(29) | 68.27(19) | O(22)#5-Tb(3)-O(14)#6 | 80.14(17) |
| O(8)-Tb(2)-O(29) | 140.82(17) | O(21)#1-Tb(3)-O(30) | 146.71(19) |
| O(17)-Tb(2)-O(7) | 78.10(16) | O(21)#1-Tb(3)-O(13) | 75.45(18) |
| O(3)-Tb(2)-O(7) | 75.55(18) | O(13)-Tb(3)-O(30) | 137.21(19) |
| O(4)#4-Tb(2)-O(7) | 125.65(16) | O(22)#5-Tb(3)-O(30) | 72.91(19) |
| O(27)-Tb(2)-O(7) | 74.6(2) | O(14)#6-Tb(3)-O(30) | 76.41(17) |

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|-----------------------|------------|-----------------------|------------|
| O(28)-Tb(2)-O(7) | 140.35(18) | O(21)#1-Tb(3)-O(5) | 85.91(17) |
| O(8)-Tb(2)-O(7) | 52.54(14) | O(13)-Tb(3)-O(5) | 78.15(19) |
| O(29)-Tb(2)-O(7) | 137.26(17) | O(22)#5-Tb(3)-O(5) | 133.81(17) |
| O(17)-Tb(2)-O(3) | 90.36(19) | O(14)#6-Tb(3)-O(5) | 145.49(17) |
| O(17)-Tb(2)-O(4)#4 | 154.12(19) | O(13)-Tb(3)-O(30) | 137.21(19) |
| O(3)-Tb(2)-O(4)#4 | 104.67(17) | O(30)-Tb(3)-O(5) | 104.7(2) |
| O(17)-Tb(2)-O(27) | 96.0(2) | O(21)#1-Tb(3)-O(6) | 133.13(16) |
| O(3)-Tb(2)-O(27) | 147.4(2) | O(13)-Tb(3)-O(6) | 75.53(17) |
| O(22)#5-Tb(3)-O(6) | 84.38(16) | O(12)#2-Tb(4)-O(15)#8 | 79.72(16) |
| O(14)#6-Tb(3)-O(6) | 149.19(16) | O(33)-Tb(4)-O(15)#8 | 128.58(18) |
| O(30)-Tb(3)-O(6) | 73.62(18) | O(19)-Tb(4)-O(32) | 146.9(2) |
| O(5)-Tb(3)-O(6) | 52.52(16) | O(20)#7-Tb(4)-O(32) | 77.0(2) |
| O(21)#1-Tb(3)-O(31) | 80.83(19) | O(12)#2-Tb(4)-O(32) | 107.4(2) |
| O(19)-Tb(4)-O(20)#7 | 105.81(17) | O(33)-Tb(4)-O(32) | 72.6(2) |
| O(19)-Tb(4)-O(12)#2 | 85.07(18) | O(15)#8-Tb(4)-O(32) | 72.6(2) |
| O(20)#7-Tb(4)-O(12)#2 | 153.07(18) | O(19)-Tb(4)-O(34) | 72.51(17) |
| O(19)-Tb(4)-O(33) | 140.40(19) | O(20)#7-Tb(4)-O(34) | 76.83(18) |
| O(20)#7-Tb(4)-O(33) | 80.33(18) | O(12)#2-Tb(4)-O(34) | 83.41(17) |
| O(12)#2-Tb(4)-O(33) | 76.01(18) | O(33)-Tb(4)-O(34) | 71.01(18) |
| O(19)-Tb(4)-O(15)#8 | 79.99(18) | O(15)#8-Tb(4)-O(34) | 148.78(18) |
| O(20)#7-Tb(4)-O(15)#8 | 125.92(17) | O(32)-Tb(4)-O(34) | 138.00(18) |
| O(19)-Tb(4)-O(16)#8 | 74.21(17) | O(15)#8-Tb(4)-O(16)#8 | 52.88(14) |
| O(20)#7-Tb(4)-O(16)#8 | 76.53(16) | O(32)-Tb(4)-O(16)#8 | 74.5(2) |
| O(12)#2-Tb(4)-O(16)#8 | 130.40(15) | O(34)-Tb(4)-O(16)#8 | 129.09(15) |
| O(33)-Tb(4)-O(16)#8 | 143.21(18) | | |

Eu:Tb=1/3

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|---------------|----------|---------------|----------|
| Tb(1)-O(1)#1 | 2.339(4) | Tb(3)-O(21)#1 | 2.296(5) |
| Tb(1)-O(10)#2 | 2.365(5) | Tb(3)-O(13) | 2.338(5) |
| Tb(1)-O(9)#3 | 2.375(4) | Tb(3)-O(14)#5 | 2.399(4) |
| Tb(1)-O(2) | 2.409(5) | Tb(3)-O(22)#6 | 2.402(4) |
| Tb(1)-O(26) | 2.427(5) | Tb(3)-O(30) | 2.410(6) |
| Tb(1)-O(24) | 2.459(5) | Tb(3)-O(5) | 2.452(5) |
| Tb(1)-O(23) | 2.474(5) | Tb(3)-O(6) | 2.456(5) |
| Tb(1)-O(25) | 2.474(6) | Tb(3)-O(31) | 2.471(5) |
| Tb(1)-O(1) | 2.836(5) | Tb(4)-O(19) | 2.309(5) |
| Tb(2)-O(17) | 2.292(5) | Tb(4)-O(20)#7 | 2.313(5) |
| Tb(2)-O(4)#4 | 2.324(5) | Tb(4)-O(12)#2 | 2.323(5) |
| Tb(2)-O(3) | 2.327(5) | Tb(4)-O(33) | 2.439(5) |
| Tb(2)-O(27) | 2.346(6) | Tb(4)-O(15)#8 | 2.451(5) |
| Tb(2)-O(28) | 2.468(5) | Tb(4)-O(32) | 2.450(6) |
| Tb(2)-O(8) | 2.473(5) | Tb(4)-O(34) | 2.465(5) |
| Tb(2)-O(29) | 2.482(5) | Tb(4)-O(16)#8 | 2.478(4) |

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| Tb(2)-O(7) | 2.500(4) | | |
| | | | |
| O(1)#1-Tb(1)-O(10)#2 | 74.71(17) | O(2)-Tb(1)-O(25) | 68.53(2) |
| O(9)#3-Tb(1)-O(1) | 67.56(15) | O(26)-Tb(1)-O(25) | 75.8(2) |
| O(2)-Tb(1)-O(1) | 48.91(14) | O(24)-Tb(1)-O(25) | 106.8(2) |
| O(26)-Tb(1)-O(1) | 137.56(16) | O(23)-Tb(1)-O(25) | 69.9(2) |
| O(24)-Tb(1)-O(1) | 142.32(17) | O(1)#1-Tb(1)-C(60) | 108.80(19) |
| O(23)-Tb(1)-O(1) | 124.36(18) | O(10)#2-Tb(1)-C(60) | 72.64(19) |
| O(25)-Tb(1)-O(1) | 105.11(18) | O(6)-Tb(3)-O(31) | 101.18(18) |
| O(9)#3-Tb(1)-C(60) | 153.59(19) | O(19)-Tb(4)-O(20)#7 | 105.79(17) |
| O(1)#1-Tb(1)-O(1) | 77.74(16) | O(19)-Tb(4)-O(12)#2 | 84.77(18) |
| O(10)#2-Tb(1)-O(1) | 69.37(15) | O(20)#7-Tb(4)-O(12)#2 | 152.99(19) |
| O(17)-Tb(2)-O(4)#4 | 154.03(19) | O(19)-Tb(4)-O(33) | 140.52(19) |
| O(17)-Tb(2)-O(3) | 90.04(2) | O(20)#7-Tb(4)-O(33) | 80.35(18) |
| O(4)#4-Tb(2)-O(3) | 104.90(18) | O(12)#2-Tb(4)-O(33) | 76.15(19) |
| O(17)-Tb(2)-O(27) | 96.3(2) | O(19)-Tb(4)-O(15)#8 | 80.06(18) |
| O(4)#4-Tb(2)-O(27) | 82.6(2) | O(20)#7-Tb(4)-O(15)#8 | 126.17(17) |
| O(3)-Tb(2)-O(27) | 147.3(2) | O(12)#2-Tb(4)-O(15)#8 | 79.64(17) |
| O(17)-Tb(2)-O(28) | 78.80(17) | O(33)-Tb(4)-O(15)#8 | 128.35(18) |
| O(4)#4-Tb(2)-O(28) | 85.31(18) | O(19)-Tb(4)-O(32) | 146.8(2) |
| O(3)-Tb(2)-O(28) | 73.03(19) | O(20)#7-Tb(4)-O(32) | 76.9(2) |
| O(27)-Tb(2)-O(28) | 139.6(2) | O(12)#2-Tb(4)-O(32) | 108.0(2) |
| O(17)-Tb(2)-O(8) | 130.03(16) | O(33)-Tb(4)-O(32) | 72.6(2) |
| O(4)#4-Tb(2)-O(8) | 75.50(17) | O(15)#8-Tb(4)-O(32) | 72.6(2) |
| O(3)-Tb(2)-O(8) | 71.84(18) | O(19)-Tb(4)-O(34) | 72.7(18) |
| O(27)-Tb(2)-O(8) | 79.77(19) | O(20)#7-Tb(4)-O(34) | 76.53(17) |
| O(28)-Tb(2)-O(8) | 133.57(17) | O(12)#2-Tb(4)-O(34) | 83.35(17) |
| O(17)-Tb(2)-O(29) | 80.21(19) | O(33)-Tb(4)-O(34) | 71.02(18) |
| O(4)#4-Tb(2)-O(29) | 74.86(19) | O(15)#8-Tb(4)-O(34) | 148.99(18) |
| O(3)-Tb(2)-O(29) | 141.37(19) | O(32)-Tb(4)-O(34) | 137.8(2) |
| O(27)-Tb(2)-O(29) | 71.2(2) | O(19)-Tb(4)-O(16)#8 | 74.14(17) |
| O(28)-Tb(2)-O(29) | 68.43(18) | O(20)#7-Tb(4)-O(16)#8 | 76.75(17) |
| O(8)-Tb(2)-O(29) | 140.75(17) | O(12)#2-Tb(4)-O(16)#8 | 130.26(17) |
| O(17)-Tb(2)-O(7) | 78.28(17) | O(33)-Tb(4)-O(16)#8 | 143.24(17) |
| O(4)#4-Tb(2)-O(7) | 125.60(17) | O(15)#8-Tb(4)-O(16)#8 | 52.94(14) |
| O(3)-Tb(2)-O(7) | 75.56(18) | O(32)-Tb(4)-O(16)#8 | 74.4(2) |
| O(27)-Tb(2)-O(7) | 74.46(2) | O(34)-Tb(4)-O(16)#8 | 129.14(15) |
| O(28)-Tb(2)-O(7) | 140.75(18) | O(21)#1-Tb(3)-O(13) | 75.53(18) |
| O(8)-Tb(2)-O(7) | 52.46(15) | O(21)#1-Tb(3)-O(14)#5 | 77.69(17) |
| O(29)-Tb(2)-O(7) | 136.82(17) | O(13)-Tb(3)-O(14)#5 | 125.00(16) |
| O(22)#6-Tb(3)-O(30) | 73.29(19) | O(21)#1-Tb(3)-O(22)#6 | 121.92(18) |
| O(21)#1-Tb(3)-O(5) | 85.83(18) | O(13)-Tb(3)-O(22)#6 | 75.05(18) |
| O(13)-Tb(3)-O(5) | 78.22(19) | O(14)#5-Tb(3)-O(22)#6 | 79.99(17) |

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| O(14)#5-Tb(3)-O(5) | 145.58(17) | O(21)#1-Tb(3)-O(30) | 146.64(19) |
| O(22)#6-Tb(3)-O(5) | 133.81(17) | O(13)-Tb(3)-O(30) | 137.27(19) |
| O(30)-Tb(3)-O(5) | 104.5(2) | O(14)#5-Tb(3)-O(30) | 76.30(18) |
| O(13)-Tb(3)-O(31) | 142.11(19) | O(21)#1-Tb(3)-O(6) | 133.01(17) |
| O(14)#5-Tb(3)-O(31) | 76.73(17) | O(13)-Tb(3)-O(6) | 75.45(17) |
| O(22)#6-Tb(3)-O(31) | 142.79(19) | O(14)#5-Tb(3)-O(6) | 149.01(17) |
| O(30)-Tb(3)-O(31) | 73.2(2) | O(22)#6-Tb(3)-O(6) | 84.42(17) |
| O(21)#1-Tb(3)-O(31) | 80.8(2) | O(30)-Tb(3)-O(6) | 73.60(19) |
| O(5)-Tb(3)-O(31) | 70.88(18) | O(21)#1-Tb(3)-O(31) | 80.78(2) |
| O(5)-Tb(3)-O(6) | 52.49(17) | | |

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|----------------------|------------|--------------------|------------|
| Tb(1)-O(1)#1 | 2.320(4) | Tb(3)-O(21)#1 | 2.286(4) |
| Tb(1)-O(10)#2 | 2.352(4) | Tb(3)-O(13) | 2.327(4) |
| Tb(1)-O(9)#3 | 2.372(4) | Tb(3)-O(14)#5 | 2.381(4) |
| Tb(1)-O(2) | 2.399(4) | Tb(3)-O(22)#6 | 2.387(4) |
| Tb(1)-O(26) | 2.417(5) | Tb(3)-O(30) | 2.407(5) |
| Tb(1)-O(24) | 2.448(4) | Tb(3)-O(5) | 2.438(4) |
| Tb(1)-O(25) | 2.453(5) | Tb(3)-O(31) | 2.441(5) |
| Tb(1)-O(23) | 2.466(5) | Tb(3)-O(6) | 2.450(4) |
| Tb(1)-O(1) | 2.847(5) | Tb(4)-O(19) | 2.295(4) |
| Tb(2)-O(17) | 2.281(4) | Tb(4)-O(20)#7 | 2.308(4) |
| Tb(2)-O(3) | 2.297(4) | Tb(4)-O(12)#2 | 2.311(4) |
| Tb(2)-O(4)#4 | 2.315(4) | Tb(4)-O(33) | 2.429(5) |
| Tb(2)-O(27) | 2.338(5) | Tb(4)-O(15)#8 | 2.438(4) |
| Tb(2)-O(28) | 2.453(5) | Tb(4)-O(32) | 2.432(5) |
| Tb(2)-O(29) | 2.463(4) | Tb(4)-O(34) | 2.449(4) |
| Tb(2)-O(8) | 2.470(4) | Tb(4)-O(16)#8 | 2.472(4) |
| Tb(2)-O(7) | 2.489(4) | | |
| | | | |
| O(24)-Tb(1)-O(1) | 142.41(16) | O(17)-Tb(2)-O(3) | 90.17(18) |
| O(1)#1-Tb(1)-O(10)#2 | 74.96(15) | O(17)-Tb(2)-O(4)#4 | 154.05(17) |
| O(1)#1-Tb(1)-O(9)#3 | 79.67(15) | O(3)-Tb(2)-O(4)#4 | 104.38(16) |
| O(10)#2-Tb(1)-O(9)#3 | 133.39(14) | O(17)-Tb(2)-O(27) | 96.2(2) |
| O(1)#1-Tb(1)-O(2) | 125.55(15) | O(3)-Tb(2)-O(27) | 147.56(19) |
| O(10)#2-Tb(1)-O(2) | 76.42(16) | O(4)#4-Tb(2)-O(27) | 83.04(19) |
| O(9)#3-Tb(1)-O(2) | 87.96(16) | O(17)-Tb(2)-O(28) | 78.70(16) |
| O(1)#1-Tb(1)-O(26) | 82.34(19) | O(3)-Tb(2)-O(28) | 72.87(18) |
| O(10)#2-Tb(1)-O(26) | 139.48(18) | O(4)#4-Tb(2)-O(28) | 85.13(16) |
| O(9)#3-Tb(1)-O(26) | 72.32(16) | O(27)-Tb(2)-O(28) | 139.58(19) |
| O(25)-Tb(1)-O(1) | 105.65(17) | O(17)-Tb(2)-O(29) | 80.29(18) |
| O(23)-Tb(1)-O(1) | 123.76(17) | O(3)-Tb(2)-O(29) | 141.10(18) |
| C(60)-Tb(1)-O(1) | 137.80(16) | O(4)#4-Tb(2)-O(29) | 74.89(17) |

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| O(28)-Tb(2)-O(29) | 68.30(17) | O(27)-Tb(2)-O(29) | 71.31(18) |
| O(17)-Tb(2)-O(8) | 130.30(15) | O(27)-Tb(2)-O(7) | 74.40(18) |
| O(3)-Tb(2)-O(8) | 71.94(17) | O(28)-Tb(2)-O(7) | 140.78(17) |
| O(4)#4-Tb(2)-O(8) | 75.27(15) | O(29)-Tb(2)-O(7) | 136.93(15) |
| O(27)-Tb(2)-O(8) | 79.84(17) | O(8)-Tb(2)-O(7) | 52.70(13) |
| O(28)-Tb(2)-O(8) | 133.49(15) | O(21)#1-Tb(3)-O(13) | 75.53(16) |
| O(29)-Tb(2)-O(8) | 140.45(16) | O(21)#1-Tb(3)-O(14)#5 | 77.68(15) |
| O(17)-Tb(2)-O(7) | 78.32(15) | O(13)-Tb(3)-O(14)#5 | 124.90(15) |
| O(3)-Tb(2)-O(7) | 75.86(16) | O(21)#1-Tb(3)-O(22)#6 | 122.07(16) |
| O(4)#4-Tb(2)-O(7) | 125.69(16) | O(20)#7-Tb(4)-O(34) | 76.50(16) |
| O(13)-Tb(3)-O(22)#6 | 75.29(16) | O(12)#2-Tb(4)-O(34) | 83.33(16) |
| O(14)#5-Tb(3)-O(22)#6 | 79.83(15) | O(33)-Tb(4)-O(34) | 70.91(17) |
| O(21)#1-Tb(3)-O(30) | 146.76(17) | O(15)#8-Tb(4)-O(34) | 149.17(17) |
| O(13)-Tb(3)-O(30) | 137.14(17) | O(32)-Tb(4)-O(34) | 137.43(19) |
| O(14)#5-Tb(3)-O(30) | 76.40(16) | O(19)-Tb(4)-O(16)#8 | 73.87(16) |
| O(22)#6-Tb(3)-O(30) | 72.95(17) | O(20)#7-Tb(4)-O(16)#8 | 76.72(15) |
| O(21)#1-Tb(3)-O(5) | 85.49(17) | O(12)#2-Tb(4)-O(16)#8 | 130.26(15) |
| O(13)-Tb(3)-O(5) | 77.99(17) | O(33)-Tb(4)-O(16)#8 | 143.48(16) |
| O(14)#5-Tb(3)-O(5) | 145.65(16) | O(15)#8-Tb(4)-O(16)#8 | 53.12(13) |
| O(22)#6-Tb(3)-O(5) | 134.01(16) | O(32)-Tb(4)-O(16)#8 | 74.75(19) |
| O(30)-Tb(3)-O(5) | 104.86(19) | O(34)-Tb(4)-O(16)#8 | 129.06(14) |
| O(21)#1-Tb(3)-O(31) | 80.55(18) | O(20)#7-Tb(4)-O(32) | 76.8(2) |
| O(13)-Tb(3)-O(31) | 142.05(18) | O(12)#2-Tb(4)-O(32) | 108.1(2) |
| O(14)#5-Tb(3)-O(31) | 76.69(16) | O(33)-Tb(4)-O(32) | 72.5(2) |
| O(22)#6-Tb(3)-O(31) | 142.62(18) | O(15)#8-Tb(4)-O(32) | 72.8(2) |
| O(30)-Tb(3)-O(31) | 73.5(2) | O(19)-Tb(4)-O(34) | 72.85(17) |
| O(5)-Tb(3)-O(31) | 71.09(18) | O(19)-Tb(4)-O(15)#8 | 80.21(17) |
| O(21)#1-Tb(3)-O(6) | 133.06(15) | O(20)#7-Tb(4)-O(15)#8 | 126.20(16) |
| O(13)-Tb(3)-O(6) | 75.54(16) | O(12)#2-Tb(4)-O(15)#8 | 79.57(15) |
| O(14)#5-Tb(3)-O(6) | 148.97(15) | O(33)-Tb(4)-O(15)#8 | 128.12(17) |
| O(22)#6-Tb(3)-O(6) | 84.46(15) | O(19)-Tb(4)-O(32) | 146.94(19) |
| O(30)-Tb(3)-O(6) | 73.46(17) | O(20)#7-Tb(4)-O(12)#2 | 153.02(17) |
| O(5)-Tb(3)-O(6) | 52.73(15) | O(19)-Tb(4)-O(33) | 140.54(17) |
| O(31)-Tb(3)-O(6) | 101.34(17) | O(20)#7-Tb(4)-O(33) | 80.51(17) |
| O(19)-Tb(4)-O(20)#7 | 105.65(16) | O(12)#2-Tb(4)-O(33) | 76.03(17) |
| O(19)-Tb(4)-O(12)#2 | 84.87(17) | | |

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| Tb(1)-O(1)#1 | 2.318(5) | Tb(2)-O(7) | 2.487(5) |
| Tb(1)-O(10)#2 | 2.341(5) | Tb(3)-O(21)#1 | 2.286(5) |
| Tb(1)-O(9)#3 | 2.363(5) | Tb(3)-O(13) | 2.317(5) |
| Tb(1)-O(2) | 2.388(5) | Tb(3)-O(14)#5 | 2.374(5) |
| Tb(1)-O(26) | 2.398(6) | Tb(3)-O(22)#6 | 2.379(5) |

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| Tb(1)-O(24) | 2.437(5) | Tb(3)-O(30) | 2.393(6) |
| Tb(1)-O(23) | 2.460(6) | Tb(3)-O(5) | 2.429(6) |
| Tb(1)-O(25) | 2.470(6) | Tb(3)-O(31) | 2.442(6) |
| Tb(1)-O(1) | 2.816(6) | Tb(3)-O(6) | 2.452(6) |
| Tb(2)-O(17) | 2.274(5) | Tb(4)-O(19) | 2.286(6) |
| Tb(2)-O(3) | 2.297(5) | Tb(4)-O(20)#7 | 2.301(5) |
| Tb(2)-O(4)#4 | 2.304(5) | Tb(4)-O(12)#2 | 2.303(5) |
| Tb(2)-O(27) | 2.328(6) | Tb(4)-O(33) | 2.425(6) |
| Tb(2)-O(8) | 2.457(5) | Tb(4)-O(15)#8 | 2.431(5) |
| Tb(2)-O(28) | 2.457(6) | Tb(4)-O(32) | 2.444(7) |
| Tb(2)-O(29) | 2.460(6) | Tb(4)-O(34) | 2.455(6) |
| Tb(4)-O(16)#8 | 2.459(5) | | |
| | | | |
| O(1)#1-Tb(1)-O(10)#2 | 74.80(19) | O(3)-Tb(2)-O(27) | 147.8(2) |
| O(1)#1-Tb(1)-O(9)#3 | 79.76(19) | O(4)#4-Tb(2)-O(27) | 82.8(2) |
| O(10)#2-Tb(1)-O(9)#3 | 133.70(18) | O(17)-Tb(2)-O(8) | 130.37(19) |
| O(1)#1-Tb(1)-O(2) | 125.23(19) | O(3)-Tb(2)-O(8) | 71.9(2) |
| O(10)#2-Tb(1)-O(2) | 76.3(2) | O(4)#4-Tb(2)-O(8) | 75.04(19) |
| O(9)#3-Tb(1)-O(2) | 88.2(2) | O(27)-Tb(2)-O(8) | 80.0(2) |
| O(1)#1-Tb(1)-O(26) | 82.8(2) | O(17)-Tb(2)-O(28) | 78.8(2) |
| O(10)#2-Tb(1)-O(26) | 139.5(2) | O(3)-Tb(2)-O(28) | 73.0(2) |
| O(9)#3-Tb(1)-O(26) | 72.1(2) | O(4)#4-Tb(2)-O(28) | 85.4(2) |
| O(2)-Tb(1)-O(26) | 142.9(2) | O(27)-Tb(2)-O(28) | 139.2(2) |
| O(1)#1-Tb(1)-O(24) | 84.7(2) | O(8)-Tb(2)-O(28) | 133.70(18) |
| O(10)#2-Tb(1)-O(24) | 74.4(2) | O(17)-Tb(2)-O(29) | 80.0(2) |
| O(9)#3-Tb(1)-O(24) | 140.77(19) | O(3)-Tb(2)-O(29) | 141.0(2) |
| O(2)-Tb(1)-O(24) | 129.49(19) | O(4)#4-Tb(2)-O(29) | 75.2(2) |
| O(26)-Tb(1)-O(24) | 70.3(2) | O(27)-Tb(2)-O(29) | 71.2(2) |
| O(1)#1-Tb(1)-O(23) | 133.69(19) | O(8)-Tb(2)-O(29) | 140.6(2) |
| O(10)#2-Tb(1)-O(23) | 77.3(2) | O(28)-Tb(2)-O(29) | 68.1(2) |
| O(9)#3-Tb(1)-O(23) | 143.8(2) | O(17)-Tb(2)-O(7) | 78.36(19) |
| O(2)-Tb(1)-O(23) | 81.7(2) | O(3)-Tb(2)-O(7) | 76.0(2) |
| O(26)-Tb(1)-O(23) | 95.7(3) | O(4)#4-Tb(2)-O(7) | 125.43(19) |
| O(24)-Tb(1)-O(23) | 52.3(2) | O(27)-Tb(2)-O(7) | 74.6(2) |
| O(1)#1-Tb(1)-O(25) | 150.3(2) | O(8)-Tb(2)-O(7) | 52.68(16) |
| O(10)#2-Tb(1)-O(25) | 134.5(2) | O(28)-Tb(2)-O(7) | 140.9(2) |
| O(9)#3-Tb(1)-O(25) | 74.8(2) | O(29)-Tb(2)-O(7) | 136.86(19) |
| O(2)-Tb(1)-O(25) | 69.4(2) | O(21)#1-Tb(3)-O(13) | 75.0(2) |
| O(26)-Tb(1)-O(25) | 75.2(3) | O(21)#1-Tb(3)-O(14)#5 | 77.5(2) |
| O(24)-Tb(1)-O(25) | 105.7(3) | O(13)-Tb(3)-O(14)#5 | 124.68(18) |
| O(23)-Tb(1)-O(25) | 69.2(3) | O(21)#1-Tb(3)-O(22)#6 | 121.97(19) |
| O(1)#1-Tb(1)-O(1) | 77.70(18) | O(13)-Tb(3)-O(22)#6 | 75.6(2) |
| O(10)#2-Tb(1)-O(1) | 69.24(17) | O(14)#5-Tb(3)-O(22)#6 | 79.9(2) |

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| O(9)#3-Tb(1)-O(1) | 67.93(17) | O(21)#1-Tb(3)-O(30) | 146.8(2) |
| O(2)-Tb(1)-O(1) | 48.67(17) | O(13)-Tb(3)-O(30) | 137.6(2) |
| O(26)-Tb(1)-O(1) | 137.88(18) | O(14)#5-Tb(3)-O(30) | 76.8(2) |
| O(24)-Tb(1)-O(1) | 142.5(2) | O(22)#6-Tb(3)-O(30) | 73.3(2) |
| O(23)-Tb(1)-O(1) | 124.5(2) | O(21)#1-Tb(3)-O(5) | 85.7(2) |
| O(25)-Tb(1)-O(1) | 105.9(2) | O(13)-Tb(3)-O(5) | 78.2(2) |
| O(17)-Tb(2)-O(3) | 90.6(2) | O(14)#5-Tb(3)-O(5) | 145.4(2) |
| O(17)-Tb(2)-O(4)#4 | 154.2(2) | O(22)#6-Tb(3)-O(5) | 134.1(2) |
| O(3)-Tb(2)-O(4)#4 | 104.2(2) | O(30)-Tb(3)-O(5) | 104.2(2) |
| O(17)-Tb(2)-O(27) | 95.9(3) | O(21)#1-Tb(3)-O(6) | 132.8(2) |
| O(13)-Tb(3)-O(6) | 75.5(2) | O(14)#5-Tb(3)-O(6) | 149.4(2) |
| O(22)#6-Tb(3)-O(6) | 84.4(2) | O(19)-Tb(4)-O(34) | 72.5(2) |
| O(30)-Tb(3)-O(6) | 73.6(2) | O(20)#7-Tb(4)-O(34) | 77.2(2) |
| O(5)-Tb(3)-O(6) | 52.7(2) | O(12)#2-Tb(4)-O(34) | 82.6(2) |
| O(31)-Tb(3)-O(6) | 102.1(2) | O(33)-Tb(4)-O(34) | 70.8(2) |
| O(19)-Tb(4)-O(20)#7 | 105.3(2) | O(15)#8-Tb(4)-O(34) | 148.2(2) |
| O(19)-Tb(4)-O(12)#2 | 85.1(2) | O(32)-Tb(4)-O(34) | 137.9(2) |
| O(20)#7-Tb(4)-O(12)#2 | 153.0(2) | O(19)-Tb(4)-O(16)#8 | 73.8(2) |
| O(19)-Tb(4)-O(33) | 140.6(2) | O(20)#7-Tb(4)-O(16)#8 | 76.7(2) |
| O(20)#7-Tb(4)-O(33) | 79.9(2) | O(21)#1-Tb(3)-O(31) | 80.4(2) |
| O(12)#2-Tb(4)-O(33) | 76.6(2) | O(13)-Tb(3)-O(31) | 141.9(2) |
| O(19)-Tb(4)-O(15)#8 | 79.8(2) | O(14)#5-Tb(3)-O(31) | 76.2(2) |
| O(20)#7-Tb(4)-O(15)#8 | 126.2(2) | O(22)#6-Tb(3)-O(31) | 142.5(2) |
| O(12)#2-Tb(4)-O(15)#8 | 79.7(2) | O(30)-Tb(3)-O(31) | 73.4(2) |
| O(33)-Tb(4)-O(15)#8 | 129.2(2) | O(5)-Tb(3)-O(31) | 71.2(2) |
| O(19)-Tb(4)-O(32) | 147.1(2) | O(12)#2-Tb(4)-O(16)#8 | 130.36(19) |
| O(20)#7-Tb(4)-O(32) | 77.3(2) | O(33)-Tb(4)-O(16)#8 | 143.1(2) |
| O(33)-Tb(4)-O(32) | 72.3(3) | O(15)#8-Tb(4)-O(16)#8 | 52.97(17) |
| O(15)#8-Tb(4)-O(32) | 73.1(2) | O(32)-Tb(4)-O(16)#8 | 75.1(2) |
| O(34)-Tb(4)-O(16)#8 | 129.39(18) | | |