

## **A single component white electroluminescent device fabricated from a metallo-organic terbium complex**

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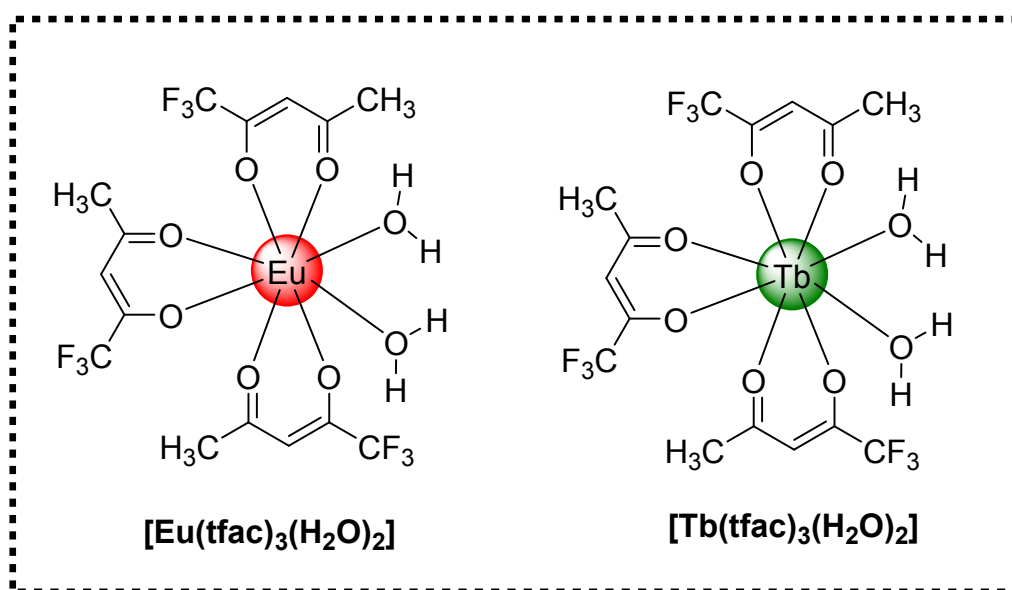
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### Synthesis of $[\text{Ln}(\text{tfac})_3(\text{H}_2\text{O})_2]$ (Ln: Eu and Tb)

Binary hydrated  $[\text{Ln}(\text{tfac})_3(\text{H}_2\text{O})_2]$  complexes (**Chart S1**) were synthesized by the method reported by one us; instead of acetylacetone, hemi-fluorinated Htfac was used. Briefly,  $\text{LnCl}_3 \cdot 6\text{H}_2\text{O}$  (Eu- 2.39 g, 6.57 mmol; Tb- 2.40 g, 6.57 mmol) aqueous solution was added dropwise through a dropping funnel to a solution of ammonium salt of tfac (2.0 g, 19.97 mmol). The white precipitate formed was filtered, washed with copious amount of deionized water and dried in vacuum over  $\text{P}_4\text{O}_{10}$ .

$[\text{Eu}(\text{tfac})_3(\text{H}_2\text{O})_2]$  Calculated for  $\text{C}_{15}\text{H}_{16}\text{EuF}_9\text{O}_8$ : C, 27.84; H, 2.49 found C, 27.50; H, 2.35; FT-IR (solid; $\text{cm}^{-1}$ ) -  $\nu(\text{O-H}) \sim 3,209 - 3,503(\text{b})$ ;  $\nu(\text{C=O}) \sim 1,613(\text{s})$ ;  $\nu(\text{C=C}) \sim 1,532(\text{m})$

$[\text{Tb}(\text{tfac})_3(\text{H}_2\text{O})_2]$  Calculated for  $\text{C}_{15}\text{H}_{16}\text{TbF}_9\text{O}_8$ : C, 27.54; H, 2.47 found C, 27.40; H, 2.20; FT-IR (solid; $\text{cm}^{-1}$ ) -  $\nu(\text{O-H}) \sim 3,209 - 3,503(\text{b})$ ;  $\nu(\text{C=O}) \sim 1,614(\text{s})$ ;  $\nu(\text{C=C}) \sim 1,531(\text{m})$ .



**Chart S1:** Chemical structures of binary hydrated  $[\text{Ln}(\text{tfac})_3(\text{H}_2\text{O})_2]$  complexes.

### Molecular Structure Determination by Single-Crystal X-ray Crystallography

For each of the two structures  $[\text{Ln}(\text{tfac})_3(\text{DPEPO})]$  (Ln: Eu(**Eu-1**) and Tb(**Tb-2**)) the crystals were cooled to 150 K using an Oxford Diffraction Cryojet low-temperature apparatus. The data reduction including an empirical absorption correction using the SCALE3 ABSPACK scaling

algorithm was performed using the CrysAlisPro software package.<sup>1</sup> The crystal structures were solved by direct methods using SIR-97,<sup>2</sup> and refined using SHELXTL<sup>3</sup> within the OLEX2<sup>4</sup> software package. The non-hydrogen atoms were refined anisotropically. The hydrogen atoms were placed in idealized positions and refined with a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{N})$ . In each structure one of the CF<sub>3</sub> groups was severely disordered. The group was modelled as two, partial occupancy CF<sub>3</sub> groups with a common C atom, and refined so that the occupancy of the two disordered components summed to unity. The structures were refined to convergence.

#### **Determination of photoluminescence quantum yield (PLQY) of Tb-2.**

The absolute PLQY of **Tb-2** in the solid-state and in DCM solution were determined by using a calibrated integrating sphere on a C-9920-02 instrument. The excitation wavelength was 335 nm and the data were measured within the range 450-700 nm. For solid-state measurements, the powder was pressed directly while for the DCM solution 10 mg of **Tb-2** was dissolved in 1 mL of DCM.

Table S 1. Crystal data and structure refinement for **Eu-1** and **Tb-2** complexes.

| Identification code                            | Eu-1                                                                           | Tb-2                                                                           |
|------------------------------------------------|--------------------------------------------------------------------------------|--------------------------------------------------------------------------------|
| CCDC number                                    | 1942486                                                                        | 1942487                                                                        |
| Empirical formula                              | C <sub>51</sub> H <sub>40</sub> EuF <sub>9</sub> O <sub>9</sub> P <sub>2</sub> | C <sub>51</sub> H <sub>40</sub> TbF <sub>9</sub> O <sub>9</sub> P <sub>2</sub> |
| Formula weight                                 | 1181.73                                                                        | 1188.69                                                                        |
| Temperature/K                                  | 150.00(10)                                                                     | 149.6(9)                                                                       |
| Crystal system                                 | triclinic                                                                      | triclinic                                                                      |
| Space group                                    | P-1                                                                            | P-1                                                                            |
| a/Å                                            | 12.9046(3)                                                                     | 12.9304(3)                                                                     |
| b/Å                                            | 13.7184(3)                                                                     | 13.7121(3)                                                                     |
| c/Å                                            | 16.8199(4)                                                                     | 16.7959(4)                                                                     |
| $\alpha/^\circ$                                | 94.511(2)                                                                      | 94.449(2)                                                                      |
| $\beta/^\circ$                                 | 110.592(2)                                                                     | 110.577(2)                                                                     |
| $\gamma/^\circ$                                | 110.126(2)                                                                     | 110.301(2)                                                                     |
| Volume/Å <sup>3</sup>                          | 2548.76(11)                                                                    | 2546.39(11)                                                                    |
| Z                                              | 2                                                                              | 2                                                                              |
| $\rho_{\text{calc}}/\text{g/cm}^3$             | 1.540                                                                          | 1.550                                                                          |
| $\mu/\text{mm}^{-1}$                           | 1.380                                                                          | 1.538                                                                          |
| F(000)                                         | 1184.0                                                                         | 1188.0                                                                         |
| Crystal size/mm <sup>3</sup>                   | 0.4 × 0.3 × 0.3                                                                | 0.3 × 0.3 × 0.3                                                                |
| Radiation                                      | MoK $\alpha$ ( $\lambda$ = 0.71073)                                            | MoK $\alpha$ ( $\lambda$ = 0.71073)                                            |
| 2 $\theta$ range for data collection/ $^\circ$ | 8.38 to 54.968                                                                 | 8.384 to 54.968                                                                |
| Index ranges                                   | -16 ≤ h ≤ 16, -17 ≤ k ≤ 17, -21 ≤ l ≤ 21                                       | -16 ≤ h ≤ 16, -17 ≤ k ≤ 17, -21 ≤ l ≤ 21                                       |
| Reflections collected                          | 55605                                                                          | 40032                                                                          |
| Independent reflections                        | 11495 [ $R_{\text{int}}$ = 0.0514, $R_{\text{sigma}}$ = 0.0403]                | 11461 [ $R_{\text{int}}$ = 0.0521, $R_{\text{sigma}}$ = 0.0510]                |
| Data/restraints/parameters                     | 11495/36/680                                                                   | 11461/36/680                                                                   |
| Goodness-of-fit on F <sup>2</sup>              | 1.073                                                                          | 1.026                                                                          |
| Final R indexes [ $I \geq 2\sigma(I)$ ]        | $R_1$ = 0.0314, $wR_2$ = 0.0668                                                | $R_1$ = 0.0348, $wR_2$ = 0.0765                                                |
| Final R indexes [all data]                     | $R_1$ = 0.0408, $wR_2$ = 0.0715                                                | $R_1$ = 0.0458, $wR_2$ = 0.0818                                                |
| Largest diff. peak/hole / e Å <sup>-3</sup>    | 1.27/-0.71                                                                     | 1.32/-1.13                                                                     |

Table S 2 . Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for **Eu-1**.  $U_{\text{eq}}$  is defined as 1/3 of the trace of the orthogonalised  $U_{ij}$  tensor.

| Atom | x          | y          | z          | U(eq)     |
|------|------------|------------|------------|-----------|
| Eu1  | 950.3(2)   | 2220.0(2)  | 2215.4(2)  | 20.36(5)  |
| P1   | 1910.8(6)  | 5200.1(5)  | 2372.8(4)  | 22.45(14) |
| P2   | -1940.2(6) | 2611.1(6)  | 2012.8(4)  | 23.98(15) |
| F1   | 3374(12)   | 1514(6)    | 207(14)    | 116(6)    |
| F2   | 4226(5)    | 2850(13)   | 1236(5)    | 87(4)     |
| F3   | 3311(9)    | 2969(13)   | -4(10)     | 110(5)    |
| F1A  | 3868(10)   | 1929(16)   | 1093(8)    | 109(4)    |
| F2A  | 3745(15)   | 3260(7)    | 642(15)    | 138(7)    |
| F3A  | 3031(8)    | 1806(14)   | -213(6)    | 109(5)    |
| F4   | 2535(2)    | -448(2)    | 4200.7(17) | 85.3(9)   |
| F5   | 2836(2)    | -718(2)    | 3041.8(17) | 74.0(7)   |
| F6   | 3723(2)    | 814.0(19)  | 3884.4(15) | 61.4(6)   |
| F7   | 1993(2)    | 1875(3)    | 5744.2(16) | 111.3(13) |
| F8   | 631(3)     | 2447(2)    | 5176.7(16) | 78.5(8)   |
| F9   | 370(2)     | 899.1(19)  | 4651.5(15) | 70.3(7)   |
| O1   | 1447.4(16) | 4016.3(14) | 2110.2(11) | 23.7(4)   |
| O2   | -746.5(17) | 2574.7(15) | 2166.9(12) | 26.2(4)   |
| O3   | -686.4(17) | 4564.7(15) | 1601.2(12) | 27.5(4)   |
| O4   | -280.1(17) | 1486.9(15) | 685.0(12)  | 27.1(4)   |
| O5   | 2200.9(18) | 2424.2(16) | 1428.5(13) | 31.3(4)   |
| O6   | -566.5(18) | 487.0(15)  | 2048.3(12) | 30.7(4)   |
| O7   | 1908.6(18) | 1028.5(15) | 2670.8(12) | 28.9(4)   |
| O8   | 2981.5(18) | 3258.7(16) | 3318.6(13) | 32.3(5)   |
| O9   | 950.9(17)  | 2217.6(15) | 3626.2(11) | 27.8(4)   |
| C1   | -161(3)    | 1220(2)    | 2.9(17)    | 29.1(6)   |
| C2   | 976(3)     | 1454(3)    | -32.5(19)  | 36.5(7)   |
| C3   | 2039(3)    | 2040(2)    | 669.1(19)  | 31.6(6)   |
| C4   | -1272(3)   | 670(3)     | -828.5(19) | 39.6(8)   |
| C5   | 3203(4)    | 2306(4)    | 525(3)     | 51.5(9)   |
| C6   | -564(3)    | -261(2)    | 2430.3(19) | 34.2(7)   |
| C7   | 492(3)     | -388(2)    | 2948(2)    | 37.3(7)   |
| C8   | 1622(3)    | 253(2)     | 3016.4(18) | 31.7(7)   |
| C9   | -1764(3)   | -1069(3)   | 2335(2)    | 50.2(9)   |
| C10  | 2677(3)    | -22(3)     | 3541(2)    | 43.5(8)   |
| C11  | 3547(3)    | 3220(3)    | 4077(2)    | 37.8(7)   |
| C12  | 2979(3)    | 2757(3)    | 4625(2)    | 41.3(8)   |
| C13  | 1762(3)    | 2316(2)    | 4359.9(18) | 32.5(7)   |

|     |          |         |            |          |
|-----|----------|---------|------------|----------|
| C14 | 4911(3)  | 3692(4) | 4428(3)    | 62.4(11) |
| C15 | 1226(3)  | 1880(3) | 4995(2)    | 47.2(9)  |
| C16 | 3455(3)  | 5802(2) | 2517.0(19) | 30.1(6)  |
| C17 | 3900(3)  | 5162(3) | 2185(2)    | 39.3(7)  |
| C18 | 5050(3)  | 5599(3) | 2191(3)    | 53.7(10) |
| C19 | 5740(3)  | 6675(3) | 2534(3)    | 55.1(10) |
| C20 | 5318(3)  | 7314(3) | 2876(2)    | 50.6(9)  |
| C21 | 4180(3)  | 6885(3) | 2875(2)    | 41.2(8)  |
| C22 | 1111(2)  | 5739(2) | 1533.6(16) | 23.2(5)  |
| C23 | 1671(3)  | 6446(2) | 1111.2(18) | 27.8(6)  |
| C24 | 987(3)   | 6741(2) | 409.9(18)  | 31.3(6)  |
| C25 | -254(3)  | 6344(2) | 129.8(18)  | 32.6(7)  |
| C26 | -825(3)  | 5650(2) | 541.3(18)  | 30.0(6)  |
| C27 | -134(3)  | 5352(2) | 1235.3(17) | 24.9(6)  |
| C28 | 1758(3)  | 5644(2) | 3345.2(17) | 27.7(6)  |
| C29 | 1894(3)  | 6686(2) | 3597(2)    | 38.3(7)  |
| C30 | 1750(4)  | 6998(3) | 4341(2)    | 48.4(9)  |
| C31 | 1451(4)  | 6270(3) | 4826(2)    | 49.3(9)  |
| C32 | 1297(3)  | 5232(3) | 4574(2)    | 45.3(8)  |
| C33 | 1464(3)  | 4917(2) | 3839.5(19) | 34.2(7)  |
| C34 | -1221(3) | 4793(2) | 2123.1(17) | 27.5(6)  |
| C35 | -1126(3) | 5811(3) | 2396.9(19) | 35.5(7)  |
| C36 | -1672(3) | 5960(3) | 2942(2)    | 44.6(8)  |
| C37 | -2301(3) | 5126(3) | 3212(2)    | 46.8(9)  |
| C38 | -2394(3) | 4106(3) | 2939.2(19) | 37.3(7)  |
| C39 | -1852(3) | 3920(2) | 2386.4(17) | 27.2(6)  |
| C40 | -2962(2) | 2167(2) | 879.8(17)  | 27.9(6)  |
| C41 | -3585(3) | 2746(3) | 447(2)     | 37.3(7)  |
| C42 | -4367(3) | 2345(3) | -432(2)    | 47.0(9)  |
| C43 | -4530(3) | 1376(3) | -855(2)    | 46.9(9)  |
| C44 | -3925(3) | 796(3)  | -434(2)    | 46.8(9)  |
| C45 | -3130(3) | 1192(3) | 435(2)     | 38.2(7)  |
| C46 | -2689(3) | 1752(2) | 2574.6(18) | 29.5(6)  |
| C47 | -3917(3) | 1454(3) | 2358(2)    | 44.9(8)  |
| C48 | -4461(3) | 839(3)  | 2826(2)    | 54.8(10) |
| C49 | -3789(4) | 507(3)  | 3492(2)    | 52.2(10) |
| C50 | -2581(4) | 788(3)  | 3705(2)    | 46.0(9)  |
| C51 | -2015(3) | 1415(2) | 3245.0(19) | 34.6(7)  |

Table S 3. Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for **Eu-1**. The Anisotropic displacement factor exponent takes the form:  $2\pi^2[h^2a^2U_{11}+2hka^*b^*U_{12}+\dots]$ .

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|------|----------|----------|----------|----------|----------|----------|
| Eu1  | 24.16(7) | 17.77(7) | 17.76(7) | 6.00(5)  | 8.28(5)  | 6.54(5)  |
| P1   | 24.4(3)  | 17.7(3)  | 22.1(3)  | 7.0(3)   | 7.8(3)   | 5.8(3)   |
| P2   | 23.1(3)  | 27.0(4)  | 22.0(3)  | 8.1(3)   | 10.7(3)  | 8.1(3)   |
| F1   | 94(8)    | 57(4)    | 238(17)  | -2(7)    | 122(10)  | 27(4)    |
| F2   | 39(3)    | 145(11)  | 61(4)    | -5(5)    | 27(3)    | 16(4)    |
| F3   | 91(6)    | 163(12)  | 154(9)   | 126(9)   | 96(7)    | 71(7)    |
| F1A  | 61(5)    | 188(13)  | 120(8)   | 60(8)    | 45(5)    | 81(7)    |
| F2A  | 141(11)  | 67(5)    | 235(16)  | -1(8)    | 165(13)  | -10(6)   |
| F3A  | 69(4)    | 206(15)  | 60(4)    | -22(5)   | 39(3)    | 60(6)    |
| F4   | 80.7(18) | 130(2)   | 86.7(18) | 87.0(18) | 48.2(15) | 61.8(18) |
| F5   | 83.8(18) | 67.2(16) | 89.2(18) | 14.1(14) | 31.7(15) | 55.1(15) |
| F6   | 51.3(13) | 59.3(15) | 71.2(15) | 24.8(12) | 13.6(11) | 28.6(12) |
| F7   | 72.2(18) | 206(4)   | 48.0(14) | 74.1(19) | 18.3(13) | 42(2)    |
| F8   | 107(2)   | 86.7(19) | 62.0(15) | 13.3(14) | 56.7(15) | 39.7(17) |
| F9   | 98.5(19) | 54.5(15) | 57.9(14) | 22.5(12) | 46.0(14) | 13.5(14) |
| O1   | 24.4(10) | 19.2(9)  | 25.5(9)  | 7.5(8)   | 9.6(8)   | 6.5(8)   |
| O2   | 27.4(10) | 24.9(10) | 26.7(10) | 9.9(8)   | 11.6(8)  | 9.3(8)   |
| O3   | 33.1(11) | 22.2(10) | 33(1)    | 10.9(8)  | 18.8(9)  | 11.0(9)  |
| O4   | 33.4(11) | 25.1(10) | 21.5(9)  | 5.3(8)   | 11.3(8)  | 10.0(9)  |
| O5   | 32.8(11) | 32.6(11) | 29.4(10) | 7.6(9)   | 15.6(9)  | 10.8(9)  |
| O6   | 34.1(11) | 22.9(10) | 26.9(10) | 6.5(8)   | 10.1(9)  | 4.1(9)   |
| O7   | 39.2(12) | 22.5(10) | 30.4(10) | 10.1(8)  | 18.2(9)  | 13.2(9)  |
| O8   | 30.2(11) | 28.0(11) | 29.6(11) | 10.7(9)  | 5.9(9)   | 6.7(9)   |
| O9   | 31.3(11) | 28.9(11) | 20.1(9)  | 6.3(8)   | 8.0(8)   | 10.7(9)  |
| C1   | 45.4(18) | 22.5(14) | 22.8(13) | 7.2(11)  | 13.2(13) | 17.6(13) |
| C2   | 48.7(19) | 43.6(19) | 28.2(15) | 8.3(13)  | 20.9(14) | 25.3(16) |
| C3   | 42.2(17) | 33.8(16) | 35.7(16) | 16.9(13) | 24.0(14) | 24.3(15) |
| C4   | 50(2)    | 37.1(18) | 23.2(15) | 1.0(13)  | 6.4(14)  | 18.1(16) |
| C5   | 50(2)    | 64(3)    | 50(2)    | 8.4(19)  | 29.6(19) | 25(2)    |
| C6   | 46.2(18) | 21.9(15) | 29.4(15) | 3.8(12)  | 20.1(14) | 3.3(14)  |
| C7   | 54(2)    | 28.3(16) | 37.0(17) | 18.0(13) | 24.1(15) | 16.3(15) |
| C8   | 50.2(19) | 26.1(15) | 27.6(14) | 10.2(12) | 20.7(14) | 19.1(14) |
| C9   | 52(2)    | 37(2)    | 51(2)    | 14.9(16) | 24.7(18) | 0.7(17)  |
| C10  | 58(2)    | 41(2)    | 45.3(19) | 23.8(16) | 25.4(17) | 27.9(18) |
| C11  | 33.4(17) | 31.2(17) | 32.5(16) | 6.6(13)  | 1.7(13)  | 6.3(14)  |
| C12  | 40.3(18) | 47(2)    | 24.4(15) | 11.6(14) | 2.4(13)  | 13.8(16) |
| C13  | 46.3(18) | 30.2(16) | 19.7(13) | 7.1(12)  | 10.8(13) | 16.0(14) |
| C14  | 33.8(19) | 74(3)    | 53(2)    | 18(2)    | 0.8(17)  | 8.4(19)  |

|     |          |          |          |          |          |          |
|-----|----------|----------|----------|----------|----------|----------|
| C15 | 55(2)    | 57(2)    | 26.3(16) | 13.2(16) | 15.3(16) | 17.9(19) |
| C16 | 24.7(14) | 27.8(15) | 31.1(15) | 11.4(12) | 7.0(12)  | 6.3(12)  |
| C17 | 28.6(16) | 31.3(17) | 53(2)    | 11.3(15) | 16.6(15) | 5.4(14)  |
| C18 | 29.8(18) | 51(2)    | 78(3)    | 14(2)    | 23.9(18) | 11.3(17) |
| C19 | 25.9(17) | 52(2)    | 76(3)    | 24(2)    | 17.1(18) | 4.7(17)  |
| C20 | 29.0(17) | 35.5(19) | 62(2)    | 16.9(17) | 2.3(16)  | -0.7(15) |
| C21 | 32.5(17) | 29.1(17) | 46.0(19) | 7.8(14)  | 5.6(14)  | 4.6(14)  |
| C22 | 32.1(15) | 18.9(13) | 18.7(12) | 4.8(10)  | 9.6(11)  | 10.8(12) |
| C23 | 35.9(16) | 22.3(14) | 28.0(14) | 8.6(11)  | 15.5(12) | 11.6(13) |
| C24 | 48.7(19) | 25.3(15) | 28.3(14) | 11.6(12) | 20.9(14) | 17.7(14) |
| C25 | 50.7(19) | 27.1(16) | 22.0(14) | 7.4(12)  | 11.5(13) | 20.3(15) |
| C26 | 33.4(16) | 25.1(15) | 28.4(14) | 4.6(12)  | 7.9(12)  | 13.1(13) |
| C27 | 33.5(15) | 18.3(13) | 24.0(13) | 5.9(11)  | 12.5(12) | 10.4(12) |
| C28 | 31.0(15) | 24.1(15) | 21.5(13) | 5.7(11)  | 6.4(11)  | 8.0(12)  |
| C29 | 54(2)    | 26.9(16) | 30.3(16) | 6.6(13)  | 14.7(15) | 13.4(15) |
| C30 | 76(3)    | 33.1(19) | 31.5(17) | 0.0(14)  | 17.6(17) | 21.8(18) |
| C31 | 75(3)    | 50(2)    | 26.5(16) | 5.2(15)  | 22.9(17) | 27(2)    |
| C32 | 65(2)    | 46(2)    | 29.6(16) | 14.2(15) | 23.0(16) | 22.3(18) |
| C33 | 45.5(18) | 27.1(16) | 27.3(15) | 7.8(12)  | 13.0(13) | 12.8(14) |
| C34 | 30.0(15) | 34.1(16) | 22.9(13) | 8.1(12)  | 10.5(11) | 17.6(13) |
| C35 | 42.8(18) | 31.8(17) | 31.9(16) | 7.1(13)  | 11.9(14) | 18.3(15) |
| C36 | 63(2)    | 45(2)    | 35.8(17) | 7.7(15)  | 20.1(17) | 34.6(19) |
| C37 | 66(2)    | 63(2)    | 36.0(18) | 15.7(17) | 30.0(17) | 43(2)    |
| C38 | 42.9(18) | 51(2)    | 30.1(16) | 16.5(14) | 20.6(14) | 25.5(16) |
| C39 | 29.0(15) | 33.6(16) | 21.4(13) | 7.8(11)  | 9.5(11)  | 15.7(13) |
| C40 | 20.8(13) | 35.3(16) | 25.1(14) | 7.1(12)  | 11.6(11) | 6.0(12)  |
| C41 | 31.9(16) | 49(2)    | 32.8(16) | 11.3(14) | 12.5(13) | 17.8(15) |
| C42 | 36.0(18) | 71(3)    | 34.1(17) | 18.1(17) | 9.8(14)  | 23.9(18) |
| C43 | 29.9(17) | 67(3)    | 28.7(16) | 1.5(16)  | 6.4(13)  | 10.1(17) |
| C44 | 37.1(18) | 52(2)    | 35.1(17) | -6.7(16) | 6.7(14)  | 11.6(17) |
| C45 | 32.5(17) | 40.4(19) | 33.6(16) | 3.9(14)  | 9.1(13)  | 10.7(15) |
| C46 | 31.8(15) | 27.7(15) | 26.9(14) | 5.8(12)  | 17.1(12) | 4.2(13)  |
| C47 | 33.7(17) | 59(2)    | 34.3(17) | 11.4(16) | 17.4(14) | 6.6(16)  |
| C48 | 40(2)    | 67(3)    | 48(2)    | 9.5(19)  | 28.3(17) | 1.0(19)  |
| C49 | 63(2)    | 42(2)    | 52(2)    | 12.5(17) | 42(2)    | 1.3(18)  |
| C50 | 67(2)    | 40(2)    | 38.7(18) | 18.0(15) | 31.8(18) | 18.4(18) |
| C51 | 42.9(18) | 32.0(17) | 34.2(16) | 12.0(13) | 22.6(14) | 12.6(14) |

Table S 4. Bond Lengths for **Eu-1** complex.

| Atom | Atom | Length/Å   |  | Atom | Atom | Length/Å |
|------|------|------------|--|------|------|----------|
| Eu1  | O1   | 2.3614(18) |  | C7   | C8   | 1.377(4) |
| Eu1  | O2   | 2.3773(19) |  | C8   | C10  | 1.529(5) |
| Eu1  | O4   | 2.4037(18) |  | C11  | C12  | 1.429(5) |
| Eu1  | O5   | 2.3842(19) |  | C11  | C14  | 1.514(5) |
| Eu1  | O6   | 2.4224(19) |  | C12  | C13  | 1.356(5) |
| Eu1  | O7   | 2.3894(19) |  | C13  | C15  | 1.522(4) |
| Eu1  | O8   | 2.437(2)   |  | C16  | C17  | 1.380(4) |
| Eu1  | O9   | 2.3729(18) |  | C16  | C21  | 1.397(4) |
| P1   | O1   | 1.4910(19) |  | C17  | C18  | 1.392(4) |
| P1   | C16  | 1.791(3)   |  | C18  | C19  | 1.381(5) |
| P1   | C22  | 1.808(3)   |  | C19  | C20  | 1.367(6) |
| P1   | C28  | 1.800(3)   |  | C20  | C21  | 1.380(5) |
| P2   | O2   | 1.489(2)   |  | C22  | C23  | 1.398(4) |
| P2   | C39  | 1.806(3)   |  | C22  | C27  | 1.385(4) |
| P2   | C40  | 1.799(3)   |  | C23  | C24  | 1.387(4) |
| P2   | C46  | 1.803(3)   |  | C24  | C25  | 1.383(4) |
| F1   | C5   | 1.293(8)   |  | C25  | C26  | 1.381(4) |
| F2   | C5   | 1.342(8)   |  | C26  | C27  | 1.385(4) |
| F3   | C5   | 1.329(8)   |  | C28  | C29  | 1.390(4) |
| F1A  | C5   | 1.312(8)   |  | C28  | C33  | 1.386(4) |
| F2A  | C5   | 1.215(9)   |  | C29  | C30  | 1.385(4) |
| F3A  | C5   | 1.276(8)   |  | C30  | C31  | 1.377(5) |
| F4   | C10  | 1.333(4)   |  | C31  | C32  | 1.378(5) |
| F5   | C10  | 1.336(4)   |  | C32  | C33  | 1.389(4) |
| F6   | C10  | 1.324(4)   |  | C34  | C35  | 1.385(4) |
| F7   | C15  | 1.302(4)   |  | C34  | C39  | 1.400(4) |
| F8   | C15  | 1.351(5)   |  | C35  | C36  | 1.379(4) |
| F9   | C15  | 1.331(4)   |  | C36  | C37  | 1.371(5) |
| O3   | C27  | 1.392(3)   |  | C37  | C38  | 1.387(5) |
| O3   | C34  | 1.370(3)   |  | C38  | C39  | 1.400(4) |
| O4   | C1   | 1.254(3)   |  | C40  | C41  | 1.387(4) |
| O5   | C3   | 1.259(3)   |  | C40  | C45  | 1.388(4) |
| O6   | C6   | 1.253(3)   |  | C41  | C42  | 1.396(4) |
| O7   | C8   | 1.258(3)   |  | C42  | C43  | 1.368(5) |
| O8   | C11  | 1.243(3)   |  | C43  | C44  | 1.368(5) |
| O9   | C13  | 1.267(3)   |  | C44  | C45  | 1.386(4) |
| C1   | C2   | 1.413(4)   |  | C46  | C47  | 1.391(4) |
| C1   | C4   | 1.503(4)   |  | C46  | C51  | 1.382(4) |
| C2   | C3   | 1.369(4)   |  | C47  | C48  | 1.382(5) |

|    |    |          |  |     |     |          |
|----|----|----------|--|-----|-----|----------|
| C3 | C5 | 1.530(5) |  | C48 | C49 | 1.372(6) |
| C6 | C7 | 1.414(5) |  | C49 | C50 | 1.371(5) |
| C6 | C9 | 1.506(4) |  | C50 | C51 | 1.393(4) |

Table S 5. Bond Angles for **Eu-1** complex.

| Atom | Atom | Atom | Angle/°    |  | Atom | Atom | Atom | Angle/°    |
|------|------|------|------------|--|------|------|------|------------|
| O1   | Eu1  | O2   | 74.89(6)   |  | O7   | C8   | C10  | 114.2(3)   |
| O1   | Eu1  | O4   | 95.11(6)   |  | C7   | C8   | C10  | 117.3(3)   |
| O1   | Eu1  | O5   | 77.81(7)   |  | F4   | C10  | F5   | 107.0(3)   |
| O1   | Eu1  | O6   | 149.27(7)  |  | F4   | C10  | C8   | 113.1(3)   |
| O1   | Eu1  | O7   | 140.04(6)  |  | F5   | C10  | C8   | 111.6(3)   |
| O1   | Eu1  | O8   | 72.48(6)   |  | F6   | C10  | F4   | 106.3(3)   |
| O1   | Eu1  | O9   | 104.71(6)  |  | F6   | C10  | F5   | 105.2(3)   |
| O2   | Eu1  | O4   | 82.26(6)   |  | F6   | C10  | C8   | 113.1(3)   |
| O2   | Eu1  | O5   | 138.87(6)  |  | O8   | C11  | C12  | 123.5(3)   |
| O2   | Eu1  | O6   | 75.81(7)   |  | O8   | C11  | C14  | 117.5(3)   |
| O2   | Eu1  | O7   | 141.07(6)  |  | C12  | C11  | C14  | 118.9(3)   |
| O2   | Eu1  | O8   | 122.60(7)  |  | C13  | C12  | C11  | 122.6(3)   |
| O4   | Eu1  | O6   | 71.85(6)   |  | O9   | C13  | C12  | 128.8(3)   |
| O4   | Eu1  | O8   | 145.75(7)  |  | O9   | C13  | C15  | 111.8(3)   |
| O5   | Eu1  | O4   | 70.13(7)   |  | C12  | C13  | C15  | 119.4(3)   |
| O5   | Eu1  | O6   | 120.56(7)  |  | F7   | C15  | F8   | 106.2(3)   |
| O5   | Eu1  | O7   | 77.16(7)   |  | F7   | C15  | F9   | 108.0(3)   |
| O5   | Eu1  | O8   | 76.01(7)   |  | F7   | C15  | C13  | 115.8(3)   |
| O6   | Eu1  | O8   | 132.95(6)  |  | F8   | C15  | C13  | 110.8(3)   |
| O7   | Eu1  | O4   | 104.93(6)  |  | F9   | C15  | F8   | 103.0(3)   |
| O7   | Eu1  | O6   | 70.65(7)   |  | F9   | C15  | C13  | 112.2(3)   |
| O7   | Eu1  | O8   | 71.56(7)   |  | C17  | C16  | P1   | 116.9(2)   |
| O9   | Eu1  | O2   | 74.19(6)   |  | C17  | C16  | C21  | 119.4(3)   |
| O9   | Eu1  | O4   | 143.67(7)  |  | C21  | C16  | P1   | 123.5(3)   |
| O9   | Eu1  | O5   | 143.33(7)  |  | C16  | C17  | C18  | 120.2(3)   |
| O9   | Eu1  | O6   | 75.75(6)   |  | C19  | C18  | C17  | 119.3(4)   |
| O9   | Eu1  | O7   | 78.83(6)   |  | C20  | C19  | C18  | 121.0(3)   |
| O9   | Eu1  | O8   | 70.30(7)   |  | C19  | C20  | C21  | 119.9(3)   |
| O1   | P1   | C16  | 110.51(13) |  | C20  | C21  | C16  | 120.2(3)   |
| O1   | P1   | C22  | 111.69(11) |  | C23  | C22  | P1   | 123.2(2)   |
| O1   | P1   | C28  | 112.69(12) |  | C27  | C22  | P1   | 118.24(19) |
| C16  | P1   | C22  | 105.18(13) |  | C27  | C22  | C23  | 118.2(2)   |
| C16  | P1   | C28  | 110.01(14) |  | C24  | C23  | C22  | 120.3(3)   |
| C28  | P1   | C22  | 106.42(13) |  | C25  | C24  | C23  | 120.1(3)   |
| O2   | P2   | C39  | 113.84(12) |  | C26  | C25  | C24  | 120.6(3)   |

|     |    |     |            |  |     |     |     |          |
|-----|----|-----|------------|--|-----|-----|-----|----------|
| O2  | P2 | C40 | 112.76(12) |  | C25 | C26 | C27 | 118.8(3) |
| O2  | P2 | C46 | 111.25(13) |  | C22 | C27 | O3  | 117.4(2) |
| C40 | P2 | C39 | 106.72(13) |  | C22 | C27 | C26 | 122.0(3) |
| C40 | P2 | C46 | 105.88(13) |  | C26 | C27 | O3  | 120.3(3) |
| C46 | P2 | C39 | 105.81(13) |  | C29 | C28 | P1  | 121.7(2) |
| P1  | O1 | Eu1 | 160.38(11) |  | C33 | C28 | P1  | 118.8(2) |
| P2  | O2 | Eu1 | 169.51(12) |  | C33 | C28 | C29 | 119.5(3) |
| C34 | O3 | C27 | 119.6(2)   |  | C30 | C29 | C28 | 120.3(3) |
| C1  | O4 | Eu1 | 138.71(19) |  | C31 | C30 | C29 | 119.9(3) |
| C3  | O5 | Eu1 | 134.95(19) |  | C30 | C31 | C32 | 120.2(3) |
| C6  | O6 | Eu1 | 133.88(19) |  | C31 | C32 | C33 | 120.3(3) |
| C8  | O7 | Eu1 | 130.58(19) |  | C28 | C33 | C32 | 119.8(3) |
| C11 | O8 | Eu1 | 134.09(19) |  | O3  | C34 | C35 | 123.3(3) |
| C13 | O9 | Eu1 | 132.49(19) |  | O3  | C34 | C39 | 115.0(2) |
| O4  | C1 | C2  | 123.1(3)   |  | C35 | C34 | C39 | 121.8(3) |
| O4  | C1 | C4  | 118.8(3)   |  | C36 | C35 | C34 | 118.6(3) |
| C2  | C1 | C4  | 118.1(3)   |  | C37 | C36 | C35 | 121.4(3) |
| C3  | C2 | C1  | 122.4(3)   |  | C36 | C37 | C38 | 119.9(3) |
| O5  | C3 | C2  | 128.7(3)   |  | C37 | C38 | C39 | 120.6(3) |
| O5  | C3 | C5  | 114.1(3)   |  | C34 | C39 | P2  | 119.8(2) |
| C2  | C3 | C5  | 117.1(3)   |  | C34 | C39 | C38 | 117.7(3) |
| F1  | C5 | F2  | 104.5(7)   |  | C38 | C39 | P2  | 122.5(2) |
| F1  | C5 | F3  | 104.9(7)   |  | C41 | C40 | P2  | 123.1(2) |
| F1  | C5 | C3  | 116.9(5)   |  | C41 | C40 | C45 | 119.6(3) |
| F2  | C5 | C3  | 115.2(4)   |  | C45 | C40 | P2  | 117.3(2) |
| F3  | C5 | F2  | 100.6(7)   |  | C40 | C41 | C42 | 119.7(3) |
| F3  | C5 | C3  | 113.0(5)   |  | C43 | C42 | C41 | 119.7(3) |
| F1A | C5 | C3  | 106.1(5)   |  | C44 | C43 | C42 | 121.1(3) |
| F2A | C5 | F1A | 109.6(9)   |  | C43 | C44 | C45 | 119.9(3) |
| F2A | C5 | F3A | 111.7(8)   |  | C44 | C45 | C40 | 120.0(3) |
| F2A | C5 | C3  | 111.8(5)   |  | C47 | C46 | P2  | 121.0(2) |
| F3A | C5 | F1A | 104.1(7)   |  | C51 | C46 | P2  | 118.9(2) |
| F3A | C5 | C3  | 112.9(5)   |  | C51 | C46 | C47 | 120.2(3) |
| O6  | C6 | C7  | 124.1(3)   |  | C48 | C47 | C46 | 120.0(3) |
| O6  | C6 | C9  | 117.6(3)   |  | C49 | C48 | C47 | 119.6(3) |
| C7  | C6 | C9  | 118.2(3)   |  | C50 | C49 | C48 | 120.8(3) |
| C8  | C7 | C6  | 122.6(3)   |  | C49 | C50 | C51 | 120.4(3) |
| O7  | C8 | C7  | 128.4(3)   |  | C46 | C51 | C50 | 119.0(3) |

Table S 6. Torsion Angles for **Eu-1** complex.

| A   | B   | C   | D   | Angle/°    |  | A   | B   | C   | D   | Angle/°   |
|-----|-----|-----|-----|------------|--|-----|-----|-----|-----|-----------|
| Eu1 | O4  | C1  | C2  | -9.4(4)    |  | C16 | P1  | O1  | Eu1 | 91.5(3)   |
| Eu1 | O4  | C1  | C4  | 173.62(19) |  | C16 | P1  | C22 | C23 | 1.9(3)    |
| Eu1 | O5  | C3  | C2  | 11.0(5)    |  | C16 | P1  | C22 | C27 | 175.3(2)  |
| Eu1 | O5  | C3  | C5  | -171.0(2)  |  | C16 | P1  | C28 | C29 | 69.9(3)   |
| Eu1 | O6  | C6  | C7  | -18.2(4)   |  | C16 | P1  | C28 | C33 | -111.8(2) |
| Eu1 | O6  | C6  | C9  | 161.3(2)   |  | C16 | C17 | C18 | C19 | 0.2(6)    |
| Eu1 | O7  | C8  | C7  | 26.8(4)    |  | C17 | C16 | C21 | C20 | 1.5(5)    |
| Eu1 | O7  | C8  | C10 | -156.2(2)  |  | C17 | C18 | C19 | C20 | 0.8(6)    |
| Eu1 | O8  | C11 | C12 | -23.9(5)   |  | C18 | C19 | C20 | C21 | -0.6(6)   |
| Eu1 | O8  | C11 | C14 | 156.0(3)   |  | C19 | C20 | C21 | C16 | -0.6(5)   |
| Eu1 | O9  | C13 | C12 | 21.2(5)    |  | C21 | C16 | C17 | C18 | -1.3(5)   |
| Eu1 | O9  | C13 | C15 | -159.9(2)  |  | C22 | P1  | O1  | Eu1 | -151.8(3) |
| P1  | C16 | C17 | C18 | 173.4(3)   |  | C22 | P1  | C16 | C17 | -106.2(2) |
| P1  | C16 | C21 | C20 | -172.8(3)  |  | C22 | P1  | C16 | C21 | 68.3(3)   |
| P1  | C22 | C23 | C24 | 173.1(2)   |  | C22 | P1  | C28 | C29 | -43.5(3)  |
| P1  | C22 | C27 | O3  | -0.4(3)    |  | C22 | P1  | C28 | C33 | 134.7(2)  |
| P1  | C22 | C27 | C26 | -174.1(2)  |  | C22 | C23 | C24 | C25 | 0.6(4)    |
| P1  | C28 | C29 | C30 | 178.9(3)   |  | C23 | C22 | C27 | O3  | 173.3(2)  |
| P1  | C28 | C33 | C32 | -177.6(3)  |  | C23 | C22 | C27 | C26 | -0.3(4)   |
| P2  | C40 | C41 | C42 | -179.7(2)  |  | C23 | C24 | C25 | C26 | -0.2(4)   |
| P2  | C40 | C45 | C44 | 178.6(3)   |  | C24 | C25 | C26 | C27 | -0.5(4)   |
| P2  | C46 | C47 | C48 | -176.8(3)  |  | C25 | C26 | C27 | O3  | -172.7(2) |
| P2  | C46 | C51 | C50 | 177.3(2)   |  | C25 | C26 | C27 | C22 | 0.8(4)    |
| O1  | P1  | C16 | C17 | 14.5(3)    |  | C27 | O3  | C34 | C35 | -7.8(4)   |
| O1  | P1  | C16 | C21 | -171.1(2)  |  | C27 | O3  | C34 | C39 | 174.0(2)  |
| O1  | P1  | C22 | C23 | -118.1(2)  |  | C27 | C22 | C23 | C24 | -0.3(4)   |
| O1  | P1  | C22 | C27 | 55.4(2)    |  | C28 | P1  | O1  | Eu1 | -32.0(4)  |
| O1  | P1  | C28 | C29 | -166.3(2)  |  | C28 | P1  | C16 | C17 | 139.6(2)  |
| O1  | P1  | C28 | C33 | 12.0(3)    |  | C28 | P1  | C16 | C21 | -46.0(3)  |
| O2  | P2  | C39 | C34 | 52.1(3)    |  | C28 | P1  | C22 | C23 | 118.6(2)  |
| O2  | P2  | C39 | C38 | -127.7(2)  |  | C28 | P1  | C22 | C27 | -68.0(2)  |
| O2  | P2  | C40 | C41 | -129.6(2)  |  | C28 | C29 | C30 | C31 | -1.2(6)   |
| O2  | P2  | C40 | C45 | 51.2(3)    |  | C29 | C28 | C33 | C32 | 0.7(5)    |
| O2  | P2  | C46 | C47 | -163.9(3)  |  | C29 | C30 | C31 | C32 | 0.2(6)    |
| O2  | P2  | C46 | C51 | 17.9(3)    |  | C30 | C31 | C32 | C33 | 1.2(6)    |
| O3  | C34 | C35 | C36 | -178.2(3)  |  | C31 | C32 | C33 | C28 | -1.6(5)   |
| O3  | C34 | C39 | P2  | -1.4(3)    |  | C33 | C28 | C29 | C30 | 0.7(5)    |
| O3  | C34 | C39 | C38 | 178.4(2)   |  | C34 | O3  | C27 | C22 | 111.7(3)  |
| O4  | C1  | C2  | C3  | -3.3(5)    |  | C34 | O3  | C27 | C26 | -74.6(3)  |

|     |     |     |     |            |  |     |     |     |     |           |
|-----|-----|-----|-----|------------|--|-----|-----|-----|-----|-----------|
| O5  | C3  | C5  | F1  | 127.1(11)  |  | C34 | C35 | C36 | C37 | 0.0(5)    |
| O5  | C3  | C5  | F2  | 3.9(10)    |  | C35 | C34 | C39 | P2  | -179.7(2) |
| O5  | C3  | C5  | F3  | -111.0(10) |  | C35 | C34 | C39 | C38 | 0.2(4)    |
| O5  | C3  | C5  | F1A | 58.7(10)   |  | C35 | C36 | C37 | C38 | 0.2(5)    |
| O5  | C3  | C5  | F2A | -60.9(14)  |  | C36 | C37 | C38 | C39 | -0.1(5)   |
| O5  | C3  | C5  | F3A | 172.1(9)   |  | C37 | C38 | C39 | P2  | 179.8(2)  |
| O6  | C6  | C7  | C8  | -6.2(5)    |  | C37 | C38 | C39 | C34 | 0.0(4)    |
| O7  | C8  | C10 | F4  | 150.4(3)   |  | C39 | P2  | O2  | Eu1 | -161.0(6) |
| O7  | C8  | C10 | F5  | -88.9(3)   |  | C39 | P2  | C40 | C41 | -3.9(3)   |
| O7  | C8  | C10 | F6  | 29.5(4)    |  | C39 | P2  | C40 | C45 | 176.9(2)  |
| O8  | C11 | C12 | C13 | 0.0(6)     |  | C39 | P2  | C46 | C47 | 72.0(3)   |
| O9  | C13 | C15 | F7  | 175.0(3)   |  | C39 | P2  | C46 | C51 | -106.2(3) |
| O9  | C13 | C15 | F8  | -64.1(4)   |  | C39 | C34 | C35 | C36 | -0.1(4)   |
| O9  | C13 | C15 | F9  | 50.4(4)    |  | C40 | P2  | O2  | Eu1 | -39.2(7)  |
| C1  | C2  | C3  | O5  | 2.3(5)     |  | C40 | P2  | C39 | C34 | -72.9(2)  |
| C1  | C2  | C3  | C5  | -175.6(3)  |  | C40 | P2  | C39 | C38 | 107.2(3)  |
| C2  | C3  | C5  | F1  | -54.6(12)  |  | C40 | P2  | C46 | C47 | -41.1(3)  |
| C2  | C3  | C5  | F2  | -177.9(9)  |  | C40 | P2  | C46 | C51 | 140.7(2)  |
| C2  | C3  | C5  | F3  | 67.2(10)   |  | C40 | C41 | C42 | C43 | 1.3(5)    |
| C2  | C3  | C5  | F1A | -123.1(10) |  | C41 | C40 | C45 | C44 | -0.5(5)   |
| C2  | C3  | C5  | F2A | 117.4(13)  |  | C41 | C42 | C43 | C44 | -1.0(5)   |
| C2  | C3  | C5  | F3A | -9.6(10)   |  | C42 | C43 | C44 | C45 | -0.1(5)   |
| C4  | C1  | C2  | C3  | 173.7(3)   |  | C43 | C44 | C45 | C40 | 0.9(5)    |
| C6  | C7  | C8  | O7  | 1.5(5)     |  | C45 | C40 | C41 | C42 | -0.5(4)   |
| C6  | C7  | C8  | C10 | -175.3(3)  |  | C46 | P2  | O2  | Eu1 | 79.5(6)   |
| C7  | C8  | C10 | F4  | -32.3(4)   |  | C46 | P2  | C39 | C34 | 174.6(2)  |
| C7  | C8  | C10 | F5  | 88.4(4)    |  | C46 | P2  | C39 | C38 | -5.3(3)   |
| C7  | C8  | C10 | F6  | -153.2(3)  |  | C46 | P2  | C40 | C41 | 108.5(3)  |
| C9  | C6  | C7  | C8  | 174.4(3)   |  | C46 | P2  | C40 | C45 | -70.6(2)  |
| C11 | C12 | C13 | O9  | 1.4(6)     |  | C46 | C47 | C48 | C49 | -1.3(6)   |
| C11 | C12 | C13 | C15 | -177.5(3)  |  | C47 | C46 | C51 | C50 | -1.0(5)   |
| C12 | C13 | C15 | F7  | -6.0(5)    |  | C47 | C48 | C49 | C50 | 0.7(6)    |
| C12 | C13 | C15 | F8  | 114.9(4)   |  | C48 | C49 | C50 | C51 | -0.3(6)   |
| C12 | C13 | C15 | F9  | -130.6(3)  |  | C49 | C50 | C51 | C46 | 0.4(5)    |
| C14 | C11 | C12 | C13 | -179.9(3)  |  | C51 | C46 | C47 | C48 | 1.4(5)    |

Table S 7. Hydrogen Atom Coordinates ( $\text{\AA}\times 10^4$ ) and Isotropic Displacement Parameters ( $\text{\AA}^2\times 10^3$ ) for **Eu-1** complex.

| Atom | x     | y     | z     | U(eq) |
|------|-------|-------|-------|-------|
| H2   | 1003  | 1195  | -563  | 44    |
| H4A  | -1973 | 345   | -690  | 59    |
| H4B  | -1170 | 116   | -1160 | 59    |
| H4C  | -1395 | 1192  | -1177 | 59    |
| H7   | 420   | -937  | 3262  | 45    |
| H9A  | -2408 | -855  | 1998  | 75    |
| H9B  | -1767 | -1107 | 2913  | 75    |
| H9C  | -1898 | -1769 | 2031  | 75    |
| H12  | 3472  | 2756  | 5198  | 50    |
| H14A | 5179  | 3192  | 4194  | 94    |
| H14B | 5250  | 3824  | 5066  | 94    |
| H14C | 5189  | 4365  | 4251  | 94    |
| H17  | 3419  | 4422  | 1952  | 47    |
| H18  | 5357  | 5160  | 1962  | 64    |
| H19  | 6521  | 6976  | 2532  | 66    |
| H20  | 5806  | 8052  | 3115  | 61    |
| H21  | 3888  | 7328  | 3117  | 49    |
| H23  | 2524  | 6725  | 1305  | 33    |
| H24  | 1372  | 7217  | 122   | 38    |
| H25  | -718  | 6551  | -350  | 39    |
| H26  | -1677 | 5382  | 352   | 36    |
| H29  | 2086  | 7186  | 3257  | 46    |
| H30  | 1859  | 7714  | 4517  | 58    |
| H31  | 1350  | 6484  | 5335  | 59    |
| H32  | 1075  | 4729  | 4905  | 54    |
| H33  | 1378  | 4205  | 3676  | 41    |
| H35  | -692  | 6396  | 2213  | 43    |
| H36  | -1611 | 6655  | 3133  | 53    |
| H37  | -2673 | 5245  | 3586  | 56    |
| H38  | -2829 | 3530  | 3129  | 45    |
| H41  | -3480 | 3412  | 748   | 45    |
| H42  | -4784 | 2743  | -735  | 56    |
| H43  | -5073 | 1101  | -1451 | 56    |
| H44  | -4049 | 124   | -737  | 56    |
| H45  | -2700 | 795   | 726   | 46    |
| H47  | -4382 | 1674  | 1889  | 54    |
| H48  | -5296 | 647   | 2687  | 66    |
| H49  | -4165 | 77    | 3809  | 63    |

|     |       |      |      |    |
|-----|-------|------|------|----|
| H50 | -2127 | 555  | 4170 | 55 |
| H51 | -1179 | 1607 | 3390 | 42 |

Table S 8. Atomic Occupancy for **Eu-1** complex.

| Atom | Occupancy  | Atom | Occupancy  | Atom | Occupancy  |
|------|------------|------|------------|------|------------|
| F1   | 0.503 (15) | F2   | 0.503 (15) | F3   | 0.503 (15) |
| F1A  | 0.497 (15) | F2A  | 0.497 (15) | F3A  | 0.497 (15) |

Table S 9. Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for **Tb-2** complex.  $U_{eq}$  is defined as 1/3 of the trace of the orthogonalised  $U_{ij}$  tensor.

| Atom | x          | y          | z          | U(eq)     |
|------|------------|------------|------------|-----------|
| Tb1  | 932.1(2)   | 2218.8(2)  | 2216.0(2)  | 21.91(5)  |
| P1   | 1904.9(7)  | 5182.4(6)  | 2371.2(5)  | 24.37(16) |
| P2   | -1930.9(7) | 2609.7(6)  | 2019.6(5)  | 25.85(17) |
| F1   | 3286(15)   | 1506(9)    | 168(14)    | 111(6)    |
| F2   | 4199(8)    | 2740(19)   | 1267(5)    | 101(6)    |
| F3   | 3347(10)   | 3044(14)   | 84(12)     | 115(6)    |
| F1A  | 3818(11)   | 1838(17)   | 1129(9)    | 108(4)    |
| F2A  | 3831(18)   | 3224(8)    | 749(18)    | 139(8)    |
| F3A  | 3037(12)   | 1798(16)   | -192(7)    | 108(7)    |
| F4   | 2487(3)    | -458(3)    | 4166.3(19) | 90.8(10)  |
| F5   | 2778(3)    | -732(2)    | 3006.0(19) | 82.2(9)   |
| F6   | 3674(2)    | 798(2)     | 3844.6(18) | 68.6(7)   |
| F7   | 1992(3)    | 1875(3)    | 5737.7(18) | 113.3(13) |
| F8   | 642(3)     | 2449(2)    | 5177.6(17) | 81.8(9)   |
| F9   | 361(3)     | 894(2)     | 4645.5(17) | 73.9(8)   |
| O1   | 1430.4(18) | 3995.6(16) | 2106.9(13) | 25.8(4)   |
| O2   | -736.4(18) | 2582.2(17) | 2175.3(13) | 28.0(4)   |
| O3   | -680.9(19) | 4563.3(16) | 1606.3(14) | 28.8(5)   |
| O4   | -287.0(19) | 1506.9(17) | 699.2(13)  | 29.4(5)   |
| O5   | 2185(2)    | 2429.8(18) | 1446.9(14) | 33.3(5)   |
| O6   | -595(2)    | 509.4(17)  | 2041.4(14) | 32.6(5)   |
| O7   | 1864(2)    | 1033.6(17) | 2652.8(14) | 30.9(5)   |
| O8   | 2950(2)    | 3245.8(17) | 3296.0(14) | 33.9(5)   |
| O9   | 939.3(19)  | 2212.5(17) | 3615.1(13) | 29.8(5)   |
| C1   | -166(3)    | 1232(2)    | 20.2(19)   | 30.3(7)   |
| C2   | 963(3)     | 1446(3)    | -15(2)     | 39.0(8)   |
| C3   | 2031(3)    | 2036(3)    | 693(2)     | 33.3(7)   |

|     |          |          |            |          |
|-----|----------|----------|------------|----------|
| C4  | -1275(4) | 684(3)   | -814(2)    | 43.5(9)  |
| C5  | 3203(4)  | 2294(4)  | 559(3)     | 58.3(11) |
| C6  | -604(3)  | -248(3)  | 2413(2)    | 36.6(8)  |
| C7  | 447(3)   | -393(3)  | 2920(2)    | 40.8(8)  |
| C8  | 1576(3)  | 248(3)   | 2991(2)    | 34.8(8)  |
| C9  | -1807(4) | -1055(3) | 2310(3)    | 51.9(10) |
| C10 | 2618(4)  | -35(3)   | 3507(3)    | 46.6(9)  |
| C11 | 3526(3)  | 3217(3)  | 4053(2)    | 39.8(8)  |
| C12 | 2968(3)  | 2756(3)  | 4609(2)    | 42.8(9)  |
| C13 | 1748(3)  | 2306(3)  | 4346(2)    | 34.0(7)  |
| C14 | 4889(4)  | 3696(4)  | 4401(3)    | 63.6(12) |
| C15 | 1215(4)  | 1869(4)  | 4983(2)    | 50.8(10) |
| C16 | 3450(3)  | 5783(3)  | 2516(2)    | 31.3(7)  |
| C17 | 3898(3)  | 5141(3)  | 2192(2)    | 41.3(8)  |
| C18 | 5039(4)  | 5579(4)  | 2203(3)    | 59.2(11) |
| C19 | 5734(4)  | 6654(4)  | 2544(3)    | 58.9(11) |
| C20 | 5315(3)  | 7294(3)  | 2882(3)    | 51.6(10) |
| C21 | 4177(3)  | 6863(3)  | 2873(2)    | 44.4(9)  |
| C22 | 1119(3)  | 5725(2)  | 1533.5(18) | 25.9(6)  |
| C23 | 1674(3)  | 6434(2)  | 1109(2)    | 30.4(7)  |
| C24 | 999(3)   | 6736(3)  | 413(2)     | 34.4(7)  |
| C25 | -235(3)  | 6343(3)  | 138(2)     | 34.3(8)  |
| C26 | -808(3)  | 5653(3)  | 549(2)     | 33.3(7)  |
| C27 | -127(3)  | 5349(2)  | 1239.6(19) | 26.2(6)  |
| C28 | 1757(3)  | 5633(2)  | 3348.7(19) | 28.9(7)  |
| C29 | 1901(3)  | 6674(3)  | 3594(2)    | 40.0(8)  |
| C30 | 1750(4)  | 6990(3)  | 4335(2)    | 50.5(10) |
| C31 | 1453(4)  | 6269(3)  | 4826(2)    | 52.6(10) |
| C32 | 1289(4)  | 5225(3)  | 4578(2)    | 48.8(10) |
| C33 | 1455(3)  | 4904(3)  | 3842(2)    | 35.9(8)  |
| C34 | -1221(3) | 4789(3)  | 2130.6(19) | 29.1(7)  |
| C35 | -1121(3) | 5811(3)  | 2401(2)    | 37.7(8)  |
| C36 | -1671(4) | 5960(3)  | 2946(2)    | 47.8(10) |
| C37 | -2298(4) | 5121(3)  | 3213(2)    | 49.3(10) |
| C38 | -2389(3) | 4103(3)  | 2944(2)    | 39.3(8)  |
| C39 | -1846(3) | 3918(3)  | 2391.9(19) | 29.9(7)  |
| C40 | -2956(3) | 2165(3)  | 884.3(19)  | 29.3(7)  |
| C41 | -3578(3) | 2738(3)  | 456(2)     | 40.5(8)  |
| C42 | -4368(3) | 2338(4)  | -418(2)    | 49.5(10) |
| C43 | -4539(3) | 1367(4)  | -852(2)    | 49.2(10) |
| C44 | -3926(3) | 796(4)   | -428(2)    | 50.7(10) |
| C45 | -3125(3) | 1186(3)  | 438(2)     | 40.3(8)  |
| C46 | -2683(3) | 1746(3)  | 2578(2)    | 32.7(7)  |

|     |          |         |         |          |
|-----|----------|---------|---------|----------|
| C47 | -3910(3) | 1445(3) | 2364(2) | 48.3(10) |
| C48 | -4451(4) | 827(4)  | 2834(3) | 57.2(12) |
| C49 | -3779(4) | 499(3)  | 3503(3) | 55.7(11) |
| C50 | -2568(4) | 785(3)  | 3720(3) | 49.9(10) |
| C51 | -2008(3) | 1416(3) | 3256(2) | 38.0(8)  |

Table S 10. Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for **Tb-2** complex. The Anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|------|----------|----------|----------|----------|----------|----------|
| Tb1  | 25.42(8) | 19.09(8) | 21.53(8) | 6.96(5)  | 9.90(6)  | 8.37(6)  |
| P1   | 26.3(4)  | 20.0(4)  | 25.5(4)  | 8.3(3)   | 9.4(3)   | 8.3(3)   |
| P2   | 24.4(4)  | 29.4(4)  | 25.6(4)  | 9.0(3)   | 12.6(3)  | 9.8(3)   |
| F1   | 113(10)  | 67(5)    | 203(17)  | 3(8)     | 124(12)  | 35(6)    |
| F2   | 43(4)    | 187(16)  | 69(5)    | 7(6)     | 33(3)    | 37(7)    |
| F3   | 84(6)    | 151(12)  | 174(11)  | 124(10)  | 93(8)    | 59(7)    |
| F1A  | 48(5)    | 162(13)  | 133(9)   | 45(8)    | 39(5)    | 59(7)    |
| F2A  | 129(14)  | 61(6)    | 250(20)  | -11(10)  | 160(15)  | -13(7)   |
| F3A  | 71(5)    | 194(19)  | 61(5)    | -18(6)   | 46(4)    | 46(8)    |
| F4   | 86(2)    | 140(3)   | 93(2)    | 92(2)    | 50.4(17) | 70(2)    |
| F5   | 94(2)    | 78(2)    | 94(2)    | 13.2(16) | 31.4(17) | 65.5(19) |
| F6   | 55.9(16) | 64.4(17) | 87.7(18) | 29.1(14) | 19.7(14) | 33.7(14) |
| F7   | 82(2)    | 206(4)   | 47.8(16) | 71(2)    | 23.1(15) | 47(2)    |
| F8   | 112(2)   | 90(2)    | 65.8(17) | 14.0(15) | 58.9(17) | 43.6(19) |
| F9   | 104(2)   | 55.4(16) | 63.6(16) | 25.0(13) | 49.4(16) | 15.9(16) |
| O1   | 25.7(11) | 22.6(10) | 31.3(11) | 9.0(9)   | 12.1(9)  | 10.8(9)  |
| O2   | 26.0(11) | 28.3(11) | 31.6(11) | 10.8(9)  | 12.7(9)  | 11.0(9)  |
| O3   | 32.2(12) | 24.4(11) | 38.4(12) | 11.0(9)  | 21.5(10) | 13.1(10) |
| O4   | 36.0(12) | 27.9(11) | 26.2(11) | 6.9(9)   | 14.2(9)  | 13.2(10) |
| O5   | 35.0(13) | 34.7(13) | 34.4(12) | 9(1)     | 18.9(10) | 13.4(10) |
| O6   | 37.6(13) | 24.6(11) | 31.1(11) | 7.4(9)   | 13.5(10) | 7.7(10)  |
| O7   | 40.8(13) | 25.4(11) | 36.4(12) | 14.0(9)  | 21.5(10) | 16.9(10) |
| O8   | 34.1(12) | 29.0(12) | 33.4(12) | 11(1)    | 9.9(10)  | 9.8(10)  |
| O9   | 34.7(12) | 30.6(12) | 23.7(11) | 7.5(9)   | 11.1(9)  | 13.2(10) |
| C1   | 47(2)    | 23.4(15) | 24.7(15) | 6.3(12)  | 12.3(14) | 21.2(15) |
| C2   | 54(2)    | 44(2)    | 33.5(18) | 8.4(15)  | 25.3(17) | 28.5(19) |
| C3   | 44(2)    | 31.5(17) | 42.0(19) | 16.9(15) | 26.7(16) | 23.2(16) |
| C4   | 57(2)    | 41(2)    | 30.1(18) | 1.3(15)  | 12.2(16) | 24.1(19) |
| C5   | 54(3)    | 73(3)    | 56(3)    | 7(2)     | 31(2)    | 28(3)    |
| C6   | 48(2)    | 23.6(16) | 34.4(17) | 4.6(14)  | 20.9(16) | 5.4(15)  |
| C7   | 57(2)    | 31.4(18) | 41.7(19) | 18.0(15) | 25.3(18) | 18.8(18) |

|     |          |          |          |          |          |          |
|-----|----------|----------|----------|----------|----------|----------|
| C8  | 58(2)    | 28.3(17) | 31.5(17) | 13.5(14) | 24.7(16) | 23.7(17) |
| C9  | 55(3)    | 36(2)    | 58(2)    | 15.6(18) | 29(2)    | 3.3(18)  |
| C10 | 63(3)    | 44(2)    | 52(2)    | 27.0(19) | 30(2)    | 34(2)    |
| C11 | 36.1(19) | 35.2(19) | 37.2(19) | 6.9(15)  | 6.2(15)  | 11.3(16) |
| C12 | 43(2)    | 47(2)    | 27.3(17) | 12.9(15) | 3.0(15)  | 15.9(18) |
| C13 | 49(2)    | 30.2(17) | 23.6(16) | 9.3(13)  | 12.1(15) | 18.7(16) |
| C14 | 34(2)    | 74(3)    | 58(3)    | 16(2)    | 2.3(19)  | 10(2)    |
| C15 | 64(3)    | 60(3)    | 28.8(19) | 15.5(18) | 19.4(18) | 24(2)    |
| C16 | 25.7(16) | 26.7(16) | 36.7(17) | 13.2(14) | 9.0(13)  | 7.4(13)  |
| C17 | 29.9(18) | 35.0(19) | 57(2)    | 12.8(17) | 18.8(16) | 9.5(16)  |
| C18 | 34(2)    | 54(3)    | 91(3)    | 18(2)    | 31(2)    | 13(2)    |
| C19 | 27(2)    | 56(3)    | 85(3)    | 25(2)    | 21(2)    | 7.9(19)  |
| C20 | 31(2)    | 34(2)    | 66(3)    | 17.0(18) | 4.4(18)  | 1.2(16)  |
| C21 | 35(2)    | 31.6(19) | 52(2)    | 8.8(16)  | 7.8(16)  | 7.2(16)  |
| C22 | 35.3(17) | 22.2(15) | 23.0(14) | 6.4(12)  | 12.8(13) | 13.3(13) |
| C23 | 38.9(18) | 24.7(16) | 32.2(16) | 8.2(13)  | 17.8(14) | 14.2(14) |
| C24 | 56(2)    | 27.0(16) | 35.0(17) | 14.7(14) | 27.6(16) | 22.2(16) |
| C25 | 55(2)    | 26.6(17) | 26.4(16) | 9.4(13)  | 13.0(15) | 25.1(16) |
| C26 | 36.9(18) | 27.9(16) | 33.0(17) | 5.6(14)  | 9.4(14)  | 15.8(15) |
| C27 | 35.8(17) | 18.6(14) | 27.4(15) | 6.0(12)  | 13.6(13) | 13.4(13) |
| C28 | 31.6(17) | 28.8(16) | 22.7(15) | 6.0(12)  | 6.5(12)  | 12.5(14) |
| C29 | 57(2)    | 30.7(18) | 31.3(17) | 8.8(14)  | 16.5(16) | 17.2(17) |
| C30 | 78(3)    | 38(2)    | 37(2)    | 3.8(16)  | 19.4(19) | 29(2)    |
| C31 | 78(3)    | 53(2)    | 31.3(19) | 5.7(17)  | 23.8(19) | 32(2)    |
| C32 | 72(3)    | 46(2)    | 33.2(19) | 16.3(17) | 26.3(19) | 23(2)    |
| C33 | 50(2)    | 30.6(17) | 29.4(17) | 10.5(14) | 15.0(15) | 18.9(16) |
| C34 | 27.4(16) | 37.9(18) | 23.3(15) | 6.4(13)  | 7.2(12)  | 17.5(14) |
| C35 | 49(2)    | 35.9(19) | 34.3(18) | 10.0(15) | 16.2(16) | 24.6(17) |
| C36 | 70(3)    | 51(2)    | 39(2)    | 10.6(18) | 22.9(19) | 42(2)    |
| C37 | 66(3)    | 67(3)    | 40(2)    | 13.2(19) | 29.4(19) | 46(2)    |
| C38 | 44(2)    | 53(2)    | 37.7(18) | 20.1(17) | 25.3(16) | 27.8(18) |
| C39 | 30.5(17) | 37.2(18) | 26.3(15) | 9.4(13)  | 11.5(13) | 17.9(15) |
| C40 | 21.3(15) | 37.2(18) | 26.8(15) | 7.6(13)  | 11.2(12) | 7.2(13)  |
| C41 | 35.2(19) | 52(2)    | 36.2(18) | 11.3(16) | 13.2(15) | 20.3(17) |
| C42 | 39(2)    | 71(3)    | 38(2)    | 16(2)    | 11.3(16) | 27(2)    |
| C43 | 30.6(19) | 74(3)    | 31.6(18) | 4.9(19)  | 7.2(15)  | 15(2)    |
| C44 | 39(2)    | 58(3)    | 39(2)    | -7.0(18) | 9.4(16)  | 11.5(19) |
| C45 | 34.9(19) | 44(2)    | 37.2(18) | 3.2(16)  | 12.4(15) | 13.6(16) |
| C46 | 33.6(18) | 32.1(17) | 30.8(16) | 5.9(14)  | 19.5(14) | 5.2(14)  |
| C47 | 34(2)    | 64(3)    | 42(2)    | 12.9(18) | 21.1(17) | 8.5(19)  |
| C48 | 40(2)    | 69(3)    | 51(2)    | 7(2)     | 29.7(19) | -2(2)    |
| C49 | 71(3)    | 46(2)    | 54(2)    | 14.6(19) | 44(2)    | 8(2)     |
| C50 | 74(3)    | 44(2)    | 46(2)    | 20.4(18) | 39(2)    | 23(2)    |

|     |       |       |          |          |          |          |
|-----|-------|-------|----------|----------|----------|----------|
| C51 | 47(2) | 39(2) | 35.3(18) | 13.7(15) | 24.3(16) | 17.3(17) |
|-----|-------|-------|----------|----------|----------|----------|

Table S 11. Bond Lengths for **Tb-2** complex.

| Atom | Atom | Length/Å  |  | Atom | Atom | Length/Å |
|------|------|-----------|--|------|------|----------|
| Tb1  | O1   | 2.334(2)  |  | C7   | C8   | 1.375(5) |
| Tb1  | O2   | 2.357(2)  |  | C8   | C10  | 1.521(5) |
| Tb1  | O4   | 2.377(2)  |  | C11  | C12  | 1.428(5) |
| Tb1  | O5   | 2.363(2)  |  | C11  | C14  | 1.515(5) |
| Tb1  | O6   | 2.399(2)  |  | C12  | C13  | 1.363(5) |
| Tb1  | O7   | 2.357(2)  |  | C13  | C15  | 1.518(5) |
| Tb1  | O8   | 2.410(2)  |  | C16  | C17  | 1.380(5) |
| Tb1  | O9   | 2.347(2)  |  | C16  | C21  | 1.393(5) |
| P1   | O1   | 1.492(2)  |  | C17  | C18  | 1.379(5) |
| P1   | C16  | 1.793(3)  |  | C18  | C19  | 1.377(6) |
| P1   | C22  | 1.802(3)  |  | C19  | C20  | 1.363(6) |
| P1   | C28  | 1.805(3)  |  | C20  | C21  | 1.377(5) |
| P2   | O2   | 1.488(2)  |  | C22  | C23  | 1.398(4) |
| P2   | C39  | 1.806(3)  |  | C22  | C27  | 1.390(4) |
| P2   | C40  | 1.802(3)  |  | C23  | C24  | 1.382(4) |
| P2   | C46  | 1.801(3)  |  | C24  | C25  | 1.376(5) |
| F1   | C5   | 1.277(11) |  | C25  | C26  | 1.377(5) |
| F2   | C5   | 1.308(10) |  | C26  | C27  | 1.380(4) |
| F3   | C5   | 1.351(10) |  | C28  | C29  | 1.383(4) |
| F1A  | C5   | 1.358(11) |  | C28  | C33  | 1.387(4) |
| F2A  | C5   | 1.193(10) |  | C29  | C30  | 1.385(5) |
| F3A  | C5   | 1.294(11) |  | C30  | C31  | 1.375(6) |
| F4   | C10  | 1.326(4)  |  | C31  | C32  | 1.380(5) |
| F5   | C10  | 1.340(5)  |  | C32  | C33  | 1.390(5) |
| F6   | C10  | 1.327(5)  |  | C34  | C35  | 1.386(4) |
| F7   | C15  | 1.309(4)  |  | C34  | C39  | 1.391(5) |
| F8   | C15  | 1.352(5)  |  | C35  | C36  | 1.384(5) |
| F9   | C15  | 1.322(5)  |  | C36  | C37  | 1.367(6) |
| O3   | C27  | 1.390(4)  |  | C37  | C38  | 1.385(5) |
| O3   | C34  | 1.378(4)  |  | C38  | C39  | 1.402(4) |
| O4   | C1   | 1.252(4)  |  | C40  | C41  | 1.378(5) |
| O5   | C3   | 1.255(4)  |  | C40  | C45  | 1.393(5) |
| O6   | C6   | 1.251(4)  |  | C41  | C42  | 1.390(5) |
| O7   | C8   | 1.259(4)  |  | C42  | C43  | 1.373(6) |
| O8   | C11  | 1.239(4)  |  | C43  | C44  | 1.367(6) |
| O9   | C13  | 1.264(4)  |  | C44  | C45  | 1.382(5) |
| C1   | C2   | 1.409(5)  |  | C46  | C47  | 1.392(5) |

|    |    |          |  |     |     |          |
|----|----|----------|--|-----|-----|----------|
| C1 | C4 | 1.504(5) |  | C46 | C51 | 1.385(5) |
| C2 | C3 | 1.377(5) |  | C47 | C48 | 1.382(5) |
| C3 | C5 | 1.534(5) |  | C48 | C49 | 1.372(6) |
| C6 | C7 | 1.419(5) |  | C49 | C50 | 1.374(6) |
| C6 | C9 | 1.504(5) |  | C50 | C51 | 1.396(5) |

Table S 12. Bond Angles for **Tb-2** complex.

| Atom | Atom | Atom | Angle/°    |  | Atom | Atom | Atom | Angle/°  |
|------|------|------|------------|--|------|------|------|----------|
| O1   | Tb1  | O2   | 74.77(7)   |  | O7   | C8   | C10  | 114.5(3) |
| O1   | Tb1  | O4   | 94.48(7)   |  | C7   | C8   | C10  | 117.3(3) |
| O1   | Tb1  | O5   | 77.47(7)   |  | F4   | C10  | F5   | 106.8(3) |
| O1   | Tb1  | O6   | 148.52(7)  |  | F4   | C10  | F6   | 106.3(3) |
| O1   | Tb1  | O7   | 140.14(7)  |  | F4   | C10  | C8   | 113.5(3) |
| O1   | Tb1  | O8   | 72.48(7)   |  | F5   | C10  | C8   | 112.2(3) |
| O1   | Tb1  | O9   | 105.10(7)  |  | F6   | C10  | F5   | 104.3(3) |
| O2   | Tb1  | O4   | 82.26(7)   |  | F6   | C10  | C8   | 113.2(3) |
| O2   | Tb1  | O5   | 139.20(7)  |  | O8   | C11  | C12  | 123.3(3) |
| O2   | Tb1  | O6   | 75.37(7)   |  | O8   | C11  | C14  | 118.0(3) |
| O2   | Tb1  | O7   | 141.34(7)  |  | C12  | C11  | C14  | 118.7(3) |
| O2   | Tb1  | O8   | 122.76(7)  |  | C13  | C12  | C11  | 122.5(3) |
| O4   | Tb1  | O6   | 71.80(7)   |  | O9   | C13  | C12  | 128.3(3) |
| O4   | Tb1  | O8   | 145.07(7)  |  | O9   | C13  | C15  | 111.9(3) |
| O5   | Tb1  | O4   | 70.70(7)   |  | C12  | C13  | C15  | 119.8(3) |
| O5   | Tb1  | O6   | 121.26(7)  |  | F7   | C15  | F8   | 105.1(3) |
| O5   | Tb1  | O8   | 74.82(8)   |  | F7   | C15  | F9   | 108.3(4) |
| O6   | Tb1  | O8   | 133.90(7)  |  | F7   | C15  | C13  | 115.6(4) |
| O7   | Tb1  | O4   | 104.93(7)  |  | F8   | C15  | C13  | 110.8(3) |
| O7   | Tb1  | O5   | 76.73(7)   |  | F9   | C15  | F8   | 103.6(4) |
| O7   | Tb1  | O6   | 71.33(8)   |  | F9   | C15  | C13  | 112.5(3) |
| O7   | Tb1  | O8   | 71.77(8)   |  | C17  | C16  | P1   | 117.2(2) |
| O9   | Tb1  | O2   | 74.29(7)   |  | C17  | C16  | C21  | 119.1(3) |
| O9   | Tb1  | O4   | 143.89(7)  |  | C21  | C16  | P1   | 123.6(3) |
| O9   | Tb1  | O5   | 142.62(8)  |  | C16  | C17  | C18  | 120.0(4) |
| O9   | Tb1  | O6   | 75.89(7)   |  | C19  | C18  | C17  | 120.0(4) |
| O9   | Tb1  | O7   | 78.99(7)   |  | C20  | C19  | C18  | 120.8(4) |
| O9   | Tb1  | O8   | 70.79(7)   |  | C19  | C20  | C21  | 119.6(4) |
| O1   | P1   | C16  | 110.73(14) |  | C20  | C21  | C16  | 120.5(4) |
| O1   | P1   | C22  | 111.64(13) |  | C23  | C22  | P1   | 123.8(2) |
| O1   | P1   | C28  | 112.71(13) |  | C27  | C22  | P1   | 118.2(2) |
| C16  | P1   | C22  | 105.00(14) |  | C27  | C22  | C23  | 117.7(3) |
| C16  | P1   | C28  | 109.88(15) |  | C24  | C23  | C22  | 120.8(3) |

|     |    |     |            |  |     |     |     |          |
|-----|----|-----|------------|--|-----|-----|-----|----------|
| C22 | P1 | C28 | 106.52(14) |  | C25 | C24 | C23 | 119.8(3) |
| O2  | P2 | C39 | 113.66(13) |  | C24 | C25 | C26 | 120.9(3) |
| O2  | P2 | C40 | 113.06(13) |  | C25 | C26 | C27 | 119.0(3) |
| O2  | P2 | C46 | 111.56(14) |  | O3  | C27 | C22 | 117.2(3) |
| C40 | P2 | C39 | 106.47(15) |  | C26 | C27 | O3  | 120.6(3) |
| C46 | P2 | C39 | 105.84(15) |  | C26 | C27 | C22 | 121.9(3) |
| C46 | P2 | C40 | 105.64(15) |  | C29 | C28 | P1  | 121.3(2) |
| P1  | O1 | Tb1 | 160.13(12) |  | C33 | C28 | P1  | 118.8(2) |
| P2  | O2 | Tb1 | 168.74(13) |  | C33 | C28 | C29 | 119.9(3) |
| C34 | O3 | C27 | 119.9(2)   |  | C30 | C29 | C28 | 120.0(3) |
| C1  | O4 | Tb1 | 138.3(2)   |  | C31 | C30 | C29 | 120.1(3) |
| C3  | O5 | Tb1 | 134.7(2)   |  | C30 | C31 | C32 | 120.2(3) |
| C6  | O6 | Tb1 | 133.7(2)   |  | C31 | C32 | C33 | 120.1(3) |
| C8  | O7 | Tb1 | 130.9(2)   |  | C28 | C33 | C32 | 119.6(3) |
| C11 | O8 | Tb1 | 134.5(2)   |  | O3  | C34 | C35 | 122.8(3) |
| C13 | O9 | Tb1 | 132.6(2)   |  | O3  | C34 | C39 | 114.9(3) |
| O4  | C1 | C2  | 123.4(3)   |  | C35 | C34 | C39 | 122.2(3) |
| O4  | C1 | C4  | 118.7(3)   |  | C36 | C35 | C34 | 118.4(3) |
| C2  | C1 | C4  | 117.8(3)   |  | C37 | C36 | C35 | 121.0(3) |
| C3  | C2 | C1  | 122.0(3)   |  | C36 | C37 | C38 | 120.4(3) |
| O5  | C3 | C2  | 128.5(3)   |  | C37 | C38 | C39 | 120.4(3) |
| O5  | C3 | C5  | 114.0(3)   |  | C34 | C39 | P2  | 119.9(2) |
| C2  | C3 | C5  | 117.5(3)   |  | C34 | C39 | C38 | 117.5(3) |
| F1  | C5 | F2  | 106.0(9)   |  | C38 | C39 | P2  | 122.6(3) |
| F1  | C5 | F3  | 106.1(8)   |  | C41 | C40 | P2  | 123.1(3) |
| F1  | C5 | C3  | 115.5(7)   |  | C41 | C40 | C45 | 119.7(3) |
| F2  | C5 | F3  | 101.5(9)   |  | C45 | C40 | P2  | 117.1(2) |
| F2  | C5 | C3  | 115.6(4)   |  | C40 | C41 | C42 | 120.0(4) |
| F3  | C5 | C3  | 111.0(5)   |  | C43 | C42 | C41 | 120.0(4) |
| F1A | C5 | C3  | 104.4(5)   |  | C44 | C43 | C42 | 120.1(3) |
| F2A | C5 | F1A | 106.6(12)  |  | C43 | C44 | C45 | 120.8(4) |
| F2A | C5 | F3A | 114.1(10)  |  | C44 | C45 | C40 | 119.3(4) |
| F2A | C5 | C3  | 114.1(6)   |  | C47 | C46 | P2  | 121.3(3) |
| F3A | C5 | F1A | 103.0(8)   |  | C51 | C46 | P2  | 118.7(3) |
| F3A | C5 | C3  | 113.2(7)   |  | C51 | C46 | C47 | 120.0(3) |
| O6  | C6 | C7  | 124.1(3)   |  | C48 | C47 | C46 | 120.0(4) |
| O6  | C6 | C9  | 117.7(3)   |  | C49 | C48 | C47 | 119.8(4) |
| C7  | C6 | C9  | 118.2(3)   |  | C48 | C49 | C50 | 120.9(4) |
| C8  | C7 | C6  | 122.4(3)   |  | C49 | C50 | C51 | 119.9(4) |
| O7  | C8 | C7  | 128.2(3)   |  | C46 | C51 | C50 | 119.4(4) |

Table S 13. Torsion Angles for **Tb-2** complex.

| A   | B   | C   | D   | Angle/°   |  | A   | B   | C   | D   | Angle/°   |
|-----|-----|-----|-----|-----------|--|-----|-----|-----|-----|-----------|
| Tb1 | O4  | C1  | C2  | -9.9(5)   |  | C16 | P1  | O1  | Tb1 | 90.9(4)   |
| Tb1 | O4  | C1  | C4  | 172.8(2)  |  | C16 | P1  | C22 | C23 | 1.7(3)    |
| Tb1 | O5  | C3  | C2  | 12.4(5)   |  | C16 | P1  | C22 | C27 | 176.1(2)  |
| Tb1 | O5  | C3  | C5  | -169.8(3) |  | C16 | P1  | C28 | C29 | 70.0(3)   |
| Tb1 | O6  | C6  | C7  | -18.1(5)  |  | C16 | P1  | C28 | C33 | -112.1(3) |
| Tb1 | O6  | C6  | C9  | 162.2(2)  |  | C16 | C17 | C18 | C19 | 0.5(6)    |
| Tb1 | O7  | C8  | C7  | 26.5(5)   |  | C17 | C16 | C21 | C20 | 1.7(5)    |
| Tb1 | O7  | C8  | C10 | -156.3(2) |  | C17 | C18 | C19 | C20 | 0.8(7)    |
| Tb1 | O8  | C11 | C12 | -23.2(5)  |  | C18 | C19 | C20 | C21 | -0.9(7)   |
| Tb1 | O8  | C11 | C14 | 156.7(3)  |  | C19 | C20 | C21 | C16 | -0.4(6)   |
| Tb1 | O9  | C13 | C12 | 22.0(5)   |  | C21 | C16 | C17 | C18 | -1.8(5)   |
| Tb1 | O9  | C13 | C15 | -159.9(2) |  | C22 | P1  | O1  | Tb1 | -152.5(3) |
| P1  | C16 | C17 | C18 | 173.4(3)  |  | C22 | P1  | C16 | C17 | -106.7(3) |
| P1  | C16 | C21 | C20 | -173.1(3) |  | C22 | P1  | C16 | C21 | 68.3(3)   |
| P1  | C22 | C23 | C24 | 173.5(2)  |  | C22 | P1  | C28 | C29 | -43.3(3)  |
| P1  | C22 | C27 | O3  | -1.1(3)   |  | C22 | P1  | C28 | C33 | 134.6(3)  |
| P1  | C22 | C27 | C26 | -174.3(2) |  | C22 | C23 | C24 | C25 | 0.6(4)    |
| P1  | C28 | C29 | C30 | 178.3(3)  |  | C23 | C22 | C27 | O3  | 173.6(2)  |
| P1  | C28 | C33 | C32 | -177.5(3) |  | C23 | C22 | C27 | C26 | 0.5(4)    |
| P2  | C40 | C41 | C42 | -179.1(3) |  | C23 | C24 | C25 | C26 | 0.2(5)    |
| P2  | C40 | C45 | C44 | 178.3(3)  |  | C24 | C25 | C26 | C27 | -0.7(5)   |
| P2  | C46 | C47 | C48 | -176.6(3) |  | C25 | C26 | C27 | O3  | -172.6(3) |
| P2  | C46 | C51 | C50 | 177.3(3)  |  | C25 | C26 | C27 | C22 | 0.3(4)    |
| O1  | P1  | C16 | C17 | 13.9(3)   |  | C27 | O3  | C34 | C35 | -7.9(4)   |
| O1  | P1  | C16 | C21 | -171.1(3) |  | C27 | O3  | C34 | C39 | 174.0(3)  |
| O1  | P1  | C22 | C23 | -118.4(3) |  | C27 | C22 | C23 | C24 | -0.9(4)   |
| O1  | P1  | C22 | C27 | 56.0(3)   |  | C28 | P1  | O1  | Tb1 | -32.6(4)  |
| O1  | P1  | C28 | C29 | -166.0(3) |  | C28 | P1  | C16 | C17 | 139.1(3)  |
| O1  | P1  | C28 | C33 | 11.9(3)   |  | C28 | P1  | C16 | C21 | -45.9(3)  |
| O2  | P2  | C39 | C34 | 52.0(3)   |  | C28 | P1  | C22 | C23 | 118.2(3)  |
| O2  | P2  | C39 | C38 | -127.9(3) |  | C28 | P1  | C22 | C27 | -67.4(3)  |
| O2  | P2  | C40 | C41 | -129.6(3) |  | C28 | C29 | C30 | C31 | -0.3(6)   |
| O2  | P2  | C40 | C45 | 51.5(3)   |  | C29 | C28 | C33 | C32 | 0.5(5)    |
| O2  | P2  | C46 | C47 | -164.2(3) |  | C29 | C30 | C31 | C32 | -0.7(7)   |
| O2  | P2  | C46 | C51 | 18.3(3)   |  | C30 | C31 | C32 | C33 | 1.6(7)    |
| O3  | C34 | C35 | C36 | -178.3(3) |  | C31 | C32 | C33 | C28 | -1.5(6)   |
| O3  | C34 | C39 | P2  | -1.5(4)   |  | C33 | C28 | C29 | C30 | 0.4(5)    |
| O3  | C34 | C39 | C38 | 178.5(3)  |  | C34 | O3  | C27 | C22 | 112.6(3)  |
| O4  | C1  | C2  | C3  | -3.9(5)   |  | C34 | O3  | C27 | C26 | -74.1(4)  |

|     |     |     |     |            |  |     |     |     |     |           |
|-----|-----|-----|-----|------------|--|-----|-----|-----|-----|-----------|
| O5  | C3  | C5  | F1  | 134.5(12)  |  | C34 | C35 | C36 | C37 | 0.0(6)    |
| O5  | C3  | C5  | F2  | 10.0(13)   |  | C35 | C34 | C39 | P2  | -179.6(2) |
| O5  | C3  | C5  | F3  | -104.8(11) |  | C35 | C34 | C39 | C38 | 0.3(5)    |
| O5  | C3  | C5  | F1A | 62.4(11)   |  | C35 | C36 | C37 | C38 | 0.3(6)    |
| O5  | C3  | C5  | F2A | -53.6(18)  |  | C36 | C37 | C38 | C39 | -0.3(6)   |
| O5  | C3  | C5  | F3A | 173.7(11)  |  | C37 | C38 | C39 | P2  | 179.9(3)  |
| O6  | C6  | C7  | C8  | -5.4(5)    |  | C37 | C38 | C39 | C34 | 0.0(5)    |
| O7  | C8  | C10 | F4  | 149.5(3)   |  | C39 | P2  | O2  | Tb1 | -162.2(6) |
| O7  | C8  | C10 | F5  | -89.4(4)   |  | C39 | P2  | C40 | C41 | -4.1(3)   |
| O7  | C8  | C10 | F6  | 28.3(4)    |  | C39 | P2  | C40 | C45 | 177.0(2)  |
| O8  | C11 | C12 | C13 | 0.1(6)     |  | C39 | P2  | C46 | C47 | 71.7(3)   |
| O9  | C13 | C15 | F7  | 175.8(4)   |  | C39 | P2  | C46 | C51 | -105.8(3) |
| O9  | C13 | C15 | F8  | -64.8(4)   |  | C39 | C34 | C35 | C36 | -0.4(5)   |
| O9  | C13 | C15 | F9  | 50.7(4)    |  | C40 | P2  | O2  | Tb1 | -40.6(7)  |
| C1  | C2  | C3  | O5  | 2.5(6)     |  | C40 | P2  | C39 | C34 | -73.1(3)  |
| C1  | C2  | C3  | C5  | -175.3(4)  |  | C40 | P2  | C39 | C38 | 107.0(3)  |
| C2  | C3  | C5  | F1  | -47.5(13)  |  | C40 | P2  | C46 | C47 | -41.0(3)  |
| C2  | C3  | C5  | F2  | -172.0(12) |  | C40 | P2  | C46 | C51 | 141.5(3)  |
| C2  | C3  | C5  | F3  | 73.2(11)   |  | C40 | C41 | C42 | C43 | 0.8(6)    |
| C2  | C3  | C5  | F1A | -119.6(10) |  | C41 | C40 | C45 | C44 | -0.6(5)   |
| C2  | C3  | C5  | F2A | 124.4(17)  |  | C41 | C42 | C43 | C44 | -0.6(6)   |
| C2  | C3  | C5  | F3A | -8.3(12)   |  | C42 | C43 | C44 | C45 | -0.3(6)   |
| C4  | C1  | C2  | C3  | 173.5(3)   |  | C43 | C44 | C45 | C40 | 0.9(6)    |
| C6  | C7  | C8  | O7  | 1.0(6)     |  | C45 | C40 | C41 | C42 | -0.2(5)   |
| C6  | C7  | C8  | C10 | -176.1(3)  |  | C46 | P2  | O2  | Tb1 | 78.3(7)   |
| C7  | C8  | C10 | F4  | -33.0(5)   |  | C46 | P2  | C39 | C34 | 174.8(3)  |
| C7  | C8  | C10 | F5  | 88.2(4)    |  | C46 | P2  | C39 | C38 | -5.1(3)   |
| C7  | C8  | C10 | F6  | -154.2(3)  |  | C46 | P2  | C40 | C41 | 108.2(3)  |
| C9  | C6  | C7  | C8  | 174.3(3)   |  | C46 | P2  | C40 | C45 | -70.7(3)  |
| C11 | C12 | C13 | O9  | 0.5(6)     |  | C46 | C47 | C48 | C49 | -1.0(6)   |
| C11 | C12 | C13 | C15 | -177.6(3)  |  | C47 | C46 | C51 | C50 | -0.2(5)   |
| C12 | C13 | C15 | F7  | -5.8(6)    |  | C47 | C48 | C49 | C50 | 0.6(6)    |
| C12 | C13 | C15 | F8  | 113.5(4)   |  | C48 | C49 | C50 | C51 | 0.0(6)    |
| C12 | C13 | C15 | F9  | -131.0(4)  |  | C49 | C50 | C51 | C46 | -0.2(5)   |
| C14 | C11 | C12 | C13 | -179.8(4)  |  | C51 | C46 | C47 | C48 | 0.8(6)    |

Table S 14. Hydrogen Atom Coordinates ( $\text{\AA} \times 10^4$ ) and Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for **Tb-2** complex.

| Atom | x     | y     | z     | U(eq) |
|------|-------|-------|-------|-------|
| H2   | 987   | 1175  | -542  | 47    |
| H4A  | -1981 | 367   | -678  | 65    |
| H4B  | -1181 | 121   | -1143 | 65    |
| H4C  | -1387 | 1205  | -1167 | 65    |
| H7   | 368   | -955  | 3222  | 49    |
| H9A  | -2450 | -868  | 1935  | 78    |
| H9B  | -1839 | -1060 | 2884  | 78    |
| H9C  | -1917 | -1765 | 2043  | 78    |
| H12  | 3466  | 2763  | 5183  | 51    |
| H14A | 5158  | 3185  | 4185  | 95    |
| H14B | 5231  | 3858  | 5040  | 95    |
| H14C | 5161  | 4354  | 4201  | 95    |
| H17  | 3421  | 4399  | 1962  | 50    |
| H18  | 5346  | 5139  | 1976  | 71    |
| H19  | 6516  | 6953  | 2543  | 71    |
| H20  | 5806  | 8033  | 3123  | 62    |
| H21  | 3885  | 7307  | 3113  | 53    |
| H23  | 2526  | 6712  | 1301  | 36    |
| H24  | 1384  | 7213  | 125   | 41    |
| H25  | -697  | 6550  | -342  | 41    |
| H26  | -1659 | 5390  | 360   | 40    |
| H29  | 2102  | 7172  | 3255  | 48    |
| H30  | 1853  | 7706  | 4505  | 61    |
| H31  | 1360  | 6490  | 5338  | 63    |
| H32  | 1063  | 4724  | 4910  | 59    |
| H33  | 1361  | 4189  | 3678  | 43    |
| H35  | -685  | 6395  | 2217  | 45    |
| H36  | -1612 | 6655  | 3138  | 57    |
| H37  | -2673 | 5238  | 3585  | 59    |
| H38  | -2824 | 3526  | 3136  | 47    |
| H41  | -3467 | 3405  | 759   | 49    |
| H42  | -4788 | 2737  | -715  | 59    |
| H43  | -5085 | 1092  | -1448 | 59    |
| H44  | -4052 | 124   | -732  | 61    |
| H45  | -2694 | 789   | 726   | 48    |
| H47  | -4376 | 1663  | 1895  | 58    |
| H48  | -5285 | 630   | 2694  | 69    |
| H49  | -4155 | 69    | 3821  | 67    |

|     |       |      |      |    |
|-----|-------|------|------|----|
| H50 | -2113 | 552  | 4184 | 60 |
| H51 | -1170 | 1618 | 3403 | 46 |

Table S 15. Atomic Occupancy for **Tb-2** complex.

| <b>Atom</b> | <b>Occupancy</b> |  | <b>Atom</b> | <b>Occupancy</b> |  | <b>Atom</b> | <b>Occupancy</b> |
|-------------|------------------|--|-------------|------------------|--|-------------|------------------|
| F1          | 0.513(18)        |  | F2          | 0.513(18)        |  | F3          | 0.513(18)        |
| F1A         | 0.487(18)        |  | F2A         | 0.487(18)        |  | F3A         | 0.487(18)        |

Table S 16 Corrected emission intensity relative to  $^5D_0 \rightarrow ^7F_1$  transition,  $R_{21}$  and CIE color coordinates of **Eu-1** and  $[\text{Eu}(\text{tfac})_3(\text{H}_2\text{O})_2]$  in the solid-state and in DCM solution at RT.

|                                                          | Corrected emission Intenisty relative to $^5\text{D}_0 \rightarrow ^7\text{F}_1$ transition |                         |                                 |                               |                                |                | $^a\text{R}_{21}$ | Color Coordinate |       |
|----------------------------------------------------------|---------------------------------------------------------------------------------------------|-------------------------|---------------------------------|-------------------------------|--------------------------------|----------------|-------------------|------------------|-------|
|                                                          | $\int 0-0$                                                                                  | $\int 0-1$              | $\int 0-2$                      | $\int 0-3$                    | $\int 0-4$                     | $\int_{total}$ |                   | x                | y     |
| [Eu(tfac) <sub>3</sub> (H <sub>2</sub> O) <sub>2</sub> ] |                                                                                             |                         |                                 |                               |                                |                |                   |                  |       |
| Solid-state                                              | 0.19<br>[17272.39]<br>(1.33%)                                                               | 1.00<br>[16875.59]<br>- | 10.61<br>[16232.29]<br>(74.35%) | 0.43<br>[15328.74]<br>(3.01%) | 2.04<br>[14314.11]<br>(14.29%) | 14.27          | 10.61             | 0.666            | 0.330 |
| DCM                                                      | 0.18<br>[17270.37]<br>(1.12%)                                                               | 1.00<br>[16871.00]<br>- | 10.38<br>[16231.59]<br>(74.14%) | 0.42<br>[15328.74]<br>(3.00%) | 2.02<br>[14317.83]<br>(14.40%) | 14.00          | 10.38             | 0.659            | 0.332 |
| Eu-1                                                     |                                                                                             |                         |                                 |                               |                                |                |                   |                  |       |
| Solid-state                                              | 0.18<br>(17259.51)<br>[1.18%]                                                               | 1.00<br>(16874.68)<br>- | 12.56<br>(16249.52)<br>[82.41%] | 0.35<br>(15325.23)<br>[2.29%] | 1.15<br>(14355.98)<br>[7.54%]  | 15.24          | 12.56             | 0.664            | 0.324 |
| DCM                                                      | 0.20<br>(17261.80)<br>[1.14%]                                                               | 1.00<br>(16872.34)<br>- | 13.76<br>(16215.69)<br>[79.50%] | 0.43<br>(15312.89)<br>[2.46%] | 2.02<br>(14328.91)<br>[11.62%] | 17.41          | 13.76             | 0.669            | 0.329 |

Table S 17. Photophysical properties of [Eu(tfac)<sub>3</sub>(H<sub>2</sub>O)<sub>2</sub>] complex in the solid-state and in DCM solution at RT.

|             | $\Omega_2$                                               | $\Omega_2$ | FWHM      | $\tau_{\text{obs}}$ | $\tau_{\text{rad}}$ | $A_R$               | $A_{NR}$ | $Q_{Eu}^{Eu}$ | $Q_{Eu}^L$ | $\eta_{\text{sen}}$ |
|-------------|----------------------------------------------------------|------------|-----------|---------------------|---------------------|---------------------|----------|---------------|------------|---------------------|
|             | ( $\times 10^{-20} \text{ cm}^{-2}$ )                    |            | (nm)      | ( $\mu\text{s}$ )   | ( $\mu\text{s}$ )   | ( $\text{s}^{-1}$ ) |          | (%)           |            |                     |
|             | [Eu(tfac) <sub>3</sub> (H <sub>2</sub> O) <sub>2</sub> ] |            |           |                     |                     |                     |          |               |            |                     |
| Solid-state | 18.60                                                    | 8.24       | 1.00;7.94 | 384                 | 1317                | 759.30              | 1844.87  | 29.16         | -          | -                   |
| DCM         | 18.25                                                    | 8.16       | 2.40;6.00 | 254                 | 1583                | 631.63              | 3305.38  | 16.04         |            |                     |

Table S 18. The key properties of double-EMLs devices with **Tb-2** at different concentrations.

| Device   | $V_{\text{turn-on}}$ (V) | $B^a$ (cd/m <sup>2</sup> ) | $\eta_c^b$ (cd/A) | $\eta_p^c$ (lm/W) | EQE  | $\text{CIE}_{x,y}^d$ |
|----------|--------------------------|----------------------------|-------------------|-------------------|------|----------------------|
| 8.0 wt%  | 3.2                      | 1248                       | 8.83              | 8.16              | 3.5% | (0.262, 0.408)       |
| 10.0 wt% | 3.3                      | 1285                       | 10.44             | 8.62              | 4.5% | (0.250, 0.427)       |
| 12.0 wt% | 3.3                      | 1341                       | 11.96             | 11.02             | 4.7% | (0.250, 0.443)       |
| 14.0 wt% | 3.2                      | 1324                       | 11.50             | 10.62             | 5.2% | (0.254, 0.430)       |
| 16.0 wt% | 3.5                      | 1259                       | 9.53              | 8.09              | 3.8% | (0.252, 0.456)       |

<sup>a</sup>The data for maximum brightness (B). <sup>b</sup> maximum current efficiency ( $\eta_c$ ). <sup>c</sup> maximum power efficiency ( $\eta_p$ ). <sup>d</sup> Commission Internationale de l'Eclairage coordinates ( $\text{CIE}_{x,y}$ ) at 10 mA/cm<sup>2</sup>.

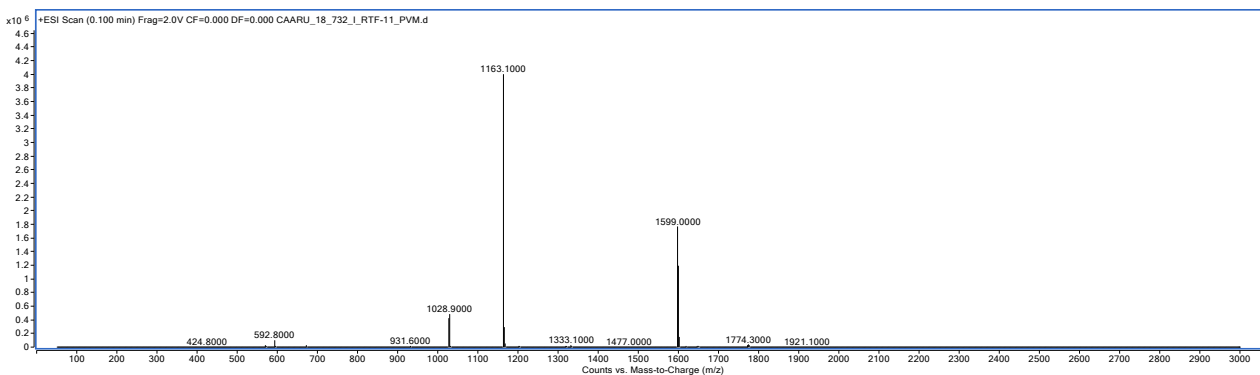


Fig. S 1. Positive mode ESI-MS spectrum of **Eu-1** complex in acetone solution.

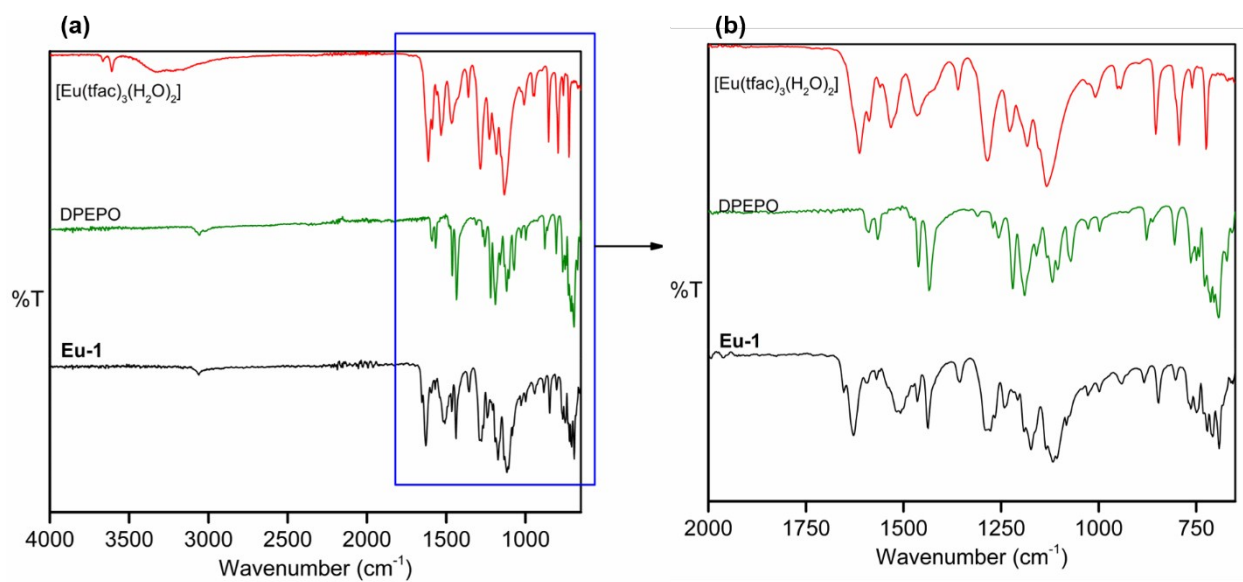


Fig. S 2. FT-IR spectra of free (a) DPEPO,  $[\text{Eu}(\text{tfac})_2(\text{H}_2\text{O})_2]$  and **Eu-1** complex and (b) a magnified view in the range between 2000 – 650  $\text{cm}^{-1}$ .

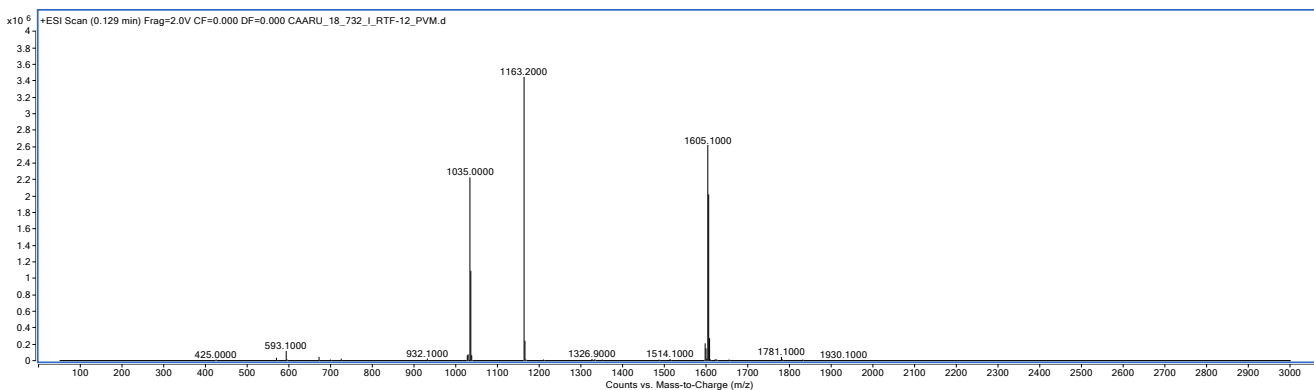


Fig. S 3. Positive mode ESI-MS spectrum of **Tb-2** complex in acetone solution.

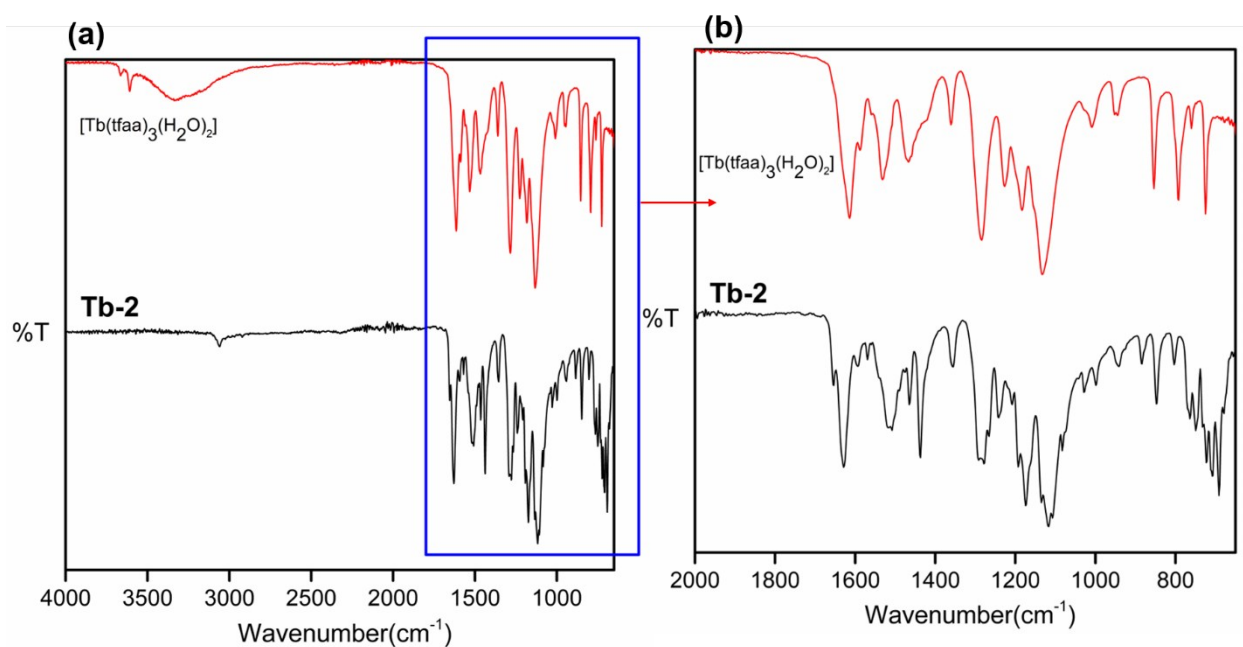


Fig. S 4. FT-IR spectra of (a)  $[\text{Tb}(\text{tfac})_2(\text{H}_2\text{O})_2]$  and **Tb-2** complex and (b) a magnified view in the range between 2000 – 650  $\text{cm}^{-1}$ .

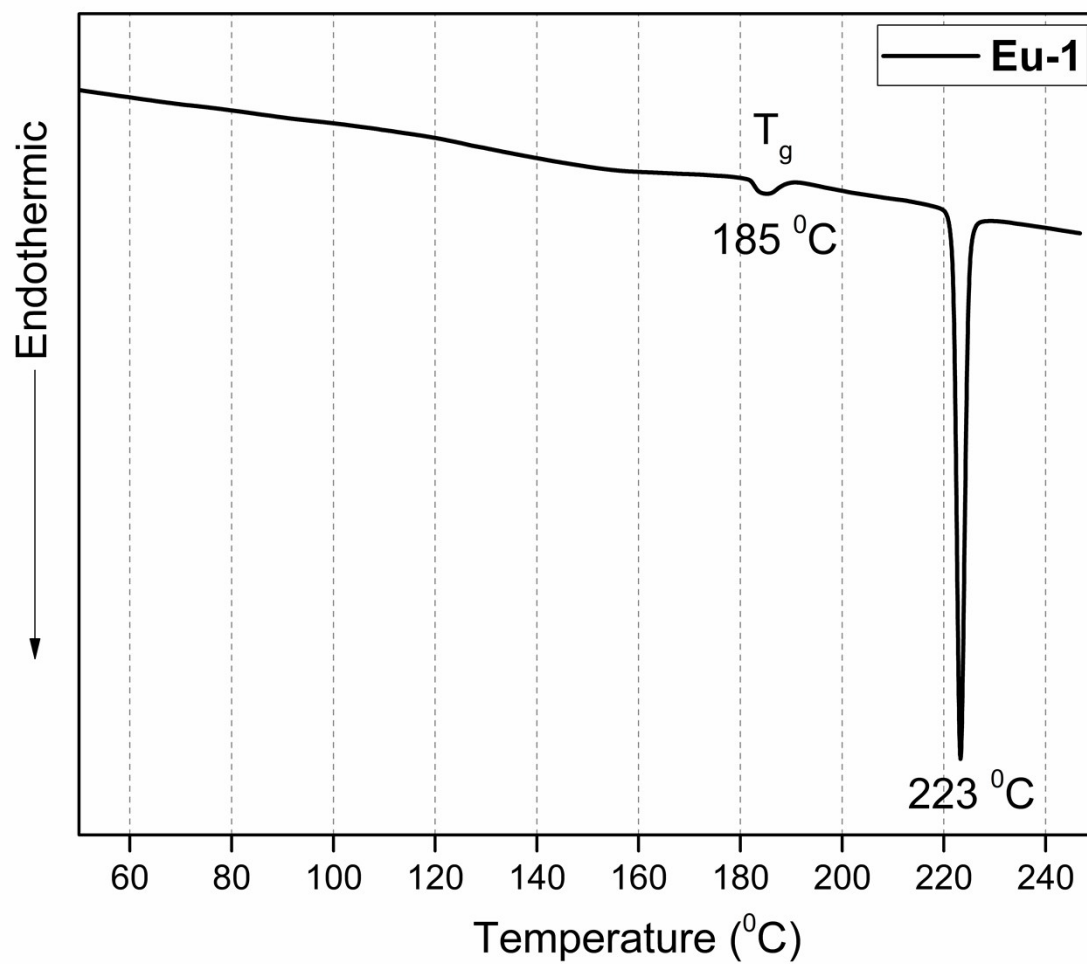


Fig. S 5. DSC curve of **Eu-1** complex recorded under dinitrogen atmosphere with heating rate 10 °C/min.

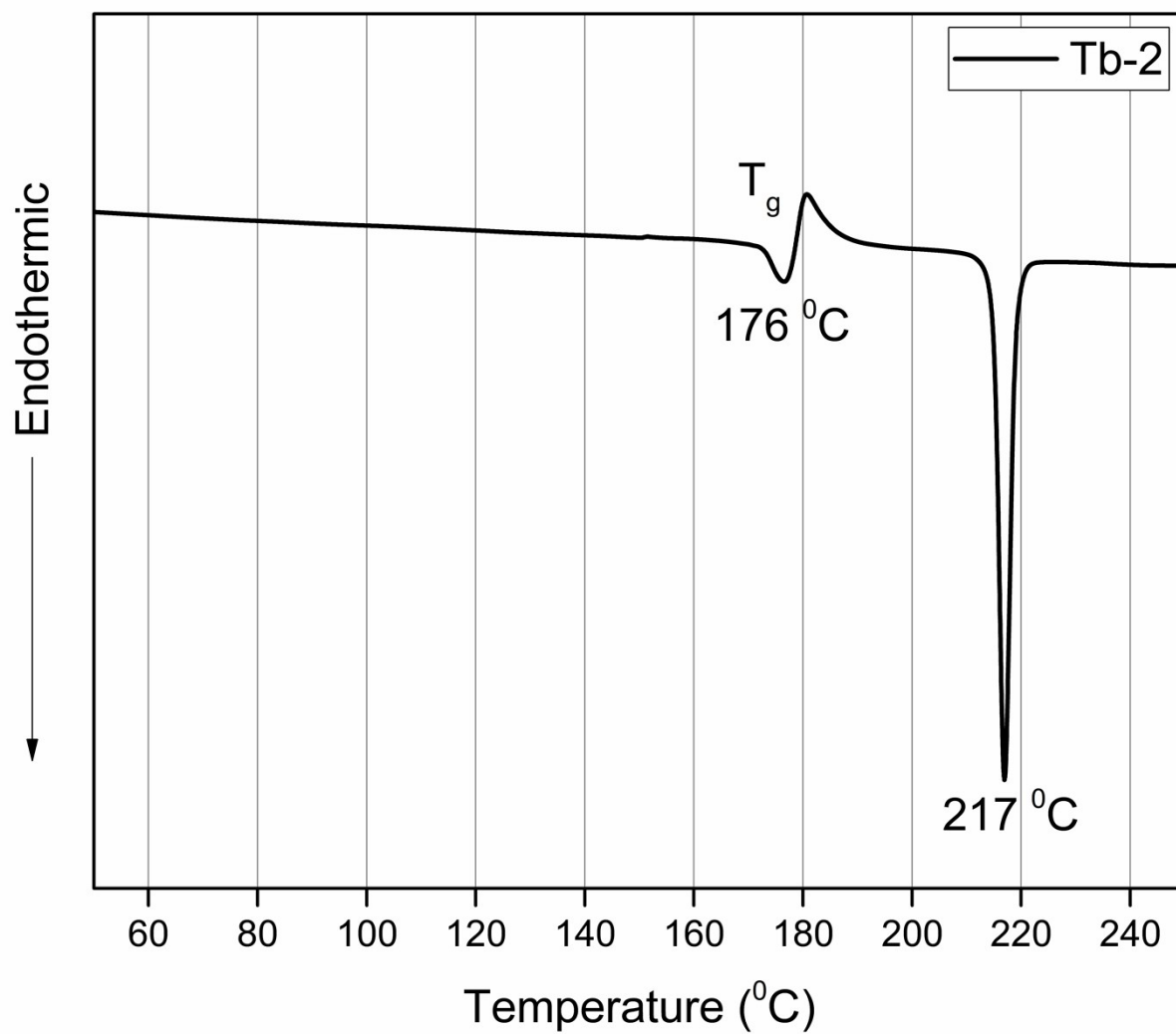


Fig. S 6. DSC curve **Tb-2** complex recorded under dinitrogen atmosphere with heating rate 10 °C/min.

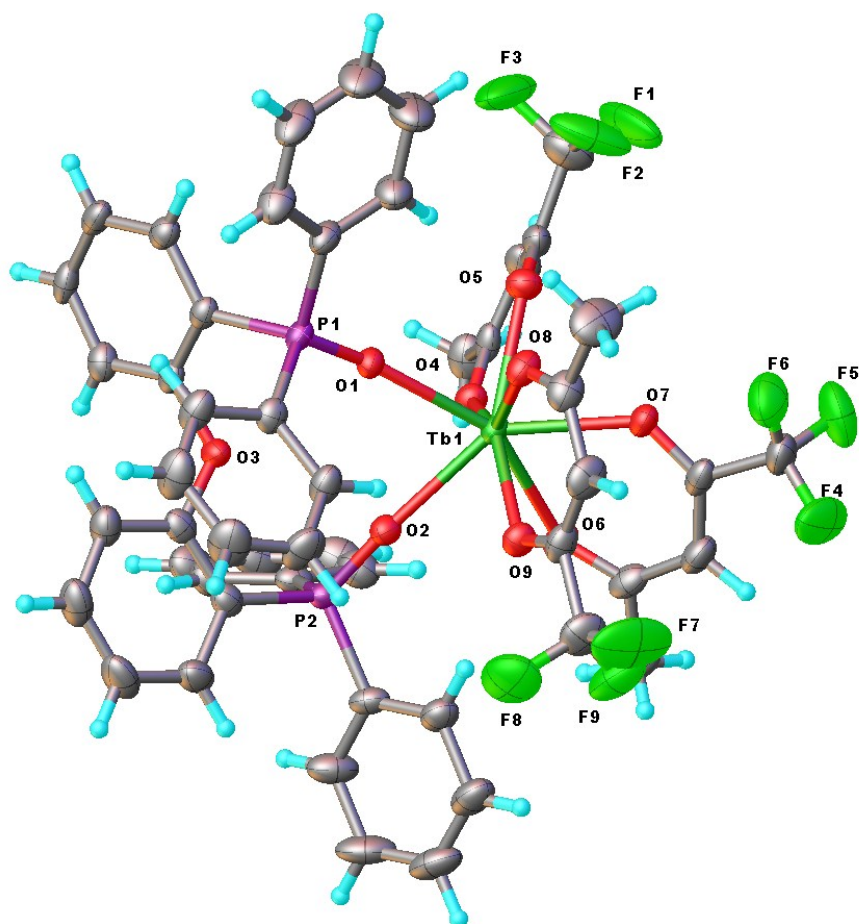


Fig. S 7. The molecular structure of **Tb-2** complex.

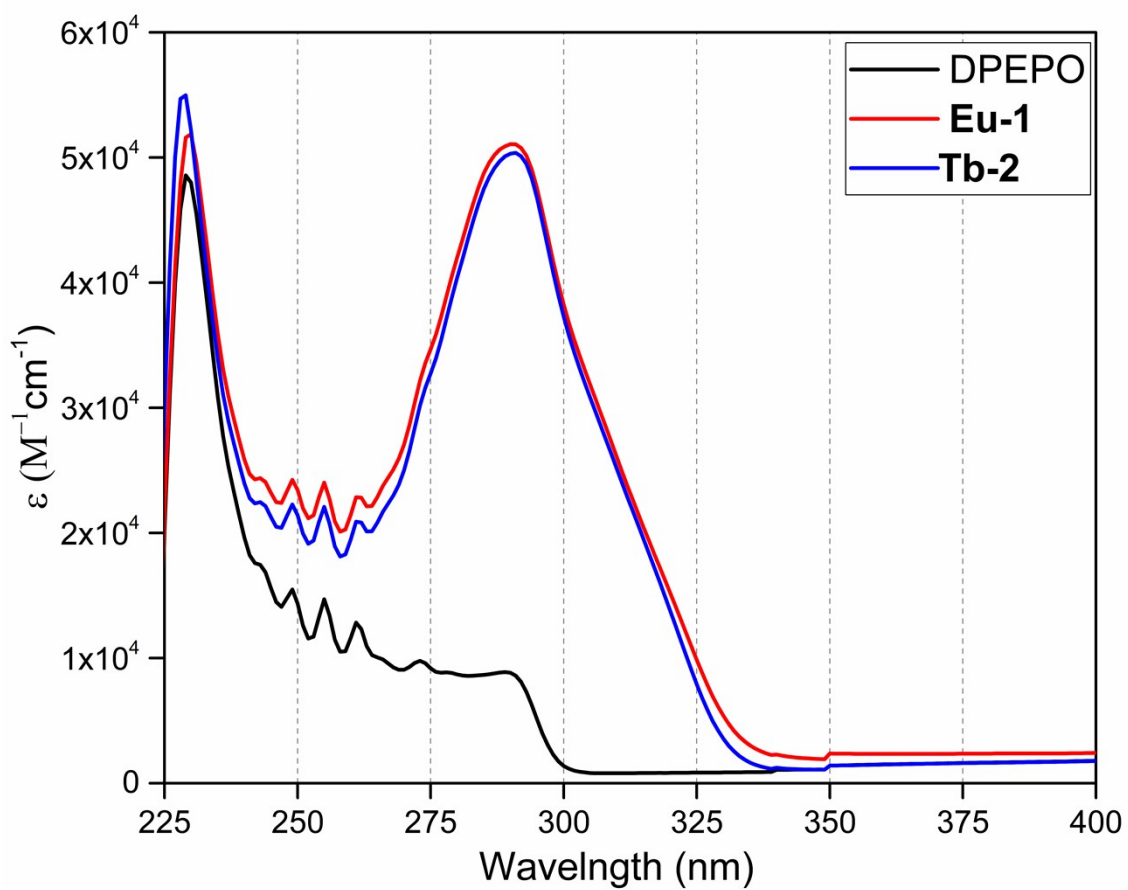


Fig. S 8. Optical absorption spectra of free DPEPO ligand, **Eu-1** and **Tb-2** complex in DCM solution.

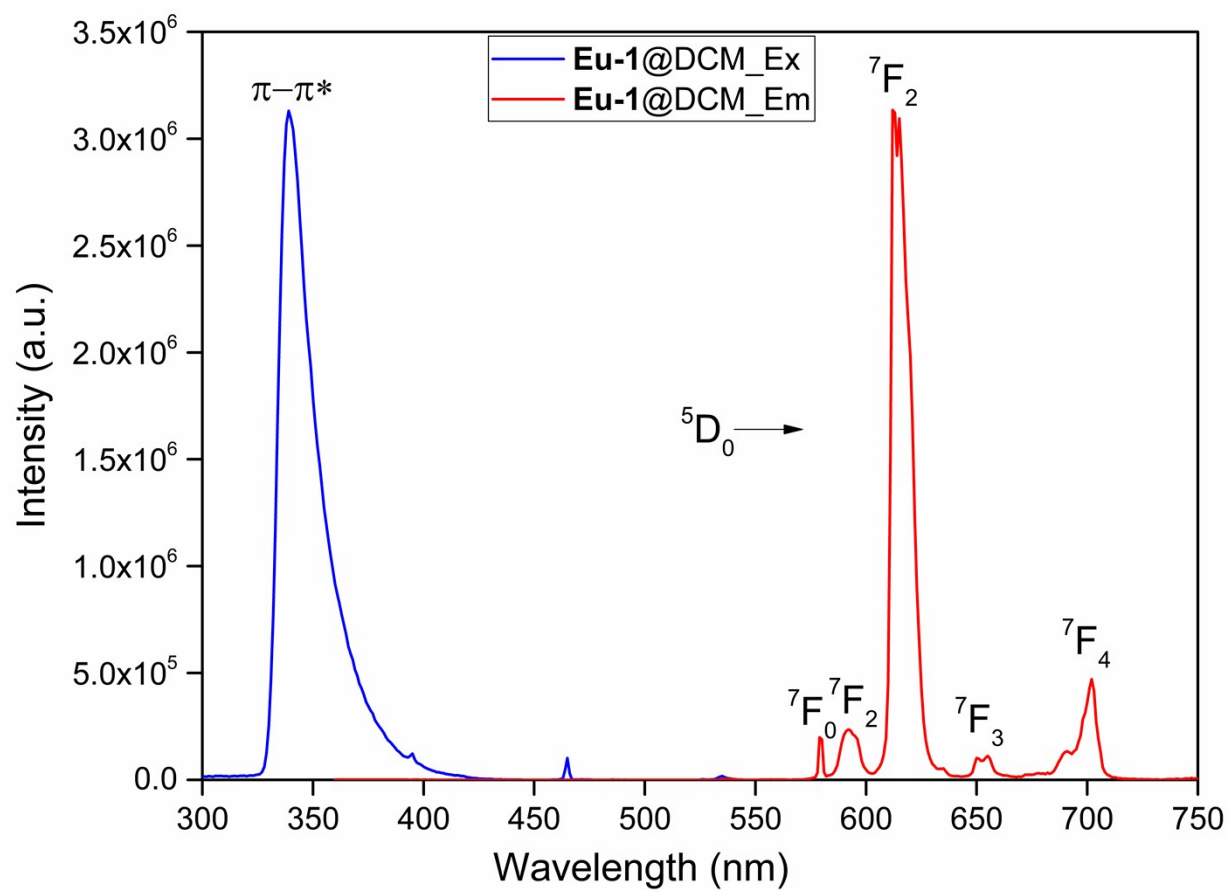


Fig. S 9. Excitation and corrected emission spectra of **Eu-1** in DCM at RT.

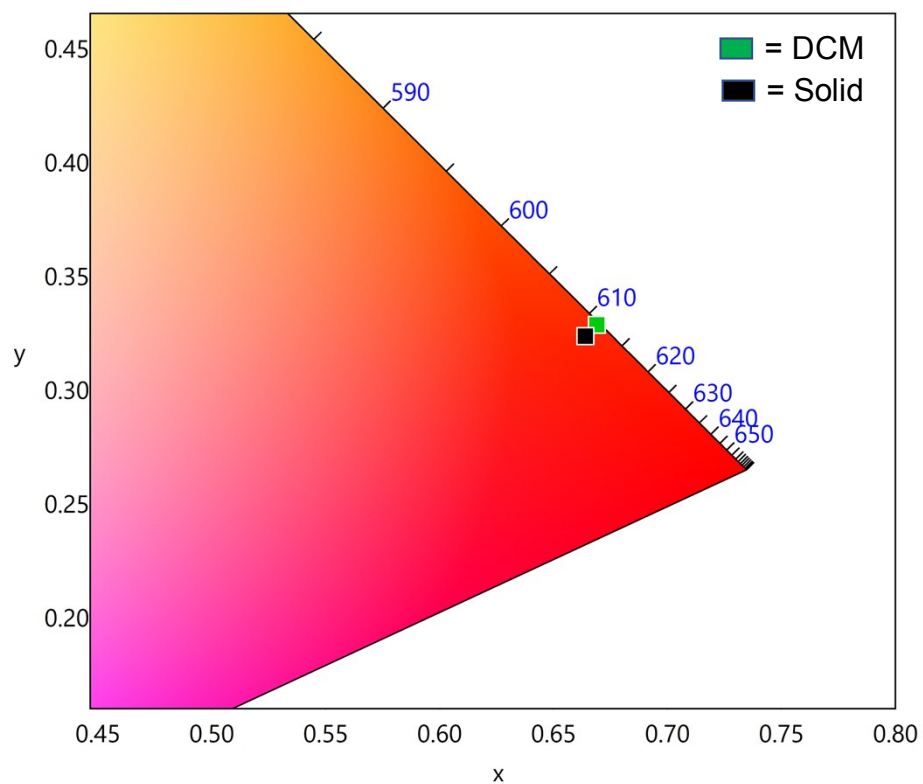


Fig. S 10. Magnified view of the 1931 CIE color coordinates of the **Eu-1** in the solid state and in DCM solution at RT.

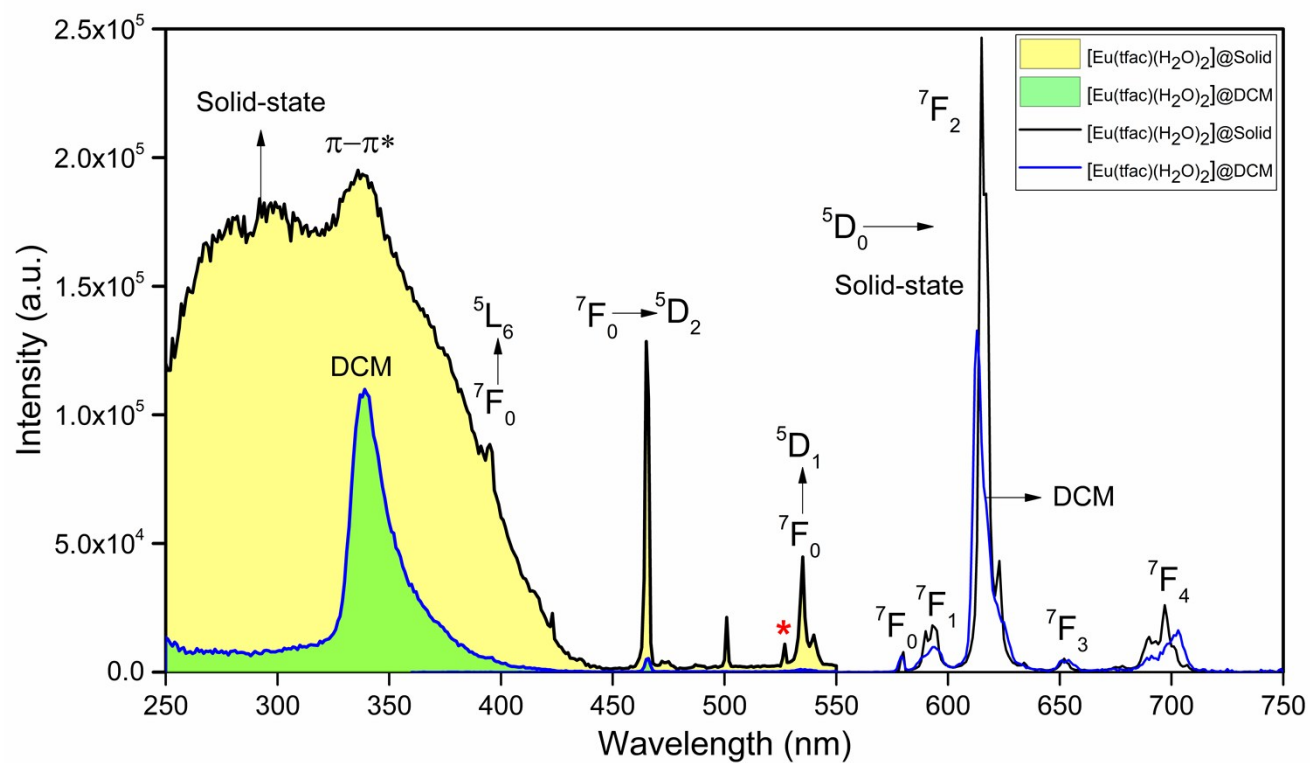


Fig. S 11. Excitation and corrected emission spectra of  $[\text{Eu}(\text{tfac})_3(\text{H}_2\text{O})_2]$  in solid-state and in DCM solution at RT.

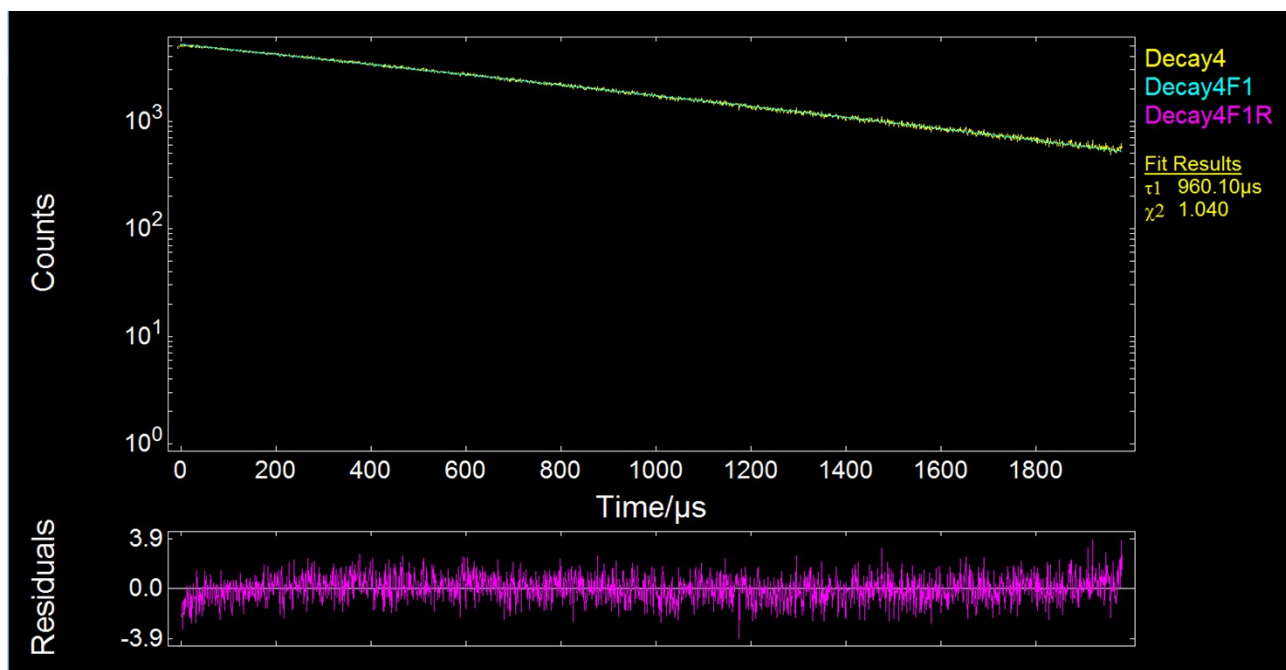


Fig. S 12. Experimental decay profile for **Eu-1** complex together with fitted curve in the solid state at RT by exciting it at  $\lambda_{\text{max}}^{\text{Ex}} \approx 359$  nm.

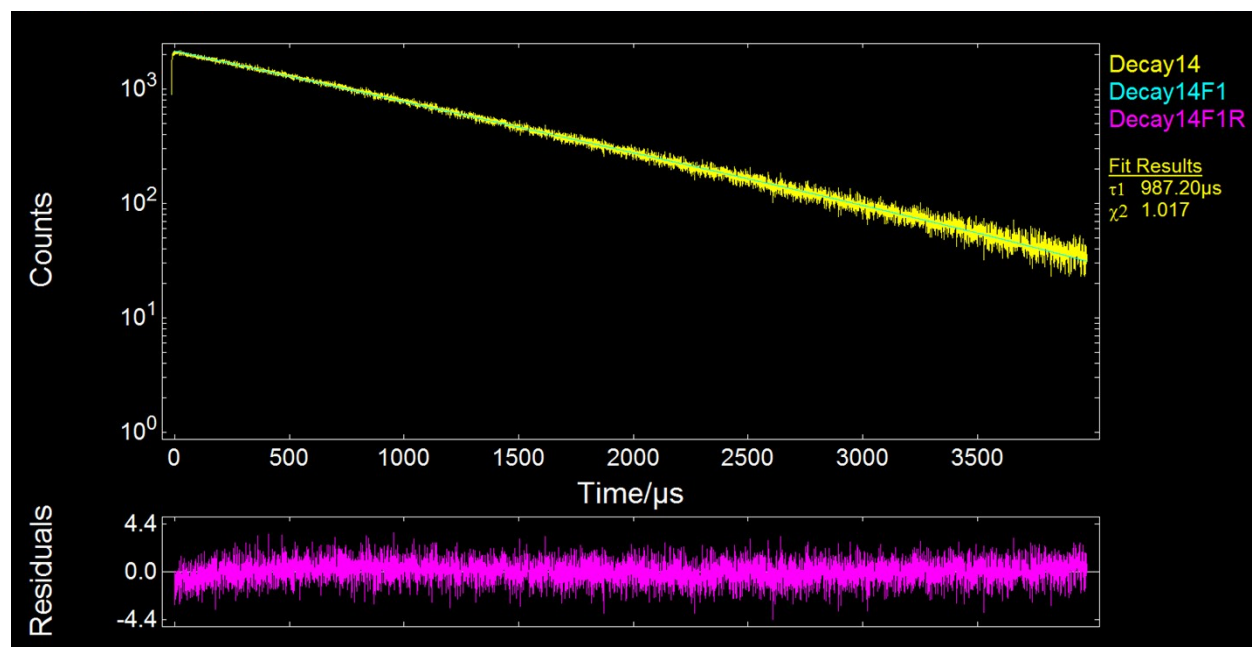


Fig. S 13. Experimental decay profile for **Eu-1** complex together with fitted curve in DCM solution at RT by exciting it at  $\lambda_{\text{max}}^{\text{Ex}} \approx 340$  nm.

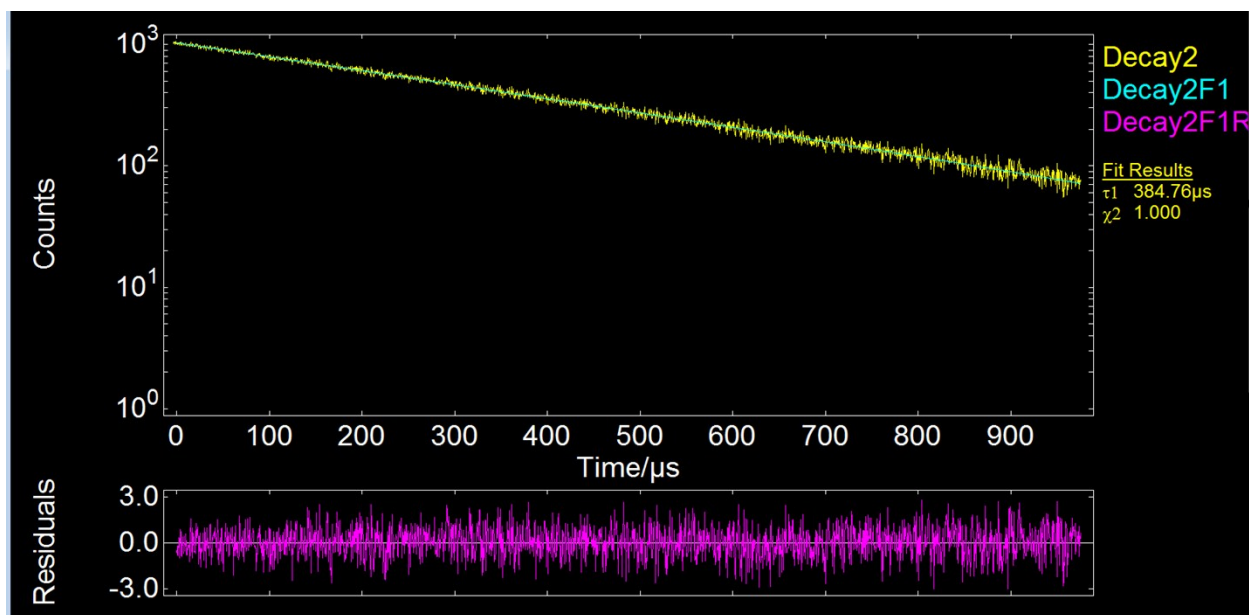


Fig. S 14. Experimental decay profile for  $[\text{Eu}(\text{tfac})_3(\text{H}_2\text{O})_2]$  complex together with fitted curve in the solid-state at RT.

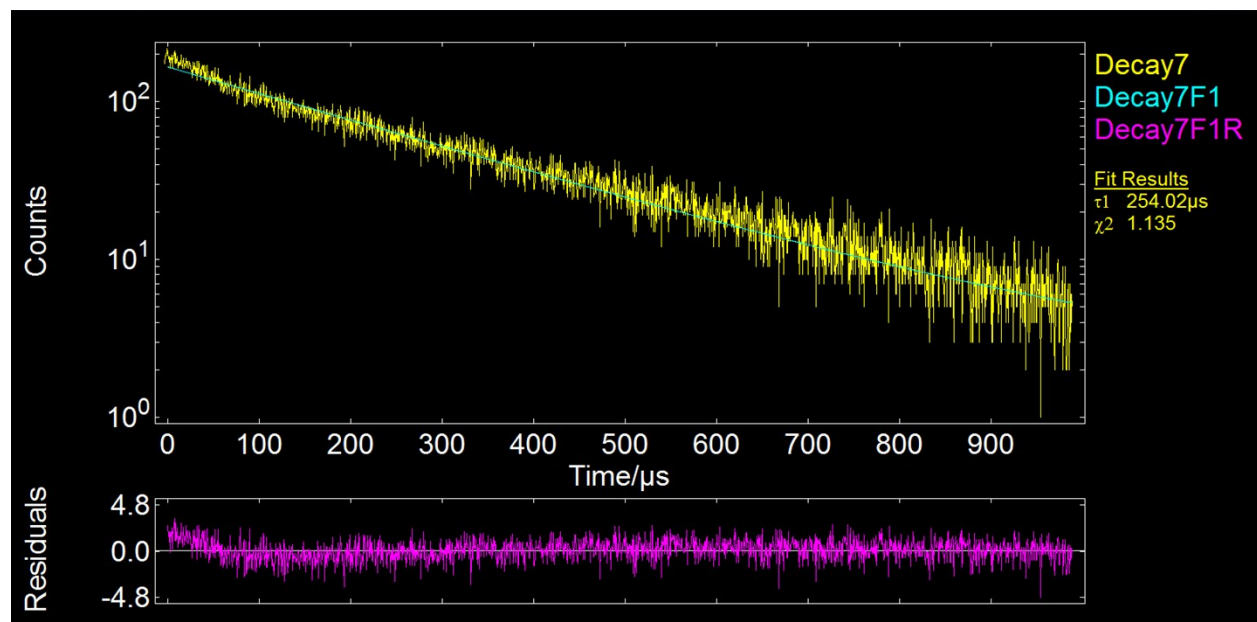


Fig. S 15. Experimental decay profile for  $[\text{Eu}(\text{tfac})_3(\text{H}_2\text{O})_2]$  complex together with fitted curve in DCM at RT.

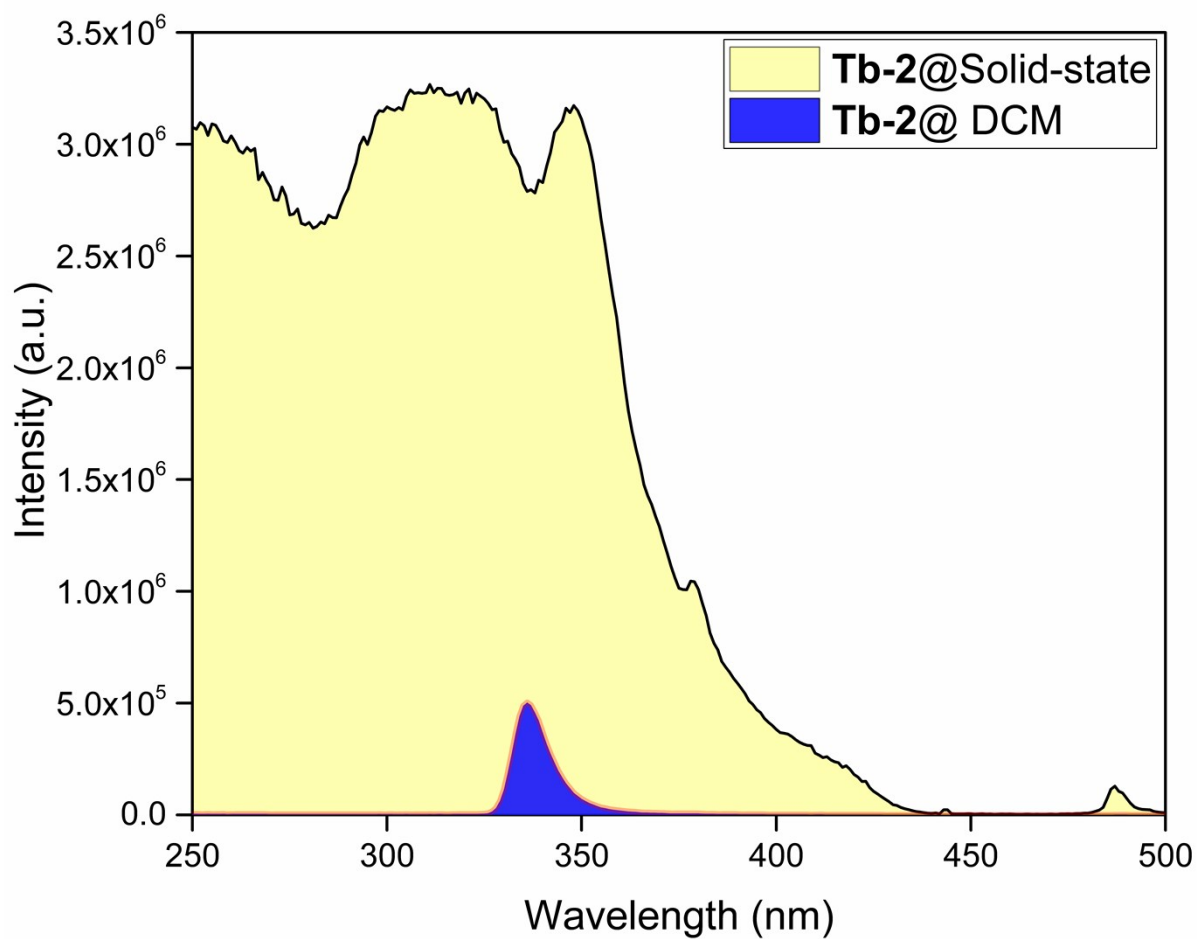


Fig. S 16. Excitation spectra of **Tb-2** complex in the solid-state and in DCM solution at RT.

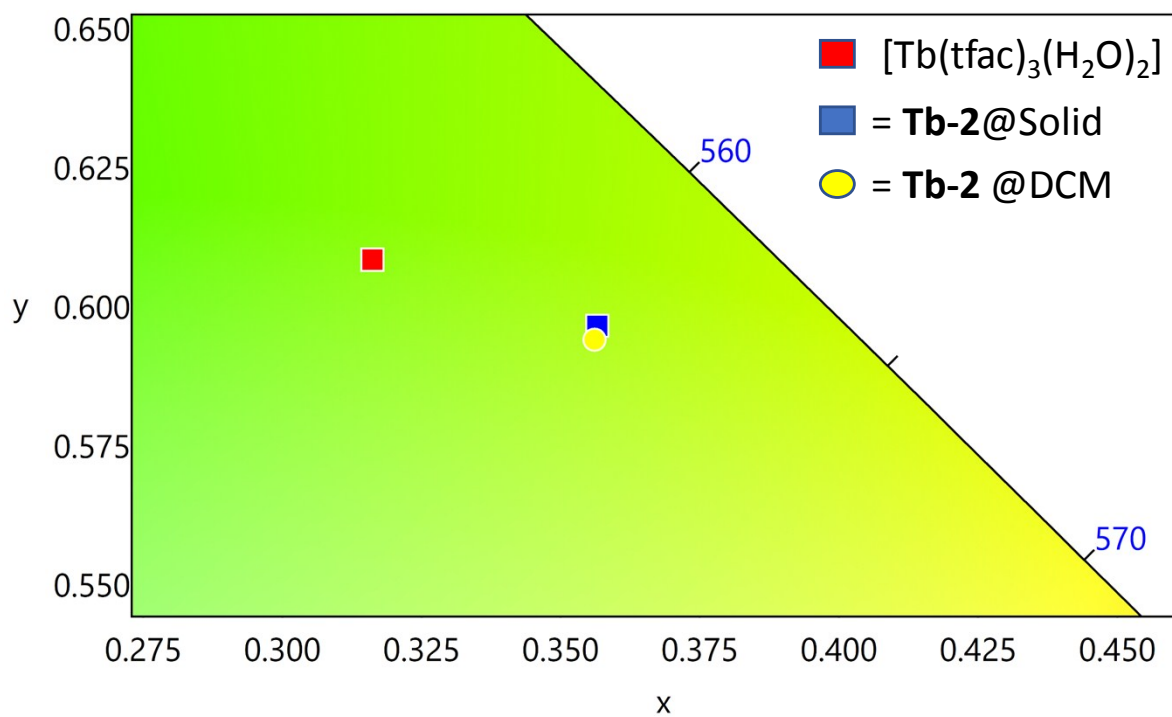


Fig. S 17. Magnified view of the 1931 CIE color coordinates of the  $[\text{Tb}(\text{tfac})_3(\text{H}_2\text{O})_2]$  and **Tb-2** complex at RT.

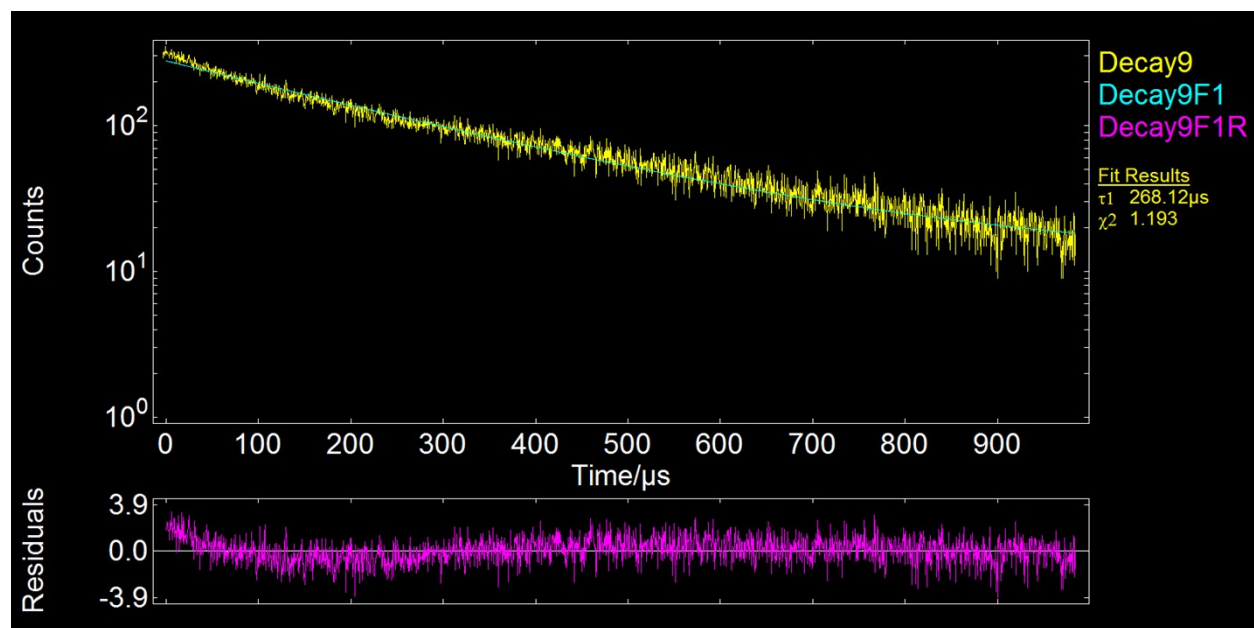


Fig. S 18. Experimental decay profile for **Tb-2** complex together with fitted curve in the solid-state at RT.

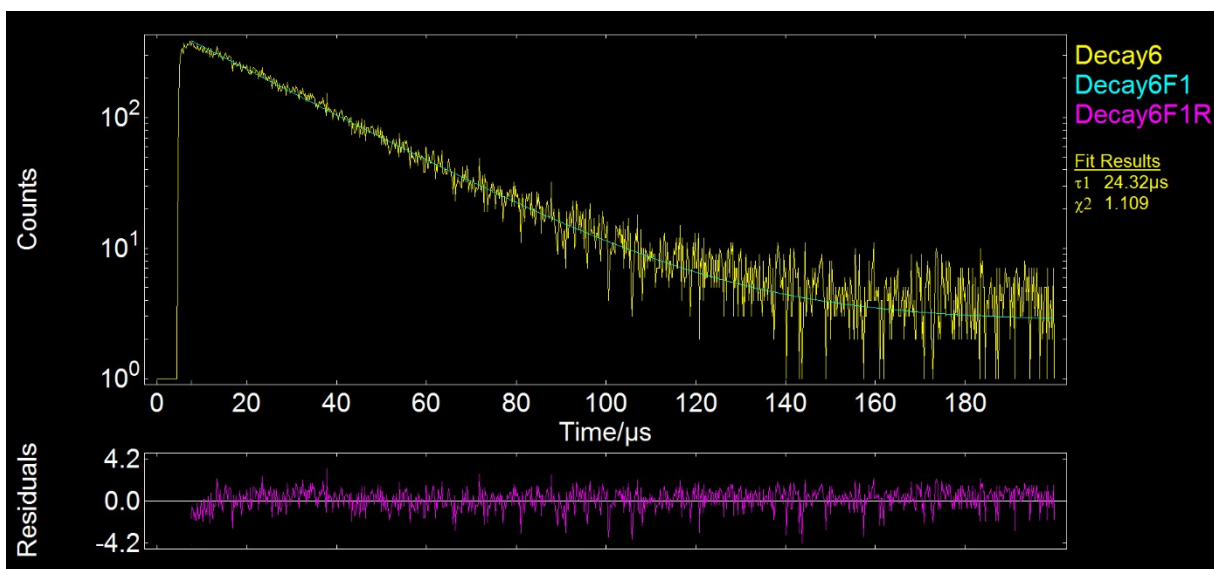


Fig. S 19. Experimental decay profile for **Tb-2** complex together with fitted curve in DCM solution at RT.

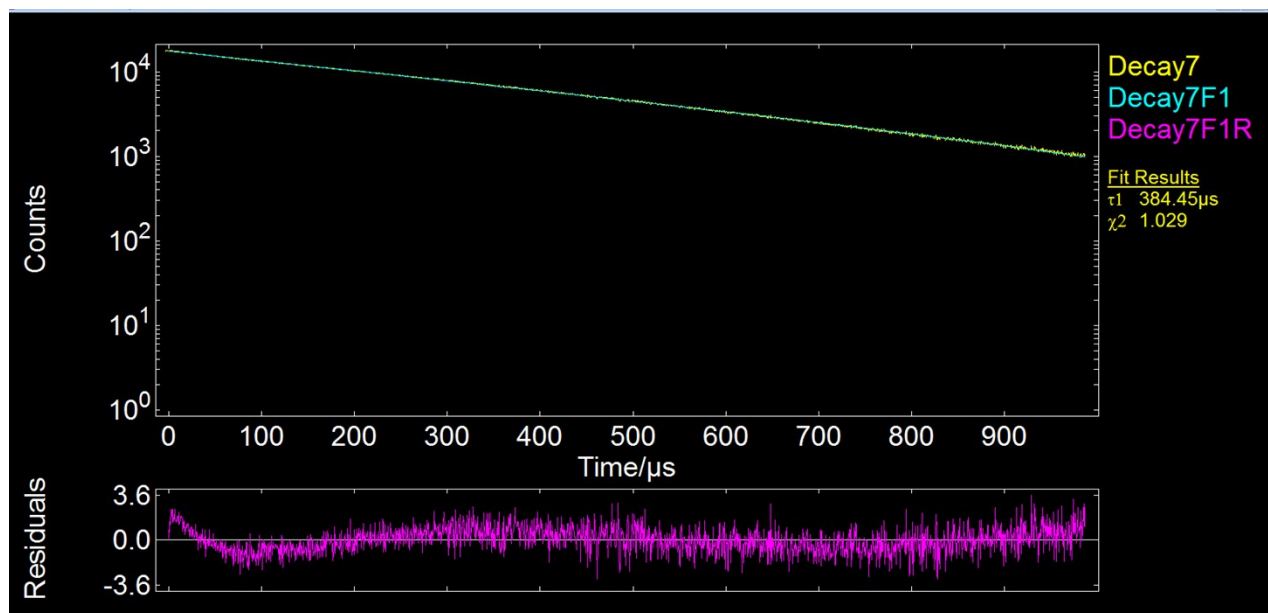


Fig. S 20. Experimental decay profile for  $[\text{Tb}(\text{tfac})_3(\text{H}_2\text{O})_2]$  complex together with fitted curve in the solid-state solution at RT.

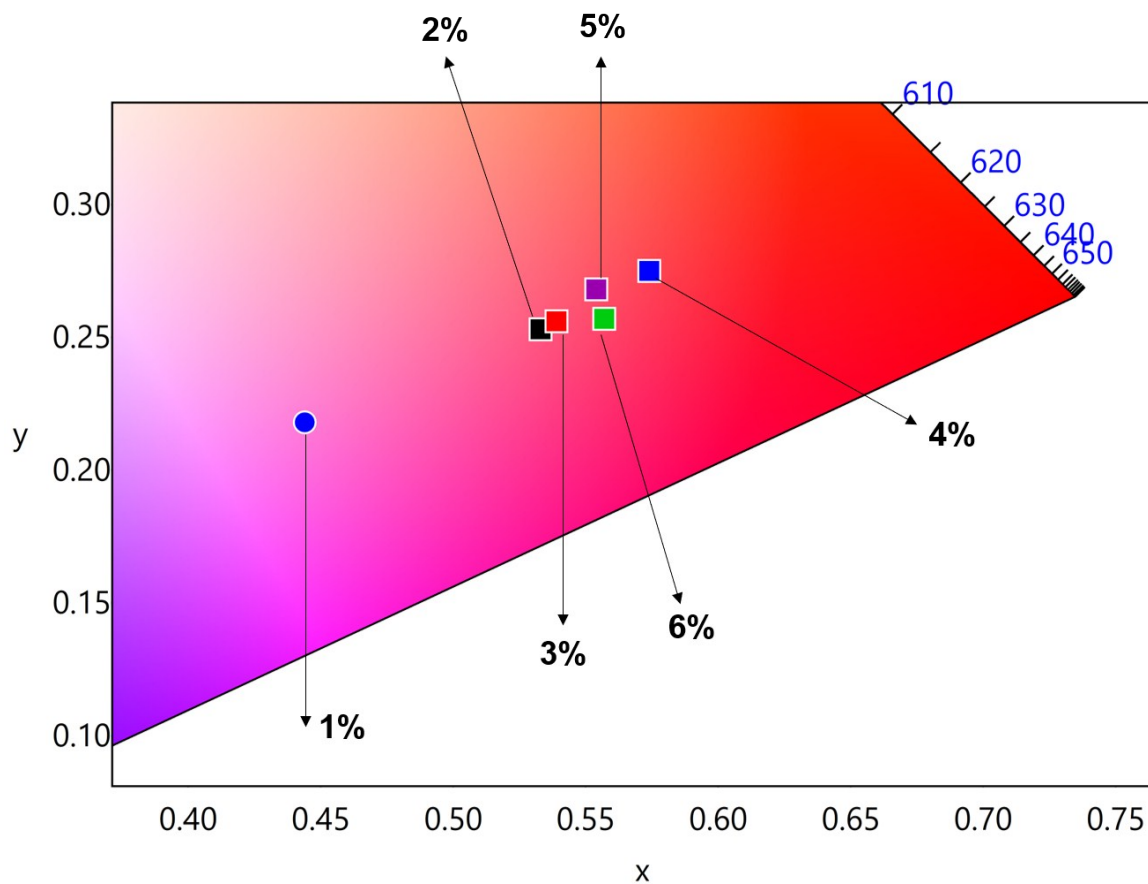


Fig. S 21. A magnified view of the CIE color coordinates at 10 mA/cm<sup>2</sup> of double-EMLs devices with different doping concentration of **Eu-1** complex.

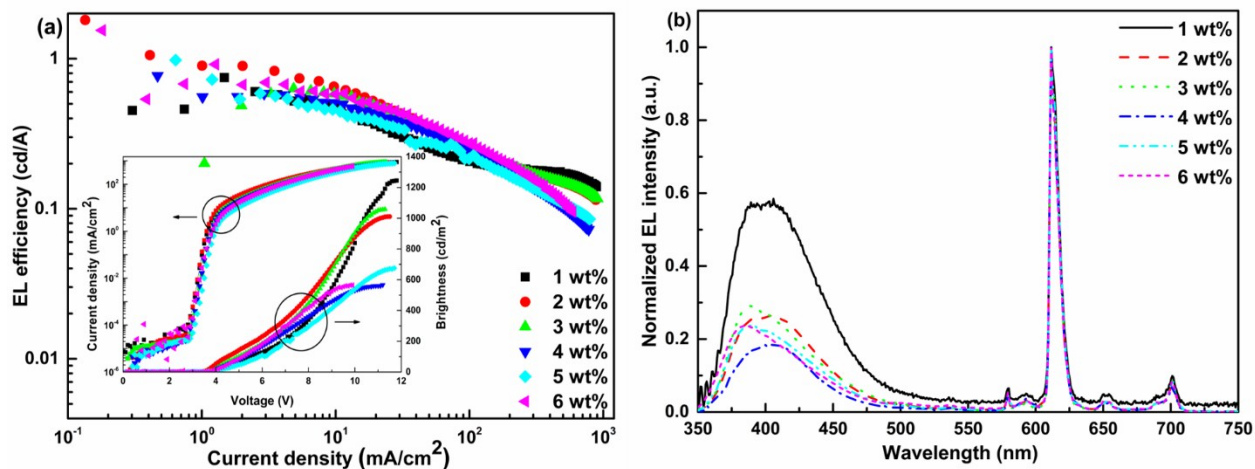


Fig. S 22. (a) EL efficiency-current density characteristics of double-EMLs devices with **Eu-1** at different doping concentrations. Inset: Current density-brightness-voltage characteristics of the double-EMLs devices with **Eu-1** at different doping concentrations. (b) Normalized EL spectra of the double-EMLs devices with **Eu-1** at different doping concentrations operating at 10 mA cm<sup>-2</sup>.

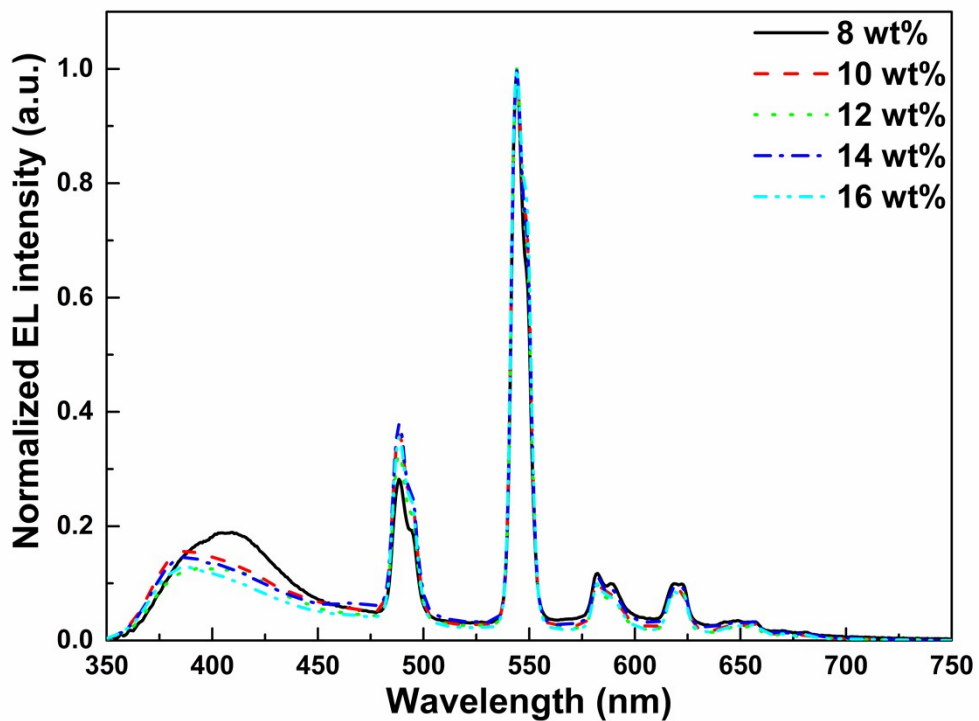


Fig. S 23. Normalized EL spectra of the double-EMLs devices with **Tb-2** at different doping concentrations operating at 10 mA cm<sup>-2</sup>.

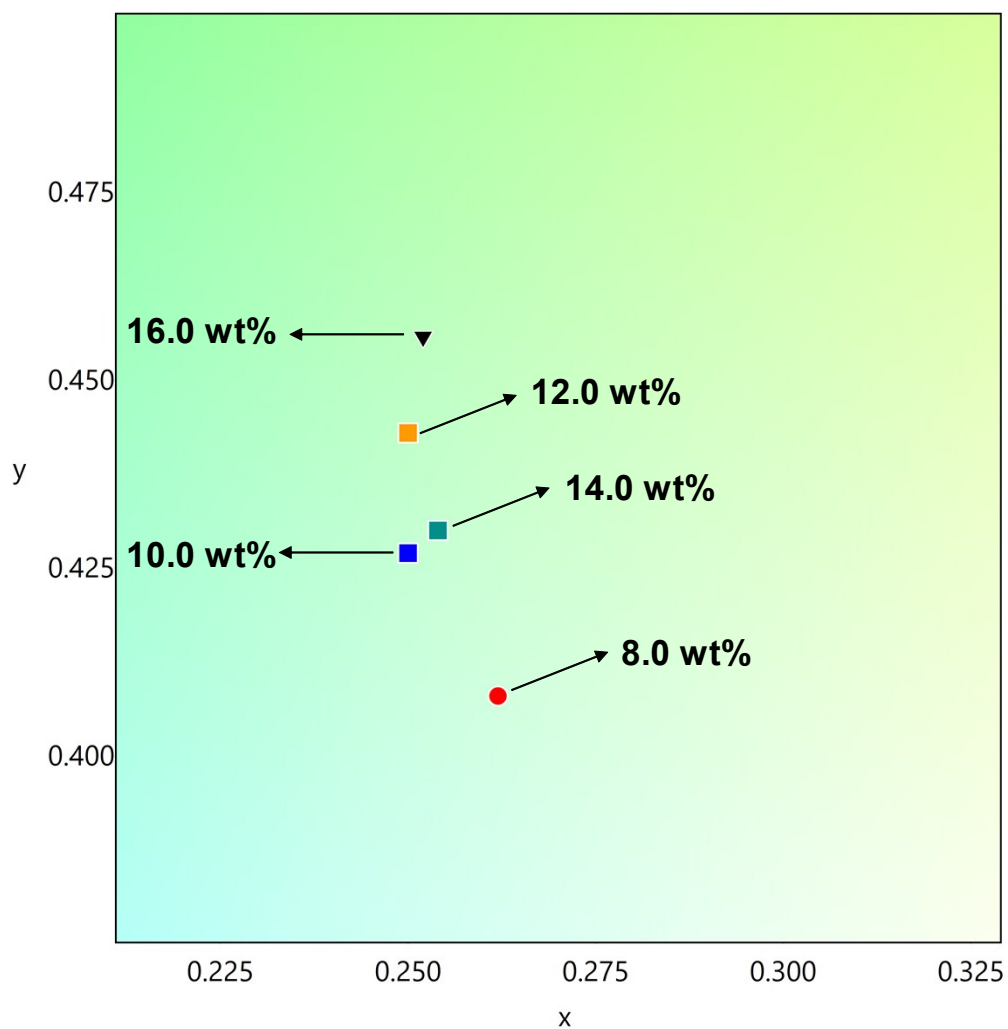


Fig. S 24. A magnified view of the CIE color coordinates at 10 mA/cm<sup>2</sup> of double-EMLs devices with different doping concentration of **Tb-2** complex.

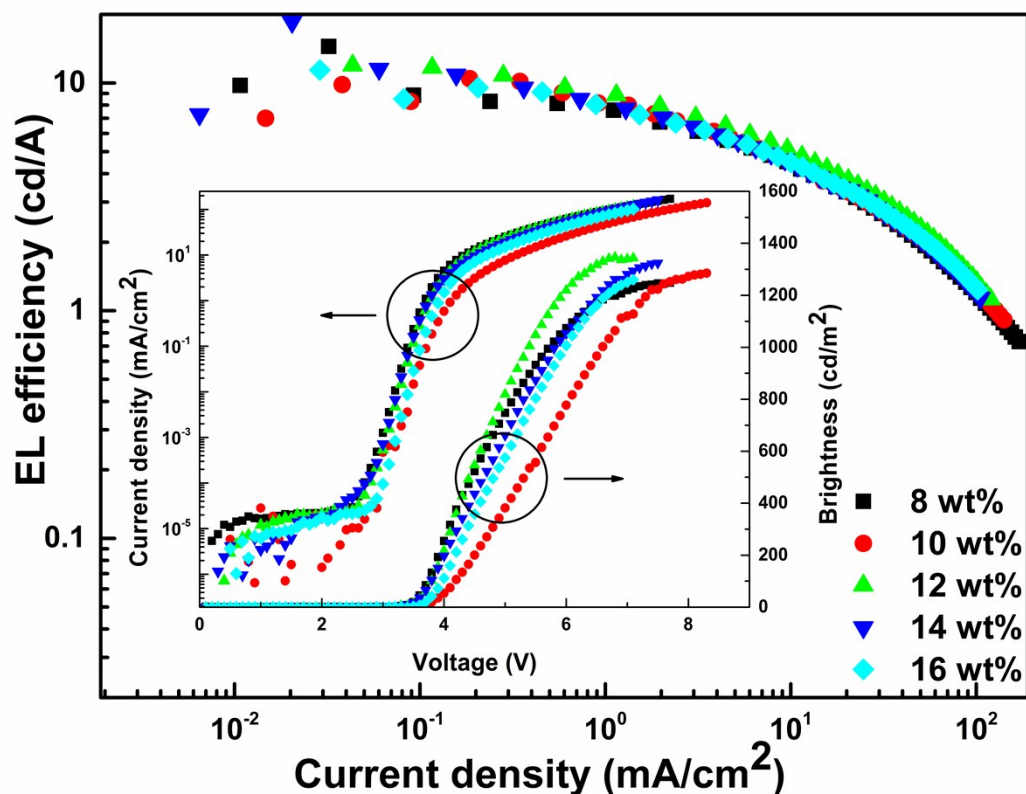


Fig. S 25. EL efficiency-current density characteristics of the double-EMLs devices with Tb-2 at different doping concentrations. Inset: Current density-brightness-voltage characteristics of the single-EML devices with Tb-2 at different doping concentrations.

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