

**Supporting Information for:**

**Multimodal Luminescence Manometer Based on a Novel Organic Complex**

**Material - Eu(bpyO<sub>2</sub>)<sub>4</sub>(PF<sub>6</sub>)<sub>3</sub>**

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*FT-IR data*

IR data of **Eu(bpyO<sub>2</sub>)<sub>4</sub>(PF<sub>6</sub>)<sub>3</sub>**, selected IR (KBr, cm<sup>-1</sup>): ν(O-H) 3434; ν(C-H) 3070, 3115; ν(N-O) 1215, 1235; ν(O-H) 1623; ν(C=C) 1509, 1479, 1427; ν(PF<sub>6</sub>) 845, 890, 555

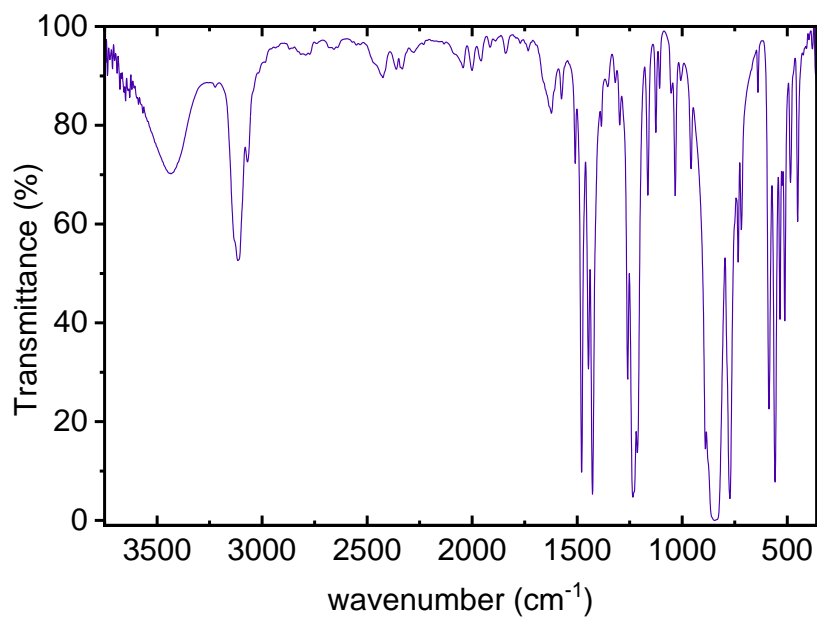


Figure S1. FT-IR spectrum for the complex studied **Eu(bpyO<sub>2</sub>)<sub>4</sub>(PF<sub>6</sub>)<sub>3</sub>**.

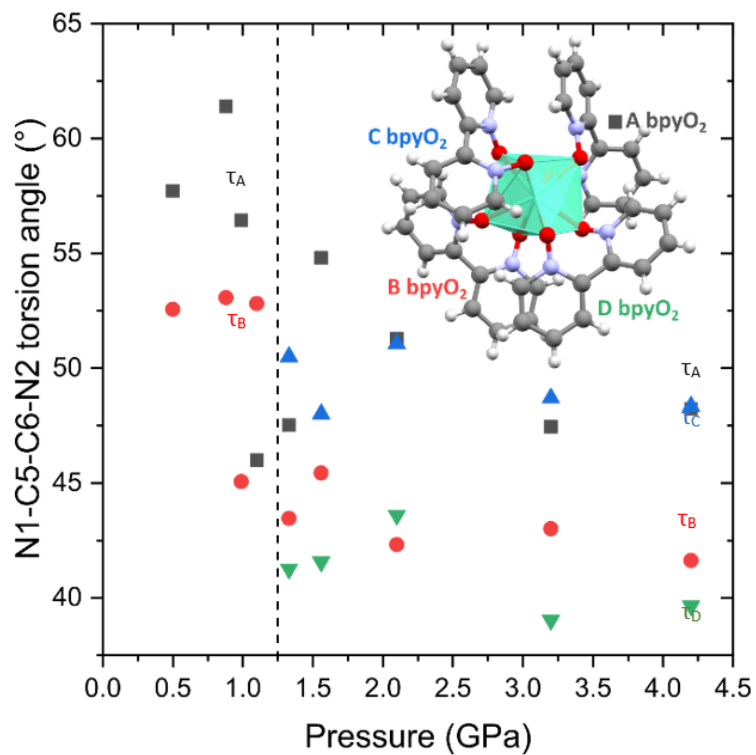
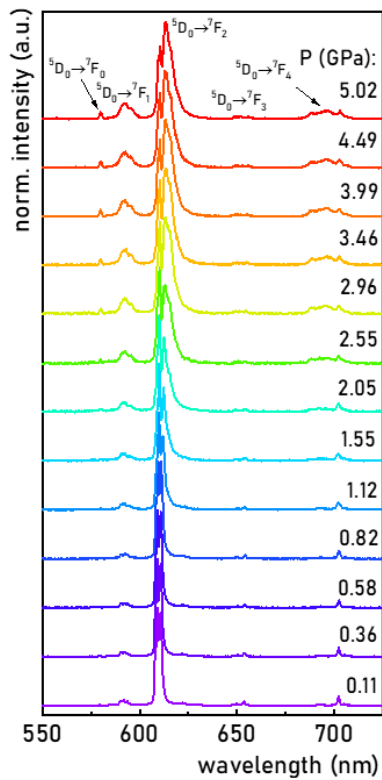
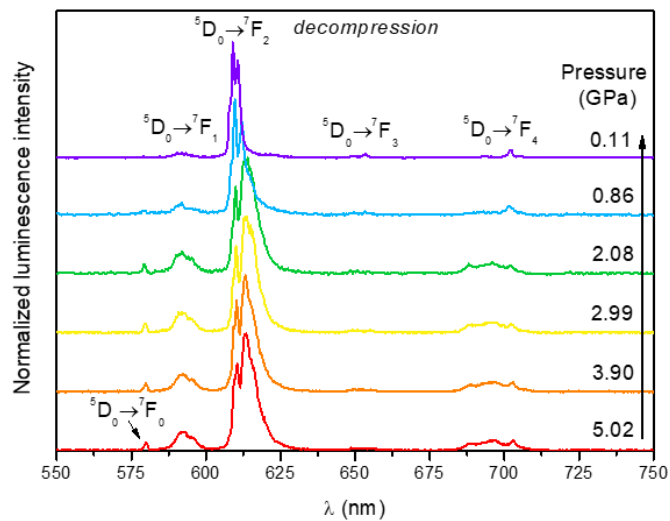


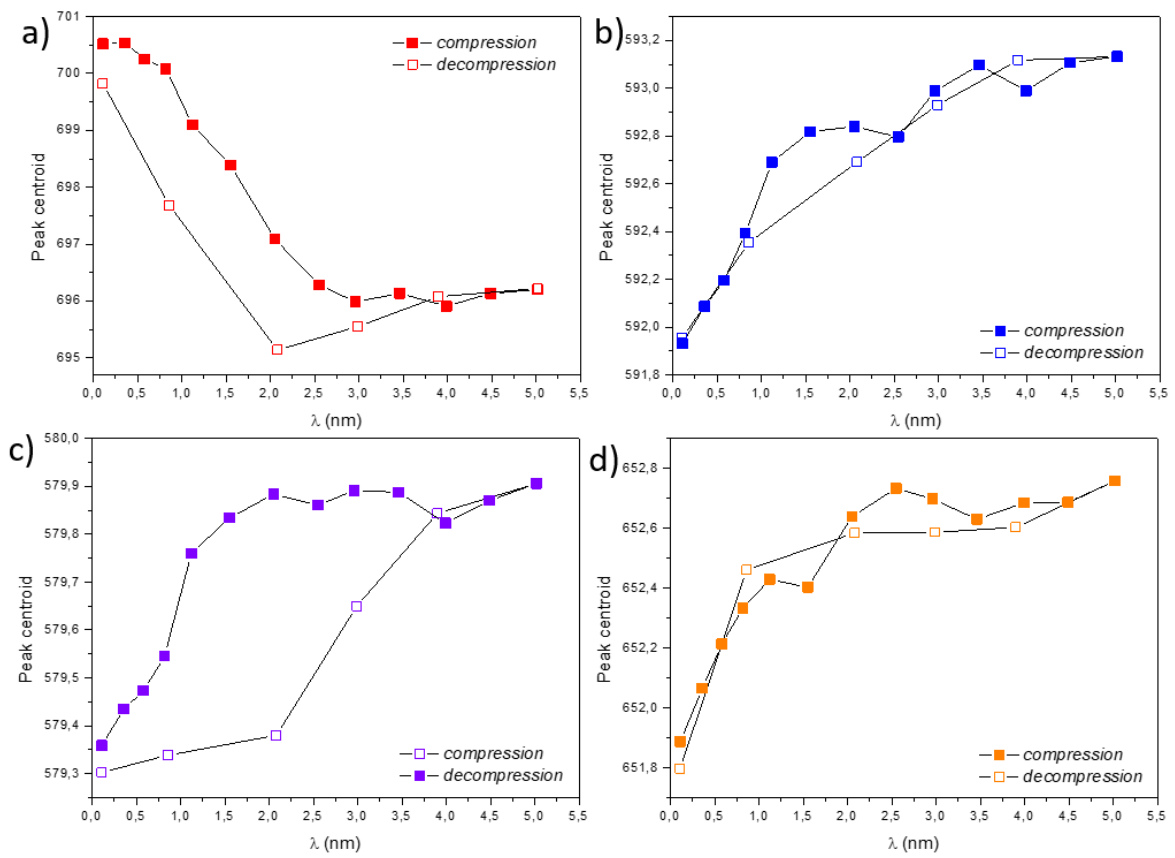
Figure S2. Changes of the N1-C5-C6-N2 torsion angles with increasing pressure. On the inset (upper right) the four independent ligands present in phase  $\beta$  were indicated.



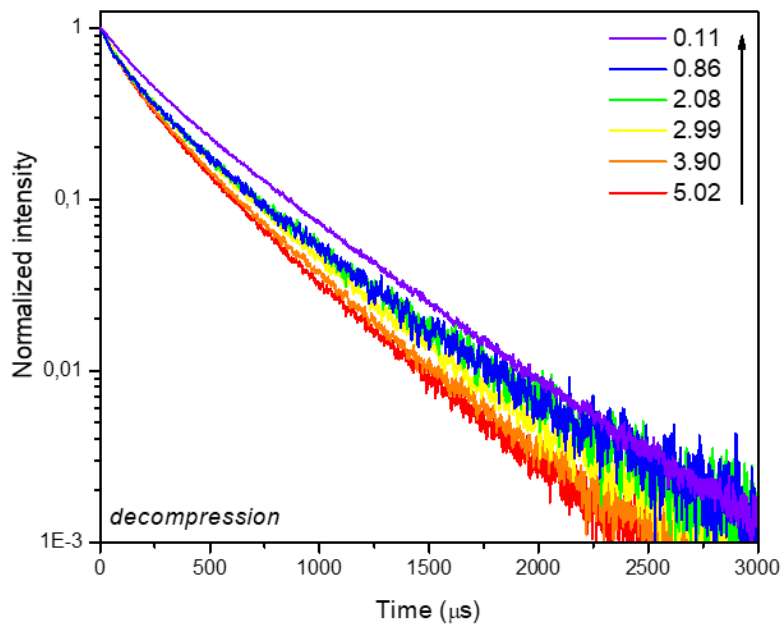
**Figure S3.** Pressure-dependent emission spectra ( $\lambda_{\text{exc}} = 328 \text{ nm}$ ) of  $\text{Eu}(\text{bpyO}_2)_4(\text{PF}_6)_3$ .



**Figure S4.** Pressure-dependent emission spectra ( $\lambda_{\text{exc}} = 328 \text{ nm}$ ) of  $\text{Eu}(\text{bpyO}_2)_4(\text{PF}_6)_3$  (decompression).



**Figure S5.** Pressure-dependent emission peak centroids of  $\text{Eu}(\text{bpyO}_2)_4(\text{PF}_6)_3$ .



**Figure S6.** Pressure-dependent luminescence decay curves ( $\lambda_{\text{exc}} = 328 \text{ nm}$ ,  $\lambda_{\text{em}} = 610 \text{ nm}$ ) of  $\text{Eu}(\text{bpyO}_2)_4(\text{PF}_6)_3$  (decompression).

**Table S1.** Detailed crystallographic data for phase  $\alpha$ .

| Pressure   |              | <b>0.001 GPa</b>  | <b>0.47 GPa</b>   | <b>0.88 GPa</b>   | <b>0.99 GPa</b>   | <b>1.10 GPa</b>   |
|--|--------------|---|---|---|---|---|
| CCDC numbers   |              | 2345591   | 2346017   | 2346018   | 2346019   | 2346020   |
| Crystal system   |              | orthorhombic  | orthorhombic  | orthorhombic  | orthorhombic  | orthorhombic  |
| Space group  |              | <i>Pbcn</i>   | <i>Pbcn</i>   | <i>Pbcn</i>   | <i>Pbcn</i>   | <i>Pbcn</i>   |
| Unit cell dimensions                                     | <i>a</i> (Å) | 13.36546(15)  | 13.0576(17)   | 12.752(19)  | 12.742(8)   | 12.7784(19)   |
|  | <i>b</i> (Å) | 24.6682(3)  | 24.507(2)   | 24.441(5)   | 24.494(15)  | 24.42(7)  |
|  | <i>c</i> (Å) | 14.94455(15)  | 14.6945(6)  | 14.444(3)   | 14.308(3)   | 14.216(2)   |
| Unit cell angles   | $\alpha$ (°) | 90  | 90  | 90  | 90  | 90  |
|  | $\beta$ (°)  | 90  | 90  | 90  | 90  | 90  |
|  | $\gamma$ (°) | 90  | 90  | 90  | 90  | 90  |
| Volume (Å <sup>3</sup> )                                 |              | 4927.25(10)   | 4702.2(8)   | 4502(7)   | 4466(4)   | 4437(13)  |
| <i>Z/Z'</i>  |              | 4/0.5   | 4/0.5   | 4/0.5   | 4/0.5   | 4/0.5   |
| Radiation $\lambda$ (Å)                                  |              | 1.54184   | 0.71073   | 0.71073   | 0.71073   | 0.71073   |
| Molecular volume (V/Z)                                   |              | 1231.81   | 1175.57   | 1125.5  | 1116.5  | 1109.25   |
| Density (g/cm <sup>3</sup> )                             |              | 1.806   | 1.892   | 1.976   | 1.993   | 2.005   |
| Absorption (mm <sup>-1</sup> )                           |              | 11.206  | 1.57  | 1.64  | 1.653   | 1.664   |
| F(000)   |              | 2648.0  | 2648.0  | 2648.0  | 2648  | 2648.0  |
| Crystal size (mm)  |              | 0.2 × 0.12 × 0.08   | 0.20 × 0.12 × 0.1   | 0.20 × 0.12 × 0.1   | 0.20 × 0.12 × 0.1   | 0.20 × 0.12 × 0.1   |
| 2 $\theta$ -range (°)                                    |              | 7.168 to 150.92   | 5.544 to 56.672   | 6.484 to 52.612   | 5.694 to 52.722   | 6.376 to 52.944   |
| Min/max indices: <i>h, k, l</i>                          |              | -13 ≤ <i>h</i> ≤ 16, -28 ≤ <i>k</i> ≤ 30, -18 ≤ <i>l</i> ≤ 18 | -11 ≤ <i>h</i> ≤ 11, -25 ≤ <i>k</i> ≤ 25, -19 ≤ <i>l</i> ≤ 18 | -5 ≤ <i>h</i> ≤ 5, -29 ≤ <i>k</i> ≤ 29, -16 ≤ <i>l</i> ≤ 17 | -11 ≤ <i>h</i> ≤ 11, -22 ≤ <i>k</i> ≤ 21, -17 ≤ <i>l</i> ≤ 17 | -15 ≤ <i>h</i> ≤ 14, -5 ≤ <i>k</i> ≤ 5, -17 ≤ <i>l</i> ≤ 17 |
| Reflect. Collected/unique                                |              | 13171/5010  | 13835/5870  | 3774/948  | 8164/1675   | 7694/932  |
| Data/restraints/parameters                               |              | 5010/0/353  | 5870/364/305  | 948/556/305   | 1675/599/305  | 932/682/305   |
| Goodness-of-fit on F <sup>2</sup>                        |              | 1.061   | 1.044   | 1.086   | 1.029   | 1.068   |
| Final R <sub>1</sub> /wR <sub>2</sub> (I > 2 $\sigma$ 1) |              | 0.0483/0.1328   | 0.0621/0.1372   | 0.0871/0.1926   | 0.1491/0.343  | 0.0910/0.1698   |
| R <sub>1</sub> /wR <sub>2</sub> (all data)               |              | 0.0539/0.1386   | 0.1365/0.1733   | 0.1740/0.2360   | 0.2437/0.4150   | 0.2012/0.2224   |
| Largest diff. peak/hole (e.Å <sup>-3</sup> )             |              | 0.88/-0.70  | 0.68/-0.66  | 0.87/-0.69  | 1.59/-1.36  | 0.44/-0.40  |

$$w = 1/(\sigma^2 F_o^2 + w_1^2 * P^2 + w_2 * P), \text{ where } P = (\text{Max}(F_o^2, 0) + 2 * F_c^2)$$

**Table S2.** Detailed crystallographic data for phase  $\beta$ .

| Pressure   |              | 1.33 GPa   | 1.46 GPa   | 2.20 GPa   | 3.20 GPa   | 4.20 GPa   |
|--|--------------|--|--|--|--|--|
| CCDC numbers   |              | 2346021  | 2346022  | 2346023  | 2346024  | 2346025  |
| Crystal system   |              | monoclinic   | monoclinic   | monoclinic   | monoclinic   | monoclinic   |
| Space group  |              | $P2_1/n$   | $P2_1/n$   | $P2_1/n$   | $P2_1/n$   | $P2_1/n$   |
| Unit cell dimensions                                     | $a$ (Å)      | 12.677(8)  | 12.651(5)  | 12.6164(6)   | 12.4995(6)   | 12.4021(7)   |
|  | $b$ (Å)      | 13.5809(9)   | 13.3972(9)   | 13.2518(6)   | 12.9103(7)   | 12.6985(5)   |
|  | $c$ (Å)      | 25.002(2)  | 24.987(11)   | 24.85(2)   | 24.69(2)   | 24.740(19)   |
| Unit cell angles   | $\alpha$ (°) | 90   | 90   | 90   | 90   | 90   |
|  | $\beta$ (°)  | 90.42(2)   | 90.86(5)   | 91.019(12)   | 91.023(14)   | 90.772(14)   |
|  | $\gamma$ (°) | 90   | 90   | 90   | 90   | 90   |
| Volume (Å <sup>3</sup> )                                 |              | 4304(3)  | 4234(3)  | 4154(4)  | 3983(4)  | 3896(3)  |
| $Z/Z'$   |              | 4/1  | 4/1  | 4/1  | 4/1  | 4/1  |
| Radiation $\lambda$ (Å)                                  |              | 0.71073  | 0.71073  | 0.71073  | 0.71073  | 0.71073  |
| Molecular volume (V/Z)                                   |              | 1076   | 1058.5   | 1038.5   | 995.75   | 974  |
| Density (g/cm <sup>3</sup> )                             |              | 2.067  | 2.101  | 1.976  | 2.232  | 2.284  |
| Absorption (mm <sup>-1</sup> )                           |              | 1.715  | 1.743  | 1.64   | 1.853  | 1.895  |
| F(000)   |              | 2648.0   | 2648.0   | 2648.0   | 2648.0   | 2648.0   |
| Crystal size (mm)  |              | 0.19 × 0.12 × 0.09   | 0.19 × 0.12 × 0.09   | 0.19 × 0.12 × 0.09   | 0.19 × 0.12 × 0.09   | 0.19 × 0.12 × 0.09   |
| 2 $\theta$ -range (°)                                    |              | 5.736 to 52.832  | 5.472 to 55.78   | 6.46 to 54.196   | 6.52 to 56.556   | 6.572 to 54.186  |
| Min/max indices: $h, k, l$                               |              | $-7 \leq h \leq 7, -16 \leq k \leq 16, -30 \leq l \leq 31$ | $-13 \leq h \leq 12, -16 \leq k \leq 17, -22 \leq l \leq 23$ | $-16 \leq h \leq 16, -16 \leq k \leq 16, -6 \leq l \leq 6$ | $-16 \leq h \leq 16, -17 \leq k \leq 17, -6 \leq l \leq 6$ | $-15 \leq h \leq 15, -16 \leq k \leq 16, -6 \leq l \leq 6$ |
| Reflect. Collected/unique                                |              | 23593/3644   | 10137/5870   | 12418/2155   | 16868/2237   | 19641/2151   |
| Data/restraints/parameters                               |              | 3644/1577/610  | 2622/1601/608  | 2155/1805/608  | 2237/1697/608  | 2151/1769/609  |
| Goodness-of-fit on F <sup>2</sup>                        |              | 1.182  | 1.053  | 1.101  | 1.067  | 1.052  |
| Final R <sub>1</sub> /wR <sub>2</sub> (I > 2 $\sigma$ 1) |              | 0.1297/0.3119  | 0.0981/0.1800  | 0.1287/0.2855  | 0.1093/0.2370  | 0.1115/0.2476  |
| R <sub>1</sub> /wR <sub>2</sub> (all data)               |              | 0.2673/0.4141  | 0.1770/0.2194  | 0.1912/0.3254  | 0.1557/0.2608  | 0.1706/0.2750  |
| Largest diff. peak/hole (e.Å <sup>-3</sup> )             |              | 0.66/-0.83   | 0.89/-0.81   | 0.90/-1.02   | 0.98/-1.08   | 0.96/-0.79   |

$$w = 1/(\sigma^2 F_o^2 + w_1^2 * P^2 + w_2 * P), \text{ where } P = (\text{Max}(F_o^2, 0) + 2 * F_c^2)$$