

**3D photoluminescent Eu(III)-MOF sensor supported by tetracarboxylate ligand for the sensitive and selective detection of Cd<sup>2+</sup> and *o*-nitrophenol**

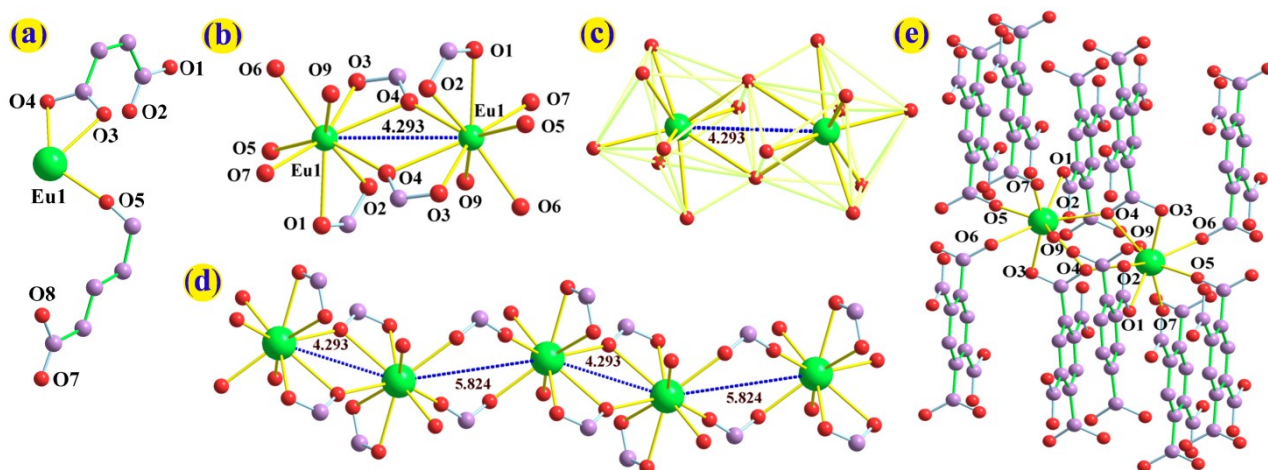
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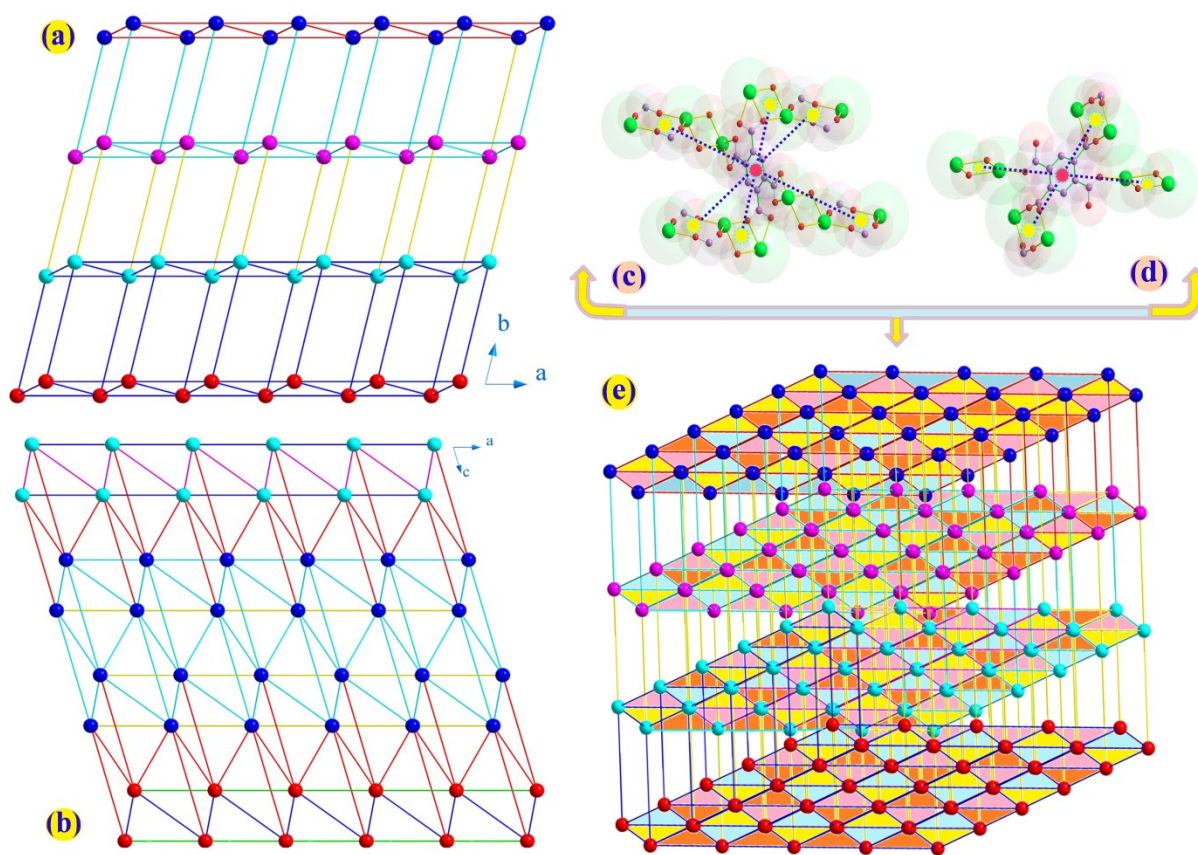
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**Figure S1:**(a) Asymmetric unit of **Cj-2**; (b) SBU of **Cj-2** (Eu...Eu = 4.293); (c) Edge sharing in SBU; (d) Linear extension of dinuclear SBUs; (e) The dinuclear unit connected with ten BTA ligands in **Cj-2**.



**Figure S2:**2D representation of (4,4) rectangular grid array nurturing by connecting Eu(III) nodes along the (a) ab and (b) ac plane; (c) Each  $\text{BTA}^{4+}$  linking six dinuclear SBUs, forming a 6-connected node (d) Each  $\text{H}_2\text{BTA}^{2-}$  linking four dinuclear Eu (III) SBUs unit is defined as a 4-connected node (e) Topological diagram of **Cj-2**.

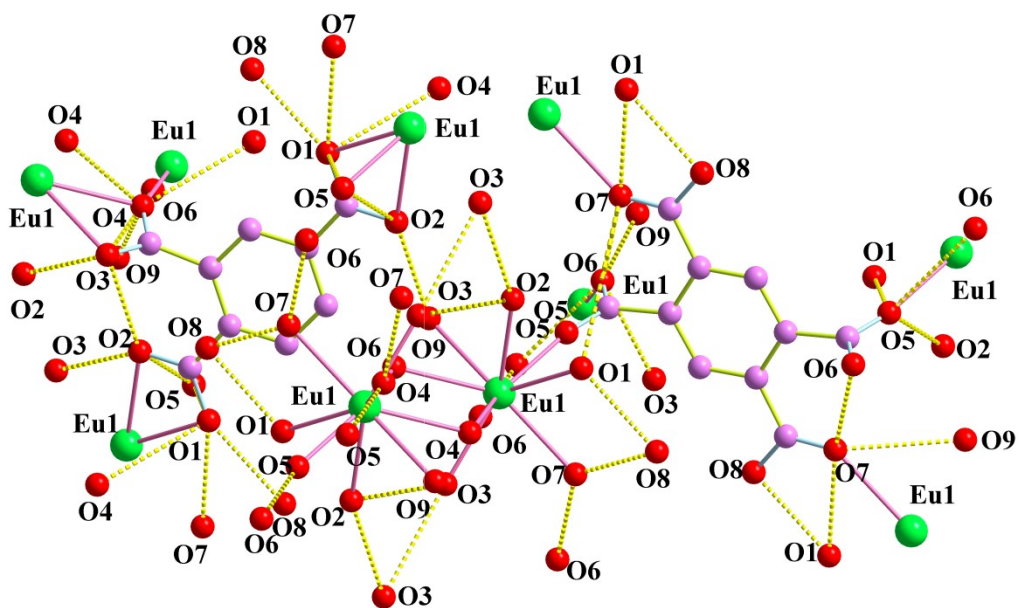


Figure S3:Hydrogen bonding positions in Cj-2

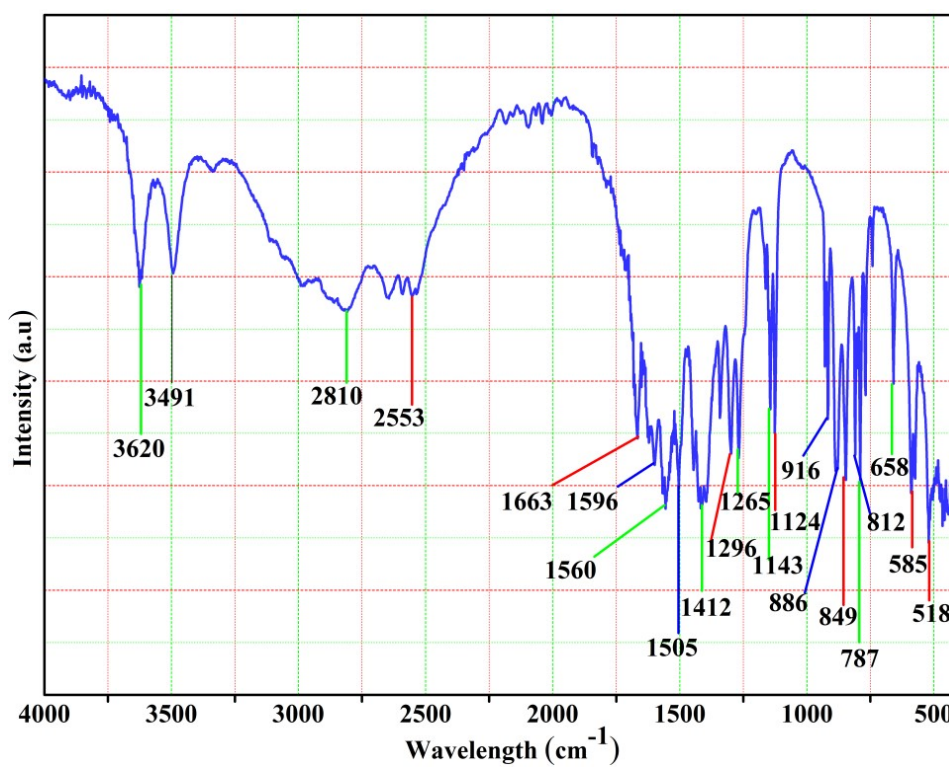
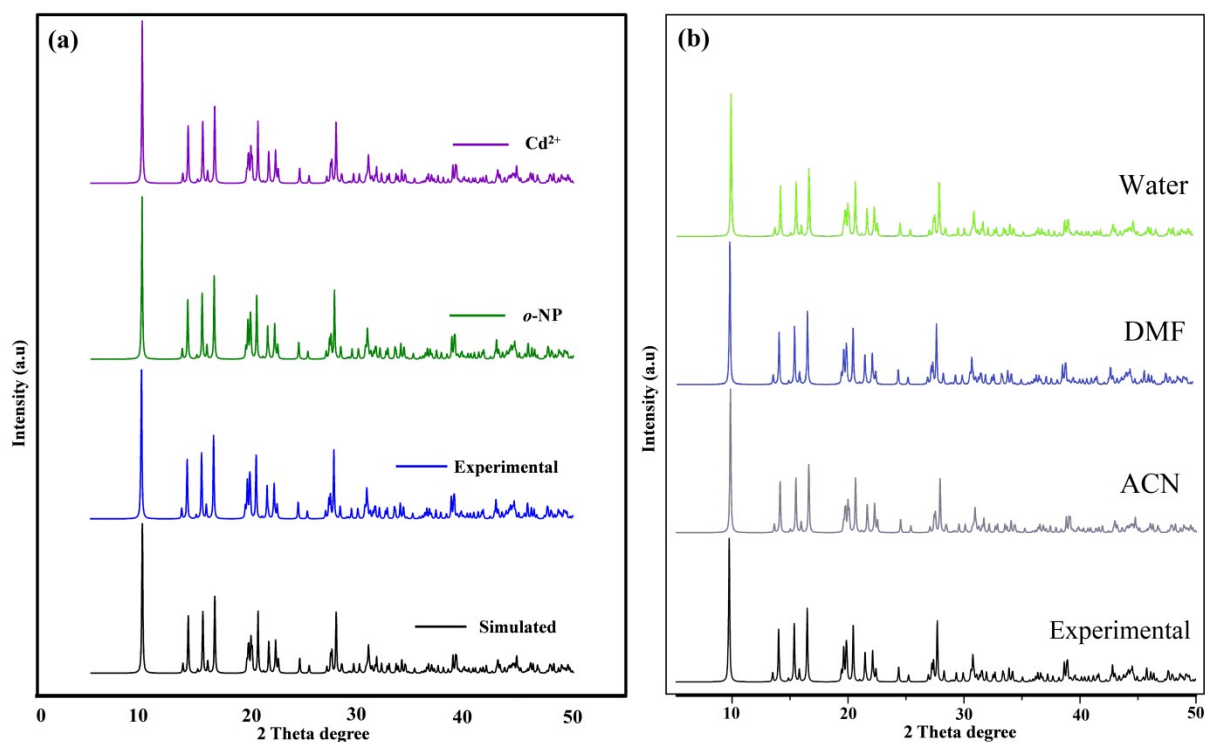
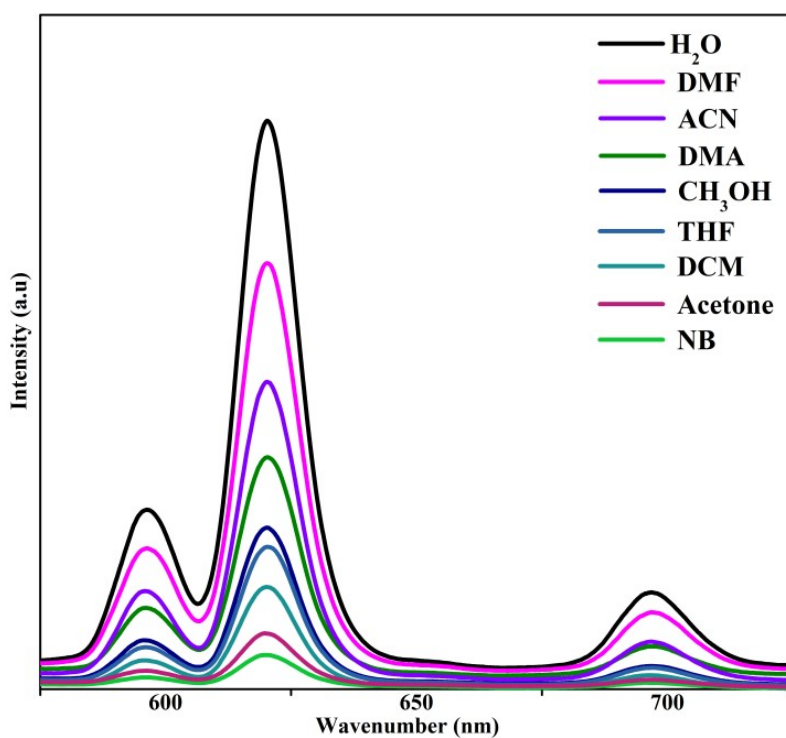


Figure S4:FTIR spectrum of Cj-2.



**Figure S5.** (a) Experimental and simulated PXR D Patterns of **Cj-2**, along with the PXR D response of recycled **Cj-2** after addition of *o*-NP, and Cd<sup>2+</sup>. (b) Experimental PXR D Patterns of **Cj-2**, along with the PXR D response of **Cj-2** in water, DMF and ACN.



**Figure S6.** Emission spectra of **Cj-2** in different solvents.

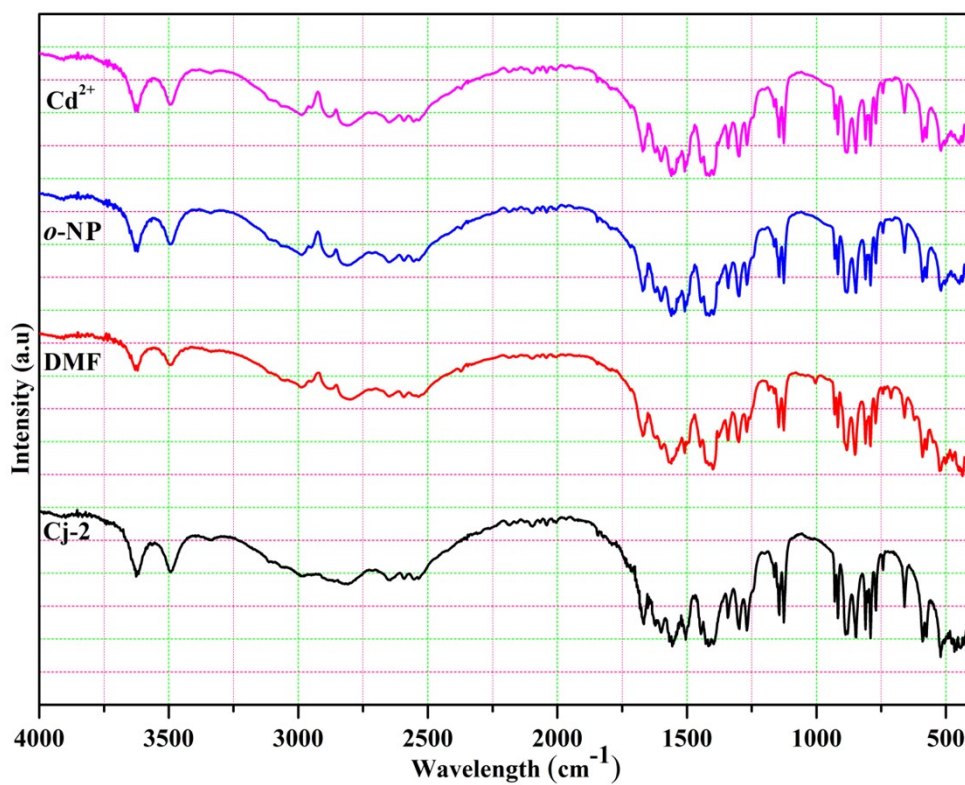


Figure S7. IR spectra of recycled Cj-2 after addition of *o*-NP, and Cd<sup>2+</sup>.

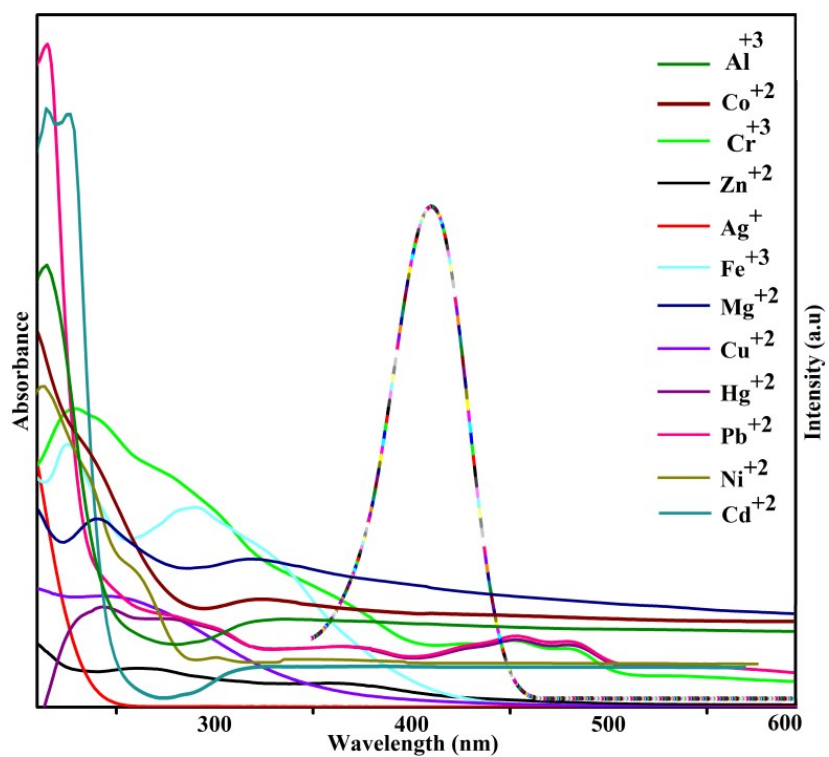
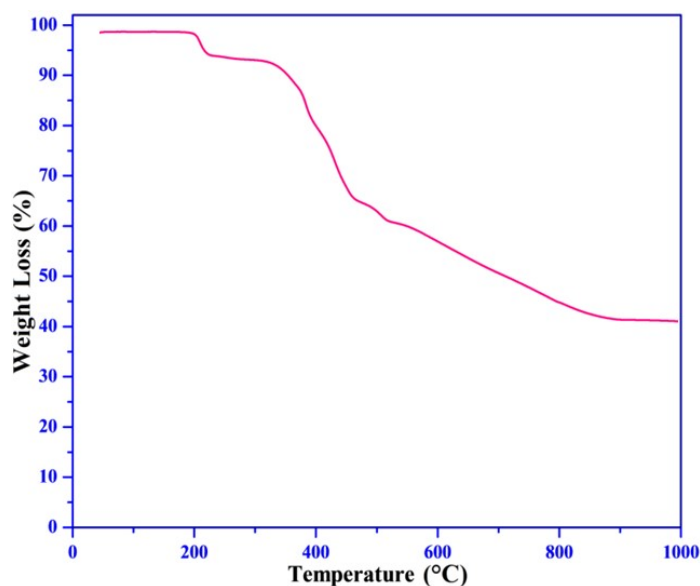


Figure S8. UV-Vis Absorption spectra of metals ions.

## Thermogravimetric Analysis



**Figure S9:** Thermogravimetric analysis curve of Cj-2.

The thermal decomposition behavior of synthesized Cj-2 was investigated using thermogravimetric analysis under an inert atmosphere ( $N_2$  gas), with a heating rate of  $10\text{ }^\circ\text{C}/\text{min}$  from  $30$  to  $950\text{ }^\circ\text{C}$ . Cj-2 demonstrates thermal stability up to  $190\text{ }^\circ\text{C}$ . Above this temperature, it undergoes two successive weight loss events between  $190$  and  $960\text{ }^\circ\text{C}$ . In the first stage, there is a  $4.27\%$  weight loss observed from  $190$  to  $270\text{ }^\circ\text{C}$ , attributed to the removal of coordinated water molecules (calculated at  $4.60\%$ ). The second decomposition stage begins at  $320\text{ }^\circ\text{C}$  and continues without a distinct endpoint within the limits of the thermal analyzer. This stage begins with a sudden weight loss followed by a gradual decline, possibly due to the structural collapse and oxidation of the organic linker (BTA). At  $690\text{ }^\circ\text{C}$ , the decomposition process results in the formation of  $\text{Eu}_2\text{O}_3$ , which remains stable up to  $950\text{ }^\circ\text{C}$ .

**Table S1: Crystal data for Cj-2****Crystallographic Information (Tables)**

|  |   |
|--|---|
| <b>Empirical formula</b>   | <b>C<sub>10</sub>H<sub>5</sub>EuO<sub>9</sub></b> |
| CCDC   | 2356125   |
| <b>Formula weight</b>  | <b>421.10</b>                                     |
| <b>Crystal system</b>  | <b>Triclinic</b>                                  |
| <b>space group</b>   | <b><i>P</i>-1</b>                                 |
| <b>Temperature (K)</b>   | <b>200(2) K</b>                                   |
| <i>a</i> (Å)   | 6.3270(7)   |
| <i>b</i> (Å)   | 9.2759(10)  |
| <i>c</i> (Å)   | 9.4488(10)  |
| <i>α</i> (deg°)  | 88.275(5)°  |
| <i>β</i> ( deg °)  | 73.972(5)°  |
| <i>γ</i> ( deg °)  | 76.714(5)°  |
| <b>Volume (Å<sup>3</sup>)</b>  | <b>518.39(10) Å<sup>3</sup></b>                   |
| <b><i>Z</i></b>  | <b>2</b>  |
| <b>Radiation type</b>  | <b>Cu Kα (λ =1.54178 Å)</b>                       |
| <b>μ (mm<sup>-1</sup>)</b>   | <b>43.843</b>                                     |
| <b>Crystal size (mm<sup>3</sup>)</b>   | <b>0.200 × 0.180 × 0.150 mm<sup>3</sup></b>       |
| <i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>  | 0.017, 0.116                                      |
| <b>No. of reflections</b>  | <b>1810</b>                                       |
| <i>R</i> <sub>int</sub>  | 0.0568  |
| (sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )  | 0.648   |
| <b><i>R</i>[<i>F</i><sup>2</sup> &gt; 2σ(<i>F</i><sup>2</sup>)], <i>wR</i>(<i>F</i><sup>2</sup>), <i>S</i></b> | <b>0.0327, 0.0875, 0.0887</b>                     |
| <b>No. of reflections</b>  | <b>75738</b>                                      |
| <b>No. of parameters</b>   | <b>190</b>  |
| <b>Δρ<sub>max</sub>, Δρ<sub>min</sub> (e Å<sup>-3</sup>)</b>   | <b>1.031, -0.894</b>                              |
| <b>Goodness-of-fit on <i>F</i><sup>2</sup></b>   | <b>1.129</b>                                      |



**Table S2: Hydrogen-bond geometry (Å, °) for Cj-2**

| Type  | Donor-H...Acceptor         | D - H    | H...A    | D...A    | D - H...A |
|-------|----------------------------|----------|----------|----------|-----------|
|       | O8-H8A...O1 <sup>i</sup>   | 0.84     | 1.73     | 2.549(6) | 164       |
|       | O9-H9A...O2 <sup>ii</sup>  | 0.85(7)  | 2.14(8)  | 2.891(6) | 147(7)    |
|       | O9-H9A...O3 <sup>ii</sup>  | 0.85(7)  | 2.31(8)  | 2.872(7) | 124(6)    |
| Intra | O9-H9A...O2 <sup>iii</sup> | 0.85(7)  | 2.59(8)  | 3.087(7) | 118(7)    |
|       | O9-H9B...O3 <sup>ii</sup>  | 0.87(10) | 2.54(13) | 2.872(7) | 104(9)    |
| Intra | C4-H4...O1 <sup>iv</sup>   | 0.95     | 2.46     | 2.782(7) | 100       |
| Intra | C8-H8...O8                 | 0.95     | 2.31     | 2.677(8) | 102       |
| Intra | C8-H8...O3 <sup>v</sup>    | 0.95     | 2.59     | 3.156(7) | 118'      |

Symmetry code(s): (i)  $-1+x, 1+y, -1+z$  (ii)  $-1+x, y, z$  (iii)  $-x, 1-y, 2-z$  (iv)  $1-x, -y, 2-z$  (v)  $1-x, -y, 2-z$

**Table S3: Selected geometric parameters (Å) for Cj-2**

|                      |           |                       |            |
|----------------------|-----------|-----------------------|------------|
| Eu1—O5               | 2.325 (4) | Eu1—O1 <sup>iii</sup> | 2.480 (4)  |
| Eu1—O9               | 2.380 (5) | Eu1—O7 <sup>iv</sup>  | 2.488 (4)  |
| Eu1—O6 <sup>i</sup>  | 2.380 (4) | Eu1—O2 <sup>iii</sup> | 2.531 (4)  |
| Eu1—O3               | 2.446 (4) | Eu1—O4                | 2.563 (4)  |
| Eu1—O4 <sup>ii</sup> | 2.454 (4) | Eu1—Eu1 <sup>ii</sup> | 4.2927 (6) |

Symmetry code(s): (i)  $-x+1, -y+1, -z+1$ ; (ii)  $-x, -y+1, -z+2$ ; (iii)  $-x+1, -y+1, -z+2$ ; (iv)  $-x, -y+2, -z+1$ .

**Table S4: Selected geometric parameters (°) for Cj-2**

|                        |             |   |             |
|------------------------|-------------|---|-------------|
| O5—Eu1—O9              | 139.63 (16) | O3—Eu1—O7 <sup>iv</sup>                 | 157.70 (14) |
| O5—Eu1—O6 <sup>i</sup> | 76.49 (14)  | O4 <sup>ii</sup> —Eu1—O7 <sup>iv</sup>  | 86.82 (14)  |
| O9—Eu1—O6 <sup>i</sup> | 66.78 (15)  | O1 <sup>iii</sup> —Eu1—O7 <sup>iv</sup> | 71.13 (14)  |

|   |                    |  |                    |
|---|--------------------|--|--------------------|
| <b>O5—Eu1—O3</b>                            | <b>80.95 (14)</b>  | <b>O5—Eu1—O2<sup>iii</sup></b>               | <b>73.50 (14)</b>  |
| <b>O9—Eu1—O3</b>                            | <b>102.58 (17)</b> | <b>O9—Eu1—O2<sup>iii</sup></b>               | <b>146.45 (14)</b> |
| <b>O6<sup>i</sup>—Eu1—O3</b>                | <b>72.59 (14)</b>  | <b>O6<sup>i</sup>—Eu1—O2<sup>iii</sup></b>   | <b>137.00 (13)</b> |
| <b>O5—Eu1—O4<sup>ii</sup></b>               | <b>145.62 (14)</b> | <b>O3—Eu1—O2<sup>iii</sup></b>               | <b>72.86 (13)</b>  |
| <b>O9—Eu1—O4<sup>ii</sup></b>               | <b>70.42 (15)</b>  | <b>O4<sup>ii</sup>—Eu1—O2<sup>iii</sup></b>  | <b>80.73 (13)</b>  |
| <b>O6<sup>i</sup>—Eu1—O4<sup>ii</sup></b>   | <b>136.89 (13)</b> | <b>O1<sup>iii</sup>—Eu1—O2<sup>iii</sup></b> | <b>51.66 (13)</b>  |
| <b>O3—Eu1—O4<sup>ii</sup></b>               | <b>112.92 (13)</b> | <b>O7<sup>iv</sup>—Eu1—O2<sup>iii</sup></b>  | <b>122.68 (13)</b> |
| <b>O5—Eu1—O1<sup>iii</sup></b>              | <b>73.14 (14)</b>  | <b>O5—Eu1—O4</b>                             | <b>128.75 (14)</b> |
| <b>O9—Eu1—O1<sup>iii</sup></b>              | <b>129.70 (17)</b> | <b>O9—Eu1—O4</b>                             | <b>76.89 (16)</b>  |
| <b>O6<sup>i</sup>—Eu1—O1<sup>iii</sup></b>  | <b>142.12 (14)</b> | <b>O6<sup>i</sup>—Eu1—O4</b>                 | <b>102.25 (13)</b> |
| <b>O3—Eu1—O1<sup>iii</sup></b>              | <b>123.14 (13)</b> | <b>O3—Eu1—O4</b>                             | <b>51.59 (12)</b>  |
| <b>O4<sup>ii</sup>—Eu1—O1<sup>iii</sup></b> | <b>73.08 (13)</b>  | <b>O4<sup>ii</sup>—Eu1—O4</b>                | <b>62.37 (15)</b>  |
| <b>O5—Eu1—O7<sup>iv</sup></b>               | <b>88.28 (15)</b>  | <b>O1<sup>iii</sup>—Eu1—O4</b>               | <b>114.30 (13)</b> |
| <b>O9—Eu1—O7<sup>iv</sup></b>               | <b>73.42 (17)</b>  | <b>O7<sup>iv</sup>—Eu1—O4</b>                | <b>142.95 (14)</b> |
| <b>O6<sup>i</sup>—Eu1—O7<sup>iv</sup></b>   | <b>85.97 (14)</b>  | <b>O2<sup>iii</sup>—Eu1—O4</b>               | <b>74.72 (13)</b>  |

**Symmetry code(s): (i)  $-x+1, -y+1, -z+1$ ; (ii)  $-x, -y+1, -z+2$ ; (iii)  $-x+1, -y+1, -z+2$ ; (iv)  $-x, -y+2, -z+1$ .**