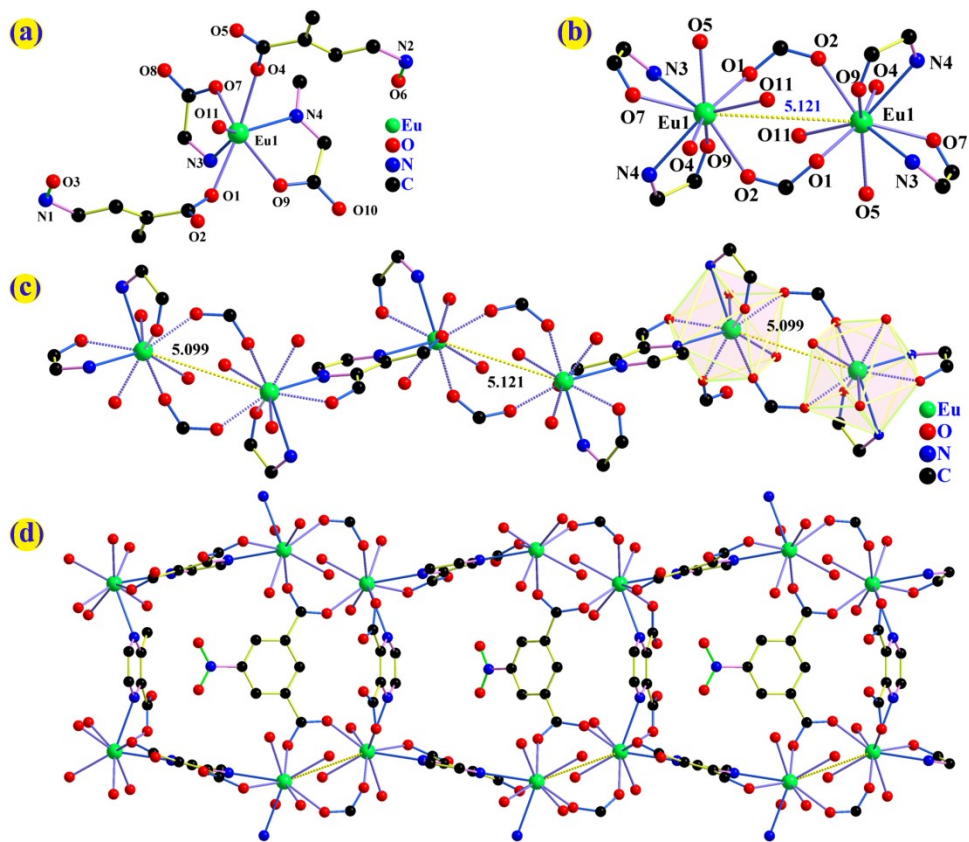


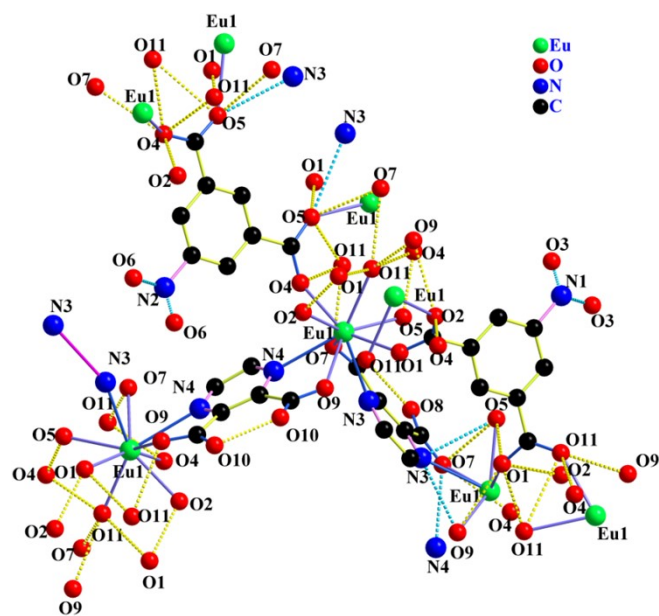
## Table of Contents

### CONTENTS

1. X-Ray Crystal structures of **Cj-3** (S1-S2)
2. FTIR spectrum of **Cj-3** (S3)
3. Experimental and simulated PXRD Patterns of **Cj-3** and recycled samples of **Cj-3** (S4)
4. Emission spectra of H<sub>2</sub>NITA and H<sub>2</sub>Pyzdc (S5)
5. Emission spectra of **Cj-3** in different solvents (S6)
6. Effect of pH on the emission spectra of **Cj-3** (S7)
7. PXRD response of **Cj-3** at different pH (2-8) (S8)
8. Recyclability of **Cj-3** after four cycles of sensing for *p*-NA and *o*-NA (S9)
9. Energy profile diagram of the 2, 3 Pyzdc ligand and NACs with calculated HOMO and LUMO energies by DFT. (S10)
10. UV-Vis Absorption spectra of metals ions (S11)
11. Variation in luminescence intensity of **Cj-3** upon incremental addition of Cr<sup>3+</sup> ions dispersed in aqueous solutions with 1M HCl (0 μl -100 μl) (S12)
12. Variation in luminescence intensity of **Cj-3** upon incremental addition of Hg<sup>2+</sup> ions dispersed in aqueous solutions with 1M HCl (0 μl -100 μl) (S13)
13. Crystallographic Information (Tables S1-S4)



**Figure S1.** Crystal structure of Cj-3: (a) asymmetric unit; (b) dinuclear  $\text{Eu}_2\text{N}_2\text{O}_{14}$  SBU; (c) representation of zig-zag rod shaped linear extension of paddle shaped SBU; (d) 2D extension of SBUs.



**Figure S2.** Hydrogen bonding positions in Cj-3

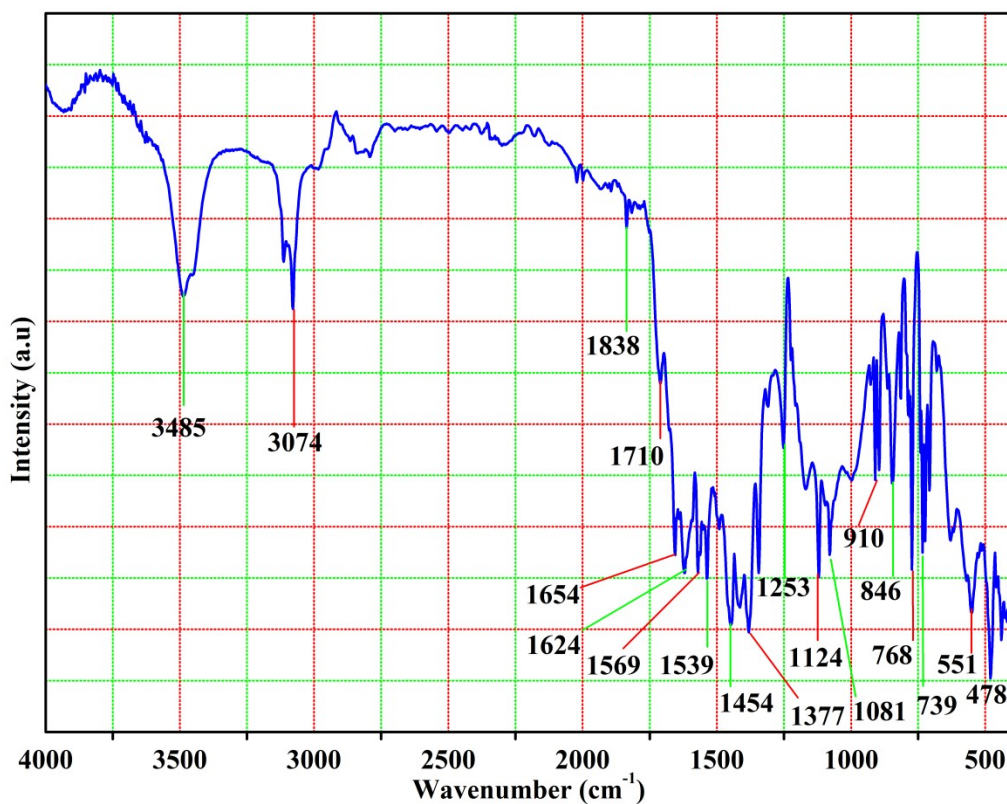


Figure S3. FTIR spectrum of Cj-3.

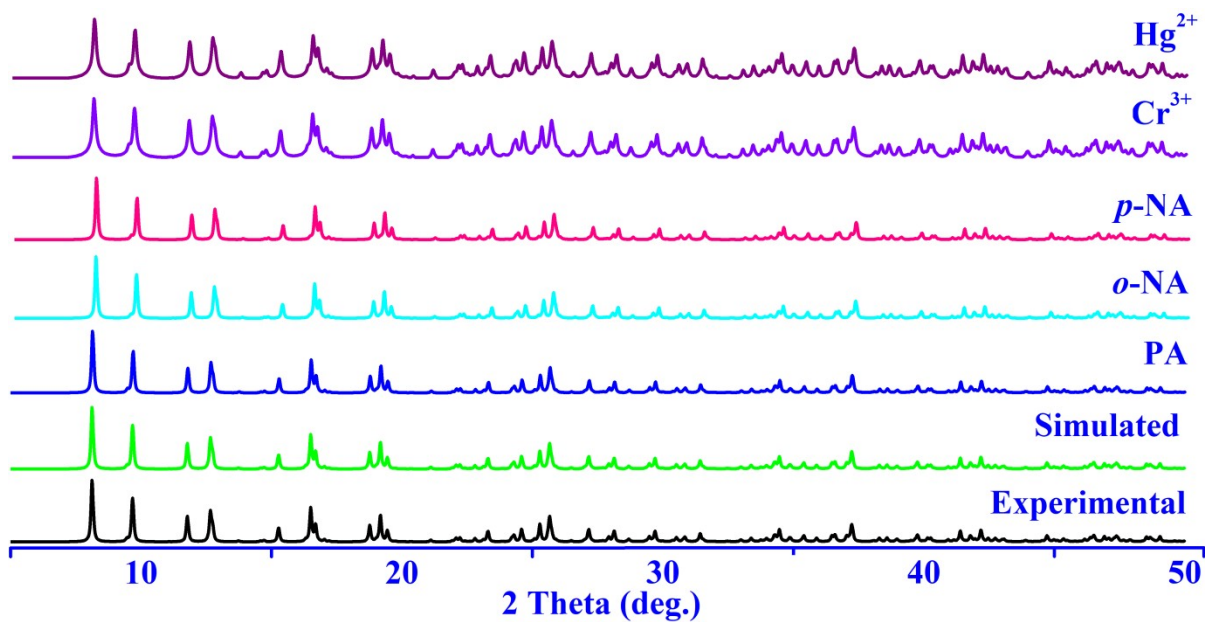
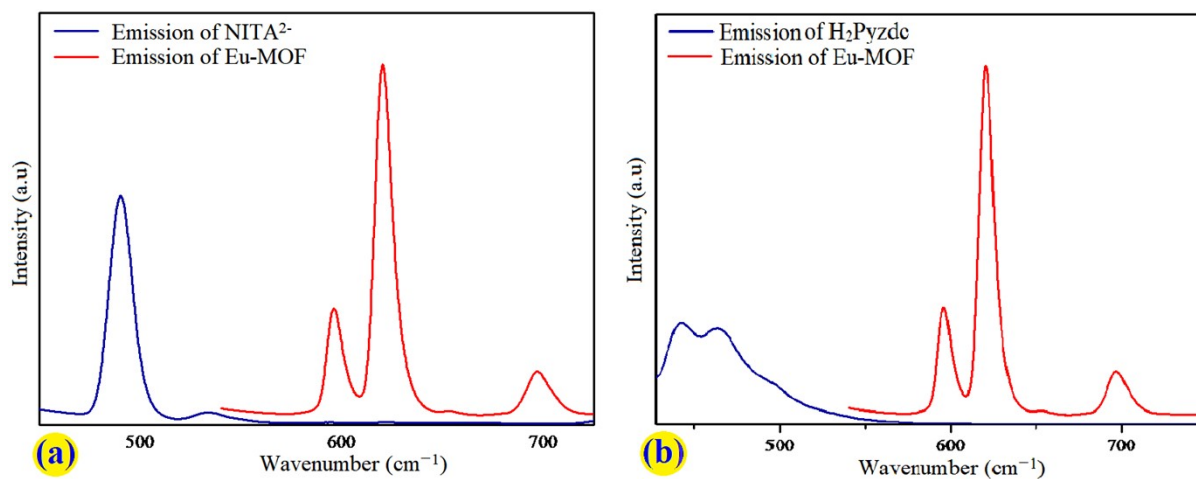
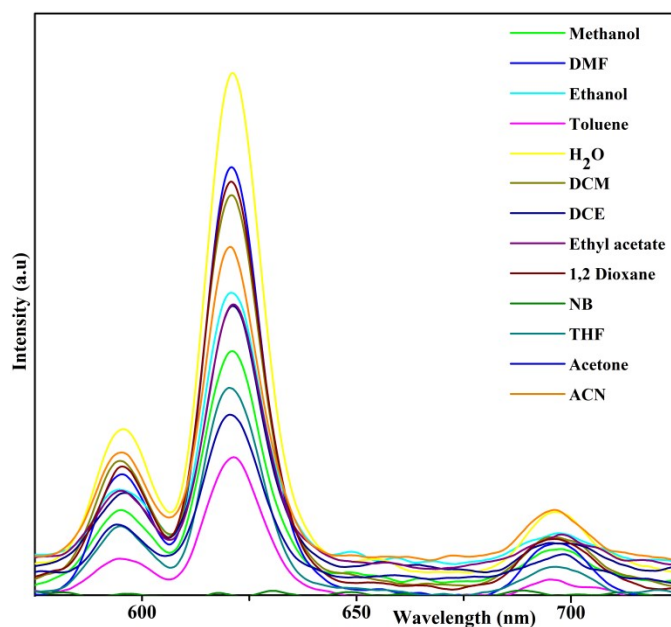


Figure S4. Experimental and simulated PXRD Patterns of Cj-3, along with the PXRD response of recycled Cj-3 after addition of PA, *p*-NA, *o*-NA, Hg<sup>2+</sup> and Cr<sup>3+</sup>.



**Figure S5.** Emission spectra of Eu-MOF and ligands; (a) Nitroisophthalic acid and (b) 2,3 Pyrazine dicarboxylic acid.



**Figure S6.** Emission spectra of Cj-3 in different solvents.

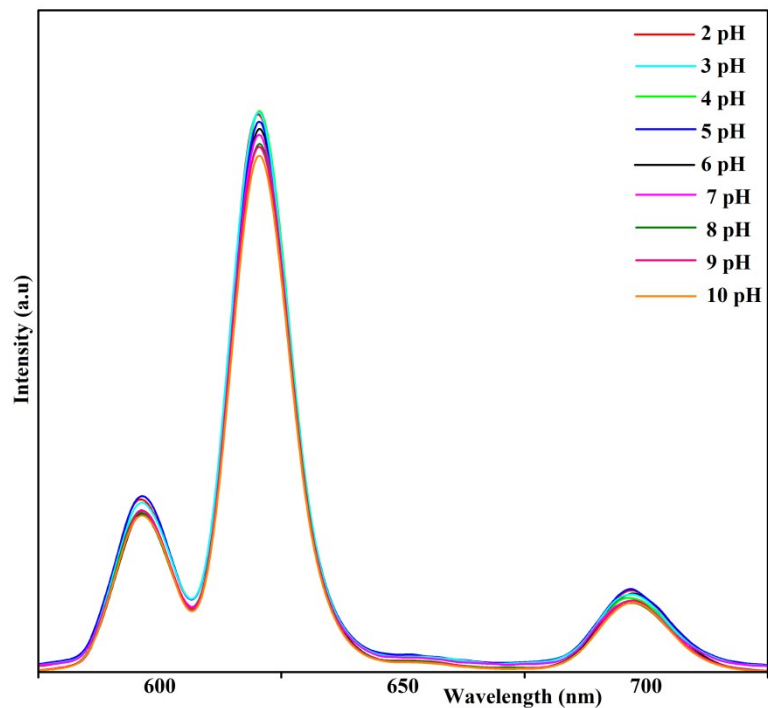


Figure S7. Effect of pH on the emission spectra of Cj-3

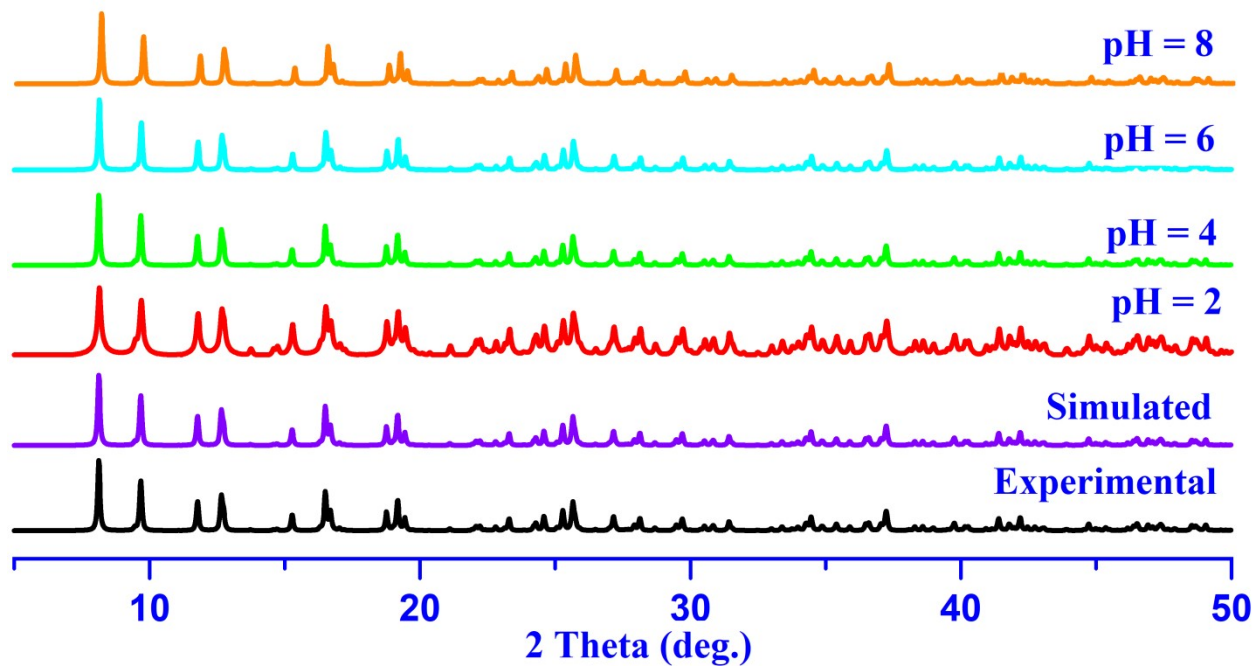
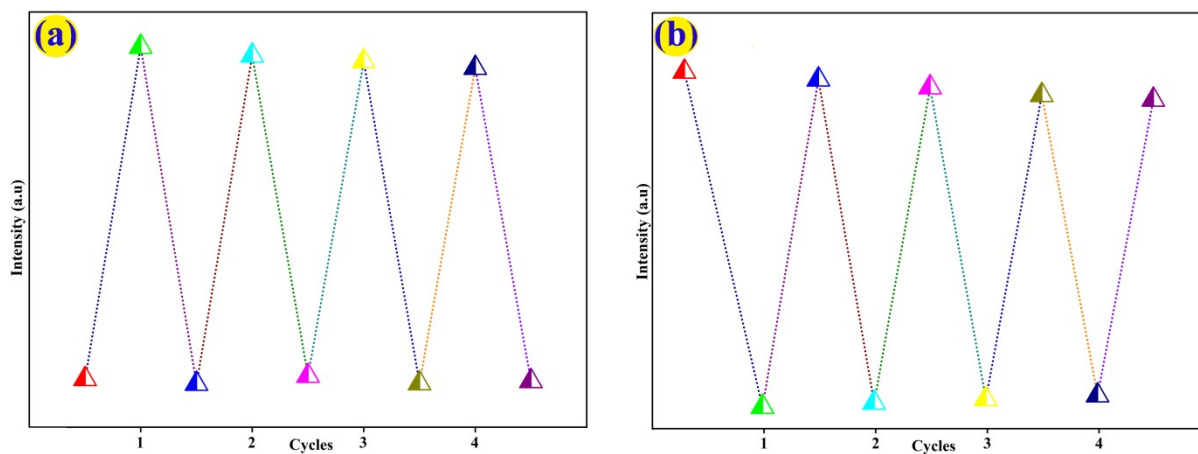
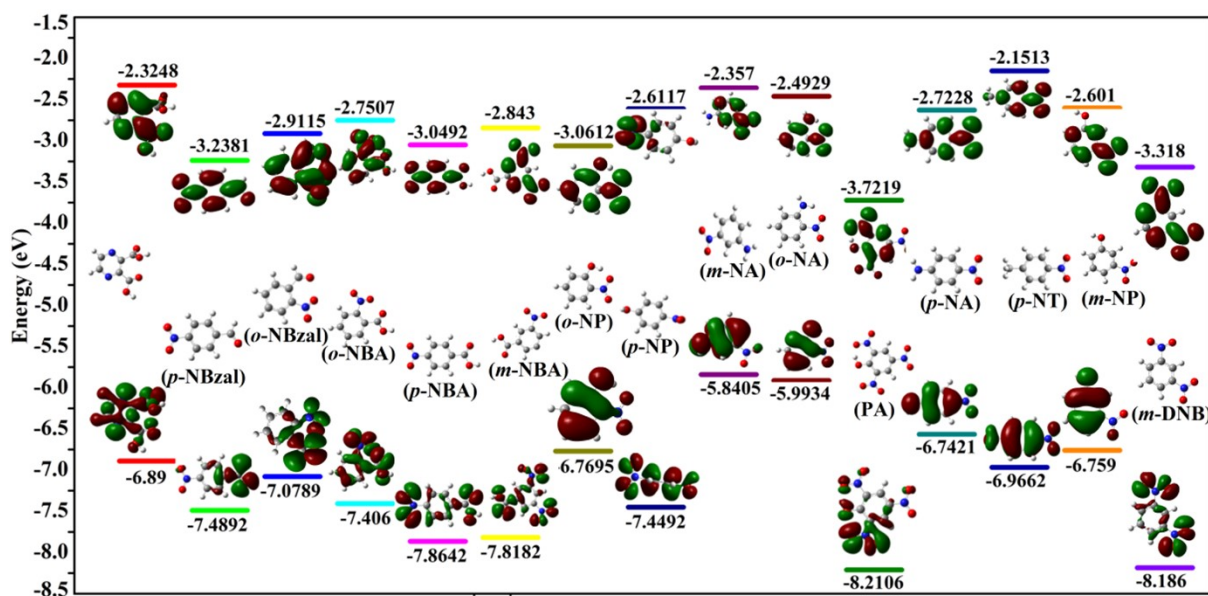


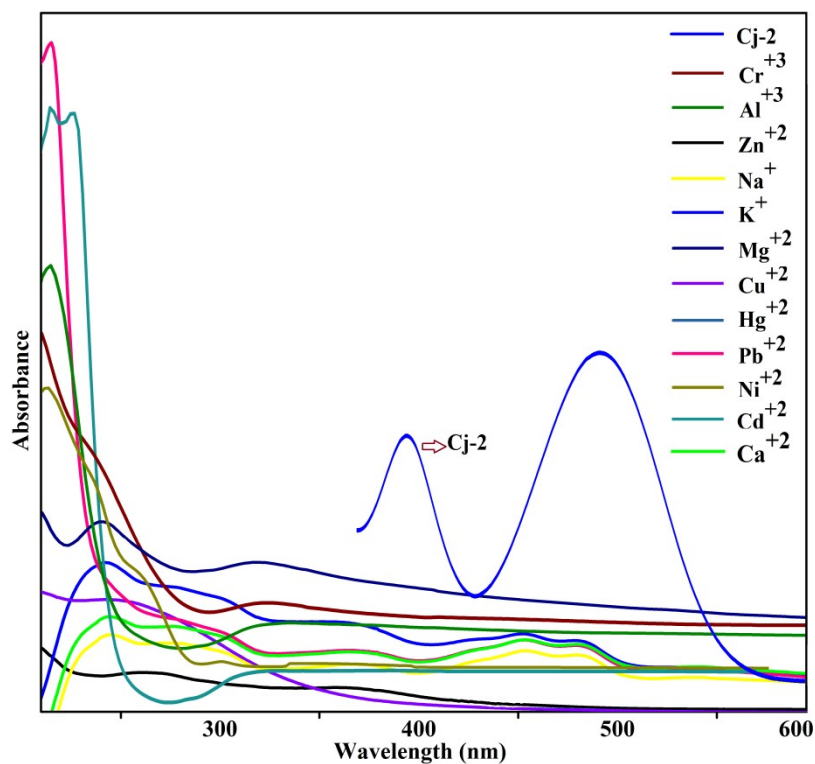
Figure S8. PXRD response of Cj-3 at different pH (2-8)



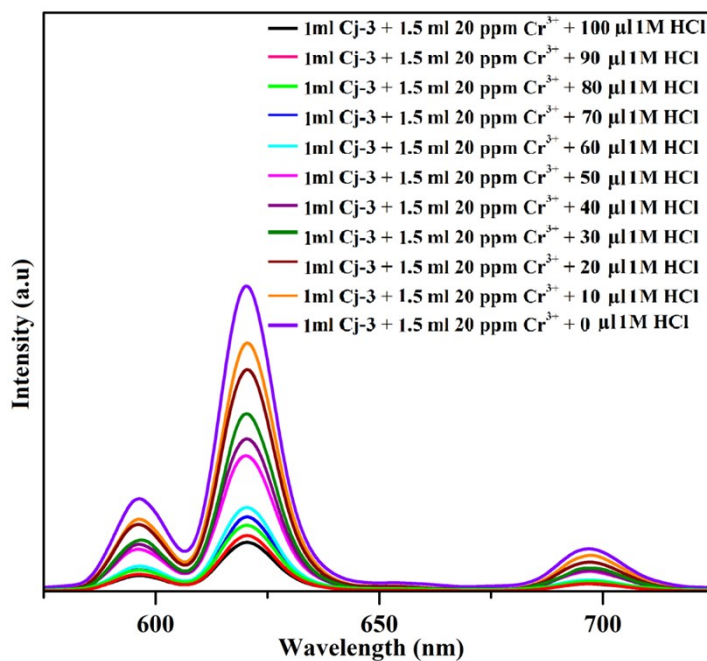
**Figure S9:** Recyclability of Cj-3 after four cycles of sensing for *p*-NA and *o*-NA



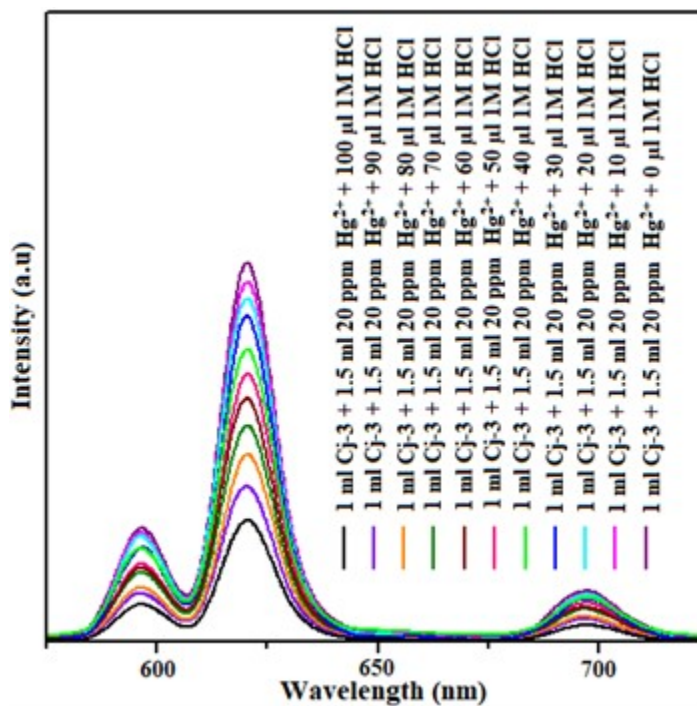
**Figure S10:** Energy profile diagram of the 2, 3 Pyzdc ligand and NACs with calculated HOMO and LUMO energies by DFT.



**Figure S11.** UV-Vis Absorption spectra of different metals ions and excitation spectra of Cj-3



**Figure S12.** Variation in luminescence intensity of Cj-3 upon incremental addition of Cr<sup>3+</sup> ions dispersed in aqueous solutions with 1M HCl (0 μl -100 μl).



**Figure S13.** Variation in luminescence intensity of **Cj-3** upon incremental addition of  $\text{Hg}^{2+}$  ions dispersed in aqueous solutions with 1M HCl (0  $\mu\text{l}$  -100  $\mu\text{l}$ ).



## Crystallographic Information (Tables)

**Table S1: Crystal data for Cj-3**

Crystal data	Cj-3
Empirical formula	$C_{14}H_8EuN_3O_{11}$
CCDC	2356631
Formula weight	546.20
Crystal system space group	orthorhombic Pbcm
Temperature (K)	293
$a$ (Å) $b$ (Å) $c$ (Å)	7.9885(4) 21.6907(12) 18.2297(10)
$\alpha$ (deg°) $\beta$ ( deg °) $\gamma$ ( deg °)	90 90 90
Volume (Å <sup>3</sup> )	33158.8(3)
$Z$	8
Radiation type	Mo K $\alpha$ ( $\lambda = 0.71073$ )
$\mu$ (mm <sup>-1</sup> )	14.048
Crystal size (mm <sup>3</sup> )	3.037 × 0.21 × 0.14
$T_{\min}$ , $T_{\max}$	0.300, 1.000
Reflections collected	27445
$R_{\text{int}}$	0.1207
Data/restraints/parameters	2859/0/272
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , $S$	0.0400, 0.0977, 1.05
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> ) Goodness-of-fit on $F^2$ F(000)	1.76, -2.01 1.052 2113.2

**Table S2: Hydrogen-bond geometry (Å, °) for Cj-3**

Type	Donor --- H...Acceptor	D - H	H...A	D...A	D - H...A
Intra	O8-H8 ...O8 <sup>i</sup>	0.82	1.58	2.399(5)	176
Intra	O11-H11A...O4 <sup>ii</sup>	0.85	2.12	2.919(4)	157
Intra	O11-H11A...O5 <sup>ii</sup>	0.85	2.52	2.863(5)	105
Intra	O11-H11A...O7 <sup>ii</sup>	0.85	2.4	2.868(5)	115
Intra	O11-H11B...O2	0.85	2.53	3.310(4)	153
Intra	O11-H11B...O1 <sup>iii</sup>	0.85	2.47	2.786(4)	103
Intra	O11-H11B...O9 <sup>iii</sup>	0.85	2.25	2.944(5)	139
	C13-H13...O8 <sup>iv</sup>	0.93	2.52	3.364(6)	150
Intra	C13-H13...O9	0.93	2.36	2.931(6)	120
Intra	C16-H16...O7	0.93	2.43	2.936(6)	114
	C16-H16...O10 <sup>v</sup>	0.93	2.54	3.377(6)	150

Symmetry code(s): (i)  $x, y, 3/2-z$  (ii)  $1-x, 1-y, 1-z$  (iii)  $-x, 1-y, 1-z$  (iv)  $-1+x, y, z$  (v)  $1+x, y, z$

**Table S3: Selected geometric parameters (Å) for Cj-3**

Eu1—O9	2.450 (3)	Eu1—O5 <sup>ii</sup>	2.417 (3)
Eu1—O11	2.425 (4)	Eu1—O1	2.380 (3)
Eu1—O4	2.358 (3)	Eu1—N3	2.635 (4)
Eu1—O2 <sup>i</sup>	2.414 (3)	Eu1—N4	2.693 (4)
Eu1—O7	2.467 (3)		

Symmetry code(s): (i)  $-x, -y+1, -z+1$ ; (ii)  $-x+1, -y+1, -z+1$ ; (iii)  $x, y, -z+1/2$ ; (iv)  $x, y, -z+3/2$ ; (v)  $x, -y+1/2, -z+1$ .

**Table S4: Selected geometric parameters (°) for Cj-3**

O11—Eu1—O9	123.70 (10)	O1—Eu1—O2 <sup>i</sup>	94.20 (11)
O4—Eu1—O9	126.72 (11)	O1—Eu1—O7	127.18 (11)
O4—Eu1—O11	76.53 (12)	O1—Eu1—O5 <sup>ii</sup>	75.03 (11)
O2 <sup>i</sup> —Eu1—O9	66.12 (11)	N3—Eu1—O9	69.67 (11)
O2 <sup>i</sup> —Eu1—O11	73.83 (12)	N3—Eu1—O11	139.19 (13)
O2 <sup>i</sup> —Eu1—O4	76.71 (13)	N3—Eu1—O4	129.84 (11)
O7—Eu1—O9	113.67 (11)	N3—Eu1—O2 <sup>i</sup>	135.53 (11)
O7—Eu1—O11	122.62 (10)	N3—Eu1—O7	60.36 (10)
O7—Eu1—O4	70.57 (11)	N3—Eu1—O5 <sup>ii</sup>	73.16 (11)
O7—Eu1—O2 <sup>i</sup>	136.90 (11)	N3—Eu1—O1	74.22 (11)
O5 <sup>ii</sup> —Eu1—O9	133.78 (10)	N4—Eu1—O9	60.12 (11)
O5 <sup>ii</sup> —Eu1—O11	72.43 (12)	N4—Eu1—O11	142.66 (14)
O5 <sup>ii</sup> —Eu1—O4	98.14 (11)	N4—Eu1—O4	75.29 (12)
O5 <sup>ii</sup> —Eu1—O2 <sup>i</sup>	146.12 (11)	N4—Eu1—O2 <sup>i</sup>	76.23 (12)
O5 <sup>ii</sup> —Eu1—O7	67.51 (11)	N4—Eu1—O7	68.98 (11)
O1—Eu1—O9	69.24 (11)	N4—Eu1—O5 <sup>ii</sup>	135.59 (12)
O1—Eu1—O11	76.27 (11)	N4—Eu1—O1	128.05 (11)
O1—Eu1—O4	152.75 (11)	N4—Eu1—N3	78.15 (13)

Symmetry code(s): (i)  $-x, -y+1, -z+1$ ; (ii)  $-x+1, -y+1, -z+1$ ; (iii)  $x, y, -z+1/2$ ; (iv)  $x, y, -z+3/2$ ; (v)  $x, -y+1/2, -z+1$ .