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# Development of a novel Cd(II) metal complex for solvent sensitive detection of Zn(II) and Mg(II) with the formation of Cd(II)-Zn(II)/Cd(II)-Mg(II) complexes and their application in effective schottky devices

Dibyendu Sathapat [a], Mainak Das[b], Manik Das[a], Uttam Kumar Das[c], Arijit Bag[d], Soumik Laha[e], Partha Pratim Roy[b], Bidhan Chandra Samanta[f], Tithi Maity[a]*

Department of Chemistry, Prabhat Kumar College, Contai, Contai, Purba Medinipur, West Bengal, India

[b] Department of Physics, Jadavpur University, Kolkata, India

[c] Department of Chemistry, School of Physical Science, Mahatma Gandhi Central University, Bihar, India.

[d]School of Natural and Applied Sciences, Maulana Abul Kalam Azad University of Technology, West Bengal, India

[e]IICB, Kolkata, West Bengal, India

[f]Mugberia Gangadhar Mahavidyalaya, Purbamedinipur, West Bengal India

Email: titlipkc2008@gmail.com

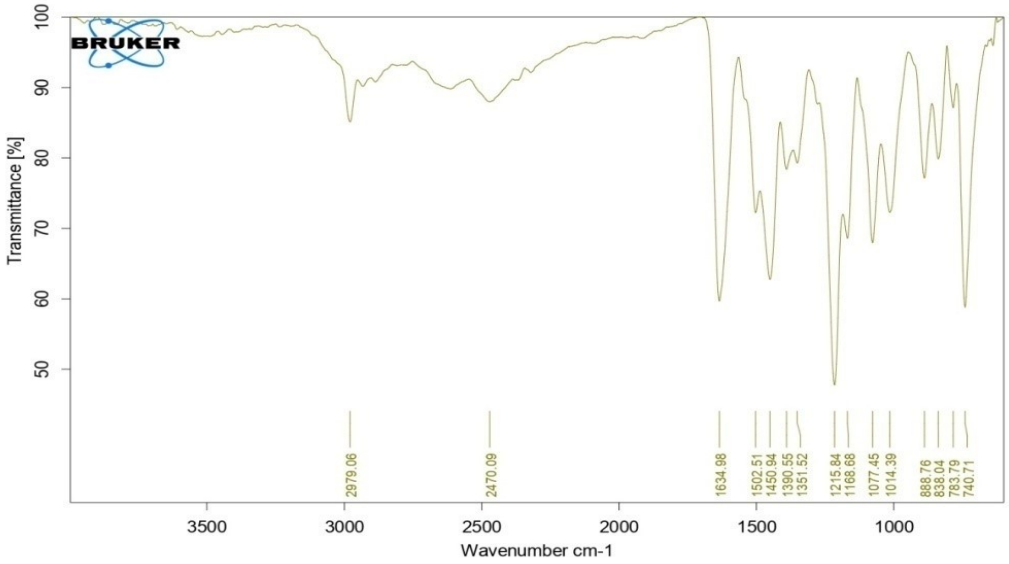


**Fig. S1**. FTIR of Complex **1**

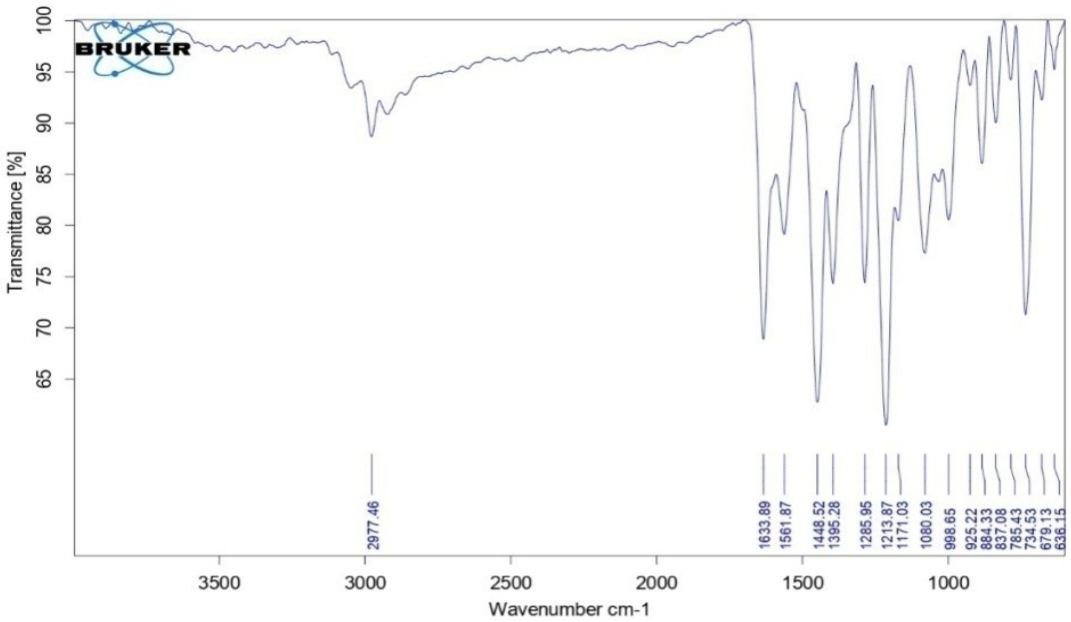


**Fig. S2**. FTIR of Complex **2**

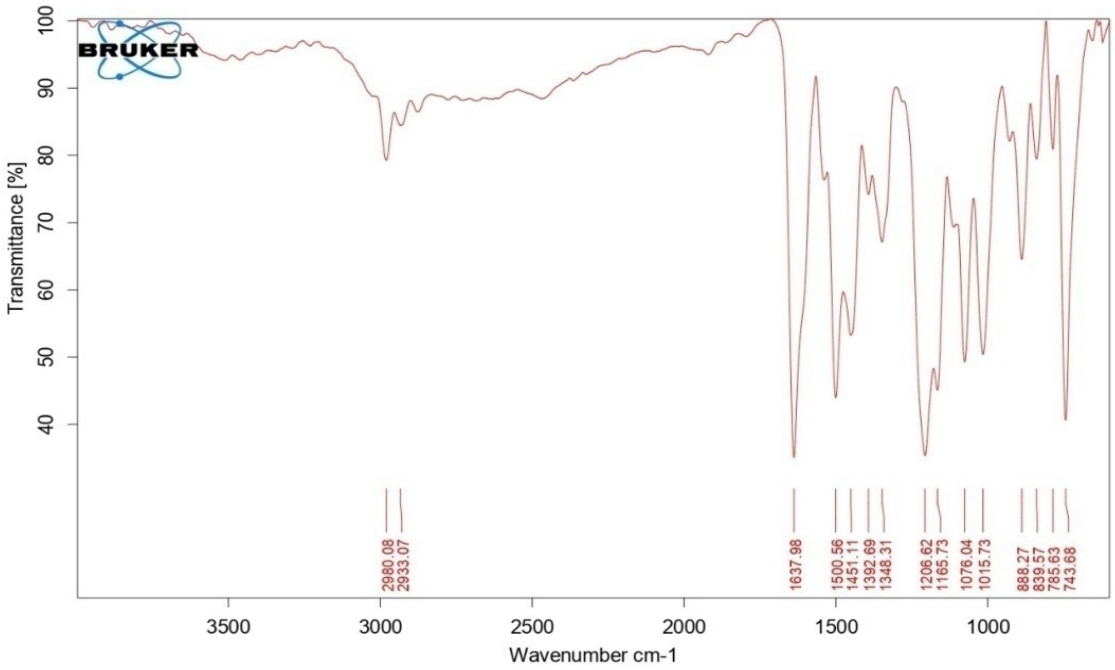


**Fig. S3**. FTIR of Complex **3**

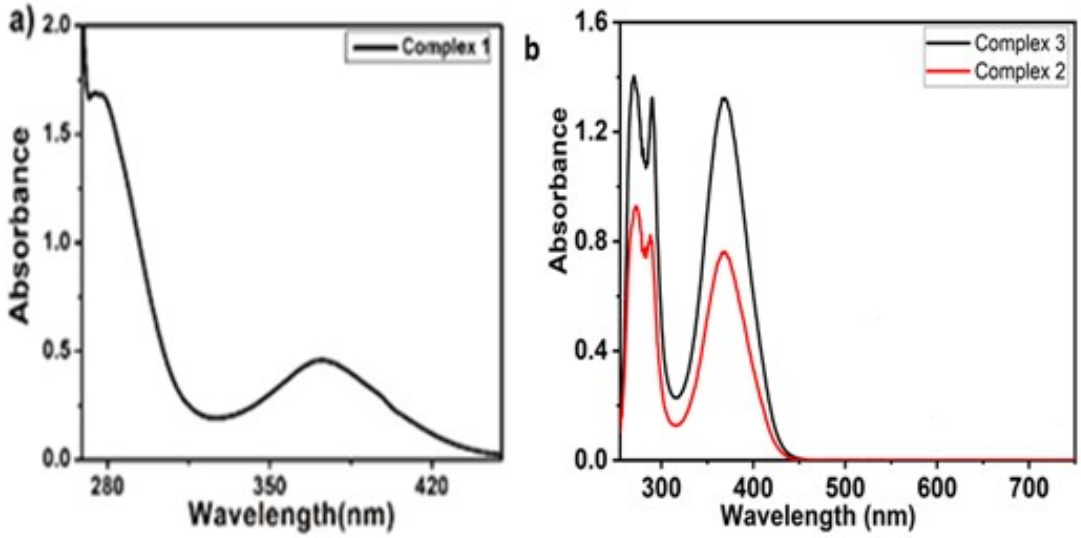


**Fig. S4**. Uv spectra of (a) Complex **1**, (b) Complex **2** and **3**

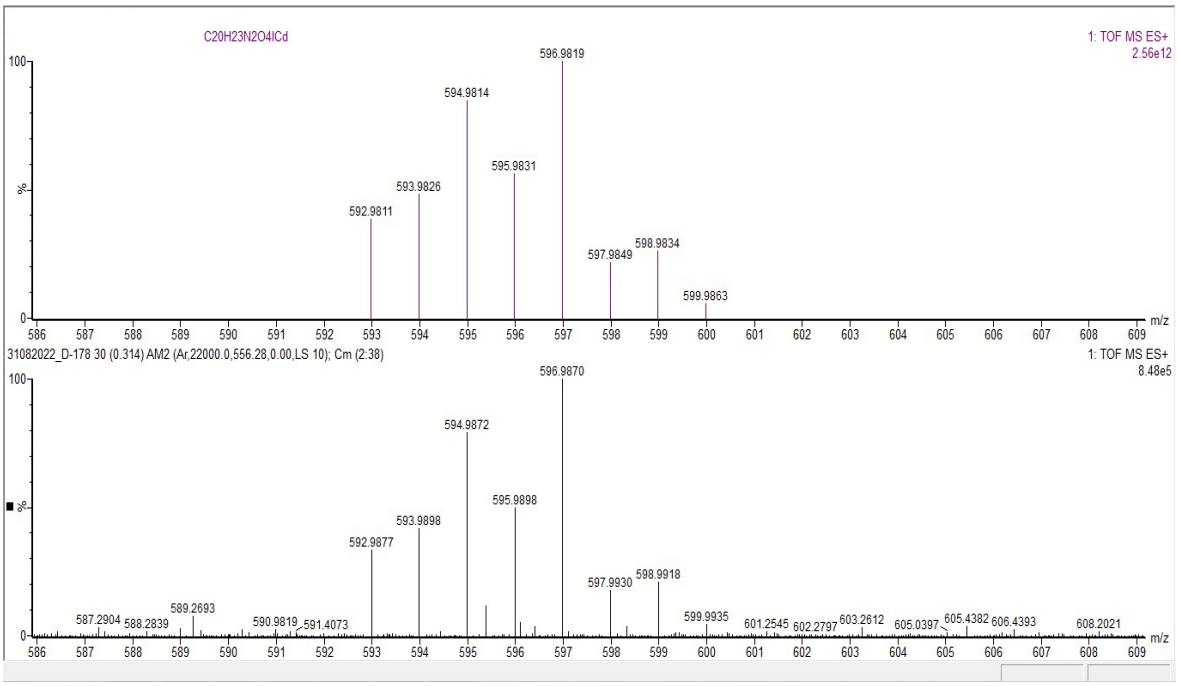


**Fig. S5**. Mass spectra of Complex **1**

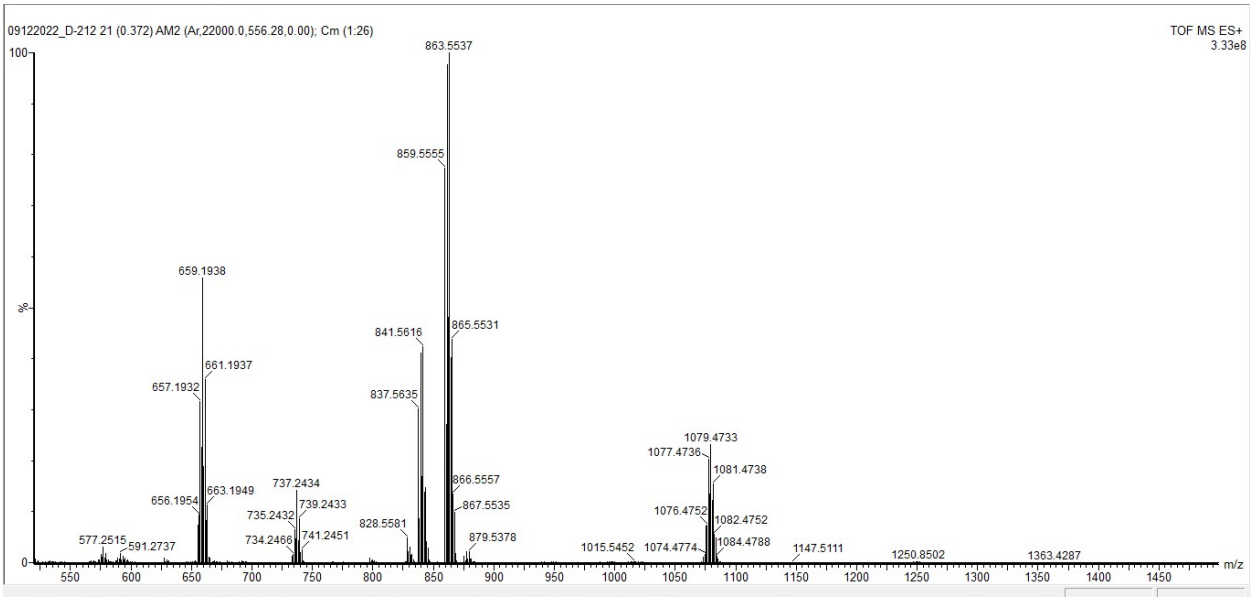


**Fig. S6**. Mass spectra of Complex **2**

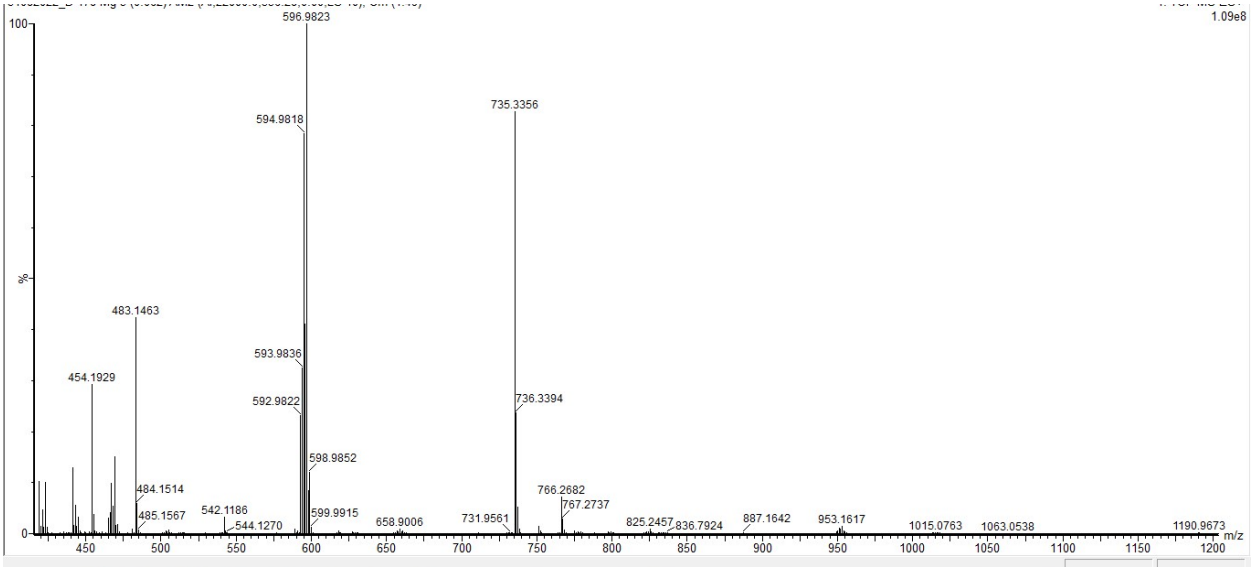


**Fig. S7**. Mass spectra of Complex **3**

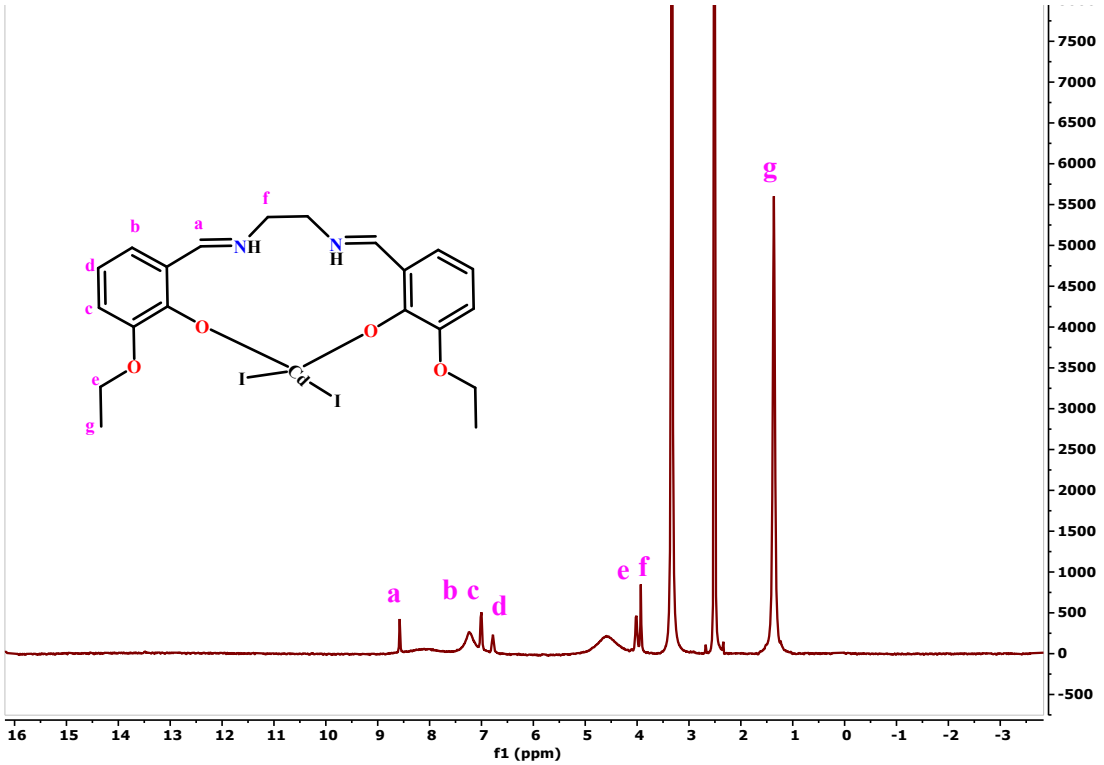


**Fig. S8:** $^{1}$H NMR spectrum of complex **1**

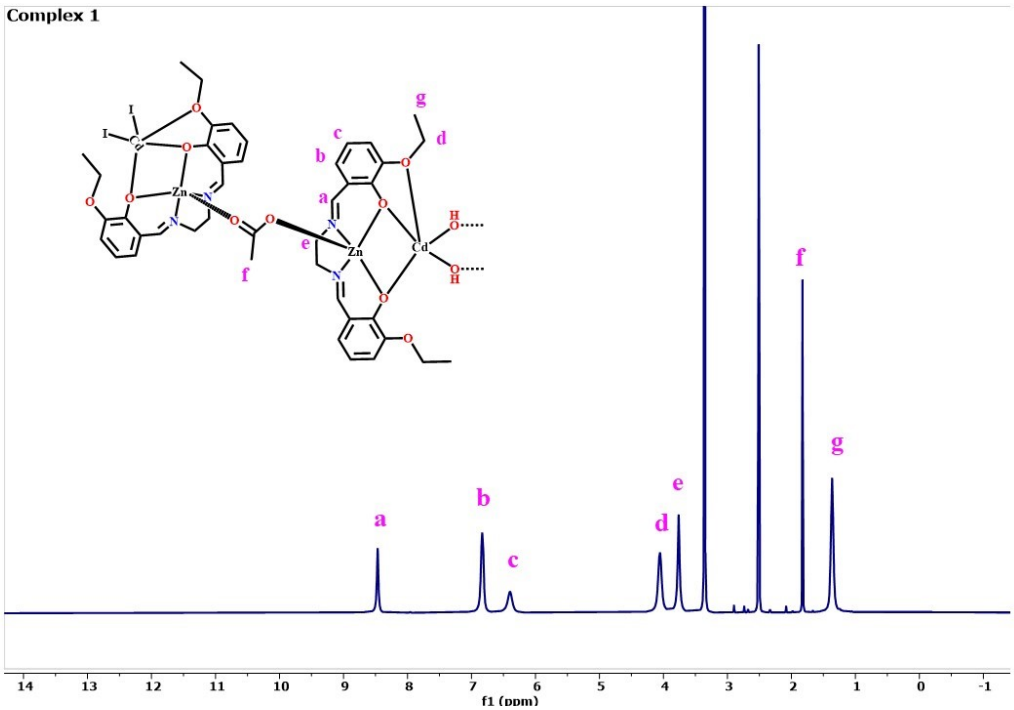


**Fig. S9:** NMR spectrum of complex **2**

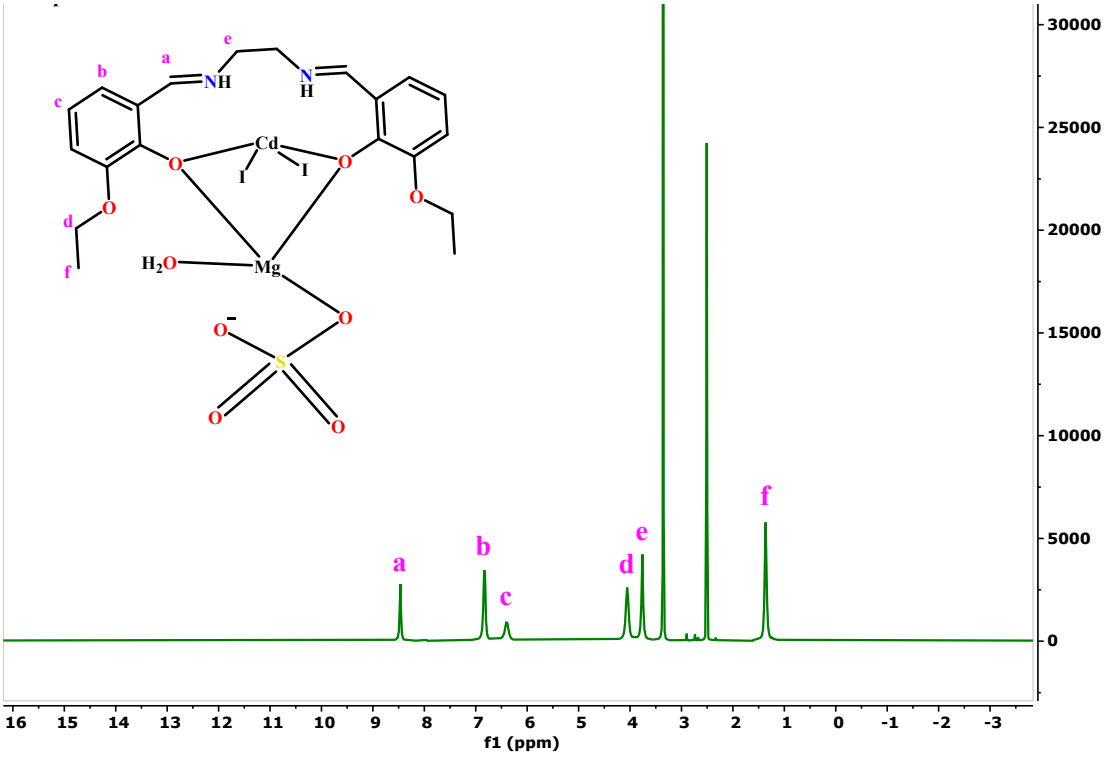


**Fig S10:** NMR spectrum of complex **3**

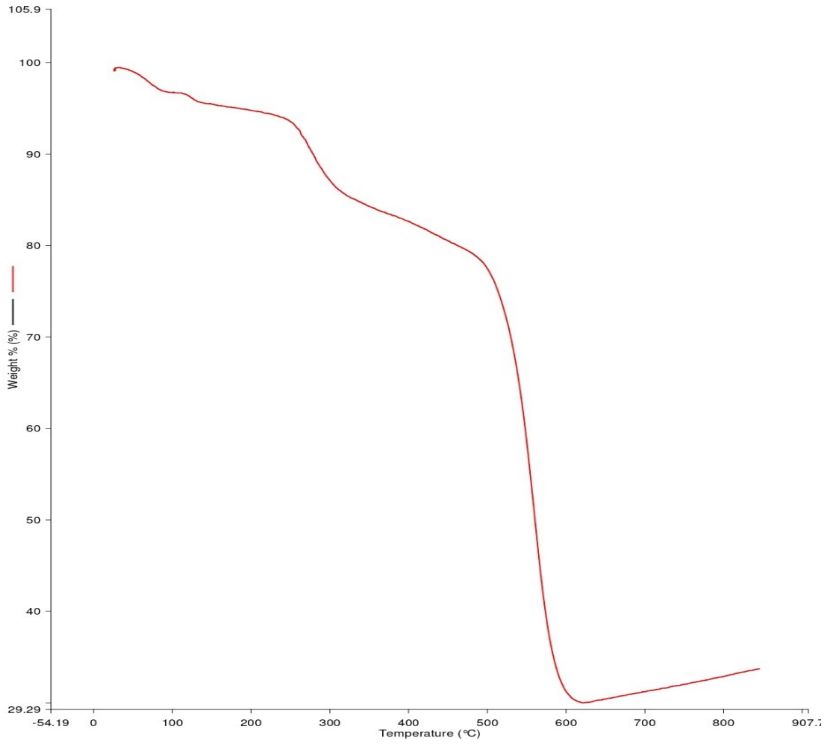


**Fig. S11:** The TGA graph for complex **2**

**TGA-DTA** plot of complex **2**
Weight loss calculation:
Monoclinic '*C* 2/c' space group, Z = 4
Therefore FW = Unitcell contents/Z
= [4 Ligand + 2 CdI2 + 6 Zn cations + 2 acetate (coordinated) + 2 oxygen atom bridged] + ~ 226 electron [SQUEEZE result]
= 2680 + (7 X 18)
= 2680 + 126 = 2806
Weight loss for 7 H2O = 126/2806
= 4.5% (experimental 4.8 %)

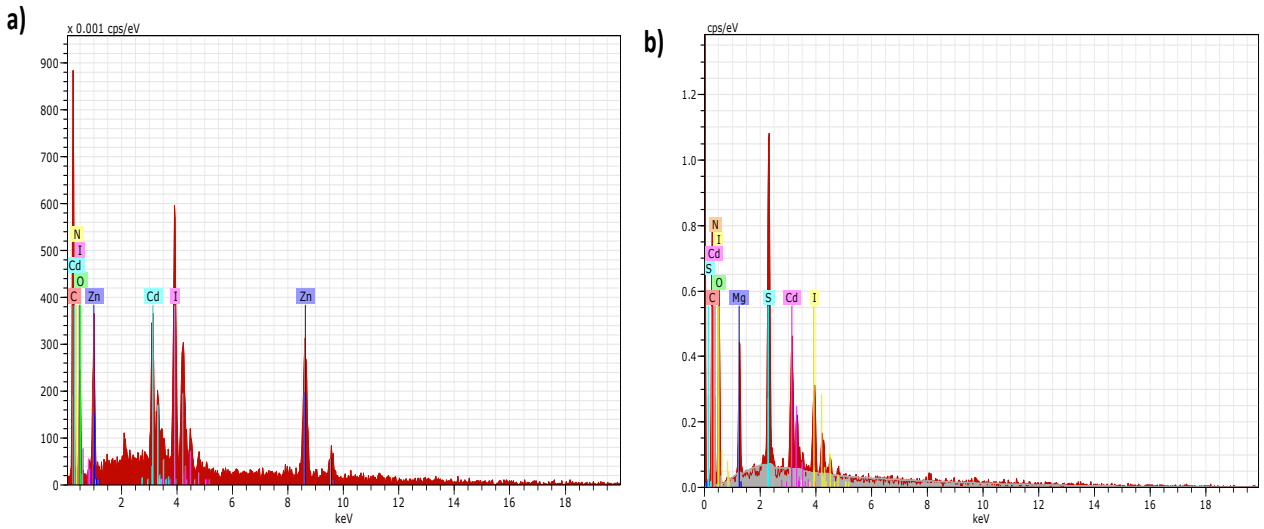


**Figure S12:** EDX result of a) complex **2** b) complex **3**

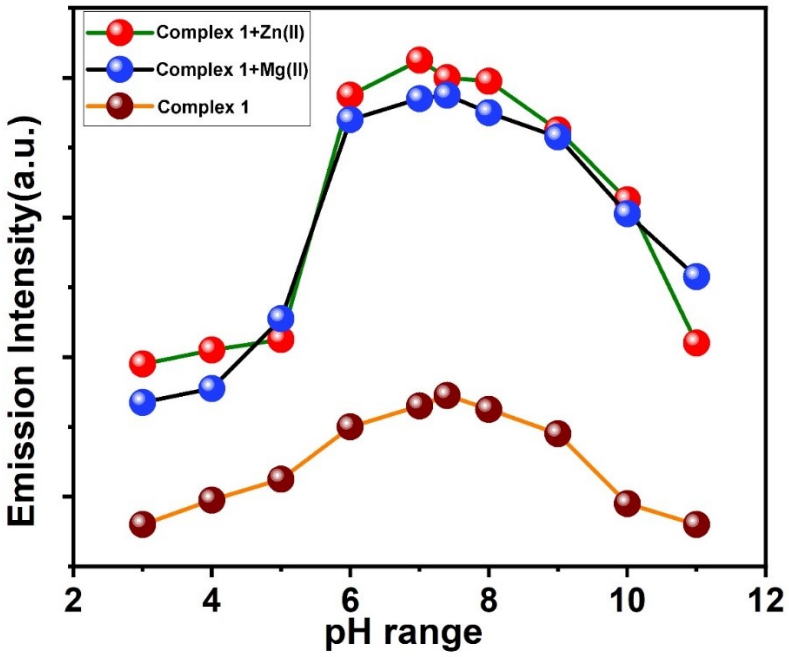


**Figure. S13**. Change of Emission Intensity of the complex **1, 2, 3** with the variation of pH

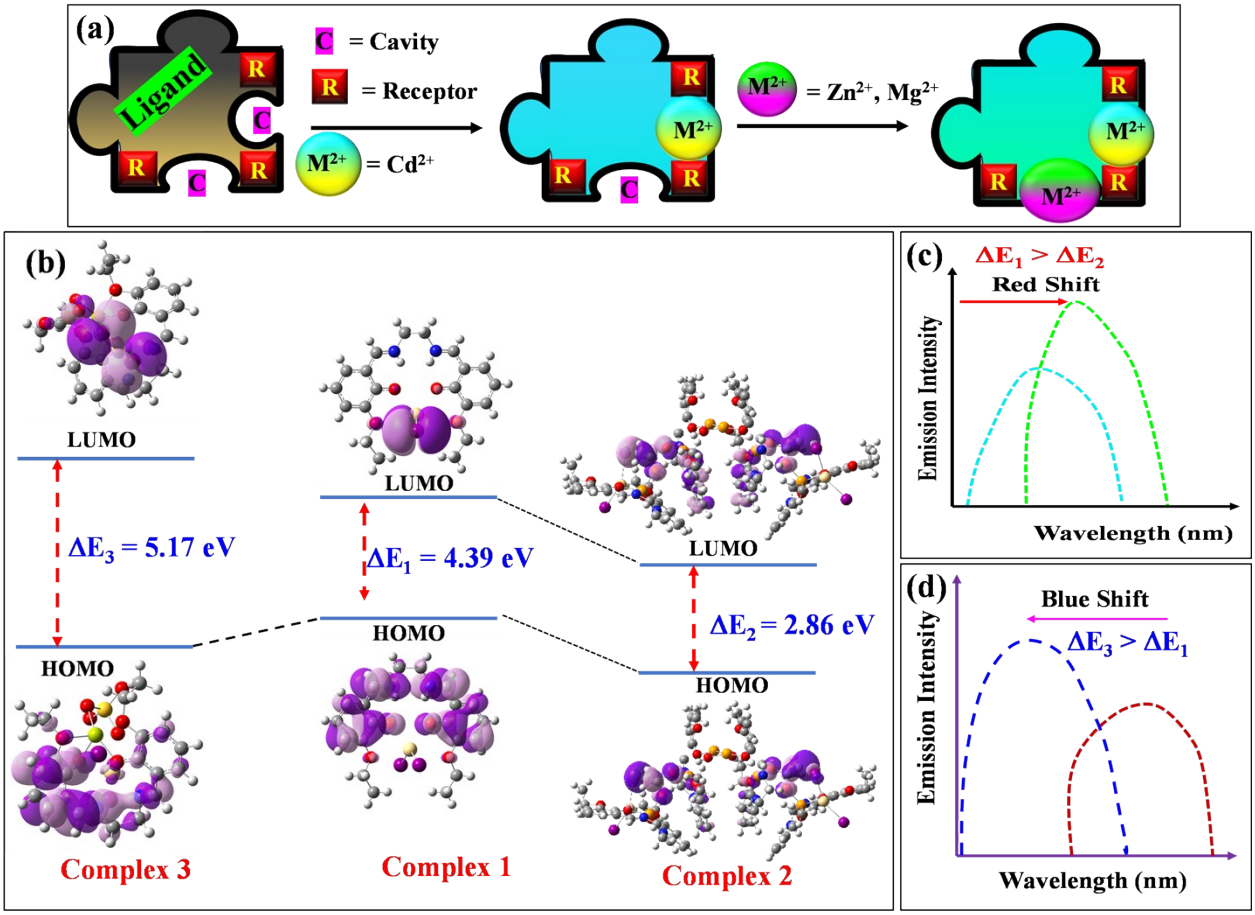


**Fig S14:** Schematic presentation of the mechanism of sensing phenomena of complex 1 towards Zn(II) and Mg(II).

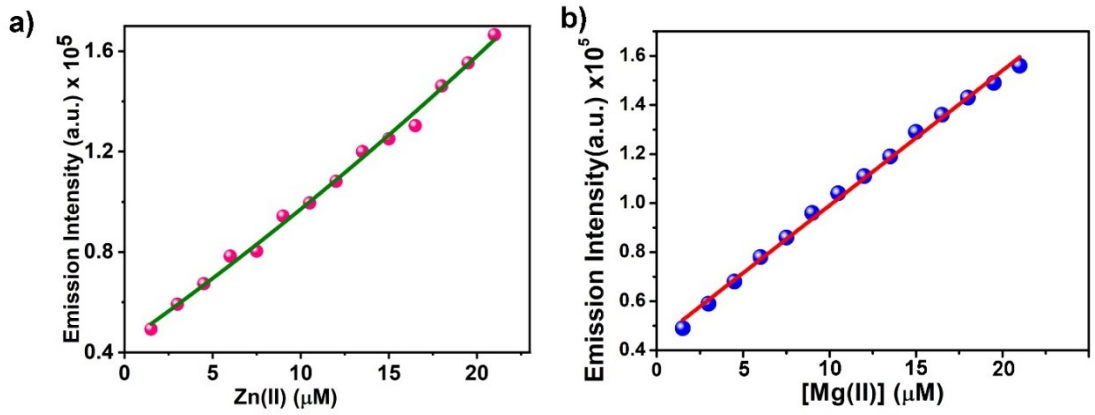


**Fig. S15:.** Change of Fluorescence intensity of complex **1** ($3\times10^{-6}$ M) by varying the concentration of (a) Zn(II) ($1.0 – 25\times10^{-6}$ M) in 9:1 ethanol-water medium and (b) Mg(II) ($1.0 – 25 \times 10^{-6}$ M) in pure HEPES buffer solution for LOD calculation purpose.

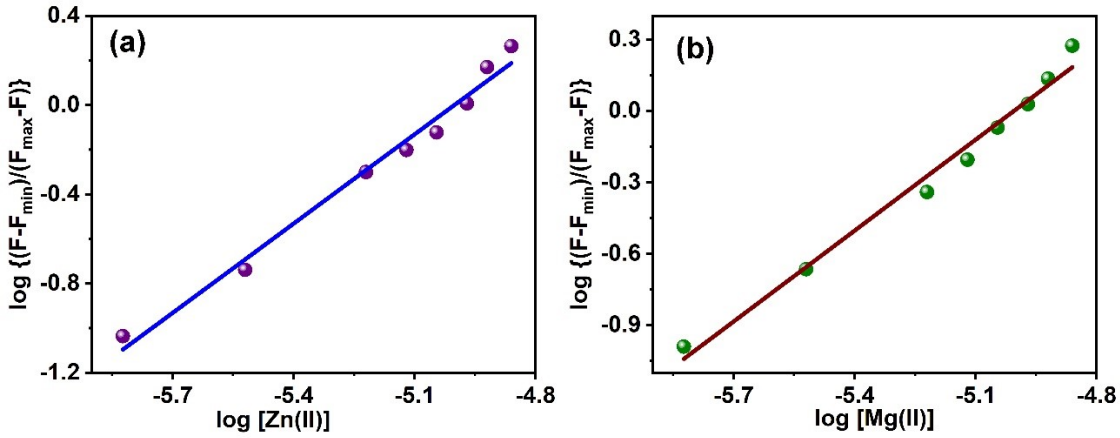


**Fig. S16:** Determination of Binding constant of (a) Complex **1** – Zn(II) and (b) Complex **1** – Mg(II) from Fluorescence titration results

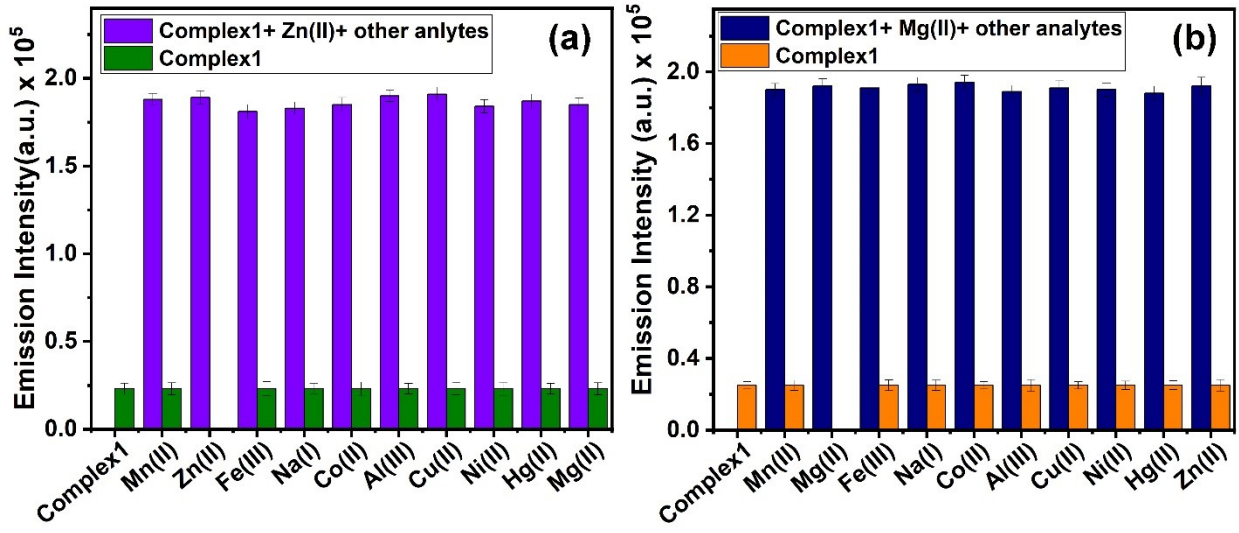


**Fig. S17:** Change of emission intensity of (a) complex**1** – Zn(II) and (b) Complex**1** – Mg(II) after the addition of several competitive metal ions.

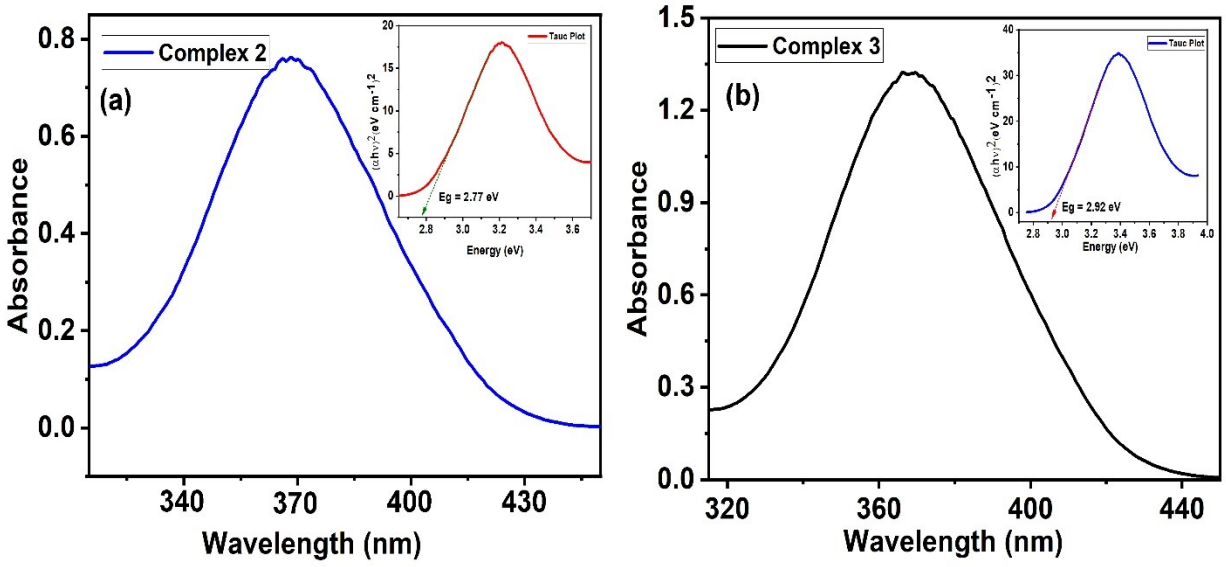


**Fig S18:** The band gap values for a) complex **2** b) complex **3** by using Tauc plot

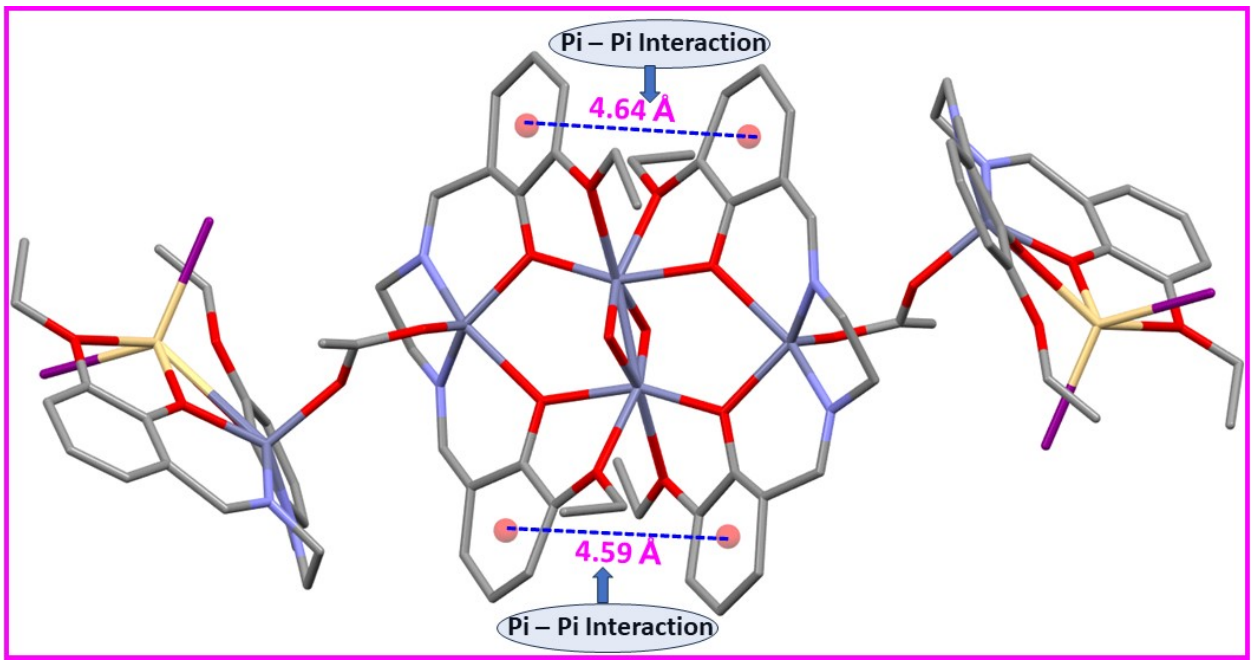


**Fig. S19:** Intramolecular **π-π** interaction in complex **2**

**Table S1:** Intra-molecular Hydrogen bonding parameter of complex **1**

| D─H•••A | D─H (Å) | H•••A (Å) | D•••A (Å) | D─H•••A (°) | Symmetry operation for A |
|---|---|---|---|---|---|
| N(1)─H(1)•••O2 | 0.900(19) | 1.81(3) | 2.565(3) | 139(3) | x, y, z |

**Table S2: C-H••• I** interaction parameter of complex **2**

| C─H•••I | C─H (Å) | H•••I (Å) | C•••I (Å) | C─H•••I (°) | Symmetry operation for A |
|---|---|---|---|---|---|
| C(19)─H(19)•••I2 | 0.9500 | 3.149 | 3.994 | 148.85 | -x+1, -y+2, -z+1 |

**Table S3:** Crystal parameters of complex **1** and **2**

| **Crystal parameters** | **Complex 1** | **Complex 2** |
|---|---|---|
| CCDC No. | 2246285 | 2246286 |
| Empirical formula | $C_{20}H_{24}N_2O_4I_2Cd$ | $C_{82.99}\ H_{95.81}\ Cd_2\ I_4\ N_8\ O_{22}\ Zn_6$ |
| Formula weight | 722.61 | 2681.93 |
| Crystal size/mm | 0.14 X 0.09 X 0.04 | 0.095 X 0.059 X 0.032 |
| Crystal system | Monoclinic | Monoclinic |
| Space group | *'P 2/n'* | *'C 2/*c *'* |
| a /Å | 8.6378(19) | 37.556(4) |
| b/Å | 11.746(3) | 12.9596(14) |
| c /Å | 11.427(3) | 27.018(3) |
| $\alpha/^0$ | 90 | 90 |
| $\beta/^0$ | 92.577(11) | 125.815(3) |

| | | |
|---|---|---|
| $\gamma/^0$ | 90 | 90 |
| Volume/Å$^3$ | 1158.2(4) | 10663.5(19) |
| Z | 2 | 4 |
| $D_{calc}$ /gcm$^{-3}$ | 2.072 | 1.669 |
| F(000) | 688 | 5247 |
| μ MoKα /mm$^{-1}$ | 3.636 | 2.938 |
| Temperature/K | 296(2) | 148.53 |
| $R_{int}$ | 0.0290 | 0.1179 |
| Range of h, k, l | -11/11, -16/14, -15/15 | -42/53, -18/17, -38/31 |
| θmin/max/° | 2.488/29.423 | 2.189/30.465 |
| Reflections collected/unique/observed [I>2σ(I)] | 14233/3200/2631 | 64906/15869/7654 |
| Data/restraints/ parameters | 3200/1/137 | 15869/0/636 |
| Goodness of fit on $F^2$ | 1.093 | 1.038 |
| Final R indices [I>2σ(I)] | $R_1$ = 0.0273 | $R_1$ = 0.1379 |
| | $wR_2$ = 0.0396 | $wR_2$ = 0.2328 |
| R indices (all data) | $R_1$ = 0.0493 | $R_1$ = 0.3471 |
| | $wR_2$ = 0.0547 | $wR_2$ = 0.4195 |