

# Supplementary Materials: Photoluminescent Coordination Polymers based on Group 12 Metals and 1H-Indazole-6-Carboxylic Acid

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### 1. Selected bond lengths and angles data.

**Table S1.** Selected bond lengths (Å) and angles (°) for complexes **1** and **2**.

Complex	1	2
M(1)···N(1)	1.984(6)	
M(1)···N(2)	1.969(7)	
M(1)···N(2A)		2.293(3)
M(1)···N(2D)		2.329(3)
M(1)···O(1)	1.935(6)	
M(1)···O(1W)	2.019(6)	
M(1)···O(2A)		2.332(2)
M(1)···O(1B)		2.374(2)
M(1)···O(1C)		2.346(2)
M(1)···O(1D)		2.258(2)
M(1)···O(2D)		2.358(2)
M(2)···N(2B)		2.332(3)
M(2)···N(2C)		2.316(3)
M(2)···O(1A)		2.320(2)
M(2)···O(1B)		2.419(3)
M(2)···O(1C)		2.349(3)
M(2)···O(1D)		2.258(2)

Complex	1	2
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N(1)-M(1)-N(2)	113.1(3)	
N(1)-M(1)-O(1)	107.7(2)	
N(1)-M(1)-O(1W)	101.0(3)	
N(2)-M(1)-O(1)	128.7(3)	
N(2)-M(1)-O(1W)	103.8(2)	
N(2A)-M(1)-N(2D)		173.40(10)
N(2B)-M(2)-N(2C)		170.76(10)
O(1)-M(1)-O(1W)	97.3(2)	
N(2A)-M(1)-O(2A)		90.31(9)
N(2A)-M(1)-O(1B)		95.49(9)
N(2A)-M(1)-O(1C)		78.08(9)
N(2A)-M(1)-O(2D)		103.31(9)
N(2D)-M(1)-O(2A)		83.09(9)
N(2D)-M(1)-O(1B)		85.83(9)
N(2D)-M(1)-O(1C)		102.89(9)
N(2D)-M(1)-O(2D)		83.16(9)
N(2B)-M(2)-O(1A)		79.11(9)
N(2B)-M(2)-O(1B)		91.68(9)
N(2B)-M(2)-O(2C)		98.75(9)
N(2B)-M(2)-O(1D)		108.91(9)
N(2C)-M(2)-O(1A)		92.24(9)
N(2C)-M(2)-O(1B)		91.41(9)
N(2C)-M(2)-O(2C)		78.08(9)
N(2C)-M(2)-O(1D)		79.57(9)
O(1C)-M(1)-O(1B)		158.86(9)
O(1C)-M(1)-O(2D)		73.64(8)
O(2A)-M(1)-O(1B)		101.09(8)
O(2A)-M(1)-O(1C)		99.08(8)
O(2A)-M(1)-O(2D)		162.54(8)
O(2D)-M(1)-O(1B)		88.58(8)
O(1A)-M(2)-O(1D)		171.45(8)
O(1A)-M(2)-O(1B)		88.97(8)
O(1A)-M(2)-O(2C)		91.70(9)
O(1B)-M(2)-O(2C)		169.48(8)
O(1B)-M(2)-O(1D)		93.63(9)
O(1D)-M(2)-O(2C)		84.27(9)

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## 2. FT-IR spectra

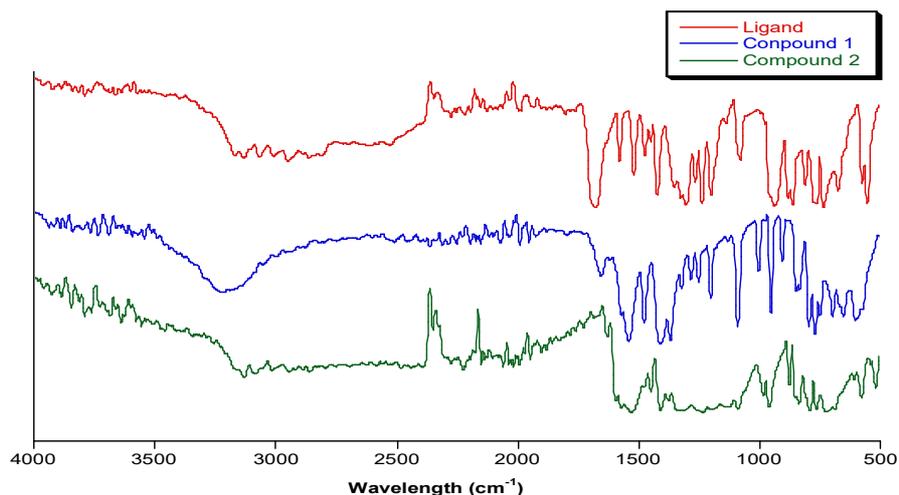


Figure S1. Infrared spectra of the ligand and compounds 1 and 2.

### 3. Luminescence properties

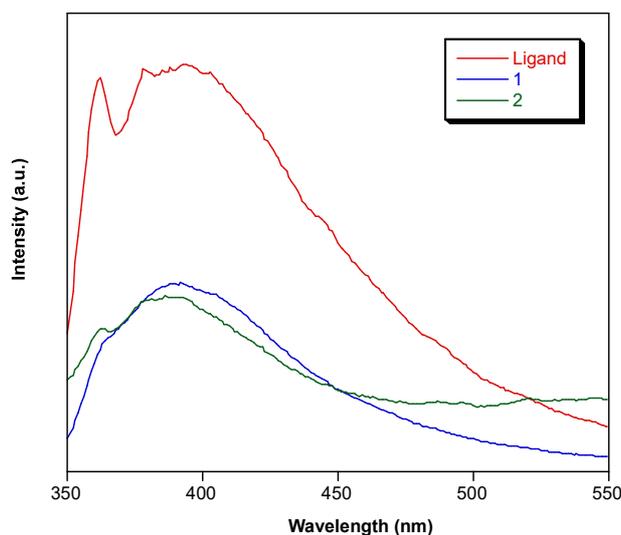
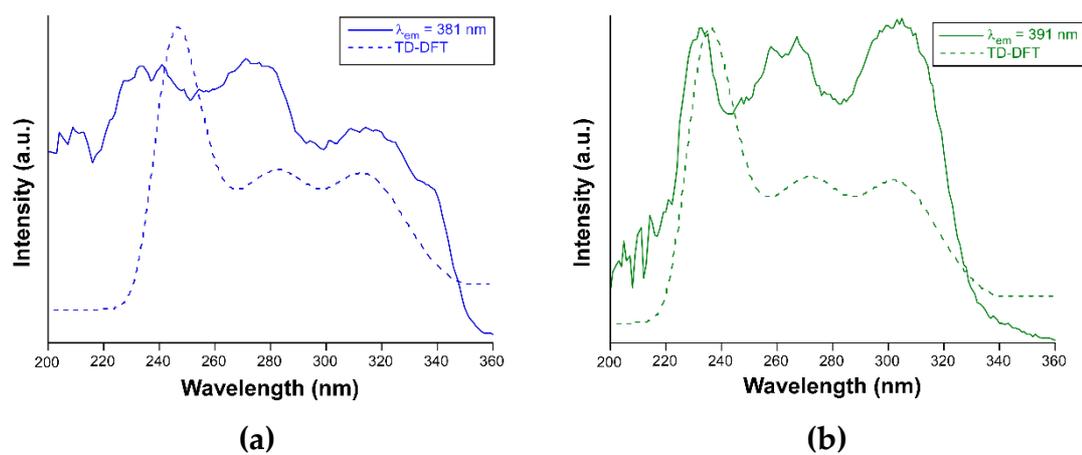
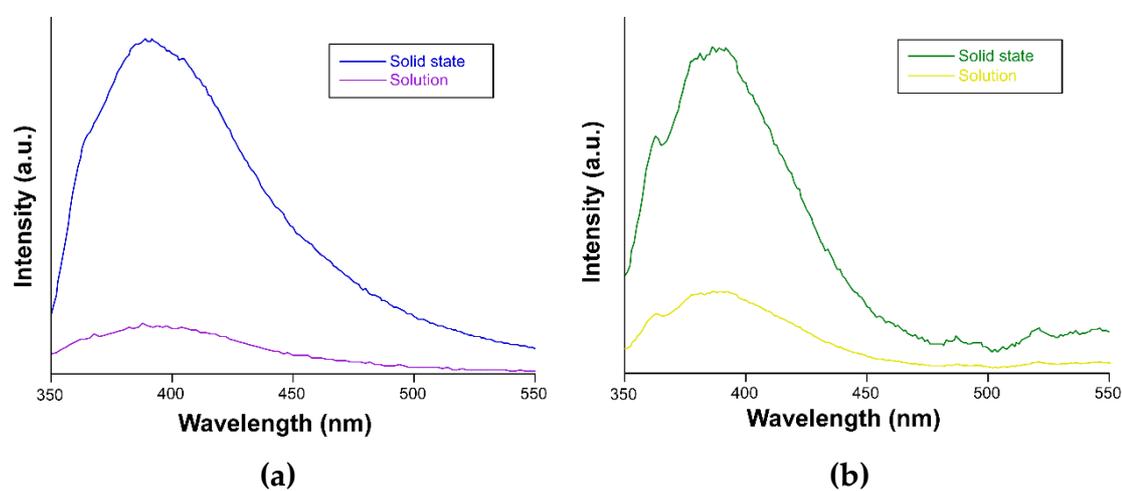


Figure S2. Emission spectra of the ligand and compounds 1 and 2 under  $\lambda_{\text{ex}} = 325$  nm.

The excitation spectra have been measured for both compounds by monitoring the emission maxima. As observed in Figure S3, both excitation spectra show a similar profile consisting of an almost regular band covering the 220–340 nm range in which three peaks (sited at ca. 235, 275 and 320 nm) are distinguished. The TD-DFT spectra calculated using X-ray models of both compounds reproduce fairly well the experimental spectra.



**Figure S3.** Experimental and TD-DFT calculated excitation spectra of compounds monitored at the emission maxima: (a)  $\lambda_{em} = 381$  nm for **1** and (b)  $\lambda_{em} = 391$  nm for **2**.



**Figure S4.** Comparative view of the photoluminescence emission spectra of compounds (a) **1** and (b) **2** in solid state and aqueous solution.

#### 4. Continuous Shape Measurements.

**Table S2.** Continuous Shape Measurements for the  $ZnN_2O_2$  coordination environment.

SP-4	1 D4h	Square
T-4	2 Td	Tetrahedron
SS-4	3 C2v	Seesaw or sawhorse‡ (cis-divacant octahedron)
vTBPY-4	4 C3v	Axially vacant trigonal bipyramid

Complex	SP-4	T-4	SS-4	vTBPY-4
1	29.137	1.086	5.417	1.705

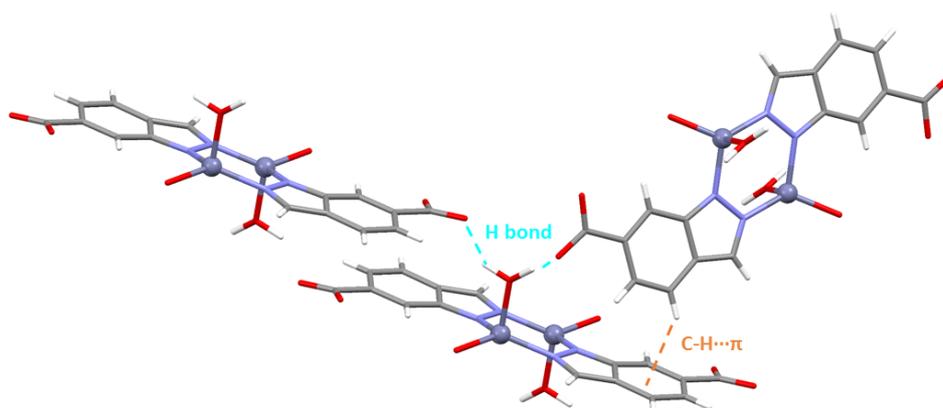
**Table S3.** Continuous Shape Measurements for the  $CdN_2O_4$  coordination environment.

HP-6	1 D6h	Hexagon
PPY-6	2 C5v	Pentagonal pyramid
OC-6	3 Oh	Octahedron
TPR-6	4 D3h	Trigonal prism
JPPY-5	5 C5v	Johnson pentagonal pyramid (J2)

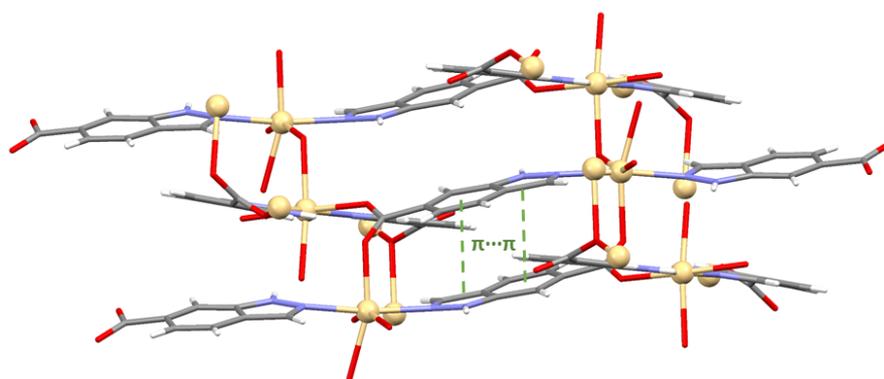
  

Complex	HP-6	PPY-6	OC-6	TPR-6	JPPY-5
2 -Cd1	28.823	19.153	2.317	9.223	23.163
2 -Cd2	29.031	27.296	1.100	14.572	19.748

#### 5. Representation of the main intermolecular interactions.



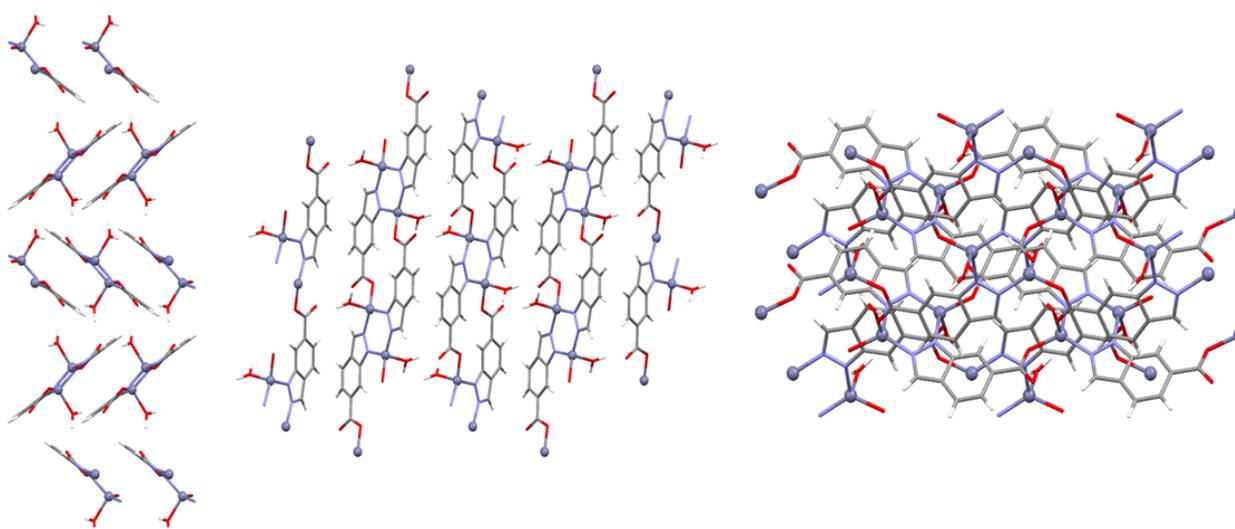
**Compound 1**



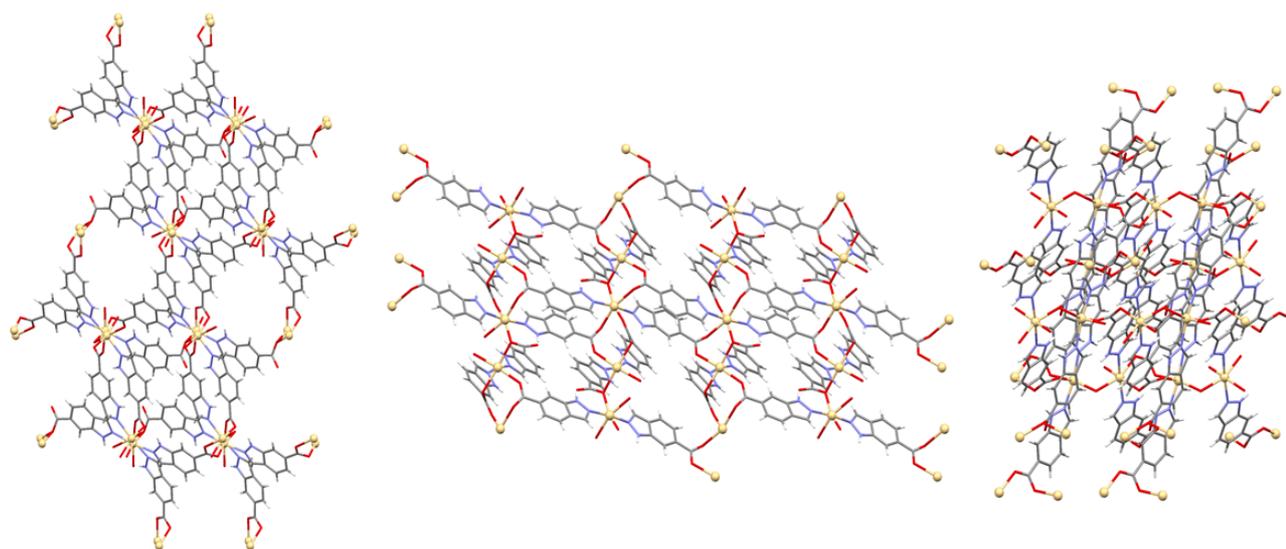
### Compound 2

**Figure S5.** The most representative intermolecular interactions and packing modes for complexes 1 (up) and 2 (down). H bonds,  $\pi \cdots \pi$  and C-H $\cdots$  $\pi$  interactions are shown with dashed blue, green and orange lines, respectively.

#### 6. Additional views of the structures.



### Compound 1



## Compound 2

Figure S6. View along a (left), b (middle) and c (right) axis of complex 1 (up) and 2 (down).

### 7. UV-Vis spectra of compounds in aqueous solution

In order to confirm the stability of the compounds in aqueous solutions, the UV-Vis spectra were measured immediately after preparing the solution and also 24 h later. As observed in the plots, both compounds present almost identical profiles showing the same bands attributed to charge transfers occurring in the complexes. It is noted that the first main band in the spectrum recorded for compound 2 is not completely solved because of the saturation. Moreover, the bands peaking in these absorbance spectra show a close resemblance to the bands recorded in the excitation spectra (Figure S3), in which the small shift may be attributed to the effect of the solvent used in these UV spectra vs the solid state use for the excitation spectra.

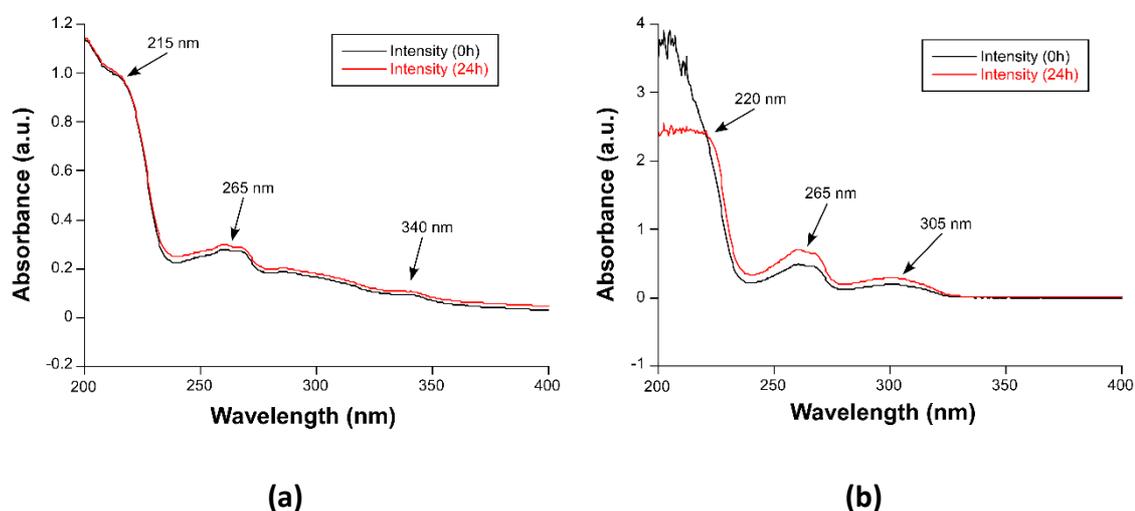


Figure S7. UV-Vis spectra of compounds (a) 1 and (b) 2 in aqueous solutions acquired at times (0 h and after 24 h).