Supplementary Information

Solvothermal Self-assembly of Cd^{2+} Coordination Polymers with Supramolecular Networks Involving N-donor Ligands and Aromatic Dicarboxylates: Synthesis, Crystal Structure and Photoluminescence Studies

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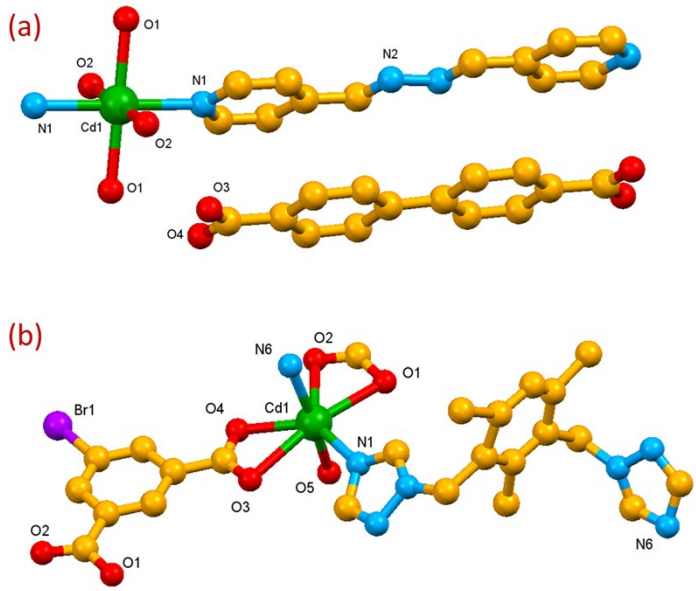

Figure S1. (a) & (b) depicting coordination environment around metal center in **CP1** and **CP2** respectively.

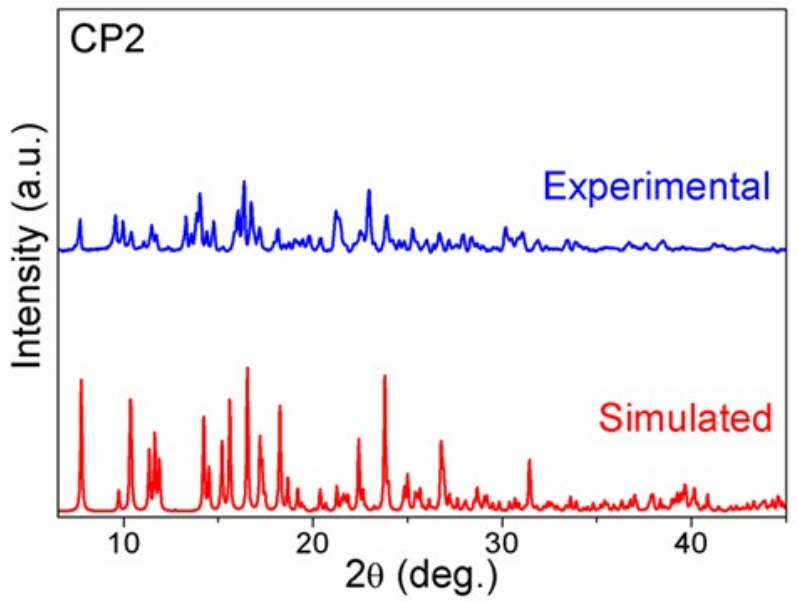

Figure S2. Experimental and simulated PXRD profiles for bulk **CP2**.

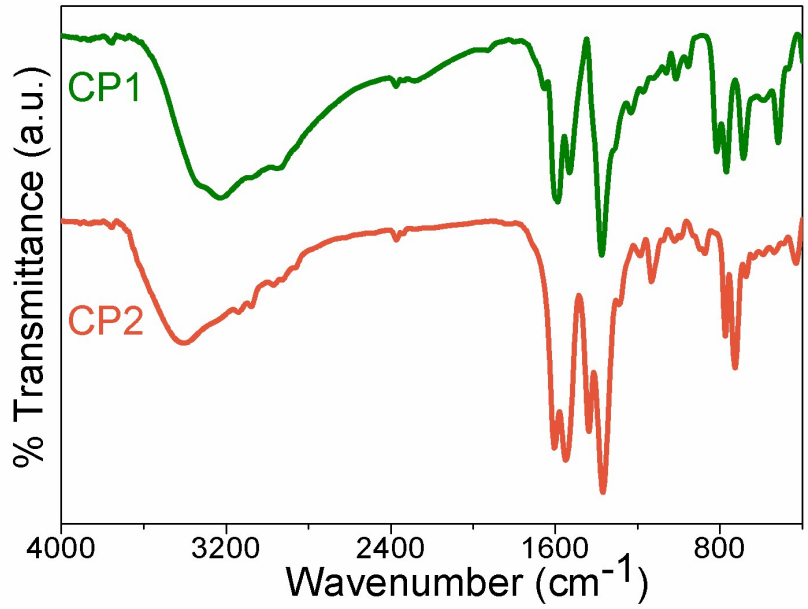

Figure S3. IR spectra recorded for compound **CP1** and **CP2** dispersed in KBr pellets in N_2 atmosphere.

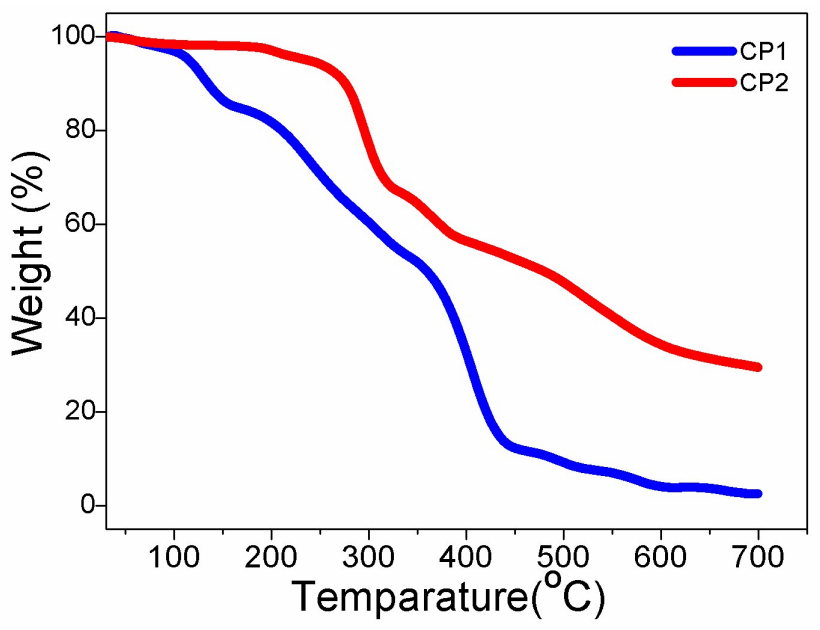

Figure S4. TGA profiles recorded for compound **CP1** and **CP2** in N_2 atmosphere.

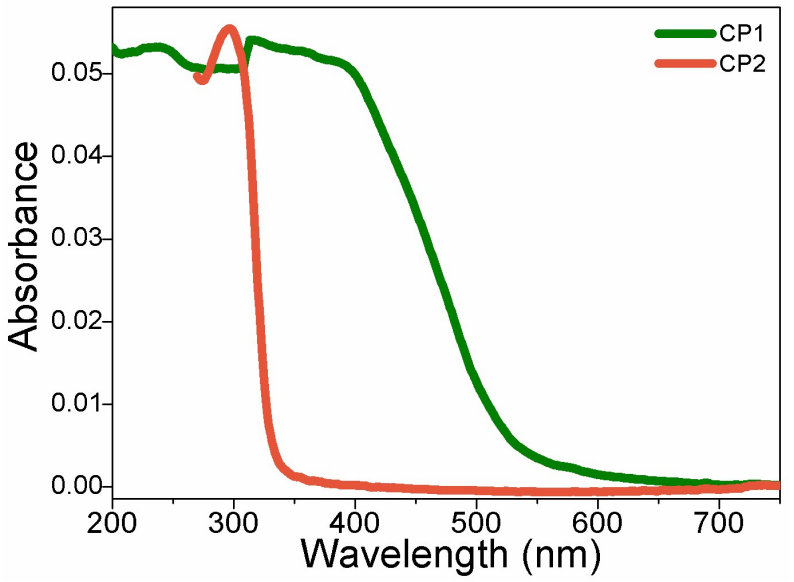

Figure S5. Solid state UV-Vis absorbance spectra for pristine samples of **CP1** and **CP2**.

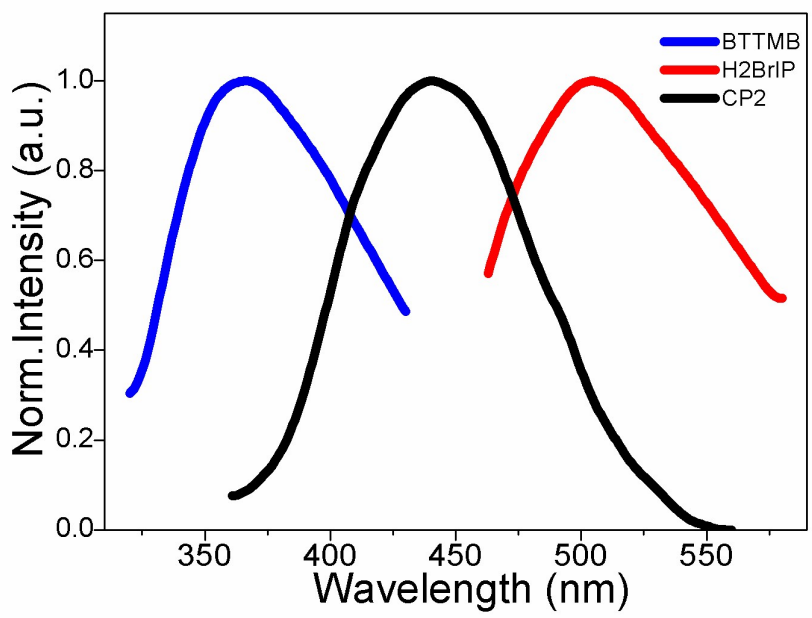

Figure S6. Photoluminescence spectra of **CP2** recorded in the solid state (λ_{ex} = 295 nm, λ_{em} = 441 nm).

S1: Calculation of Detection Limit

For calculating detection limit, acetone (0–240 µL, 4 x 10^{-2} M in ACN) stock solution was added to **CP1** (2 mg in 2 mL ACN) and fluorescent intensity was recorded. By plotting fluorescence intensity with increasing concentration of acetone, slope (m) of graph was found to be 245231 (R^2 = 0.97221). Standard deviation (σ) were calculated from five blank measurements of **CP1**. Detection limit is calculated according to the formula: Detection limit = (3σ/m), while the findings are tabulated ahead:

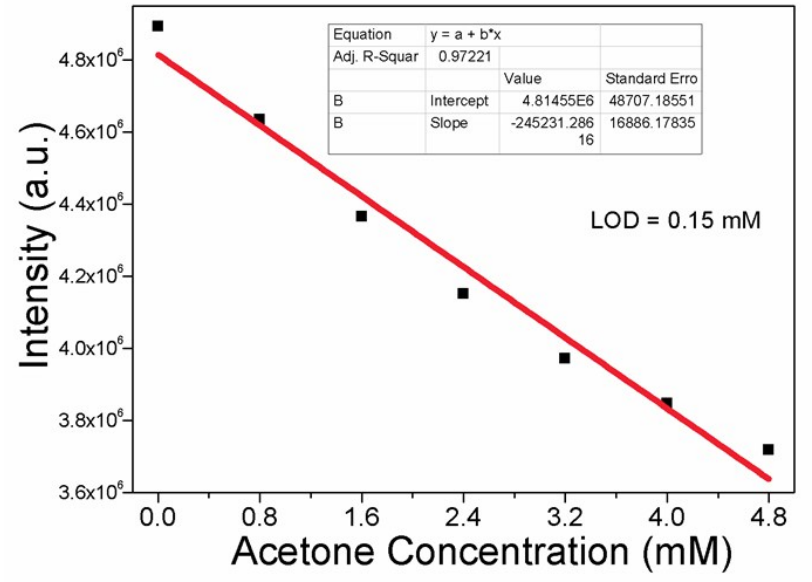

Figure S7. Linear region of fluorescence intensity of **CP1** in acetonitrile upon addition of acetone solution at λ_{em} = 342 nm upon λ_{ex} = 275 nm (R^2 = 0.97221).

Blank Readings	Fluorescence Intensity
1	4873028.66
2	4880239.61
3	4876971.58
4	4859622.16
5	4893679.91
Standard Deviation (σ)	12309.05
Slope (m)	245231
Detection limit (3σ/m)	0.15 mM

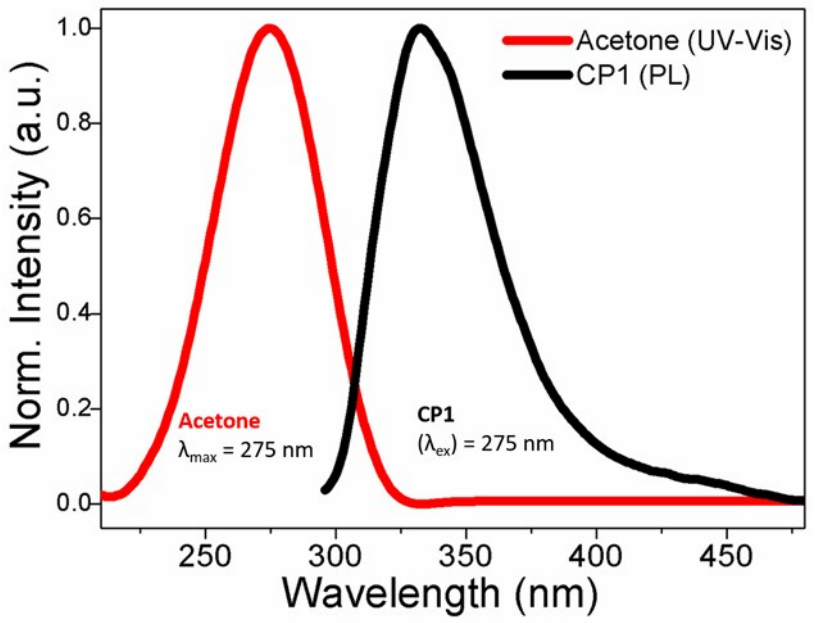

Figure S8. A spectral overlap between UV-Vis and emission spectra of acetone and **CP1** respectively.

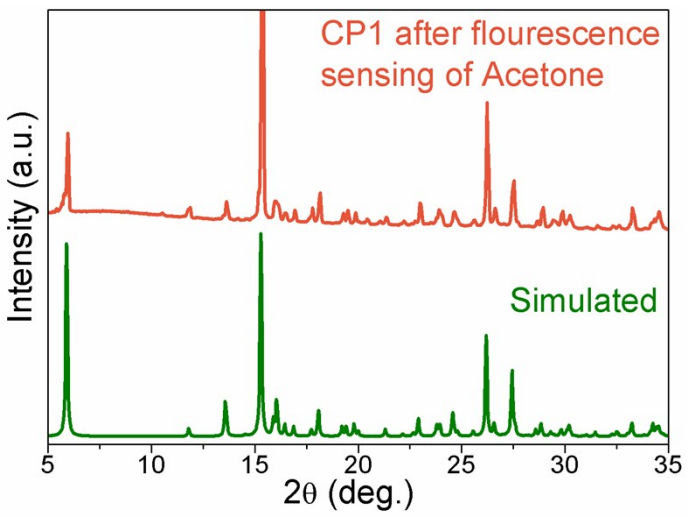

Figure S9. PXRD data of **CP1**, recorded after fluorescence experiments by Acetone in ACN.

Table S1. Crystal Data and Refinement Parameters for **CP1** and **CP2**.

Identification code	**CP1**	**CP2**
Chemical formula	$C_{26}H_{26}N_4O_8Cd$	$C_{23}H_{23}N_6O_5BrCd$
Formula weight	634.91	655.79
Crystal Colour	Yellow	Colorless
Crystal Size (mm)	0.16 x 0.14 x 0.05	0.14 x 0.11 x 0.04
Temperature (K)	293(2)	150(2)
Crystal System	Triclinic	Monoclinic
Space Group	$P\bar{1}$	$P2_1/n$
a (Å)	6.4254(11)	10.256(3)
b (Å)	7.0163(12)	15.191(4)
c (Å)	15.329(3)	17.208(4)
α(°)	101.256(3)	90
β(°)	90.381(3)	94.011(5)
γ (°)	108.064(3)	90
Z	1	4
V (Å^3)	642.7(2)	2674.4(12)
Density (Mg/m^3)	1.640	1.811
Absorption Coefficient (mm^{-1})	0.908	2.354
F(000)	322	1308
Reflections Collected	5347	4680
Independent Reflections	2741	2678
$R_{(int)}$	0.0165	0.0905
Number of parameters	230	443
S(Goodness of Fit) on F^2	1.171	1.035
Final R1/wR2 ($I>2\sigma(I)$)	0.0266/0.0700	0.0899/0.1996
Weighted R1/wR2 (all data)	0.0284/0.0801	0.1514/0.2258
CCDC Number	1521114	1521115
$R = \Sigma\|\|F_o\| - \|F_c\|\|/\Sigma\|F_o\|$; $wR = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$		

Table S2. Selected bond lengths and bond angles for **CP1** and **CP2**.

CP1			
Cd(1)-O(1)#1	2.2885(19)	Cd(1)-O(2)	2.329(2)
Cd(1)-O(1)	2.2886(19)	Cd(1)-O(2)#1	2.329(2)
Cd(1)-N(1)	2.303(2)	N(2)-N(2)#2	1.413(4)
Cd(1)-N(1)#1	2.303(2)	C(5)-C(5)#3	1.485(4)
O(1)#1-Cd(1)-O(1)	180.0	O(1)#1-Cd(1)-O(2)#1	85.83(8)
O(1)#1-Cd(1)-N(1)	93.68(7)	O(1)-Cd(1)-O(2)#1	94.17(8)
O(1)-Cd(1)-N(1)	86.32(7)	N(1)-Cd(1)-O(2)#1	86.01(8)
O(1)#1-Cd(1)-N(1)#1	86.32(7)	N(1)#1-Cd(1)-O(2)#1	93.99(8)
O(1)-Cd(1)-N(1)#1	93.68(7)	O(2)-Cd(1)-O(2)#1	180.0
N(1)-Cd(1)-N(1)#1	180.0	C(8)-N(1)-Cd(1)	121.73(16)
O(1)#1-Cd(1)-O(2)	94.17(8)	C(12)-N(1)-Cd(1)	121.01(16)
O(1)-Cd(1)-O(2)	85.83(8)	C(13)-N(2)-N(2)#2	111.0(3)
N(1)-Cd(1)-O(2)	93.99(8)	Cd(1)-O(1)-H(1C)	113(3)
N(1)#1-Cd(1)-O(2)	86.01(8)	Cd(1)-O(1)-H(1D)	113(3)
Cd(1)-O(2)-H(2D)	108(3)	Cd(1)-O(2)-H(2C)	136(3)
O(4)-C(1)-O(3)	123.7(2)	C(6)-C(5)-C(5)#3	122.1(3)
C(4)-C(5)-C(5)#3	121.5(3)		
Symmetry transformations: #1 -x+1,-y+1,-z ; #2 -x+2,-y+2,-z+1; #3 -x+2,-y+1,-z+1.			
CP2			
Cd(1)-N(1)	2.277(10)	O(4)-Cd(1)#3	2.310(8)
Cd(1)-N(6)#1	2.295(10)	N(6)-Cd(1)#4	2.295(10)
Cd(1)-O(4)#2	2.310(8)	Cd(1)-O(2)	2.375(8)
Cd(1)-O(5)	2.348(8)	Cd(1)-O(1)	2.508(7)
N(1)-Cd(1)-N(6)#1	98.1(4)	N(6)#1-Cd(1)-O(4)#2	87.8(3)
N(1)-Cd(1)-O(4)#2	131.8(3)	N(1)-Cd(1)-O(5)	93.5(3)
N(6)#1-Cd(1)-O(5)	168.4(3)	C(9)-N(1)-Cd(1)	124.5(9)
O(4)#2-Cd(1)-O(5)	84.5(3)	C(19)-N(6)-Cd(1)#4	141.9(3)
N(1)-Cd(1)-O(2)	143.7(3)	C(20)-N(6)-Cd(1)#4	124.2(17)
N(6)#1-Cd(1)-O(2)	82.5(3)	C(20A)-N(6)-Cd(1)#4	116.0(13)

O(4)#2-Cd(1)-O(2)	84.5(3)	O(3)-C(8)-O(4)	123.4(12)
O(5)-Cd(1)-O(2)	88.1(3)	O(2)-Cd(1)-O(1)	53.8(2)
N(1)-Cd(1)-O(1)	90.4(3)	C(1)-O(1)-Cd(1)	87.9(6)
N(6)#1-Cd(1)-O(1)	97.0(3)	C(1)-O(2)-Cd(1)	95.2(7)
O(4)#2-Cd(1)-O(1)	136.5(3)	C(8)-O(4)-Cd(1)#3	100.2(7)
O(5)-Cd(1)-O(1)	82.8(3)	C(10)-N(1)-Cd(1)	131.8(9)
Symmetry transformations: #1 x+1/2,-y+1/2,z-1/2; #2 x+1,y,z; #3 x-1,y,z; #4 x-1/2,-y+1/2,z+1/2.			

Table S3. Details of hydrogen bonding interactions observed in the structure of **CP1** and **CP2**.

D-H···A	**d(H···A) (Å)**	**d(D···A) (Å)**	**∠D-H···A (°)**
CP1			
O(1)-H(1C)···O(4)[1]	1.94(4)	2.662(3)	173(4)
O(1)-H(1D)···O(3)[2]	2.09(3)	2.784(3)	162(4)
O(2)-H(2C)···O(4)[3]	2.09(4)	2.726(3)	173(3)
O(2)-H(2D)···O(3)[1]	2.10(3)	2.816(3)	169(3)
C(8)-H(8)···O(1)[4]	2.36(3)	3.263(3)	151(3)
Symmetry code : 1. 1-x,1-y,-z; 2. -x,2-y,1-z; 3. 2-x,1-y,-z; 4. 1+x,y,z.			
CP2			
C(21)-H(21C)···O(2)[1]	2.59	3.271	128
C(22)-H(22A)···N(5)[2]	2.43	3.228	140
C(22)-H(22C)···N(5)[3]	2.57	3.3614	140
Symmetry code : 1. 1-x,-y,1-z; 2. -x,1-y,1-z; 3. x, y, z.			