Electronic Supplementary Information

Synthesis of Cd(II) based 1D coordination polymer by *in situ* ligand generation and fabrication of photosensitive electronic device

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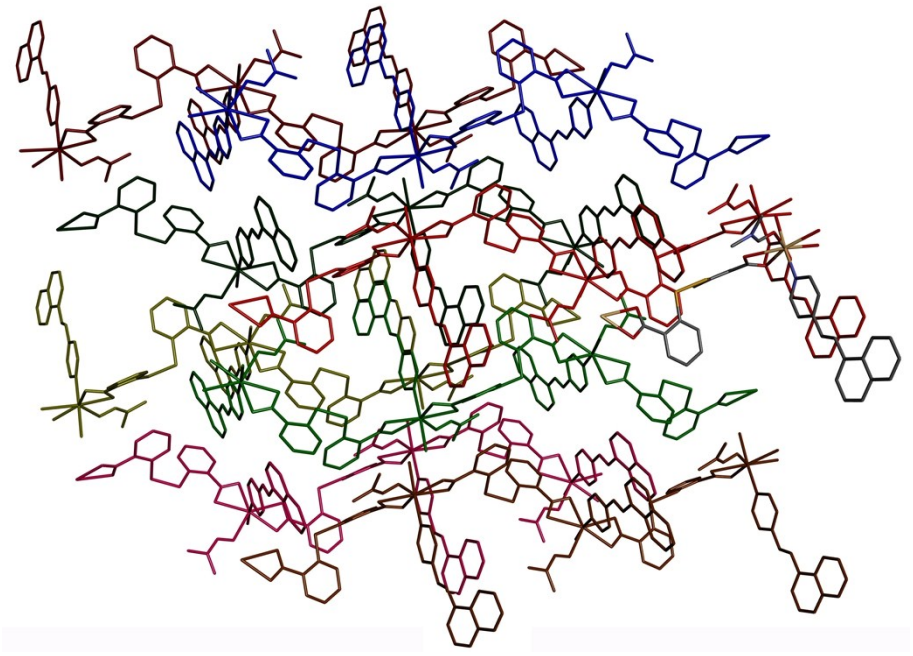

Fig. S1 A view of 3D supramolecular aggregate of the compound **1**.

Table S1 Crystal data and refinement parameters for compound **1**

Formula	$C_{34}H_{30}CdN_2O_6S_2$(**1**)
fw	739.13
crystsyst	monoclinic
space group	$P2_1/n$
a (Å)	7.7317(3)
b (Å)	17.7115(8)
c (Å)	23.3846(10)
α(deg)	90
β(deg)	99.182(2)
γ (deg)	90
V (Å^3)	3161.3(2)
Z	4
D_{calcd}(g/cm^3)	1.555
μ(mm^{-1})	0.872
λ(Å)	0.71073
data[$I > 2\sigma(I)$]/params	6201/416
GOF on F^2	1.089
final R indices[$I > 2\sigma(I)$][a,b]	$R1$ = 0.0280 $wR2$ = 0.0664

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b] $wR2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2 Selected bond lengths and bond angles in **1**

Cd01-O1	2.390(2)	O1-Cd01-N1	87.49(7)	O4a -Cd01-O5a	53.20(6)
Cd01-N1	2.304(2)	O1-Cd01-O5a	82.87(6)	O1-Cd01-O3	79.31(7)
Cd01-O2	2.273(2)	O2-Cd01-N1	96.39(8	O1-Cd01-C21	105.78(7)
Cd01-O4a	2.532(2)	O2-Cd01-O5a	143.91(6)	O2-Cd01-O3	53.33(7)
Cd01-O3	2.531(2)	O3-Cd0-C21	26.52(7)	O2-Cd01-C21	26.91(6)
Cd01-O5a	2.358(2)	O6-Cd01-N1	173.39(8)	O3-Cd01-O6	87.30(8)
Cd01-O6	2.322(2)	O6-Cd01-O5a	84.39(7)	O3-Cd01-O4a	142.89(6)
O1 -Cd01-O2	132.64(6)	N1-Cd01-O5a	90.60(7)	O6-Cd01-C21	86.90(7)
N1-Cd01-C21	98.71(7)	O1-Cd01-O6	87.61(7)	O2-Cd01-O6	90.19(8)
C21-Cd01-O4a	116.82(6)	O1-Cd01-O4a	135.73(6)	O2-Cd01-O4a	90.76(6)
O3 -Cd01-N1	96.14(8)	O3-Cd01-O5a	160.62(7)	O6 -Cd01-O4a	83.36(7)
N1-Cd01 -O4a	97.10(7)	C21-Cd01-O5a	167.47(6)	Cd01-O3-C21	86.31(14)

Symmetry Code: a = -1/2+x, 3/2-y, -1/2+z; b = 1/2+x, 3/2-y, 1/2+z

Table S3 Hydrogen bonding interactions in **1**

	D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	<D-H···A (°)
Compound **1**	O(6)-H(6A)···O(5)	0.73(4)	2.02(4)	2.727(3)	164(4)
	O(6)-H(6B)···O(1)	0.81(4)	2.17(4)	2.885(3)	149(3)

Table S4 C-H···π interactions in **1**

	C-H→ ring(j)	H···R distance (Å)	C-H···R angle(deg)	C···R distance (Å)
Compound **1**	C(30)-H(30)→R(1)	2.85	139.2	3.609
	C(11)-H(11)→R(2)	2.70	144.3	3.494

R(j) denotes the j-th ring: R(1) = C(8)/C(9)/C(10)/C(11)/C(12)/C(13); R(2)= C(22)/C(23)/C(24)/C(25)/C(26)/C(27)

Table S5 π···π interactions in **1**

	ring(j)→ring(j)	R···R distance (Å)
Compound **1**	R(3)→ R(4)	3.627

R(j) denotes the j-th ring: R(3) = C(1)/C(2)/C(3)/C(4)/C(5)/N(1); R(4)= C(12)/C(13)/C(14)/C(15)/C(16)/C(17).

Table S6 DFT table of the compound **1**

Compound **1**			
MO	Energy (eV)	Cd	Ligand
LUMO+10	-0.61	0	100
LUMO+9	-0.83	0	100
LUMO+8	-0.85	0	100
LUMO+7	-1.12	1	99
LUMO+6	-1.29	1	99
LUMO+5	-1.33	0	100
LUMO+4	-1.6	0	100
LUMO+3	-1.71	1	99
LUMO+2	-1.83	1	99
LUMO+1	-1.89	0	100
LUMO	-2.39	0	100
HOMO	-6.04	0	100
HOMO-1	-6.07	0	100
HOMO-2	-6.11	0	100
HOMO-3	-6.21	0	100
HOMO-4	-6.3	0	100
HOMO-5	-6.69	1	99
HOMO-6	-6.78	1	99
HOMO-7	-6.93	0	100
HOMO-8	-7.07	0	100
HOMO-9	-7.15	0	100
HOMO-10	-7.18	0	100
Key transition for both the compounds: HOMO-1→LUMO, Nature of transition : ILCT			

Table S7 Calculated transitions and their assignments for the compound **1**

Excitation energy (eV)	Wavelength Thro. (nm)	Oscillation frequency (f)	Key transitions	Nature of transitions
3.3605	368.94	0.4831	(62%) HOMO-1→LUMO	ILCT
3.3985	364.82	0.0704	(79%) HOMO-2→LUMO+3	ILCT
3.7297	332.42	0.0223	(84%) HOMO-3→LUMO+1	ILCT
3.8054	325.81	0.1293	(83%) HOMO-4→LUMO+1	ILCT
3.8864	319.02	0.0676	(27%) HOMO→LUMO+4	ILCT
3.8926	318.51	0.0993	(38%) HOMO-2→LUMO+4	ILCT
4.1765	296.86	0.0727	(40%) HOMO-→LUMO+5	ILCT

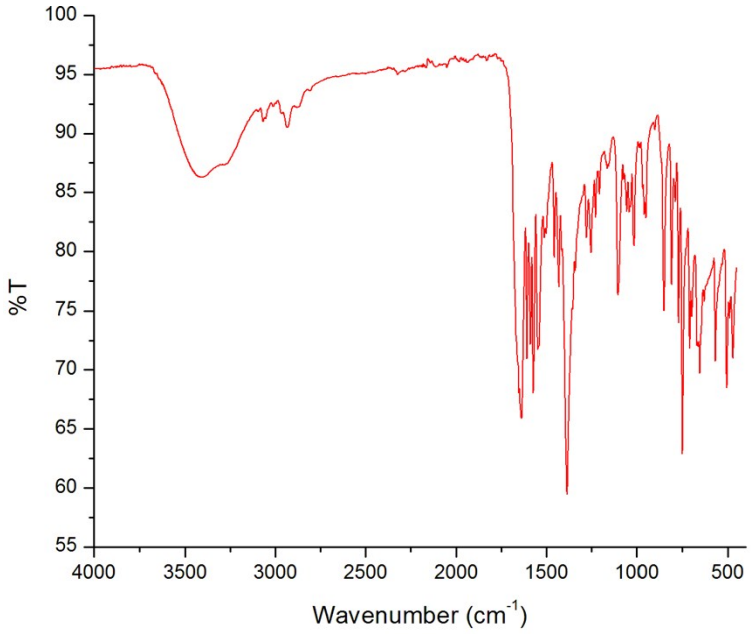

Fig. S2 FT-IR of the compound **1**.

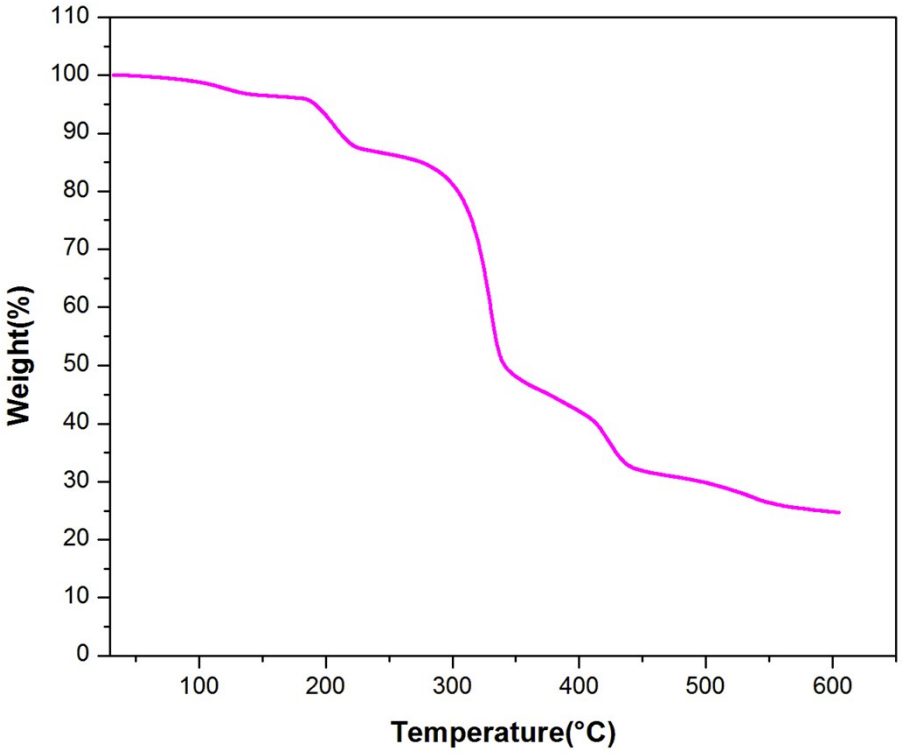

Fig. S3 TGA plot of complex **1** measured under N_2 atmosphere.

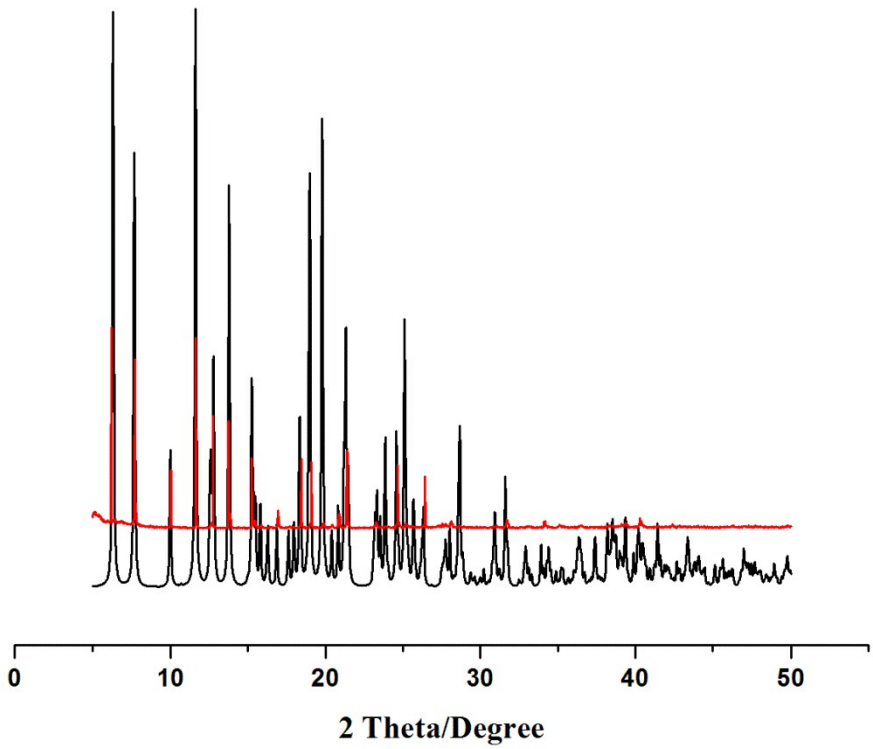

Fig. S4 Powder X-ray diffraction patterns of simulated **1** (black) and as-synthesized **1** (red).

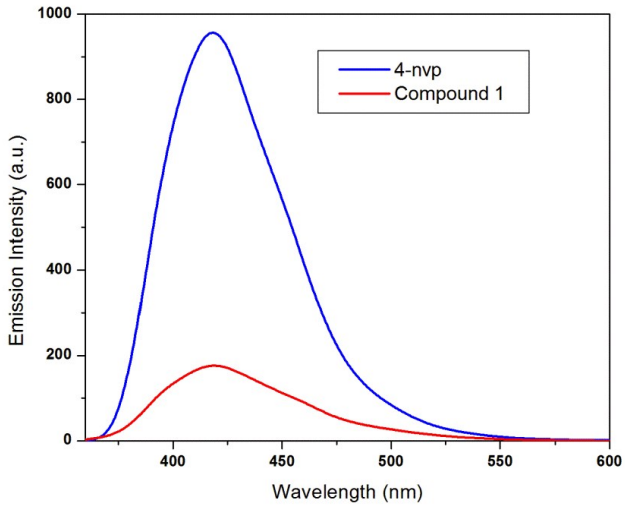

Fig. S5 Fluorescence emission spectra of 4-nvp ligand and compound **1**.

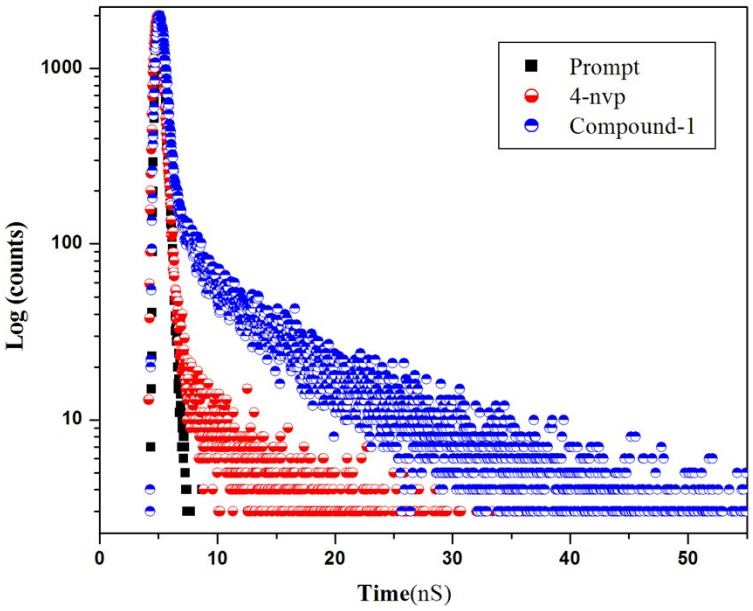

Fig. S6 Decay profile of 4-nvp ligand and compound **1**.