Electronic Supplementary Material (ESI) for Materials Advances.

Assembly of cadmium (II)-based chiral complex: crystal structure and optical properties for solid state white-light emission application

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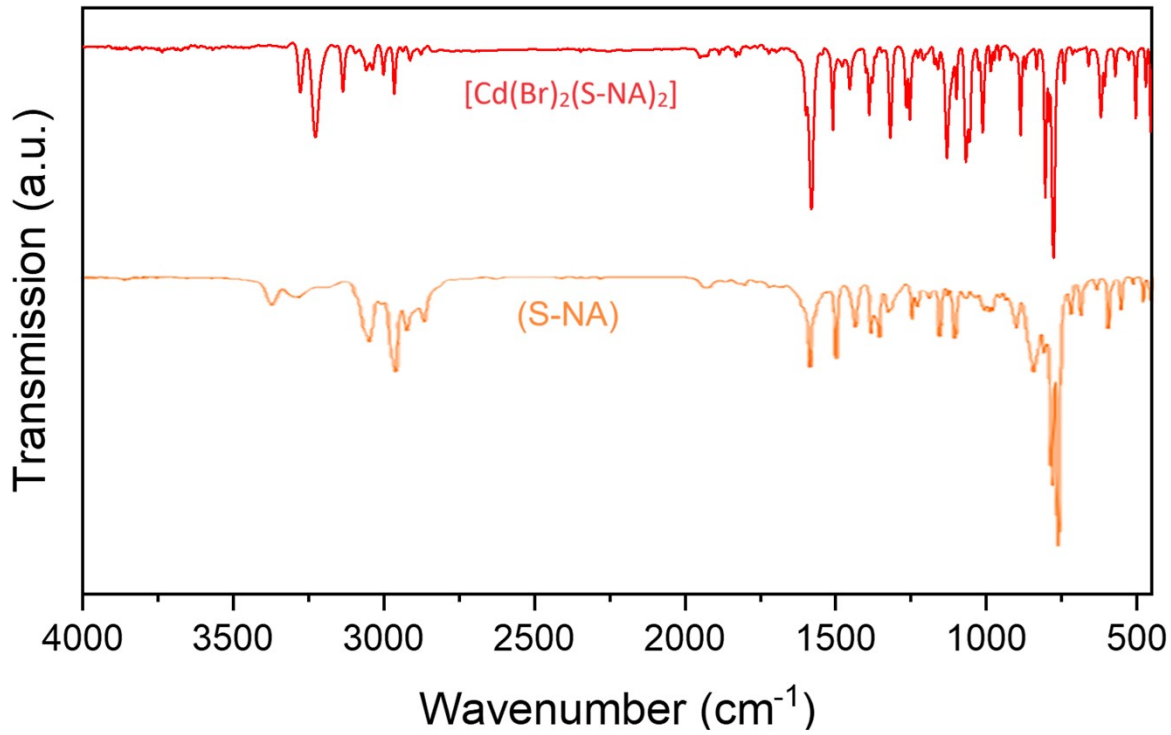

Figure S1: IR spectra of $[Cd(Br)_2(S\text{-}NA)_2]$ and (S-NA) in the region of 480-4000 cm^{-1}

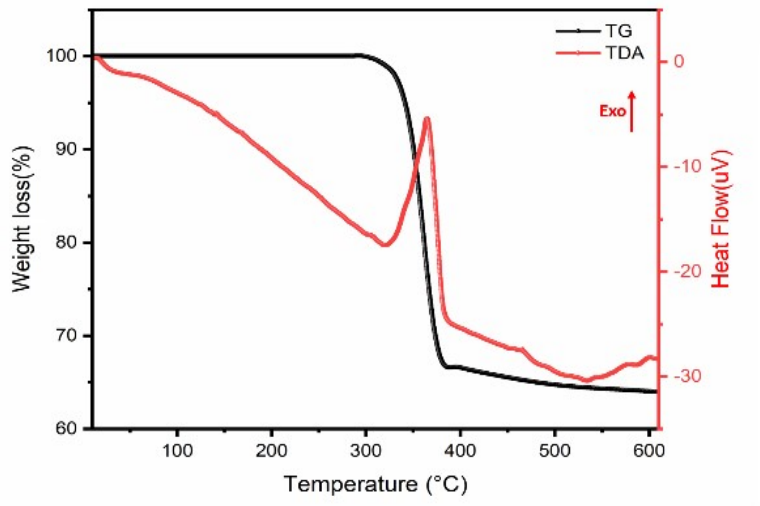

Figure S2: TGA and DTA data for $[Cd(Br)_2(S\text{-}NA)_2]$

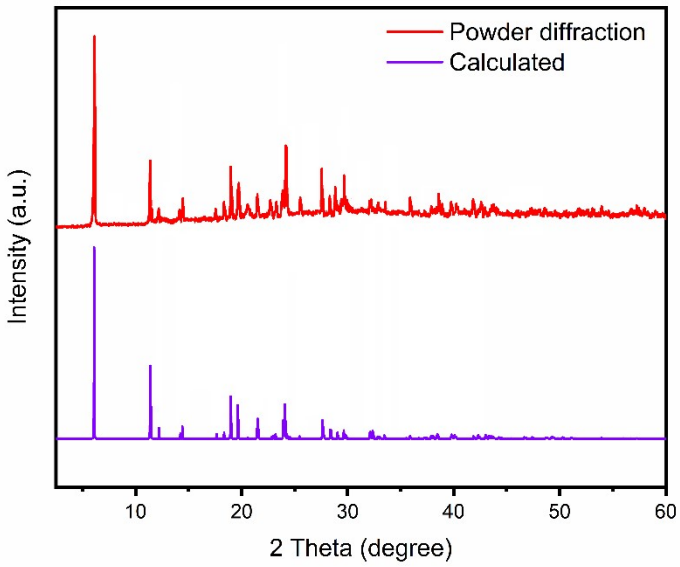

Figure S3: Poly-crystals X-ray diffraction and single crystal calculated pattern of $[Cd(Br)_2(S\text{-}NA)_2]$

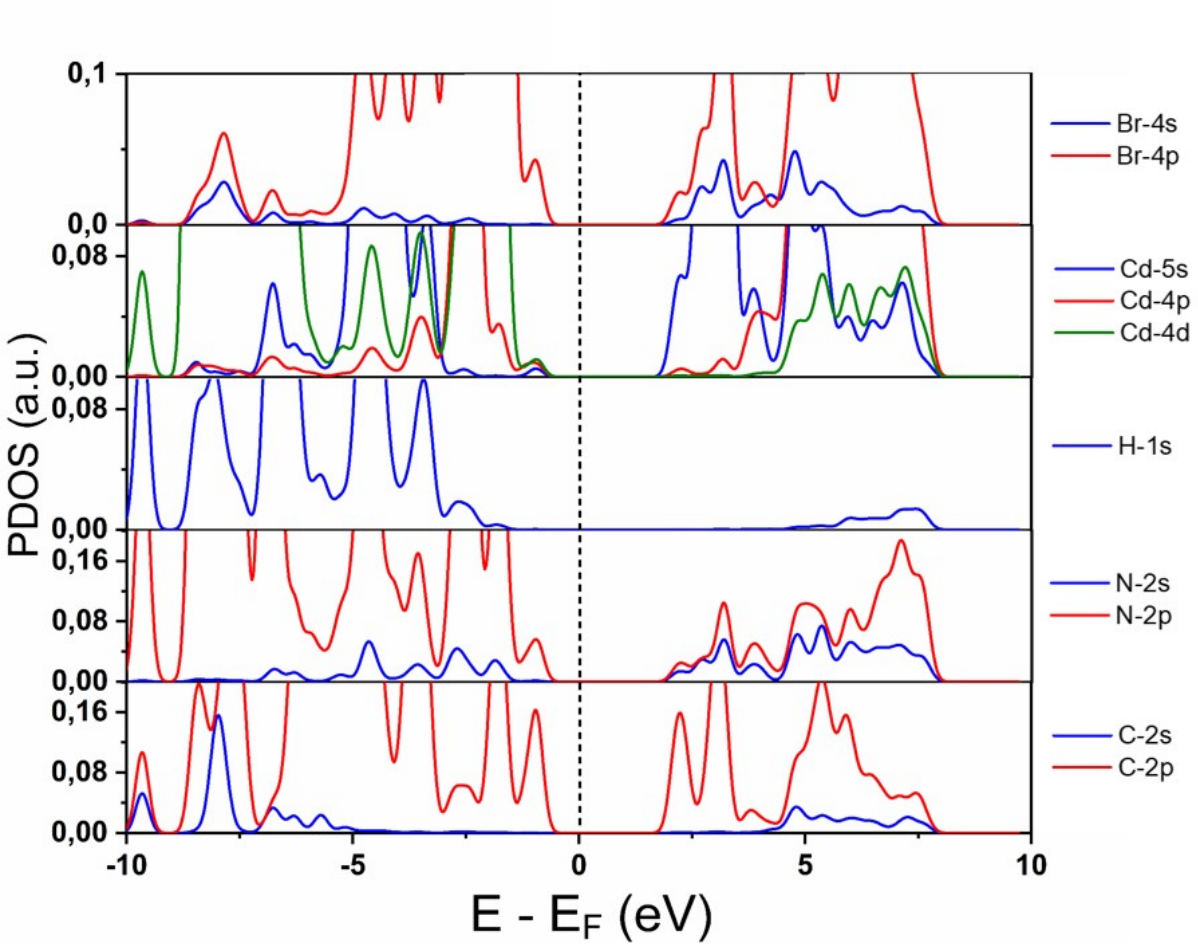

Figure S4: Zoomed PDOS

Table S1: Crystal data and structure refinement details

Crystal parameters	
Formula	$C_{24}H_{22}Br_2CdN_2$
CCDC deposition number	2081813
Formula weight	610.65
Temperature (K)	293
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	*I2*
Unit cell dimensions	
a (Å)	8.0454 (14)
b (Å)	5.1075 (6)
c (Å)	29.000 (5)
β (°)	90.722 (15)
Crystal size (mm)	0.12 × 0.15 × 0.38
V (Å³)	1191.6 (3)
Z	2
ρ_{calcd} (mg cm^{-3})	1.702
μ (mm-1)	4.28
F(000)	596
θ range for data collection (°)	2.6 - 30.9
h/k/l	-10, 11/-7, 7/-41, 41
Reflections collected	6599
Independent reflections	3521
Tmax and Tmin	0.16, 0.32
Goodness-of-fit on F2	1.09
Final R indices [I[2r(I)]	R1= 0.059 wR2= 0.176
R_{int}	0.075

Table S2: Selected bond lengths and angles (Å, º) for the compound $[Cd(Br)_2(S\text{-}NA)_2]$.

bond lengths	Å	angles	Deg °
Cd1—N1^{i}	2.259 (10)	**N1i—Cd1—N1**	103.7 (4)
Cd1—N1	2.259 (10)	**N1i—Cd1—Br1^{i}**	113.9 (2)
Cd1—Br1^{i}	2.5682 (12)	**N1—Cd1—Br1^{i}**	107.2 (2)
Cd1—Br1	2.5682 (12)	**N1i—Cd1—Br1**	107.2 (2)
		N1—Cd1—Br1	113.9 (2)
		Br1i—Cd1—Br1	110.79 (6)

Symmetry code: (i): −x+1, y, −z+1

Table S3: Hydrogen band interactions

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···Br1^{ii}	0.83 (19)	2.94 (19)	3.654 (9)	146(14)
N1—H2N···Br1^{iii}	0.83 (17)	2.77 (18)	3.475 (8)	144.2 (15)

Symmetry codes: (ii) x, y+1, z; (iii) −x+1, y+1, −z+1.