Supporting Information
For

Synthesis of isophthalic acid-carbazole coordination polymers with stacking-dependent ultralong room temperature phosphorescence and white-light emission

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X-ray Crystal Structures

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1. EXPERIMENTAL SECTION

Materials and Methods. All chemical materials were obtained from commercial sources and used without further purification. 5-(carbazol-9-yl) isophthalate (CzIP) was synthesized by following the published method.[1] Powder X-ray diffraction (PXRD) patterns were acquired on a Bruker D8 ADVANCE diffractometer with Cu Kα (λ = 1.5418 Å) radiation in the range of θ = 5−50° at room temperature. Thermogravimetric analysis (TGA) was performed on a PerkinElmer TG-7 analyzer heated from room temperature to 750 °C at a ramp rate of 5 °C/min under air atmosphere. Elemental analyses (C, H, and N) were conducted on a PerkinElmer 240C elemental analyzer. Ultraviolet-visible (UV-vis) absorption spectras were collected on a PerkinElmer Lambda 35 spectrophotometer. The luminescent and temperature-dependent phosphorescence spectra and quantum yields were measured on FLS1000 Edinburgh fluorescence spectrometer, and luminescence lifetimes were obtained on a single photon counting spectrometer with micro-second pulse lamp.

Synthesis of Compounds

Compound 1 A mixture of CzIP (15 mg, 0.065 mmol), D-Cyclopentylglycine (15 mg, 0.10 mmol) and $Zn(NO_3)_2·6H_2O$ (60 mg, 0.20 mmol) were dissolved in H_2O and DMI (8 and 2 mL), the mixture were sealed in a Teflon-lined stainless steel container and heated at 150 °C for 3 days, and then cooled to room temperature. Colorless prismatic crystals were obtained and collected by filtration. Anal. calcd (%) for $C_{20}H_{11}NO_4Zn$: C 60.80, H 2.79, N 3.55. Found (%): C 60.41, H 2.81, N 3.50.

Compound 2 CzIP (15 mg, 0.065 mmol), D-Cyclopentylglycine (15 mg, 0.10 mmol) and $Cd(SO_4)_2·8H_2O$ (50 mg, 0.06 mmol) were dissolved in H_2O and DMI (8 and 2 mL), the mixture were sealed in a Teflon-lined stainless steel container and heated at 150 °C for 3 days, and then cooled to room temperature. Colorless prismatic crystals were obtained and collected by filtration. The crystals were washed with DMF for three times to remove the surface impurities. Anal. calcd (%) for $C_{25}H_{21}CdN_3O_5$: C 53.97, H 3.78, N 7.55. Found (%): C 54.11, H 3.80, N 7.59.

Compound 3 CzIP (15 mg, 0.065 mmol), D-Cyclopentylglycine (15 mg, 0.1 mmol) and $Cd(SO_4)_2·8H_2O$ (50 mg, 0.06 mmol) were dissolved in H_2O and EtOH (8 and 2 mL), the mixture were sealed in a Teflon-lined stainless steel container and heated at 150 °C for 3 days, and then cooled to room temperature. Colorless prismatic crystals were obtained and collected by filtration.

The crystals were washed with DMF for three times to remove the surface impurities. Anal. calcd (%) for $C_{40}H_{26}Cd_2N_2O_{10}$: C 52.20, H 2.83, N 3.05. Found (%): C 52.39, H 2.88, N 3.04.

X-ray Crystal Structures

The diffraction data were measured at 293 K under nitrogen flowing with Rigaku supernova CCD system equipped with a confocal monochromated Mo-Kα radiation (λ = 0.71073 Å). The structure was solved by a direct method and refined by full-matrix least-squares using SHELX-2014[2] and Olex2.0.[3] Non-hydrogen atoms were refined with anisotropic thermal displacement coefficients. All hydrogen atoms were located on the geometrically ideal positions and refined using a riding model. CCDC 2219861–2219863 for 1-3. The crystal structure parameters were listed in Table S1.

2. Supplementary Schemes and Figure

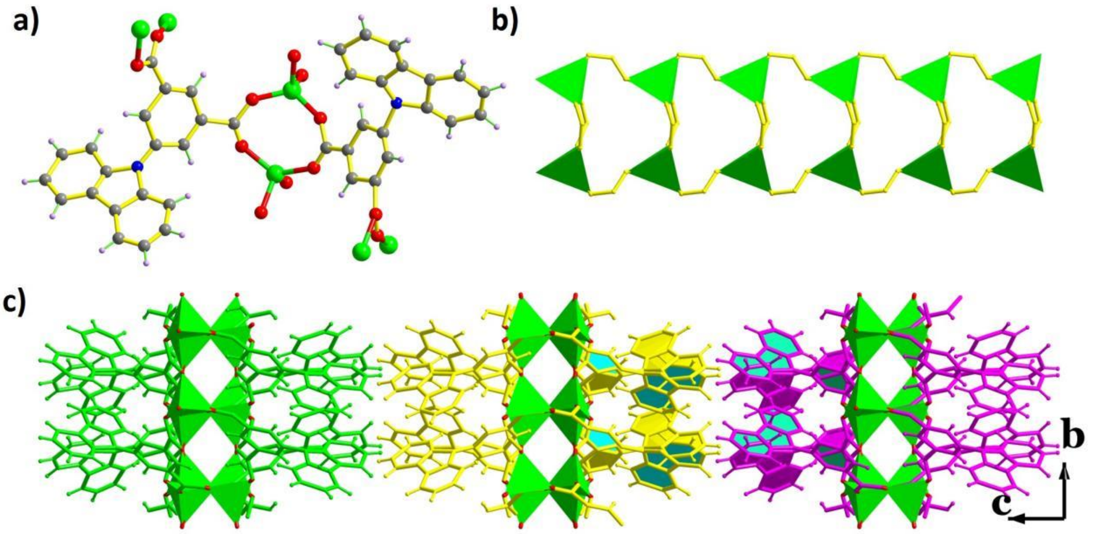


Fig. S1 (a) The coordination environment of Zn^{2+} ions in compound 1; (b) Zn^{2+} ions was connected by CzIP to form a 1D chain; (c) 2D supramolecular structure of compound 1 built of 1D chains through noncovalent interactions;the packing of carbazole groups from the adjacent layers.

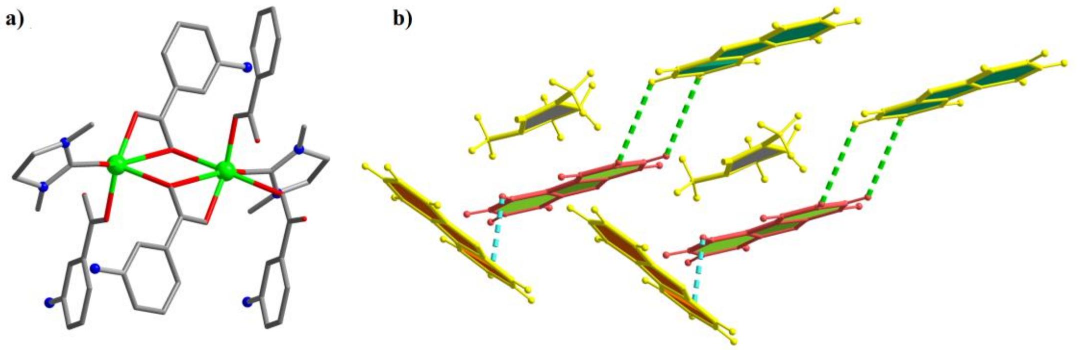
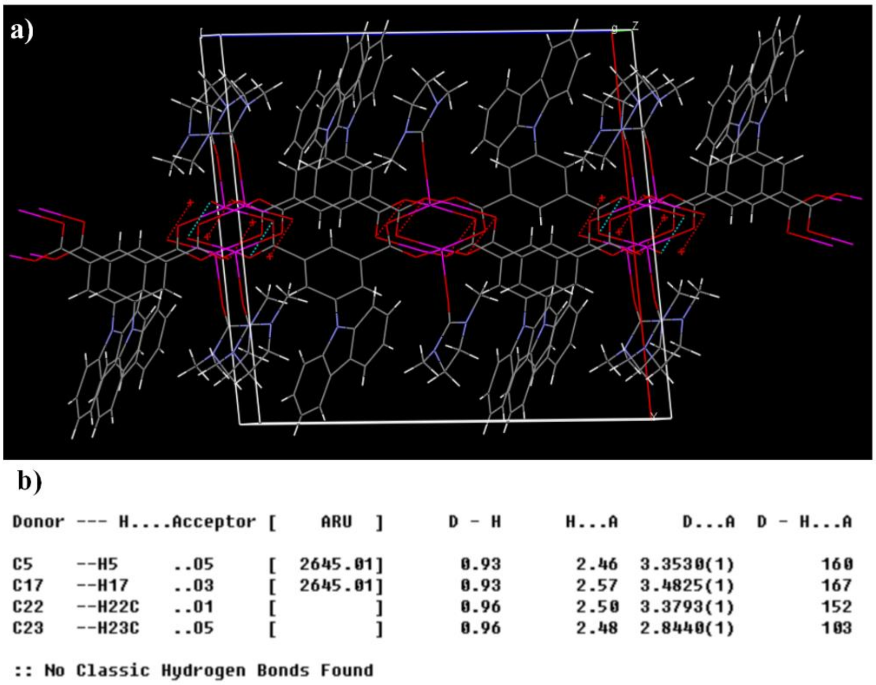


Fig. S2 (a) The coordination environment of Cd^{2+} ions in compound 2; (b) the packing of carbazole fragments.



b)

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Donor --- H....Acceptor [    ARU   ]       D - H      H...A      D...A  D - H...A

C5      --H5      ..O5       [  2645.01]        0.93       2.46  3.3530(1)        160
C17     --H17     ..O3       [  2645.01]        0.93       2.57  3.4825(1)        167
C22     --H22C    ..O1       [          ]       0.96       2.50  3.3793(1)        152
C23     --H23C    ..O5       [          ]       0.96       2.48  2.8440(1)        103

:: No Classic Hydrogen Bonds Found
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Fig. S3 The hydrogen bonds were checked by MERCURY (a) and PLATON program; (b) There are no intramolecular and intermolecular hydrogen bonds.

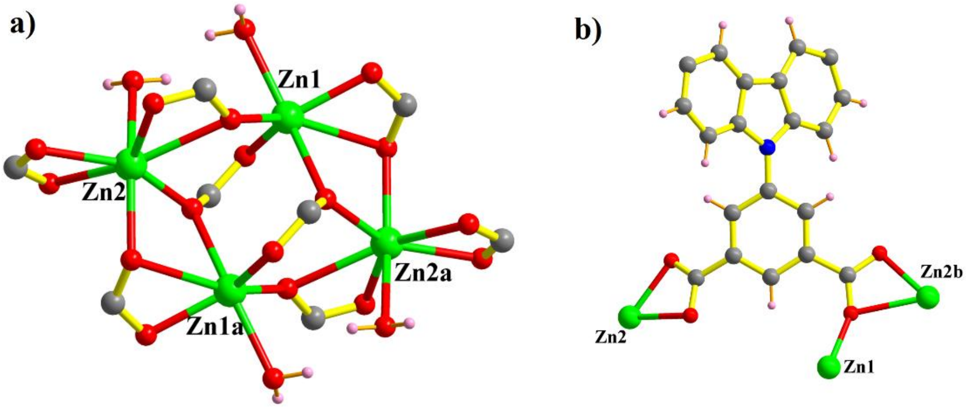

Fig. S4 (a) The coordination environment of four Zn^+ ions in compound 3; (b) the coordination mode of CzIP.

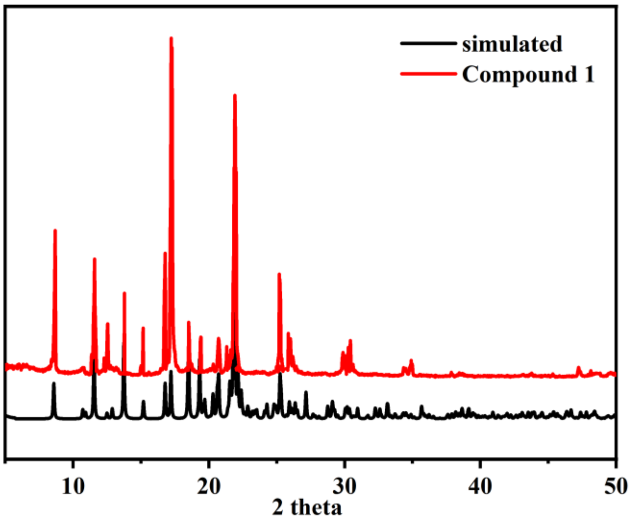

Fig. S5 The powder XRD spectra of compound 1.

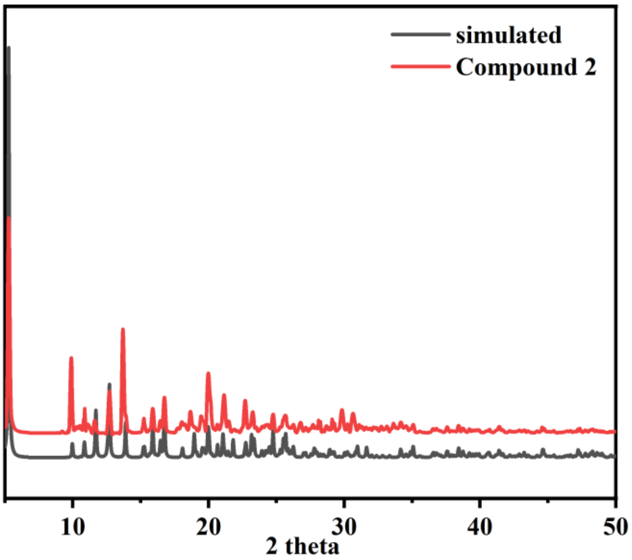

Fig. S6 The powder XRD spectra of compound 2.

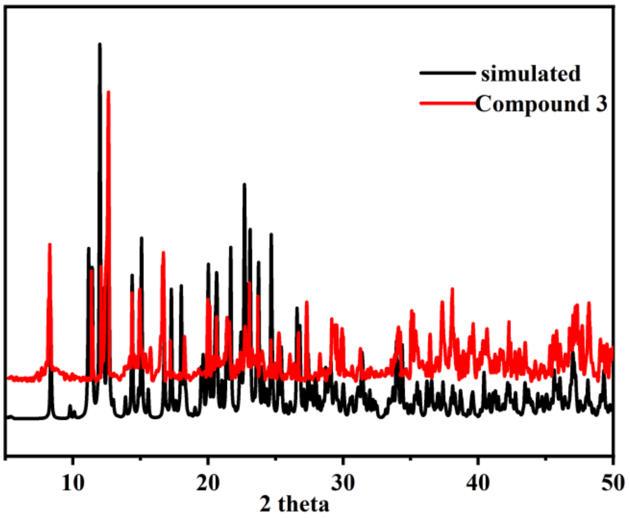

Fig.S7 The powder XRD spectra of compound 3.

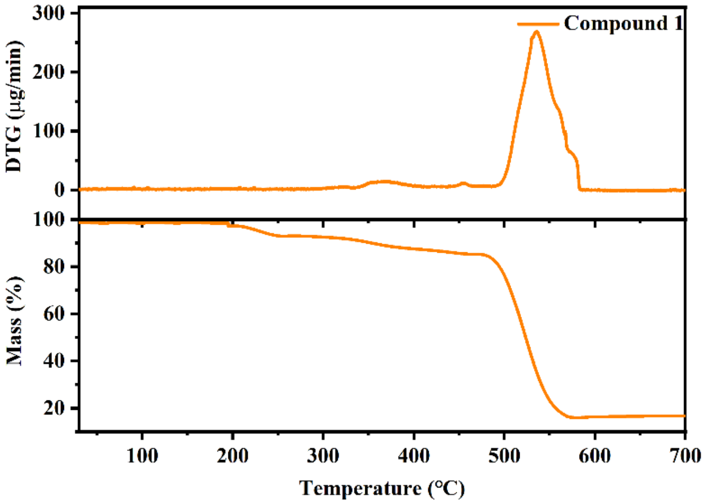

Fig. S8 TG and DTG curves of compound 1.

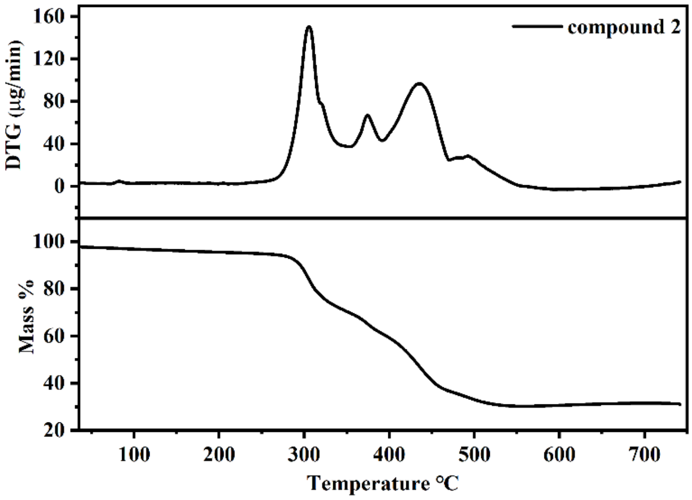

Fig. S9 TG and DTG curves of compound 2.

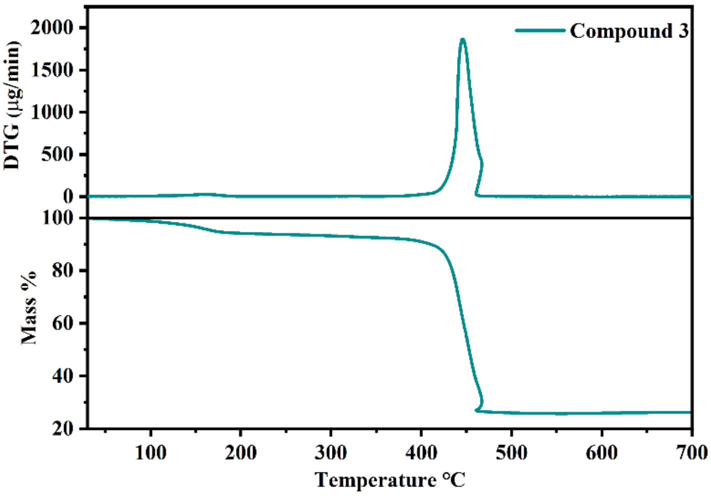

Fig. S10 TG and DTG curves of compound 3.

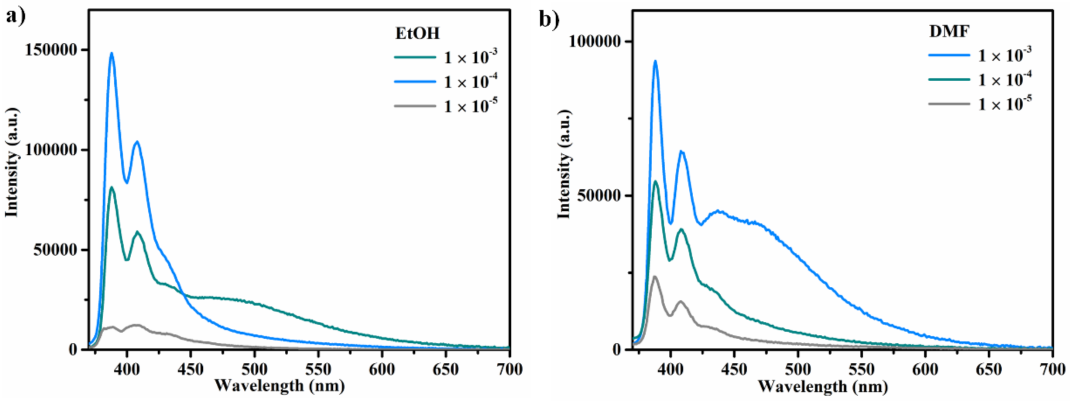

Fig. S11 The fluorescent behaviors of organic ligand CzIP in different concentrations. (a) in ethanol (EtOH) from 1×10^{-5} to 1×10^{-3} mol/L; (b) in N,N-Dimethylformamide (DMF) from 1×10^{-5} to 1×10^{-3} mol/L.

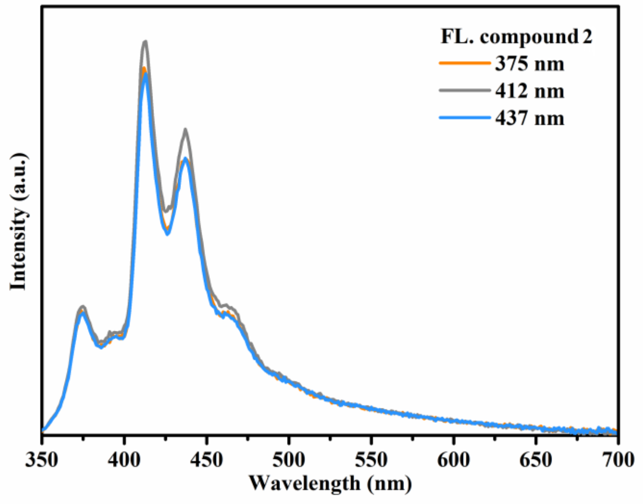

Fig. S12 Fluorescence curves of compound 2 at 375, 412 and 467 nm.

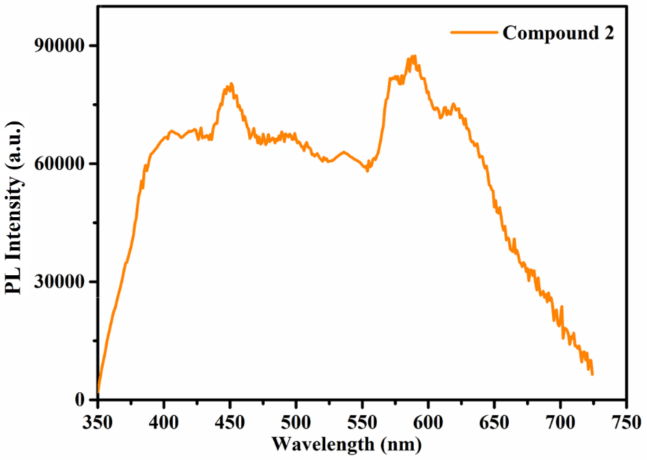

Fig. S13 Photoluminescence (PL) curves of compound 2.

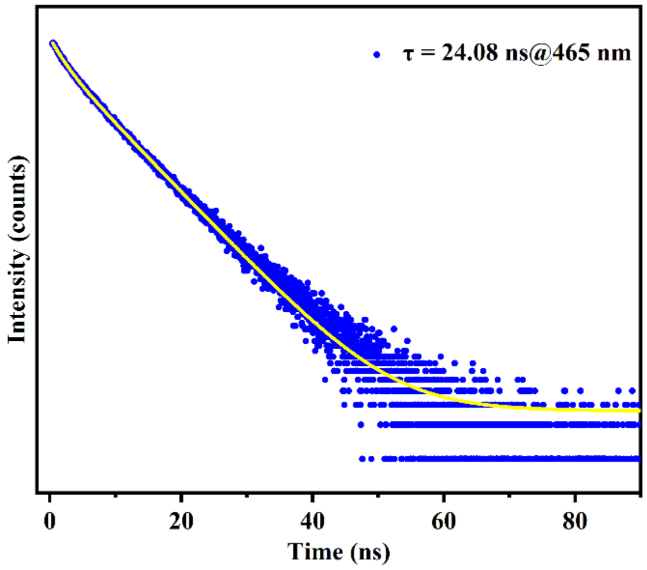

Fig. S14 Fluorescence lifetime profile of compound 1 at 465 nm.

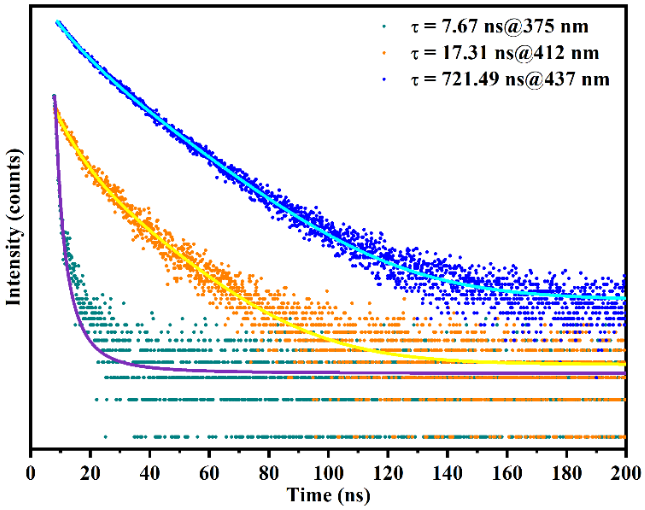

Fig. S15 Fluorescence lifetime profile of compound 2 at 375, 412 and 437 nm, respectively.

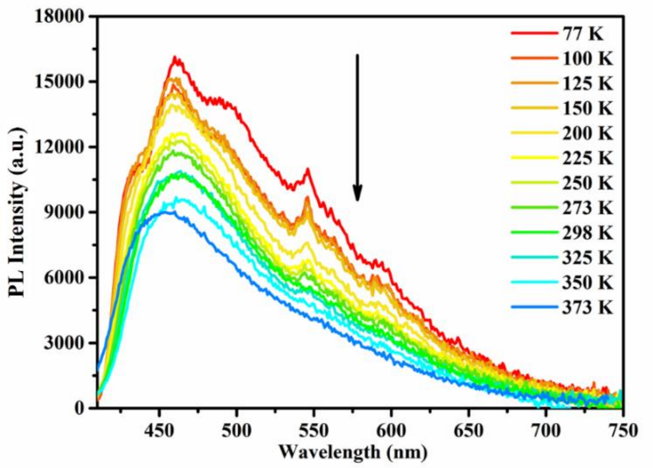

Fig. S16 Phosphorescence spectra of as prepared crystals of compound 1 under the different temperatures without door-gated instrument.

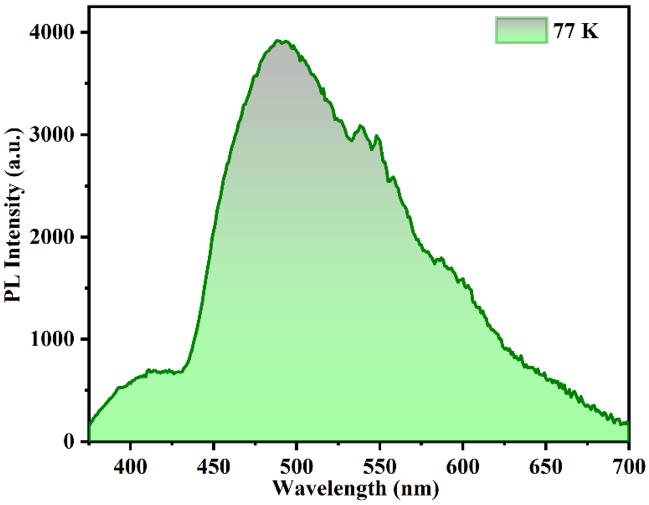

Fig. S17 Phosphorescence spectra of organic ligand compound CzIP in 1 × 10^{-5} mol/L chloroform at 77 K.

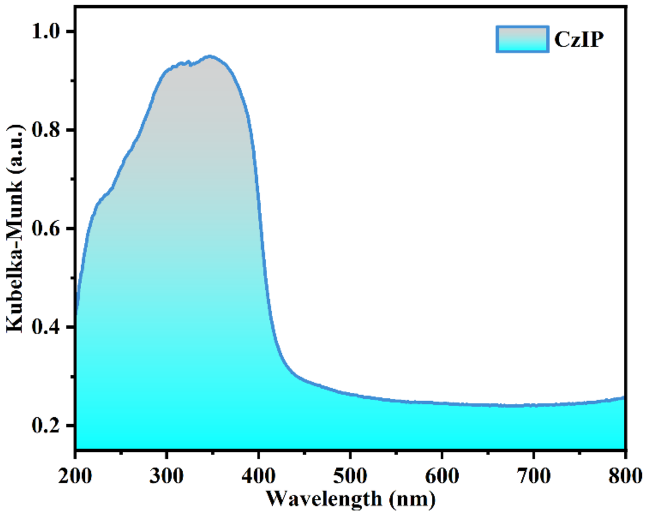

Fig. S18 UV-Visible absorption spectra of organic ligand powder under ambient conditions.

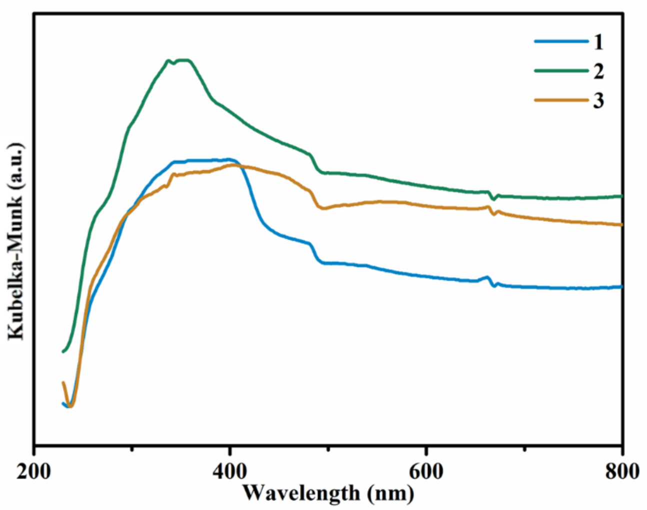

Fig. S19 UV-Visible absorption spectra of compounds 1-3 under ambient conditions.

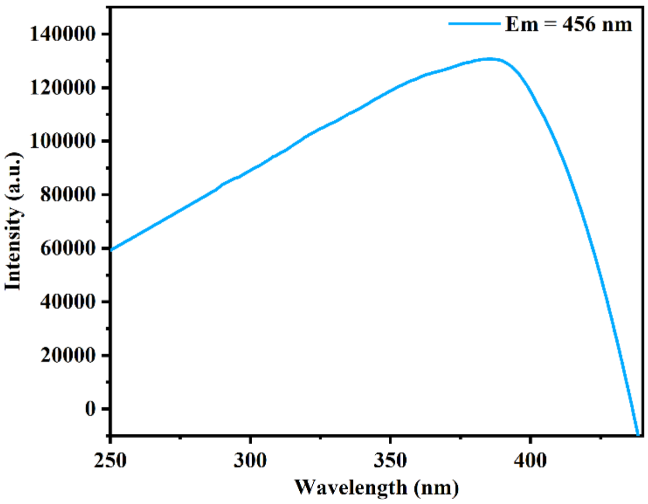

Fig. S20 Fluorescence excitation spectra of Compound 1 at Em = 456 nm.

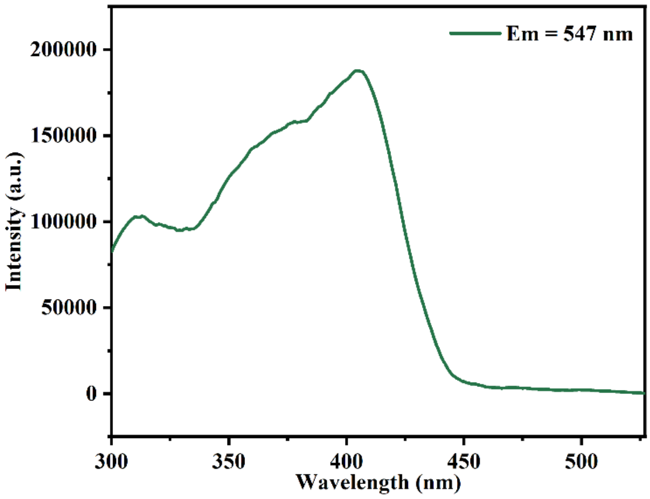

Fig. S21 Phosphorescent excitation spectra of Compound 1 at Em = 547 nm.

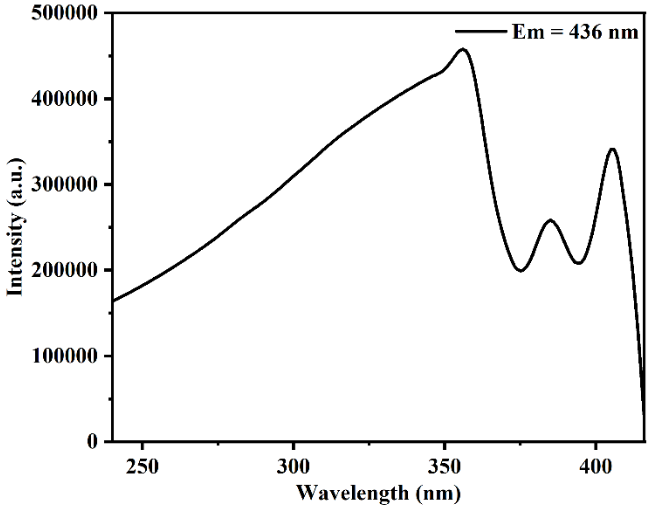

Fig. S22 Fluorescence excitation spectra of Compound 2 at Em = 436 nm.

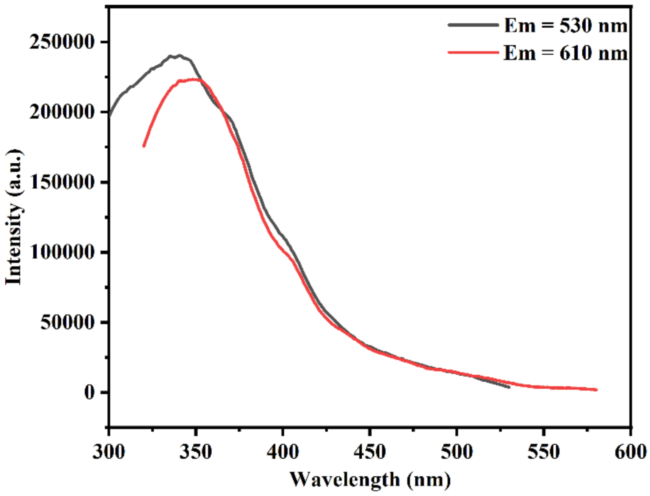

Fig. S23 Phosphorescent excitation spectra of Compound 2 at Em = 530 and 610 nm.

3. Supplementary Tables

Table S1. The crystallographic parameters of compounds 1-3.

Identification code	Compound 1	Compound 2	Compound 3
Empirical formula	$C_{20}H_{11}NO_4Zn$	$C_{25}H_{21}N_3O_5Zn$	$C_{40}H_{26}N_2O_{10}Zn_2$
Number of CCDC	2219861	2219862	2219863
Formula weight	394.67	555.85	919.43
Temperature/K	293(2)	293(2)	293(2)
Crystal system	monoclinic	monoclinic	'triclinic
Space group	$P2_1/c$	$P2_1/c$	P-1
a / Å	21.0731(17)	16.7905(5)	8.6941(3)
b / Å	4.6848(3)	7.6649(2)	10.0079(5)
c / Å	16.4494(12)	17.8041(5)	21.4461(10)
α / °	90	90	94.503(4)
β / °	103.377(8)	95.146(3)	96.145(3)
γ / °	90	90	114.370(4)
Volume/ Å^3	1579.9(2)	2282.11(12)	1674.41(13)
Z	4	4	2
ρ_{calc}g/cm^3	1.659	1.618	1.824
μ / mm^{-1}	1.582	0.999	1.338
F(000)	800	1120	912
Crystal size/ mm^3	0.08 × 0.15 × 0.16	0.10 × 0.12 × 0.16	0.10 × 0.12 × 0.16
Radiation	Mo-Kα (λ = 0.71073)	Mo-Kα (λ = 0.71073)	Mo-Kα (λ = 0.71073)
2θ range for data collection/°	5.082 to 57.000	8.276 to 55.860	7.560 to 55.176
Index ranges	$-22 \le h \le 28$, $-6 \le k \le 5$, $-18 \le l \le 22$	$-15 \le h \le 22$, $-8 \le k \le 9$, $-21 \le l \le 21$	$-10 \le h \le 9$, $-12 \le k \le 12$, $-27 \le l \le 28$
Reflections collected	3693	4751	6926
Independent reflections	2842 [R_{int} = 0.0625 R_{sigma} = 0.0946]	3827 [R_{int} = 0.0241, R_{sigma} = 0.0365]	5556 [R_{int} = 0.0242, R_{sigma} = 0.0503]
Goodness-of-fit on F^2	1.034	1.064	1.002
R_1 [I>2σ (I)]	R1 = 0.0560, wR2 = 0.1240	R1 = 0.0319, wR2 = 0.0657	R1 = 0.0340, wR2 = 0.0658
wR_2 (all data)	R1 = 0.0740, wR2 = 0.1403	R1 = 0.0446, wR2 = 0.0708	R1 = 0.0473, wR2 = 0.0706

Table S2. CIE, RGB and HSV values for the luminous colors of compounds 1.

Compound 1	CIE (x,y)	RGB	HSV	Hex codes
Phos.	0.47, 0.47	255, 195, 2	45.77, 99.22, 100	#FFC302
FL	0.25, 0.29	153, 221, 255	200, 40, 100	#99DDFF
PL	0.33, 0.36	255, 255, 226	60, 11.37, 100	#FFFFE2

Table S3. CIE, RGB and HSV values for the luminous colors of compounds 2.

Compound 2	CIE (x,y)	RGB	HSV	Hex codes
Phos.	0.47, 0.44	255, 180, 56	37.39, 78.04, 100	#FFB438
FL	0.24, 0.22	151, 162, 255	233.6, 40.78, 100	#97A2FF
PL	0.34, 0.33	255, 212, 212	0, 16.36, 100	#FFD4D4

4. References

1 M. Zhou, P. Gao,, Y. Jiang, Y. Zhou, J. Wu, X. Zhu and H. Fu, *Dyes Pigm.*, 2021, **195**, 109715.

2 G.M. Sheldrick, *Acta Crystallogr. C* 2015, **71**, 3–8.

3 L. J. Bourhis, O. V. Dolomanov, R. J. Gildea, J. A. K. Howard and H. Puschmann, *Acta Crystallogr. A*, 2015. **71**, 59–75.