

Supporting Information

Photo-facilitated aggregation and correlated color temperature adjustment of single component organic solid state white-light emitting materials

Cheng Chen,^a Xu-Hui Jin,^{a‡} Xue-Jun Zhou,^a Li-Xuan Cai,^a Ya-Jun Zhang^a and Jie Zhang*^{a,b}

^a State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, CAS, Fuzhou, Fujian 350002, P. R. China, E-mail: zhangjie@fjirsm.ac.cn

^b School of Chemistry, Beijing Institute of Technology, Beijing, 100081, P. R. China

[‡] Current address: Department of Organic Chemistry, Weizmann Institute of Science, Rehovot 76100, Israel

Additional Figures and Table

Fig. S1 The spectra data and the molecular structure of **PTP**.

Fig. S2 UV-Vis and fluorescence spectra of **PTP** and **BPTP** measured in different solvents.

Fig. S3 The electron spin resonance spectra of **BPTP** measured in solution.

Fig. S4 UV-Vis absorption spectra and fluorescence spectra of **BPTP** at different concentrations.

Fig. S5 UV-Vis spectra of **PTP** measured before and after UV light irradiation.

Fig. S6 The fluorescence spectrum of **BPTP** in thin film state.

Fig. S7 XRPD patterns of four crystalline materials.

Fig. S8 The molecular packing arrangement in four crystalline materials.

Fig. S9 Excitation spectra of four crystalline materials.

Fig. S10 Fluorescence decay curves of freshly prepared **BPTP** solution in *n*-butanol and after UV irradiation .

Fig. S11 Fluorescence decay curves of four crystalline materials.

Fig. S12 The electron spin resonance spectra of four crystalline materials.

Fig. S13 The ¹H NMR spectrum of **PTP**.

Fig. S14 The ¹H NMR spectrum of **BPT**.

Table S1. The UV spectral data of **BPTP** measured in different solvents.

Table S2. The photophysical parameters of four crystalline materials.

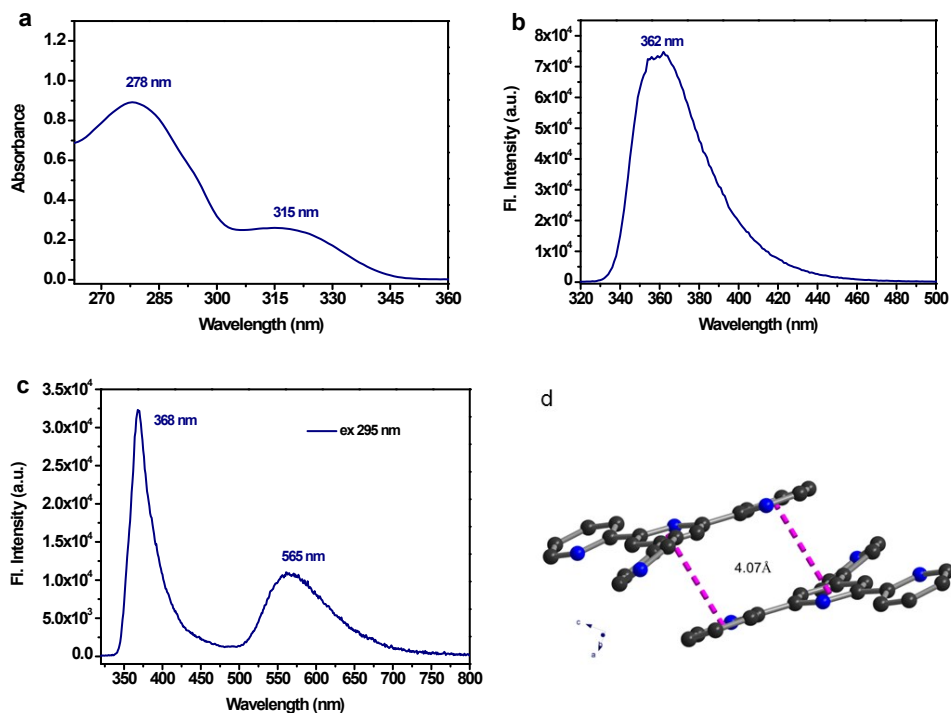


Fig. S1 (a) The UV absorption spectrum of **PTP** (2.5×10^{-5} mol/L) measured in *n*-butanol solution. (b) The fluorescence spectrum of **PTP** (2.5×10^{-5} mol/L) measured in *n*-butanol solution. (c) The solid state fluorescence spectrum of **PTP**. (d) The non-planar propeller-like conformation and the stacking mode of **PTP** in crystalline state, the closest centroid distance is 4.07 Å.

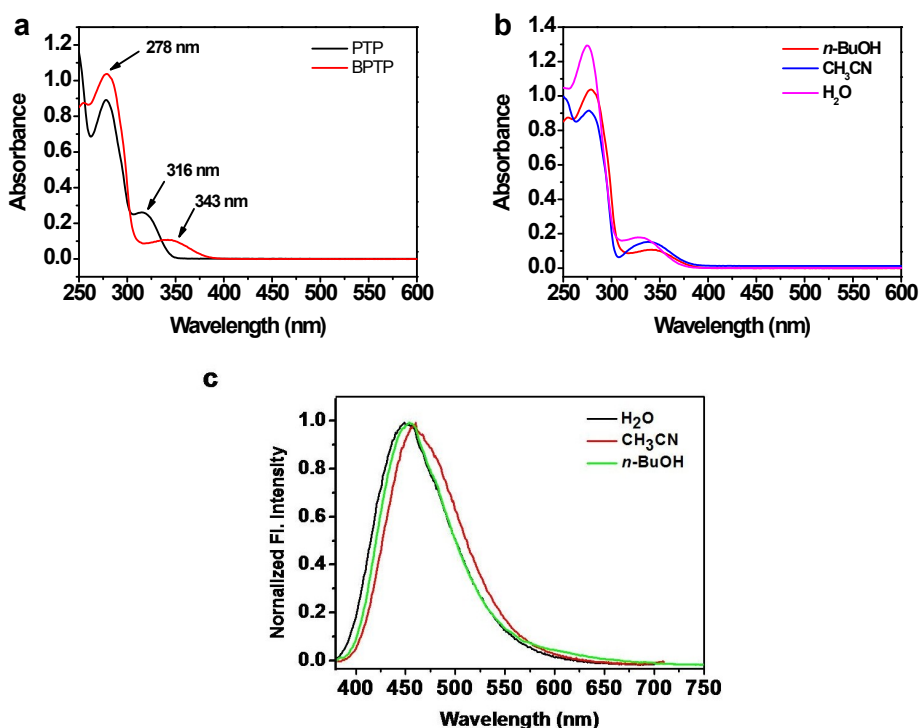


Fig. S2 (a) The UV-Vis absorption spectra of **PTP** and **BPTP** (2.5×10^{-5} mol/L) measured in *n*-butanol solution. (b) The UV-Vis absorption spectra of **BPTP** (2.5×10^{-5} mol/L) measured in *n*-butanol, acetonitrile and aqueous solutions. (c) The fluorescence spectra of **BPTP** (2.5×10^{-5} mol/L) measured in *n*-butanol, acetonitrile and aqueous solutions, and there fluorescence emission bands were at 455 nm, 460 nm and 449 nm, respectively.

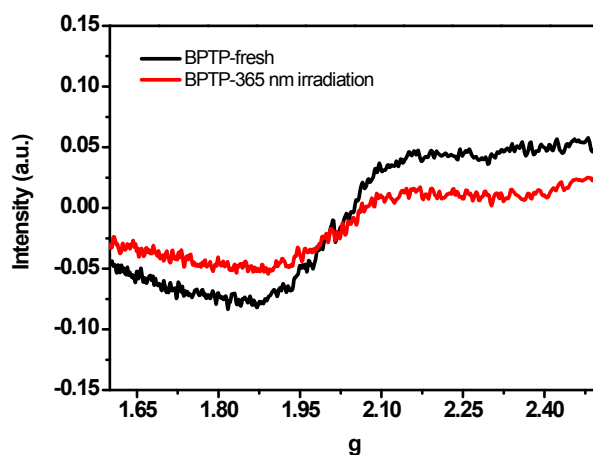


Fig. S3 The electron spin resonance spectra of **BPTP** (2.5×10^{-5} mol/L) measured in freshly prepared *n*-butanol solution (black) and after UV light (365 nm) irradiation for 100 minutes (red).

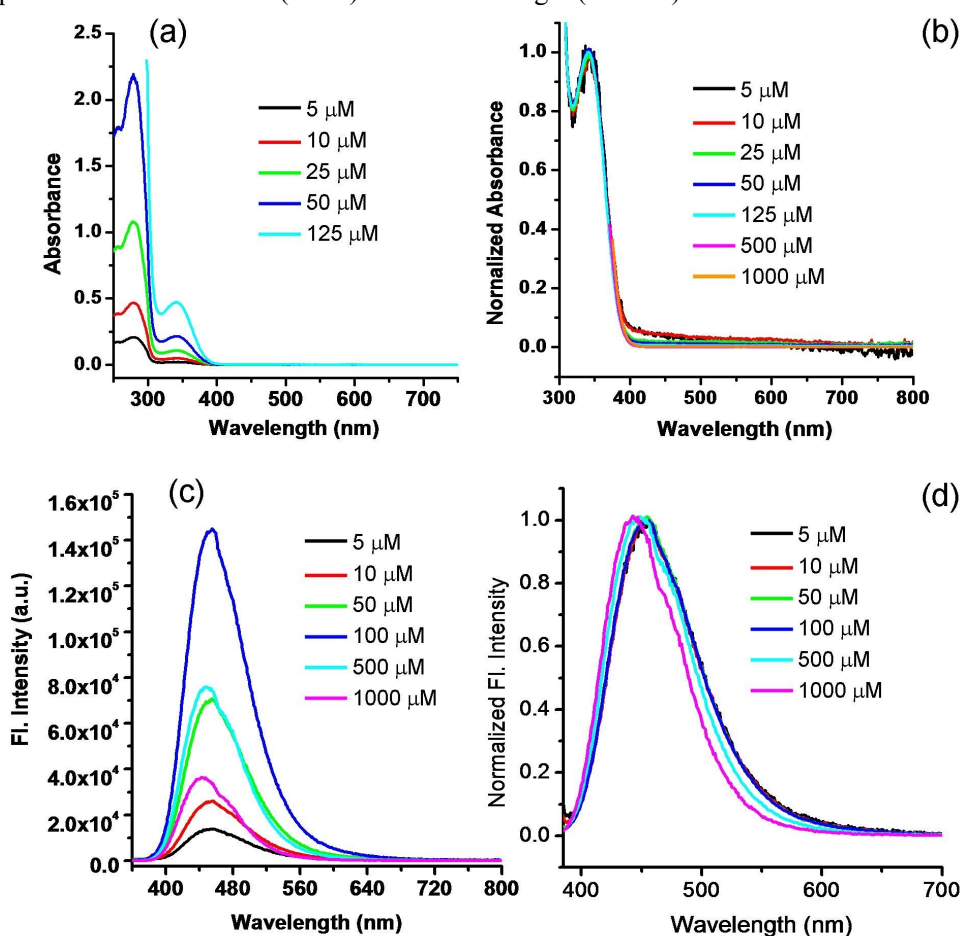


Fig. S4 (a) Concentration dependence of UV-Vis absorption spectra for **BPTP** in *n*-butanol solution. (b) Normalized adsorption spectra in the wavelength region of 300-800 nm at different concentrations. The small difference in the wavelength above 400 nm should be due to the deviation of baseline of the spectra for the sample in low concentration. (c) Fluorescence emission spectra for **BPTP** in *n*-butanol solution at different concentrations with the excitation wavelength of 345 nm. (d) Normalized emission spectra for **BPTP** in *n*-butanol solution at different concentrations with the excitation wavelength of 345 nm. The absorption spectra have little change with increasing the concentration of the solution, indicating weak intermolecular charge transition in the ground state in the absence of light irradiation, which is consistent with the observation on the fluorescence emission spectra without the emergence of the long-wavelength emission band.

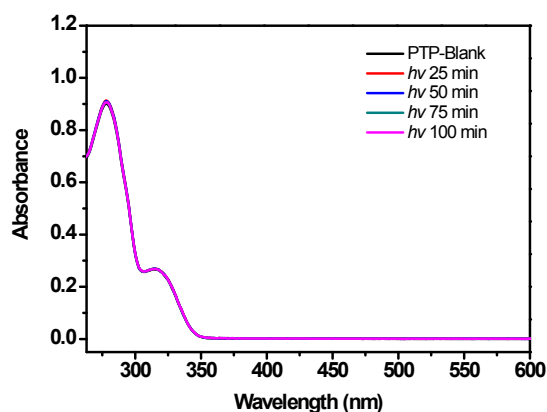


Fig. S5 The UV-Vis absorption spectra of **PTP** measured in freshly prepared *n*-butanol solution and after UV light (365 nm) irradiation.

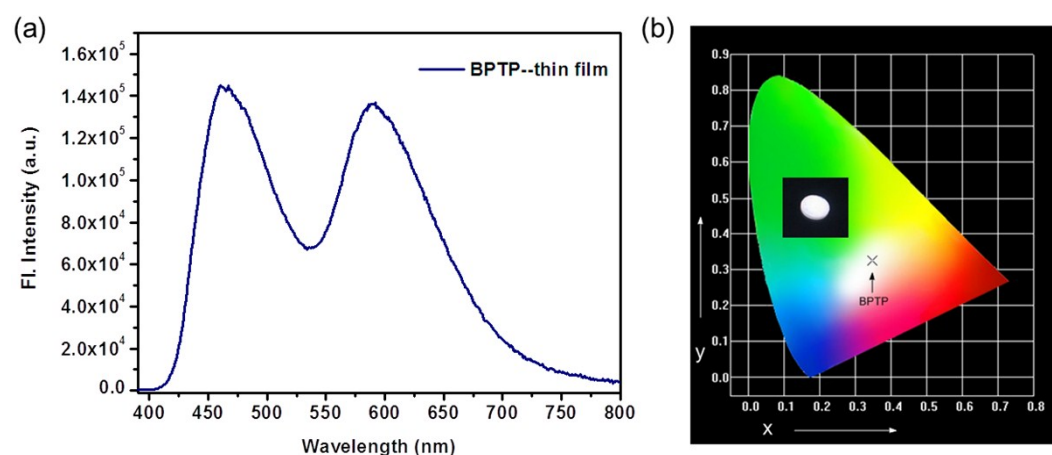


Fig. S6 (a) The fluorescence spectrum of the **BTPP** in thin film state; (b) Emission colors in a CIE 1931 chromaticity diagram: **BTPP** (0.347, 0.325). The insert photograph were taken under UV light (365 nm hand-held UV lamp, $1.2 \text{ mW}\cdot\text{cm}^{-2}$), showing the white-light emission of this material.

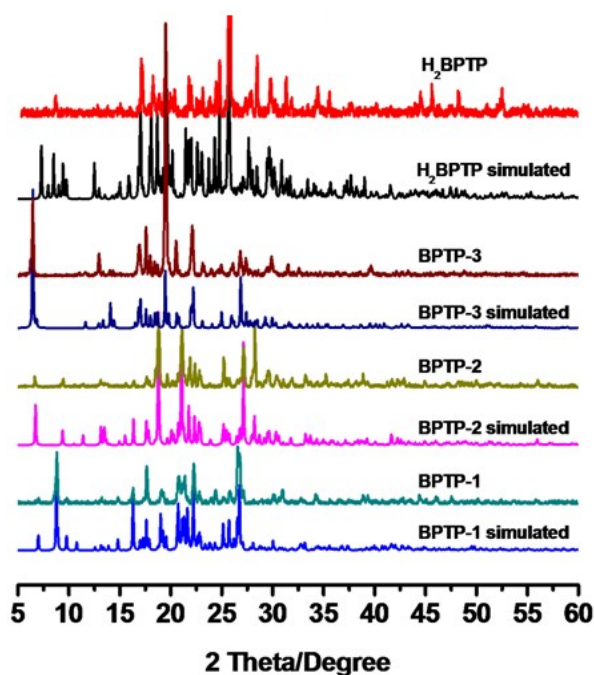


Fig. S7 The calculated and experimental XRPD patterns of four crystalline materials.

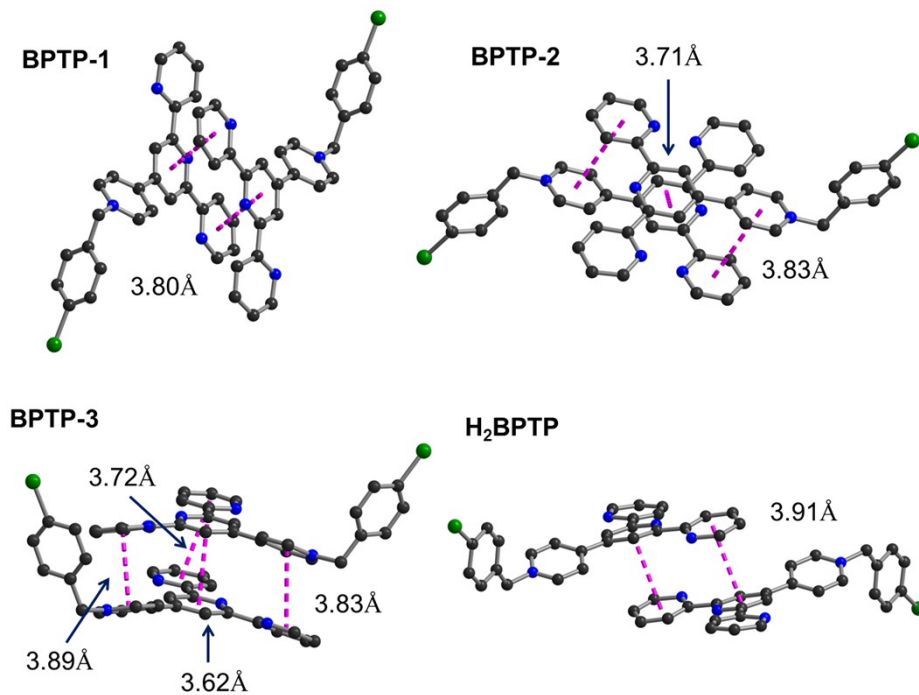


Fig. S8 The π -stacking interactions in four crystalline materials.

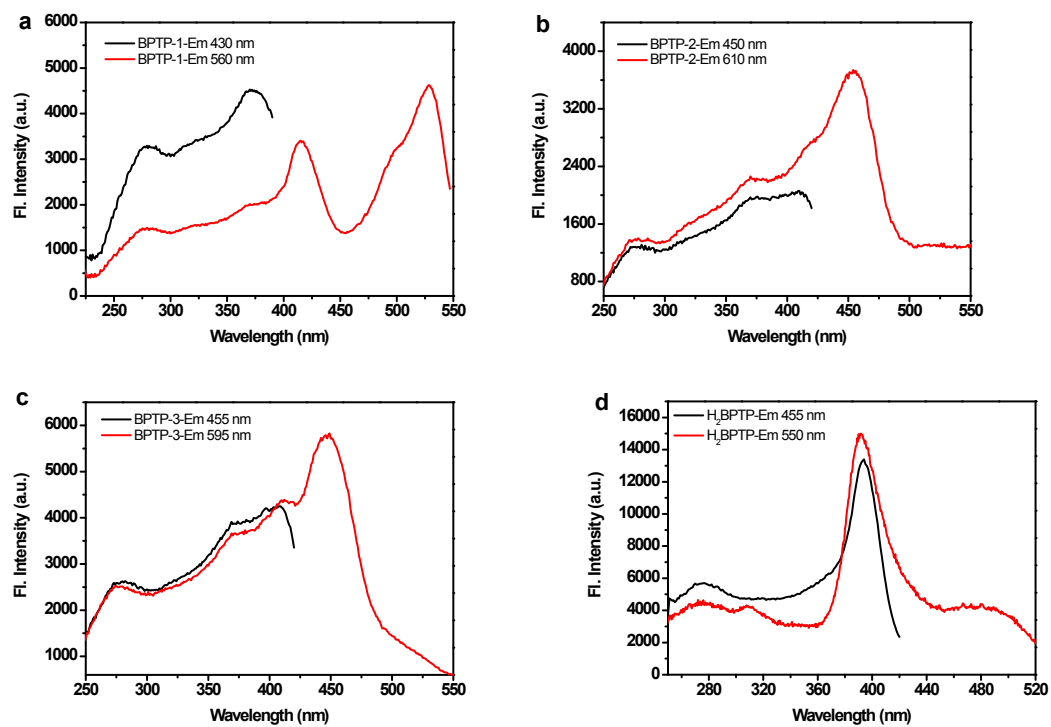


Fig. S9 Excitation spectra of four materials monitored at corresponding wavelength in crystalline states. (a) **BPTP-1**; (b) **BPTP-2**; (c) **BPTP-3** and (d) **H₂BPTP**.

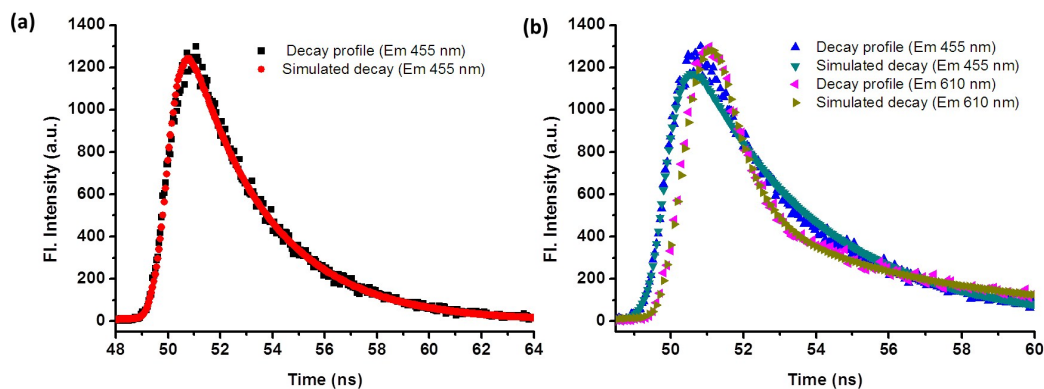


Fig. S10 Fluorescence decay curves of freshly prepared **BPTP** solution in *n*-butanol (a) and after UV irradiation (b).

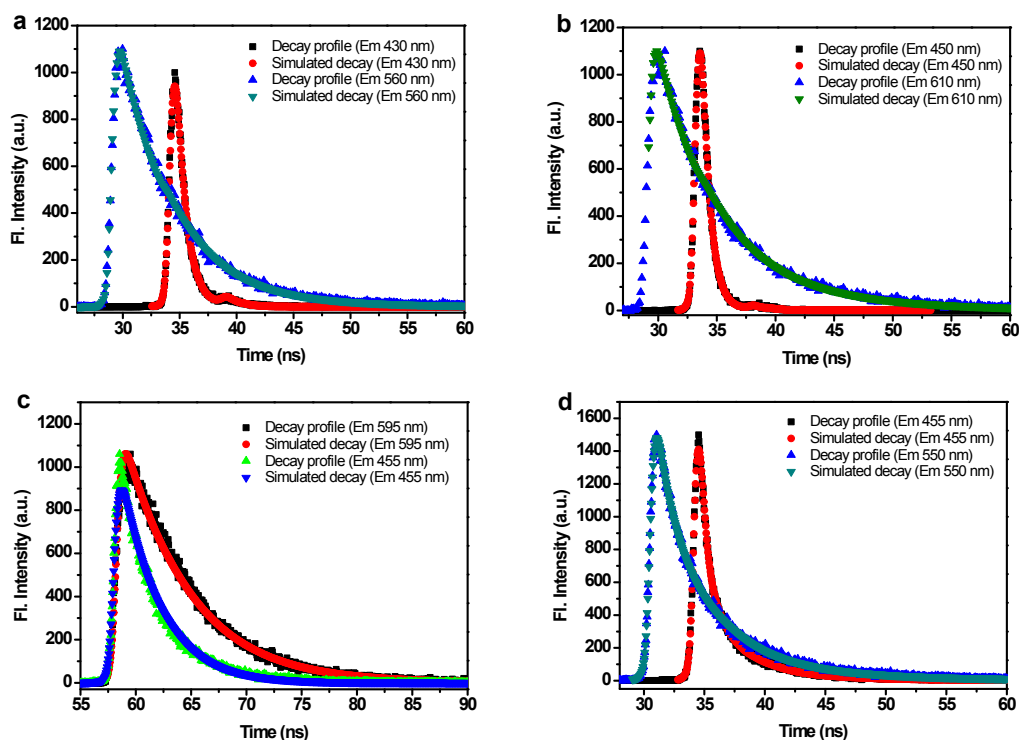


Fig. S11 Fluorescence decay curves of four crystalline materials. (a) **BPTP-1**, (b) **BPTP-2**, (c) **BPTP-3** and (d) **H₂BPTP**. $\lambda_{\text{ex}} = 345$ nm, monitoring wavelengths are shown as inset.

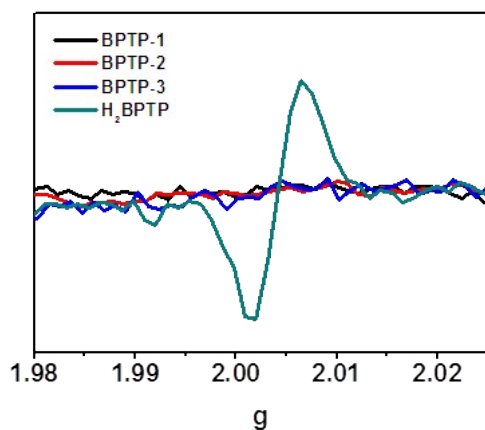


Fig. S12 The electron spin resonance spectra of **BPTP-1**, **BPTP-2**, **BPTP-3** and **H₂BPTP**.

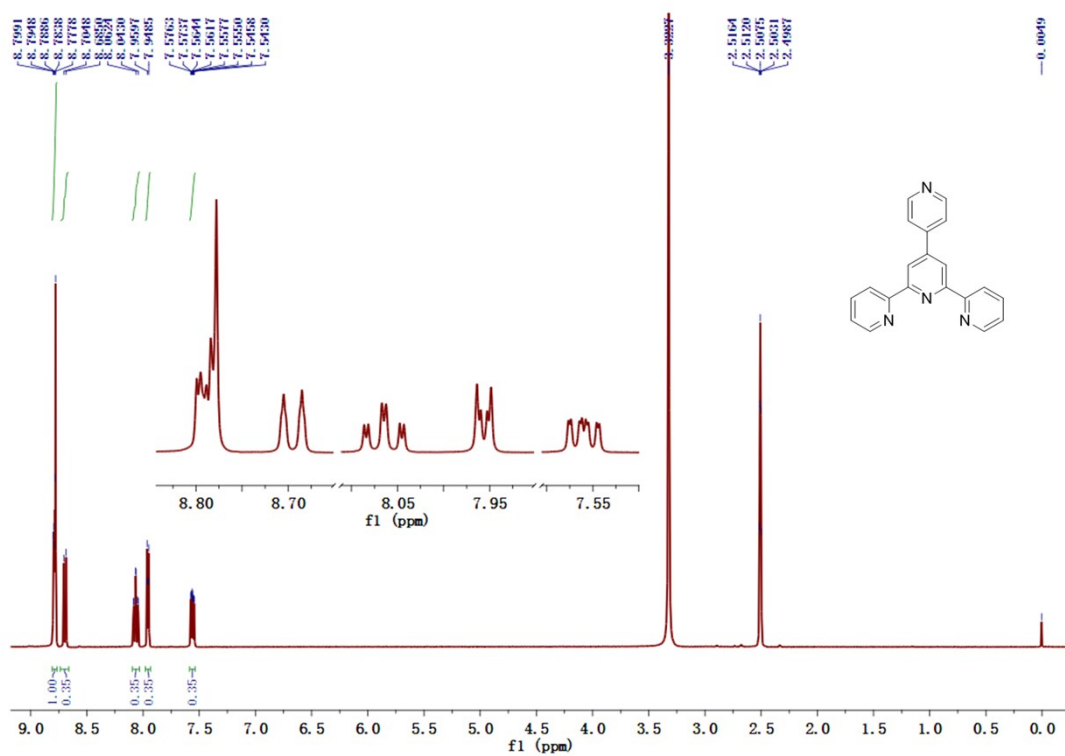


Fig. S13 The ^1H NMR spectrum of **PTP** measured in DMSO-D6 (400 MHz).

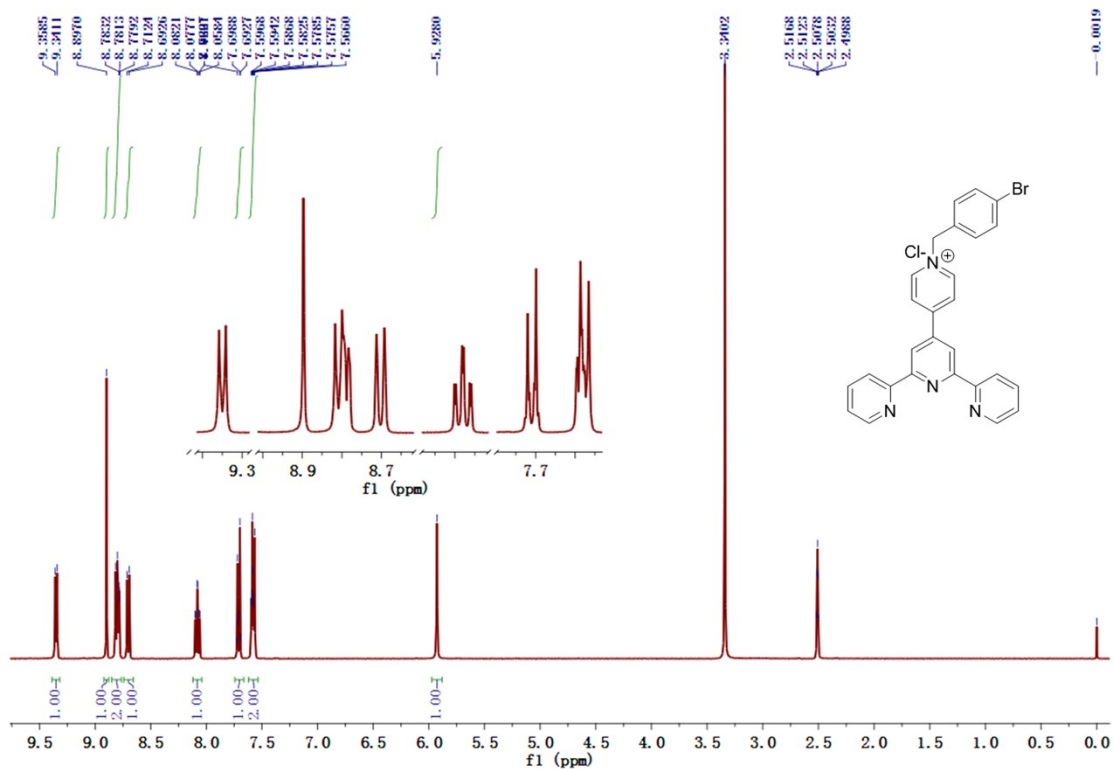


Fig. S14 ^1H NMR spectrum of **BPT** measured in DMSO-D6 (400 MHz).

Table S1. The UV-Vis absorption bands of **BPTP** (2.5×10^{-5} mol/L) measured in different solutions.

Solvent	H ₂ O	CH ₃ CN	EtOH	THF	n-BuOH	CHCl ₃
Absorption bands (nm)	274/327	277/337	278/339	277/342	278/343	278/351

Table S2. The photophysical parameters of the compounds: PL maxima (λ), PL quantum yields and decay times (Φ_{PL} , τ).

Compd	single crystal				
	λ_1 (nm)	λ_2 (nm)	τ_1 (ns) ^a	τ_2 (ns) ^b	Φ_{PL} (%)
BPTP in <i>n</i> -butanol	455 ^c		2.93(100%)		/
	455 ^d	610 ^d	3.33(100%) ^d	0.67(28.33%) ^d	/
				4.55(41.33%) ^d	
			23.03(30.35%) ^d		
BPTP-1	430	560	0.85(100%)	4.28(87.08%)	5.54
				9.86(12.92%)	
BPTP-2	450	610	0.67(100%)	4.23(62.97%)	5.46
				9.28(37.03%)	
BPTP-3	455	595	3.38(100%)	5.75(100%)	7.40
H₂BPTP	455	550	0.38(29.16%)	1.02(11.43%)	/
			1.90(42.26%)	3.68(60.39%)	
			5.48(28.60%)	9.24(28.18%)	

^a The fluorescence lifetime corresponding to the λ_1 . ^b The fluorescence lifetime corresponding to the λ_2 .

^c Freshly prepared solution. ^d after light irradiation.