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Mechanical force-induced luminescent enhancement and chromism of a nonplanar D-A phenothiazine derivative

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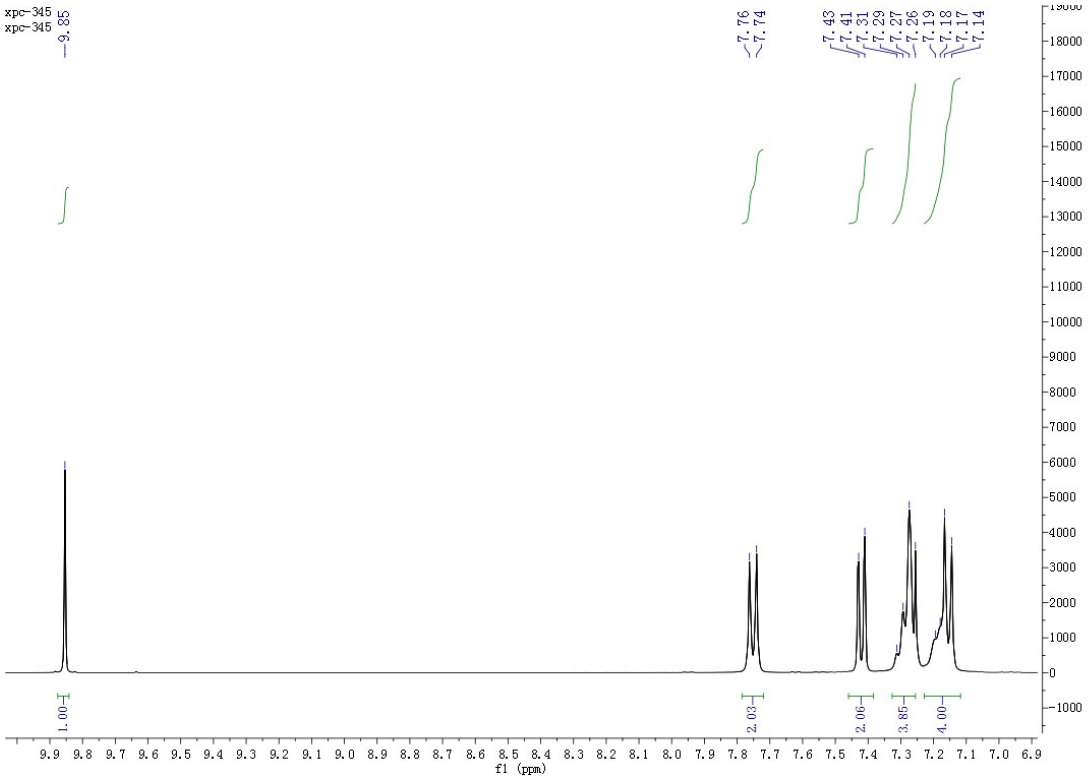

Fig. S1 ^{1}H NMR of **PBA** in $CDCl_3$.

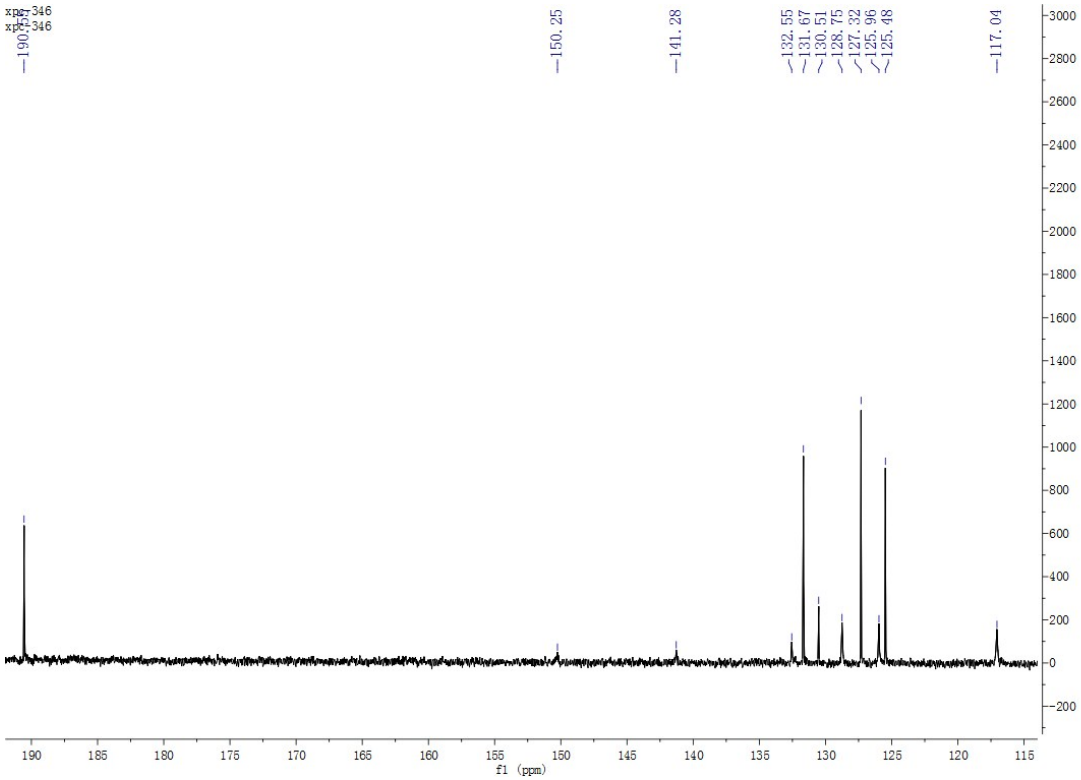

Fig. S2 ^{13}C NMR of **PBA** in $CDCl_3$.

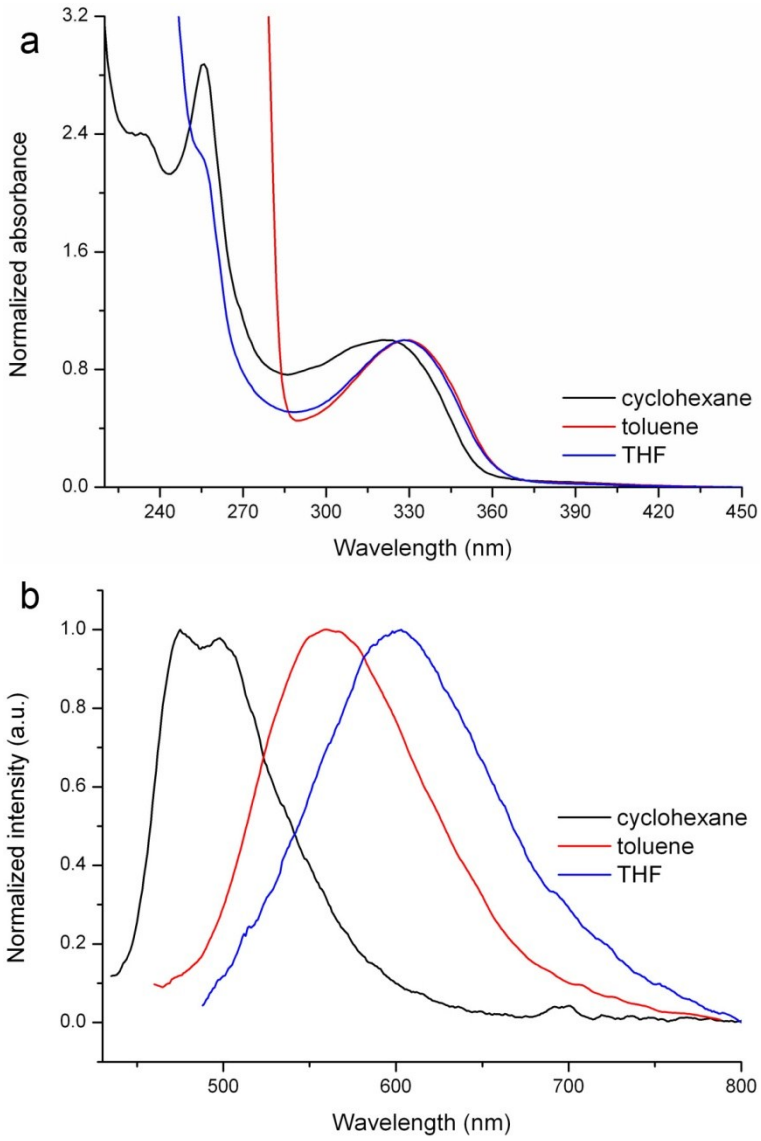

Fig. S3 Absorption (a) and fluorescence (b) spectra of **PBA** in different solvents. λ_{ex} = 340 nm.

Table S1. Computed vertical excitation spectra of **PBA** in Form A based on the optimal structure at ground state.

Excited State	Transition	Bandgap (eV)	Absorption (nm)	Oscillator strength
Triplet (T_1)	HOMO–LUMO (96.7%)	2.7086	457.74	0.0000
Singlet (S_1)	HOMO–LUMO (98.8%)	2.7360	453.17	0.0049
Triplet (T_2)	HOMO-4–LUMO (92.2%); HOMO-4–LUMO+6 (6.8%)	3.0942	400.70	0.0000
Triplet (T_3)	HOMO-2–LUMO+5 (3.9%); HOMO-1–LUMO+4 (4.2%); HOMO–LUMO+1 (29.9%) HOMO–LUMO+2 (39.1%); HOMO–LUMO+3 (14.9%)	3.2217	384.84	0.0000
Triplet (T_4)	HOMO-6–LUMO+1 (12.2%); HOMO-5–LUMO (65.2%) HOMO-3–LUMO (8.3%); HOMO-1–LUMO (4.1%)	3.4829	355.98	0.0000
Triplet (T_5)	HOMO-3–LUMO+4 (2.6%); HOMO-2–LUMO+1 (2.6%) HOMO-2–LUMO+2 (6.2%); HOMO-1–LUMO+3 (5.2%) HOMO–LUMO+1 (4.0%) HOMO–LUMO+2 (25.8%) HOMO–LUMO+3 (32.3%) HOMO–LUMO+5 (13.1%)	3.5110	353.13	0.0000
Singlet (S_2)	HOMO–LUMO+1 (94.2%); HOMO–LUMO+2 (3.5%)	3.6460	340.06 453.17	0.0010
Triplet (T_6)	HOMO–LUMO+1 (48.8%); HOMO–LUMO+2 (10.9%) HOMO–LUMO+3 (5.5%); HOMO–LUMO+4 (15.5%) HOMO–LUMO+5 (5.2%)	3.7039	334.74	0.0000
Triplet (T_7)	HOMO-3–LUMO+4 (7.0%); HOMO-2–LUMO+2 (3.1%) HOMO-1–LUMO (6.2%); HOMO-1–LUMO+2 (2.2%) HOMO-1–LUMO+3 (7.9%); HOMO–LUMO+1 (3.4%) HOMO–LUMO+2 (4.5%); HOMO–LUMO+3 (33.1%) HOMO–LUMO+3 (23.8%)	3.7261	332.74	0.0000
Triplet (T_7)	HOMO-5–LUMO (2.6%); HOMO-1–LUMO (85.9%) HOMO–LUMO+5 (2.7%)	3.7668	32.15	0.0000
Singlet (S_3)	HOMO-4–LUMO (2.1%); HOMO-1–LUMO (96.1%)	3.7696	328.90	0.0025
Singlet (S_4)	HOMO–LUMO+1 (4.4%); HOMO–LUMO+2 (70.1%) HOMO–LUMO+3 (22.4%)	3.9672	312.52	0.0023
Singlet (S_5)	HOMO–LUMO+2 (22.4%); HOMO–LUMO+3 (71.7%)	4.1546	298.43	0.0187
Singlet (S_5)	HOMO-1–LUMO+1 (4.2%); HOMO-1–LUMO+2 (6.0%) HOMO–LUMO+3 (86.1%);	4.3534	284.80	0.0578
Singlet (S_6)	HOMO-2–LUMO (98.2%)	4.5246	274.02	0.0057
Singlet (S_7)	HOMO-3–LUMO (95.8%)	4.6305	267.75	0.0179
Singlet (S_8)	HOMO–LUMO (91.6%); HOMO–LUMO (3.2%)	4.7447	261.31	0.0516

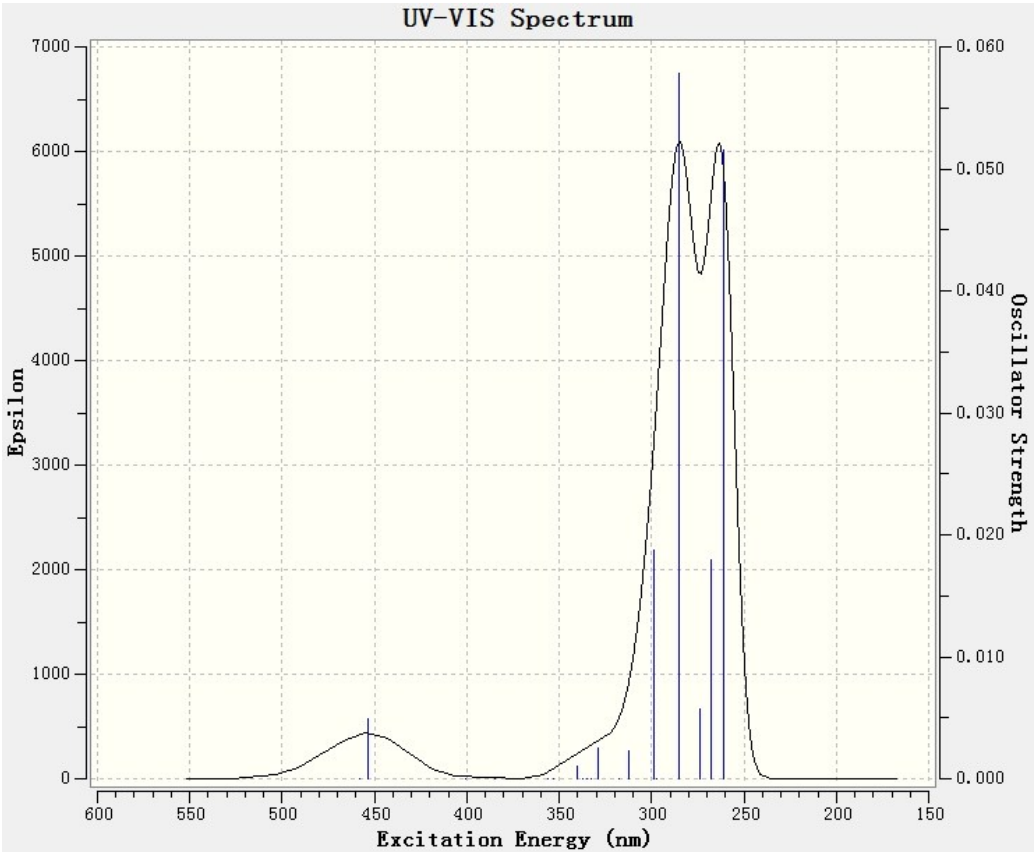

Fig. S4 Stimulated UV-Vis spectra of Form A.

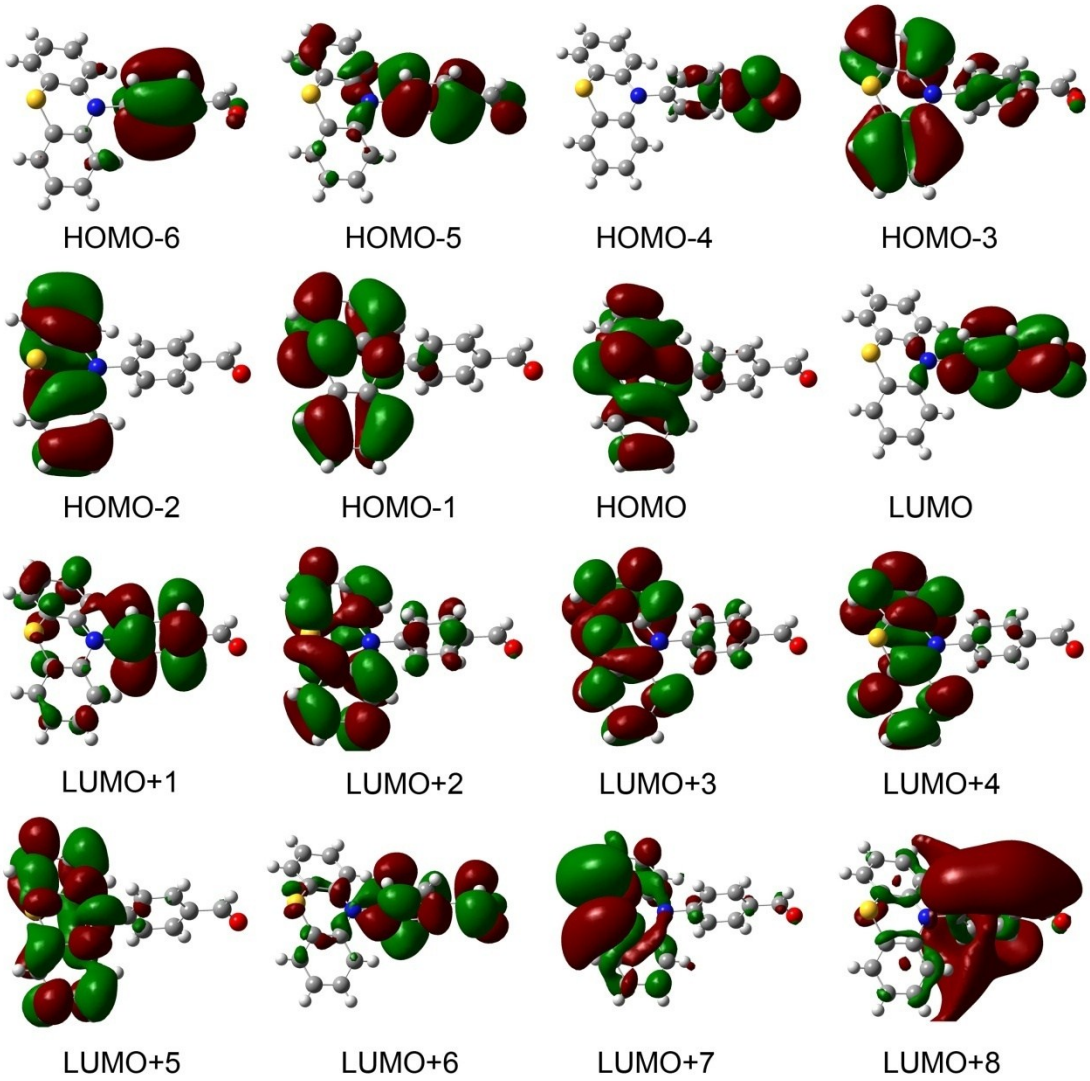

Fig. S5 Frontier molecular orbitals of Form A.

Table S2. Computed vertical excitation spectra of **PBA** in Form B based on the optimal structure at ground state.

Excited State	Transition	Bandgap (eV)	Absorption (nm)	Oscillator strength
Triplet (T_1)	HOMO-5–LUMO (3.2%) HOMO-1–LUMO (6.6%) HOMO–LUMO (81.8%)	2.8866	429.51	0.0000
Triplet (T_2)	HOMO-2–LUMO (84.8%) HOMO-2–LUMO+1 (3.5%) HOMO-2–LUMO+4 (5.2%) HOMO-2–LUMO+8 (5.2%)	3.2812	381.02	0.0000
Triplet (T_3)	HOMO-6–LUMO+2 (6.9%) HOMO-5–LUMO (3.7%) HOMO-5–LUMO+1 (5.5%) HOMO-4–LUMO+2 (4.0%) HOMO-4–LUMO+3 (6.2%) HOMO-1–LUMO (3.7%) HOMO-1–LUMO+1 (9.4%) HOMO-1–LUMO+4 (7.5%) HOMO–LUMO+1 (6.9%) HOMO–LUMO+3 (5.1%) HOMO–LUMO+4 (27.0%)	3.4564	358.71	0.0000
Triplet (T_4)	HOMO-6–LUMO+1 (98.8%) HOMO-6–LUMO+4 (7.5%) HOMO-6–LUMO+3 (2.9%) HOMO-5–LUMO (4.5%) HOMO-4–LUMO+1 (3.7%) HOMO-4–LUMO+4 (4.1%) HOMO-1–LUMO+2 (5.9%) HOMO–LUMO+2 (25.1%) HOMO–LUMO+3 (13.1%)	3.4870	355.56	0.0000
Singlet (S_1)	HOMO-2–LUMO (85.1%) HOMO-2–LUMO+1 (2.7%) HOMO-2–LUMO+4 (3.9%) HOMO-2–LUMO+8 (2.6%) HOMO–LUMO (4.4%)	3.7799	328.01	0.0159
Triplet (T_5)	HOMO-6–LUMO+2 (2.2%) HOMO-1–LUMO+1 (9.1%) HOMO-1–LUMO+4 (3.3%) HOMO–LUMO+1 (78.6%)	3.8107	325.36	0.0000
Singlet (S_2)	HOMO-2–LUMO (4.1%) HOMO–LUMO (74.0%) HOMO–LUMO+1 (29.0%) HOMO–LUMO+4 (11.4%)	3.8501	322.03	0.3274
Triplet (T_6)	HOMO-1–LUMO+5 (2.8%) HOMO–LUMO+2 (18.5%) HOMO–LUMO+3 (49.8%) HOMO–LUMO+4 (10.0%) HOMO–LUMO+5 (12.4%)	3.8517	321.89	0.0000
Triplet (T_7)	HOMO-6–LUMO+3 (3.5%) HOMO-6–LUMO+5 (2.2%) HOMO-5–LUMO+1 (8.9%) HOMO-1–LUMO (30.0%) HOMO–LUMO +1(28.0%) HOMO–LUMO (4.8%) HOMO–LUMO+1 (3.5%) HOMO–LUMO+4 (10.7%)	4.0153	308.78	0.0000
Singlet (S_3)	HOMO–LUMO+2 (88.1%) HOMO–LUMO+3 (7.1%)	4.1064	301.93	0.0015
Singlet (S_4)	HOMO–LUMO (11.7%) HOMO–LUMO+1 (73.5%) HOMO–LUMO+4 (8.5%)	4.1354	299.81	0.0890
Singlet (S_5)	HOMO-3–LUMO (2.5%) HOMO–LUMO+2 (76.2%) HOMO–LUMO+3 (81.5%) HOMO–LUMO+4 (5.2%)	4.2193	293.85	0.0104
Singlet (S_6)	HOMO-1–LUMO (52.5%) HOMO-1–LUMO+1 (2.2%) HOMO–LUMO+1 (3.7%) HOMO–LUMO+4 (36.6%)	4.3293	286.38	0.0004
Singlet (S_7)	HOMO-1–LUMO (38.9%) HOMO–LUMO (4.8%) HOMO–LUMO+3 (4.0%) HOMO–LUMO+4 (41.8%) HOMO–	4.3388	285.76	0.0999

	LUMO+5 (2.0%)			
Singlet (S_8)	HOMO-3–LUMO (20.5%) HOMO-1–LUMO+2 (3.7%) HOMO-1–LUMO+3 (5.9%) HOMO–LUMO+5 (58.2%)	4.5064	275.13	0.0064
Singlet (S_9)	HOMO-1–LUMO (4.7%) HOMO-1–LUMO+1 (88.8%)	4.5383	273.20	0.0500
Singlet (S_{10})	HOMO-3–LUMO+1 (2.4%) HOMO-1–LUMO (4.6%) HOMO-1–LUMO+2 (68.7%) HOMO-1–LUMO+3 (8.9%) HOMO–LUMO+6 (2.2%) HOMO–LUMO+5 (5.2%) HOMO–LUMO+6 (2.5%)	4.6313	267.71	0.1078

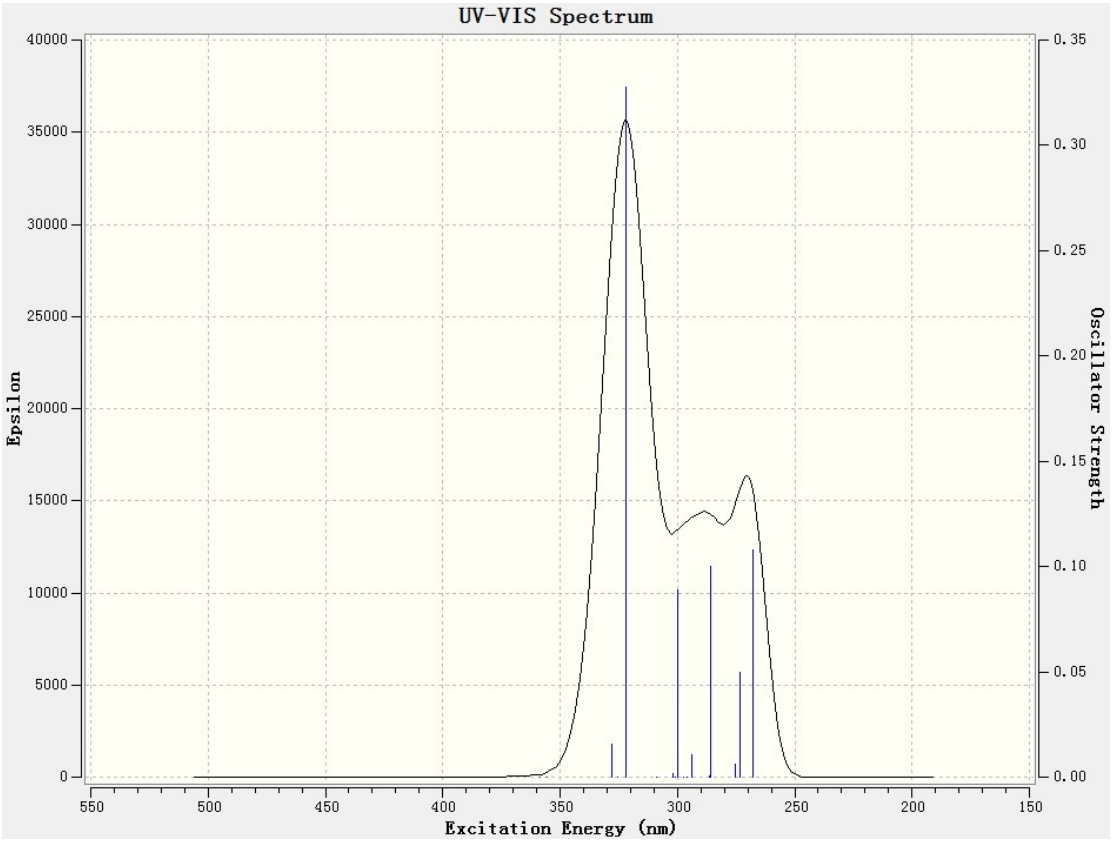

Fig. S6 Stimulated UV-Vis spectra of Form A.

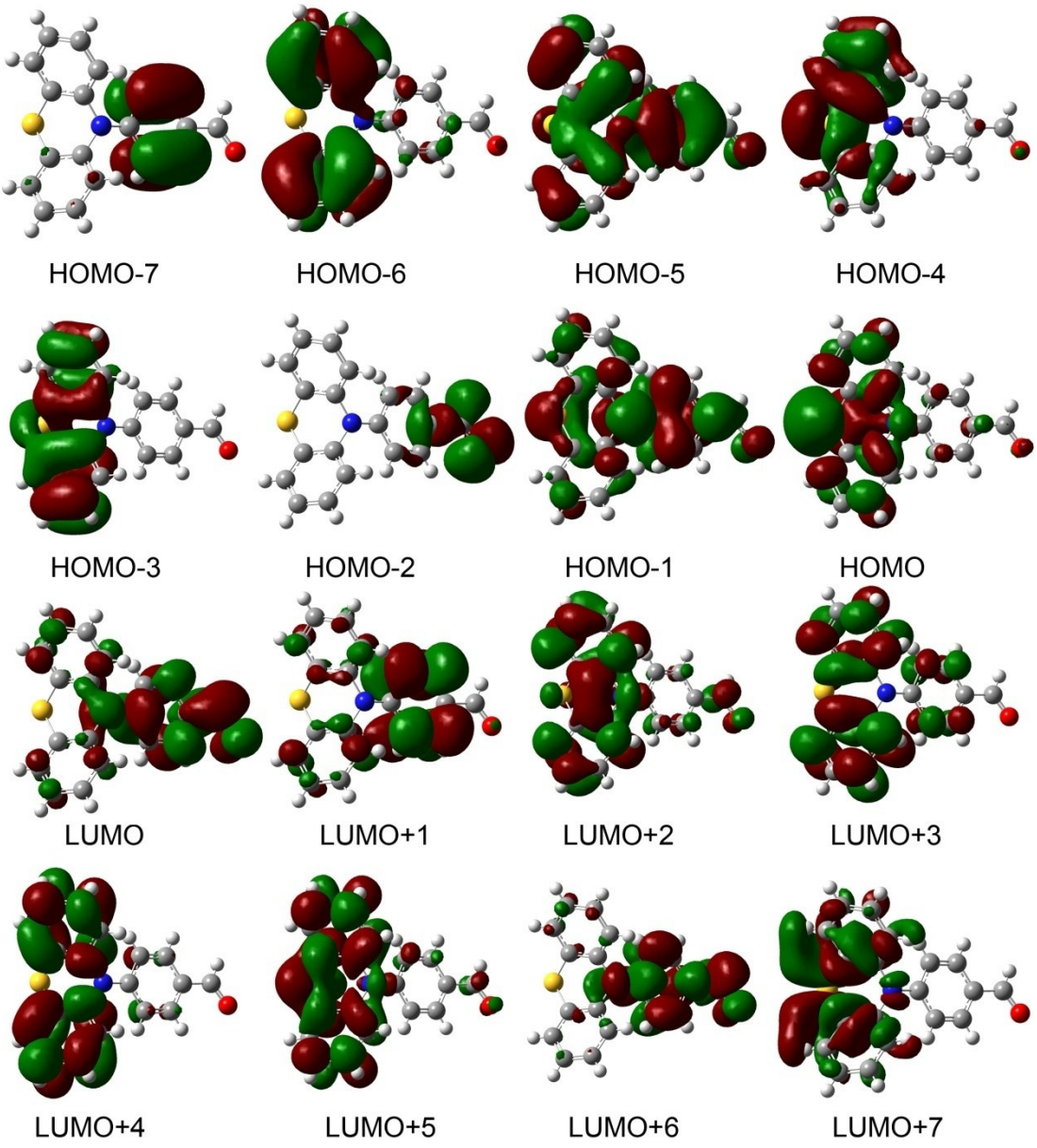

Fig. S7 Frontier molecular orbitals of Form B.

Table S3. Computed vertical excitation spectra of **PBA** in Form B in THF based on the optimal structure at ground state.

Excited State	Transition	Bandgap (eV)	Absorption (nm)	Oscillator strength
Singlet (S_1)	HOMO-1–LUMO (6.0%) ; HOMO–LUMO (85.6%) HOMO–LUMO+1 (8.4%)	3.6955	335.50	0.3401
Singlet (S_2)	HOMO-2–LUMO (87.7%) ; HOMO-2–LUMO+1 (5.0%); HOMO-2–LUMO+4 (2.5%) ; HOMO-2–LUMO+8 (4.8%)	3.7652	329.29	0.0216

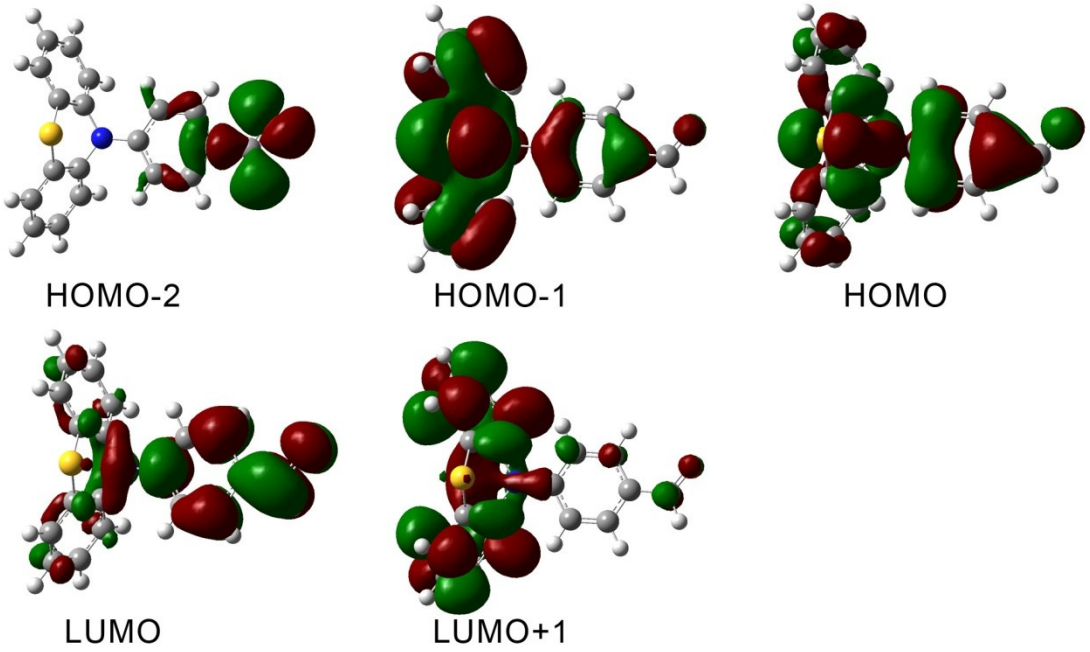

Fig. S8 Frontier molecular orbitals of Form B in THF.

Table S4. Computed vertical excitation spectra of **PBA** in Form B based on the structure in crystal.

Excited State	Transition	Bandgap (eV)	Absorption (nm)	Oscillator strength
Singlet (S_1)	HOMO–LUMO (95.7%); HOMO–LUMO+1 (4.3%)	3.7277	332.60	0.5236
Singlet (S_2)	HOMO-2–LUMO (100%); HOMO-2–LUMO+4 (2.5%) ; HOMO-2–LUMO+8 (4.8%)	3.8714	320.26	0.0072
Singlet (S_3)	HOMO-1–LUMO (60.4%) ; HOMO–LUMO+1 (39.6%);	4.1970	295.41	0.0404

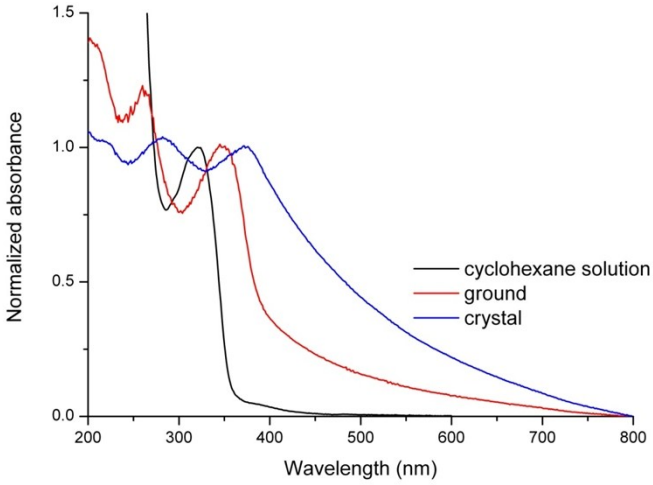

Fig. S9 UV-vis absorption spectra of solution, crystal and ground powders.

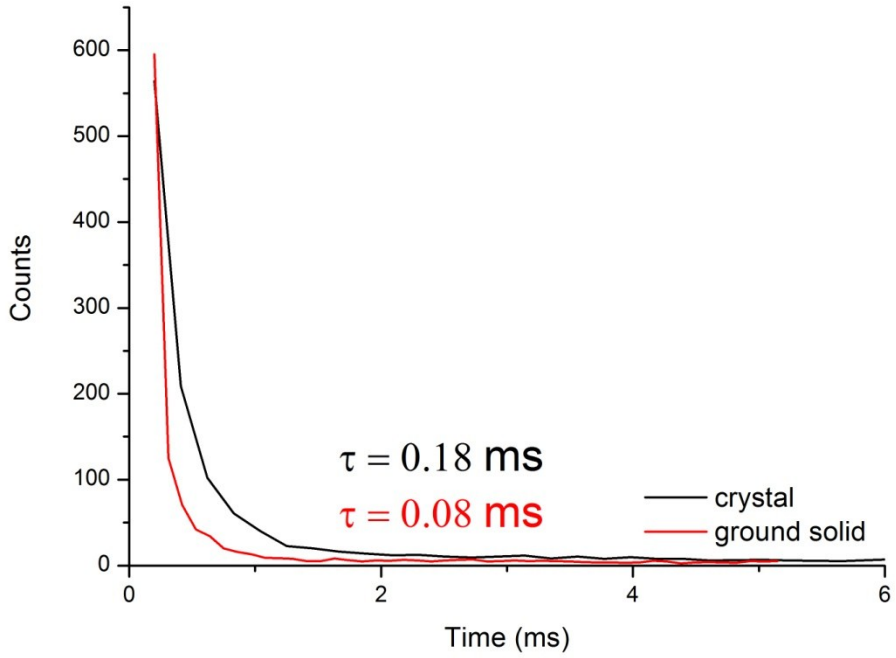

Fig. S10 Decay curves of **PBA** in crystal (λ_{em} = 550 nm) and ground solid (λ_{em} = 570 nm).

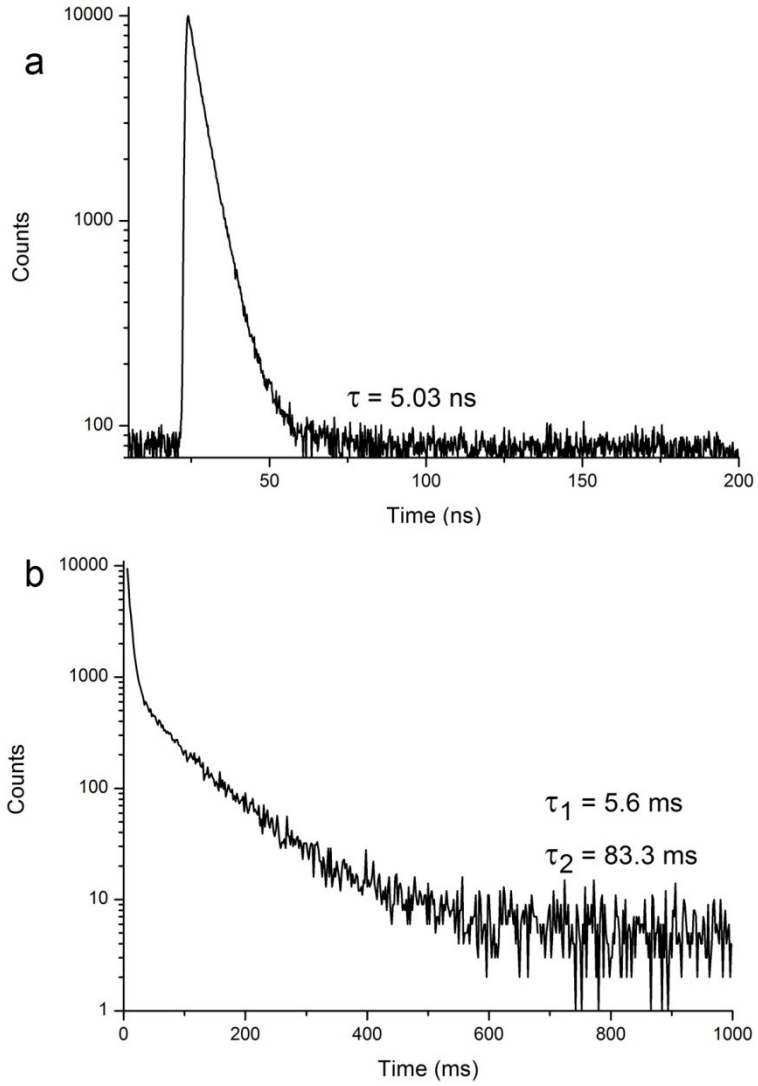

Fig. S11 Decay curves of **PBA** crystal at (a) 490 nm and (b) 550 nm with a delayed time of 0.5 ms.