Supporting Information

Near-infrared Aggregation-Induced Emission Characteristics of New *o*-Carborane Fluorophores with Large Stokes Shifts and Self-recovering Mechanochromic Luminescence

Xueyan Wu, Na Li, Chenxi Zhang, Yan Lv, Jixi Guo*

State Key Laboratory of Chemistry and Utilization of Carbon Based Energy Resources; College of Chemistry, Xinjiang University, Urumqi, 830017, Xinjiang, PR China

Email: Wuxy90@xju.edu.cn, jxguo1012@163.com,

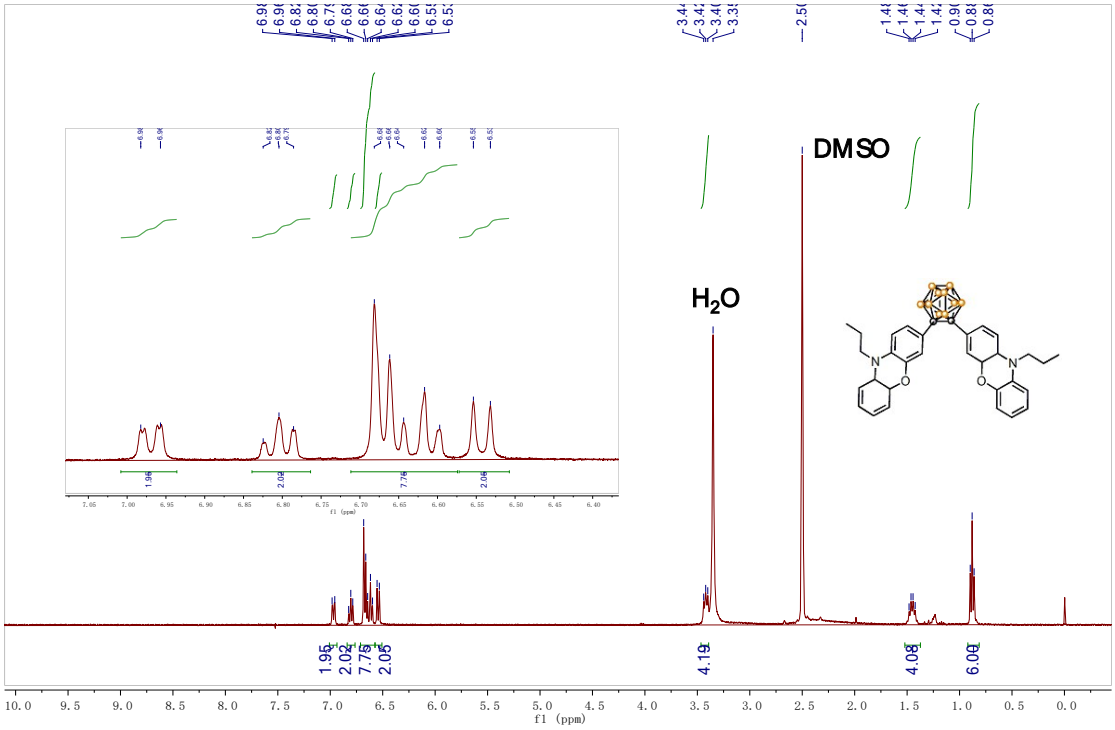

Figure S1. ^{1}H NMR spectra of **CPO** in DMSO-d_6

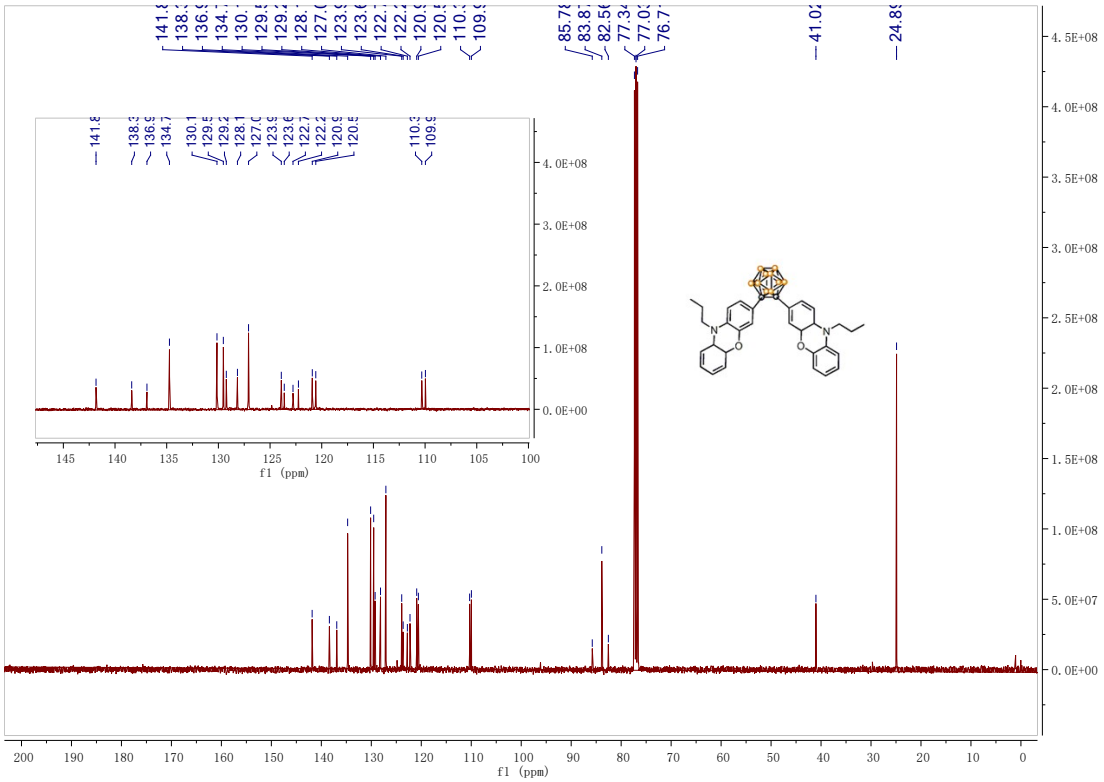

Figure S2. ^{13}C NMR spectra of **CPO** in $CDCl_3$.

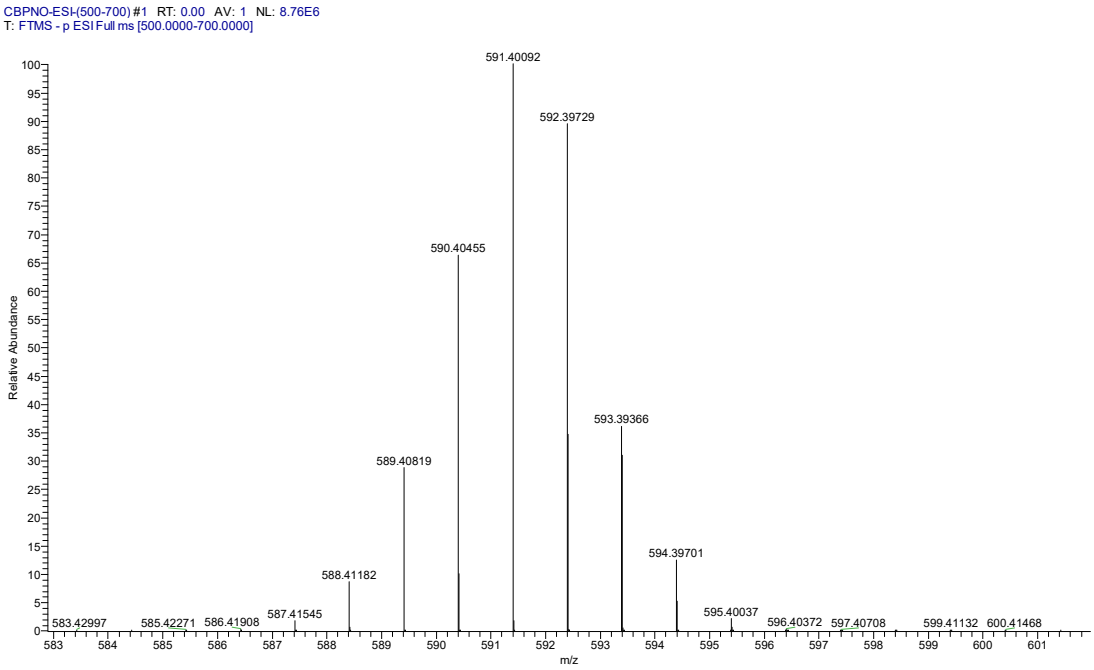

Figure S3. HRMS spectra of **CPO**

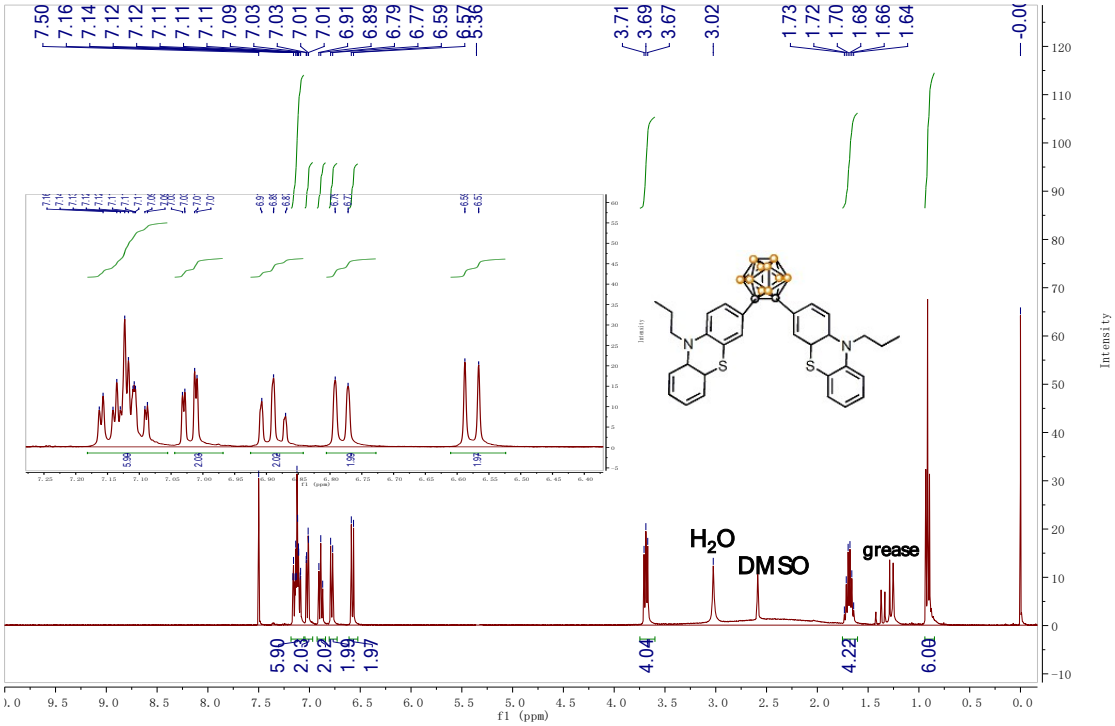

Figure S4. ^{1}H NMR spectra of CPS in $CDCl_3$ and DMSO-d_6.

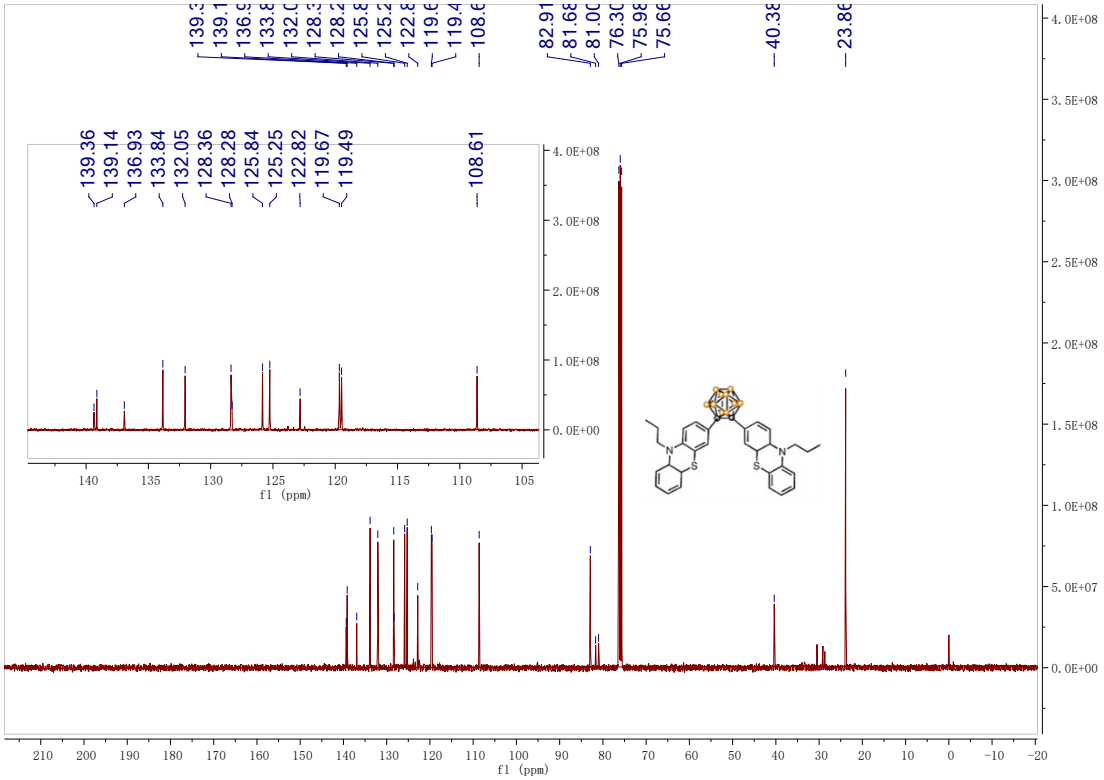

Figure S5. ^{13}C NMR spectra of CPS in $CDCl_3$.

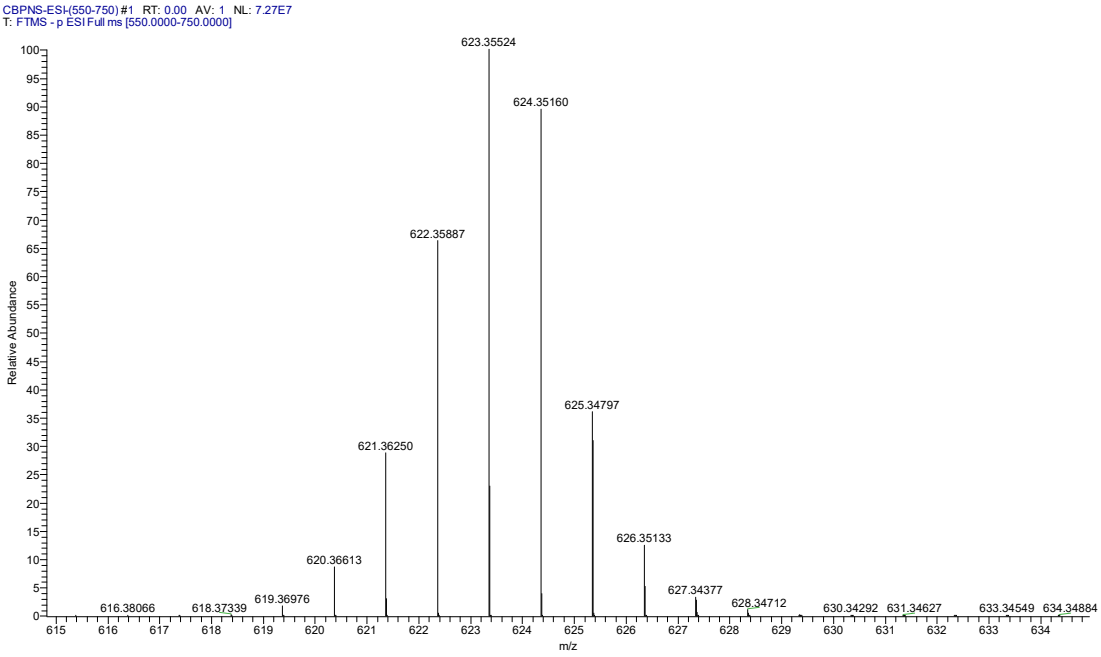

Figure S6. HRMS spectra of **CPS**

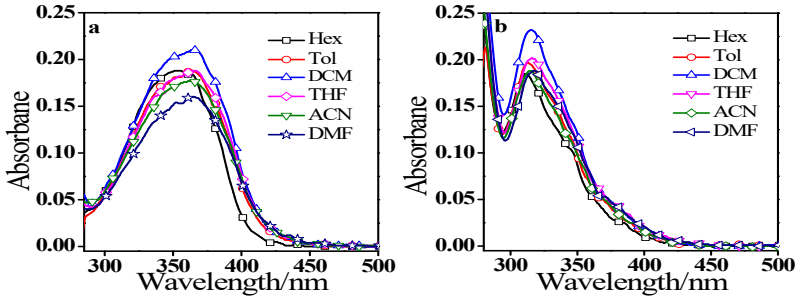

Figure S7. UV-Vis absorption spectra of (a) **CPO** and (b) **CPS** in different solvents. c = 1.0 × 10^{-5} M, 20 °C.

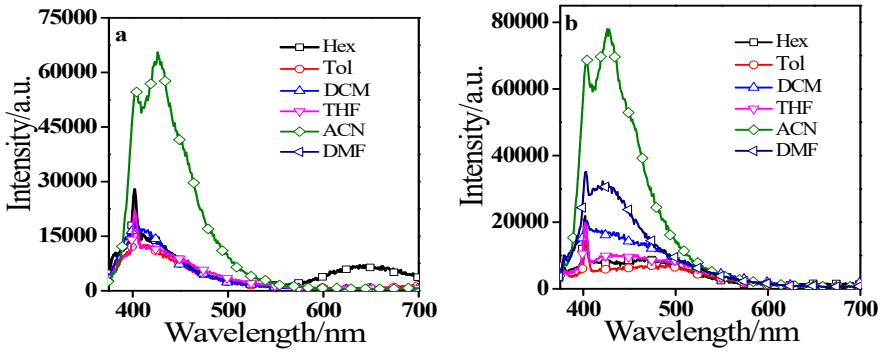

Figure S8. Fluorescence spectra of (a) **CPO** and (c) **CPS** in different solvents. (λ_{ex}=360nm), c = 1.0 × 10^{-5} M, 20 °C.

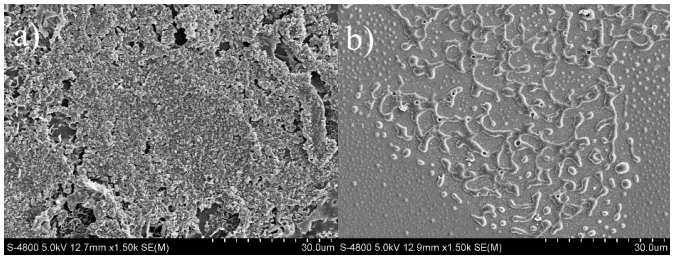

Figure S9 SEM images of (a) **CPO** and (b) **CPS** with a 99% water fraction.

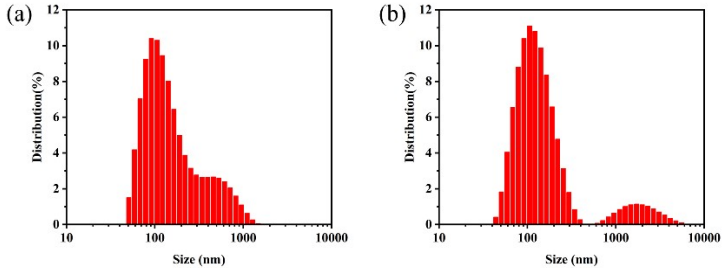

Figure S10 Size distributions of nanoparticles of (a) **CPO** and (b) **CPS** with a 99% water fraction.

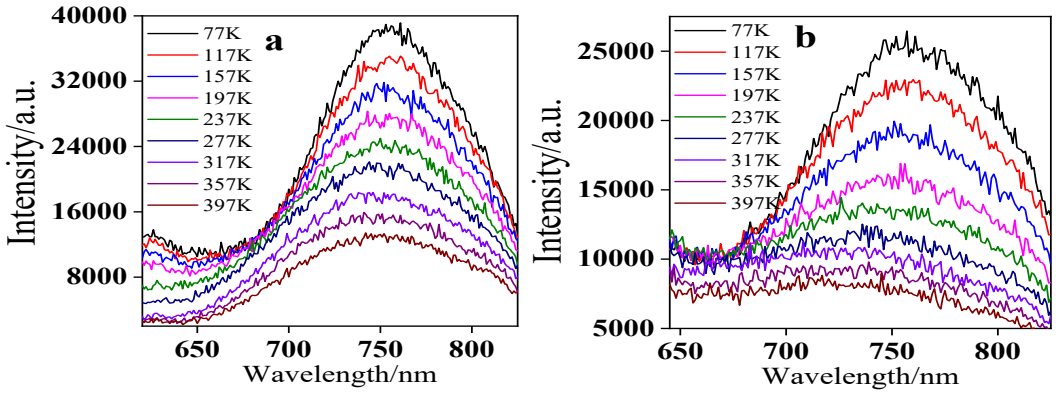

Figure S11. The normalized PL spectra of (a) **CPO** and (b) **CPS** in the solid state during heating from 77 to 397K.

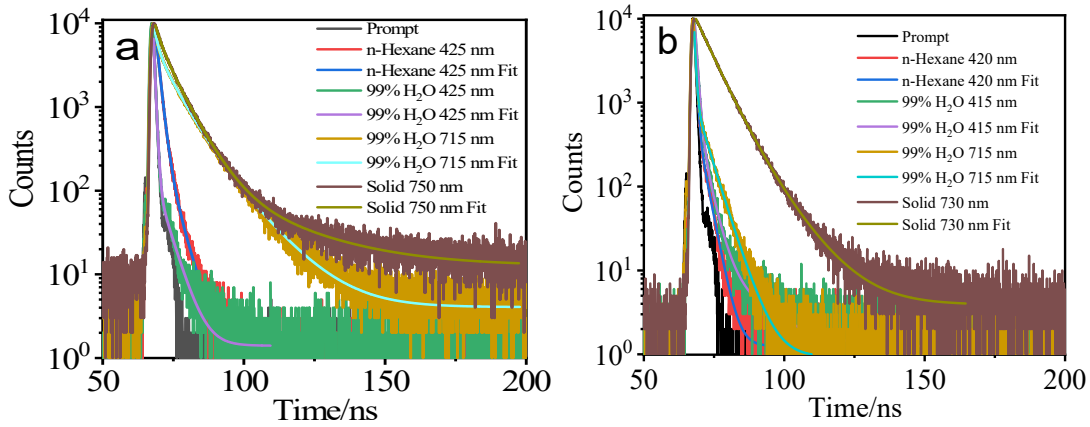

Figure S12. Decay profiles of fluorescence lifetime measurement of (a) **CPO** and (b) **CPS** in the solution, aggregation and solid state.

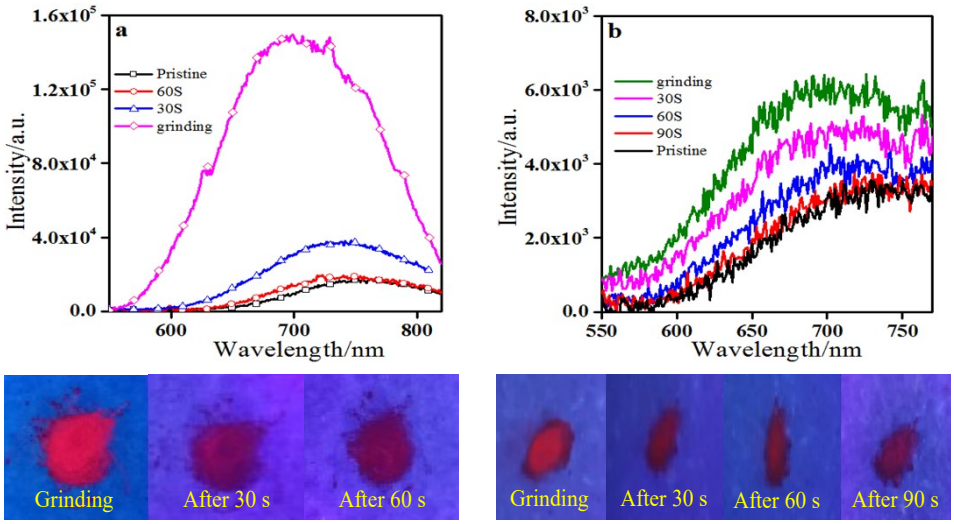

Figure S13. The self-recovering mechanochromic luminescence of (a) **CPO** and (b) **CPS** in solid at 60 ºC, and the mechanochromic luminescence photographs of **CPO** and **CPS** changes with time under day and 365 nm UV light

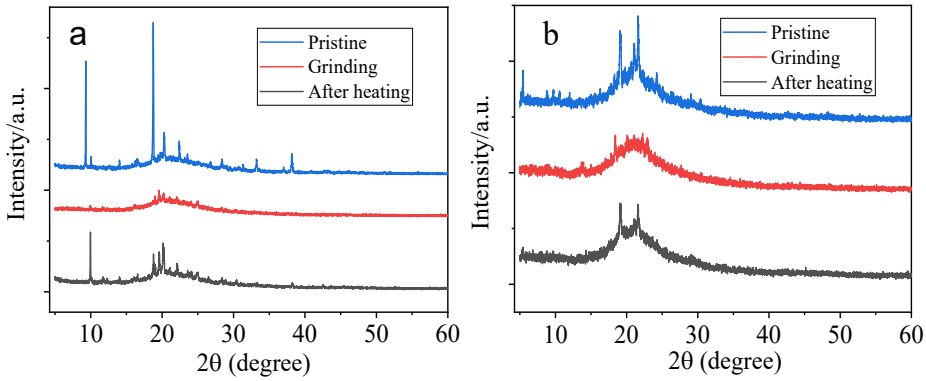

Figure S14. XRD patterns of **CPO** (a) **CPS** (b) in different solid-states: Pristine, Grinding and After heating.

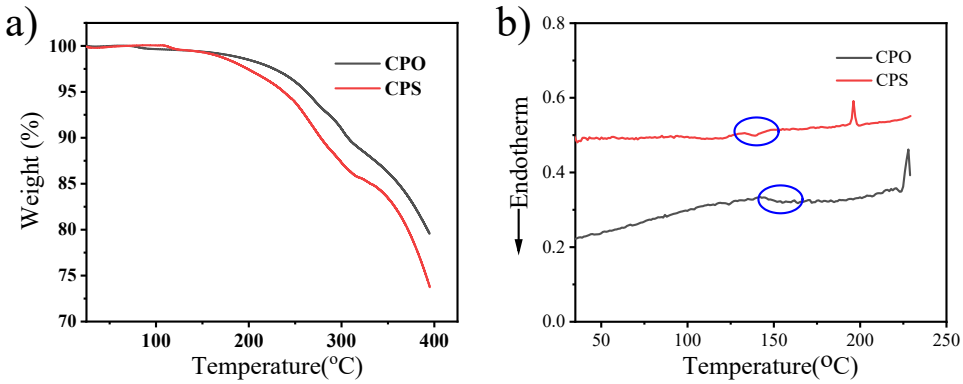

Figure S15. (a)TG and (b)DSC of **CPO** and **CPS** measured at a heating rate of 10 °C/min under N_2 atmosphere.

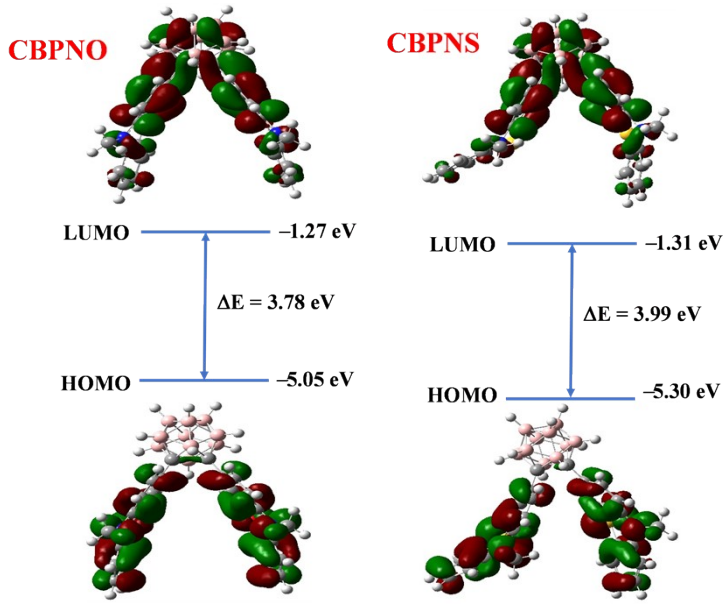

Figure S16. The electronic density contours and energy levels of the HOMOs and LUMOs of **CPO** and **CPS** were calculated by DFT at the B3LYP/6-31G(d,p) level with Gaussian 09W.

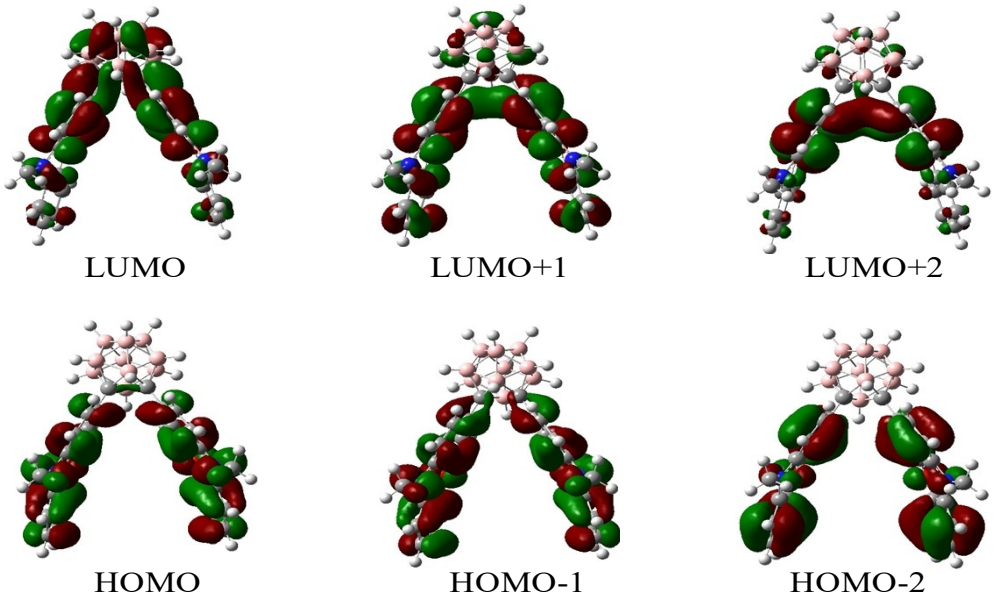

Figure S17. The theoretical calculated ground-state frontier orbitals contributions of **CPO** in gas sate using B3LYP/6-31G (d, p) level by Gaussian 09.

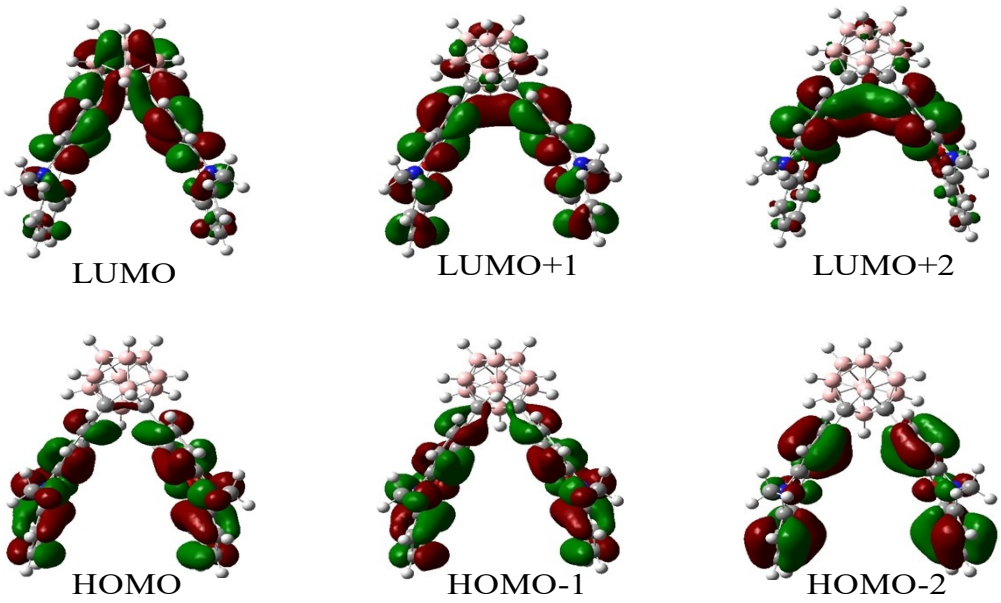

Figure S18. The theoretical calculated UV-vis absorption frontier orbitals contributions of **CPO** in gas sate estimated by TD-DFT calculation at the B3LYP/6-31G (d, p) level by Gaussian 09.

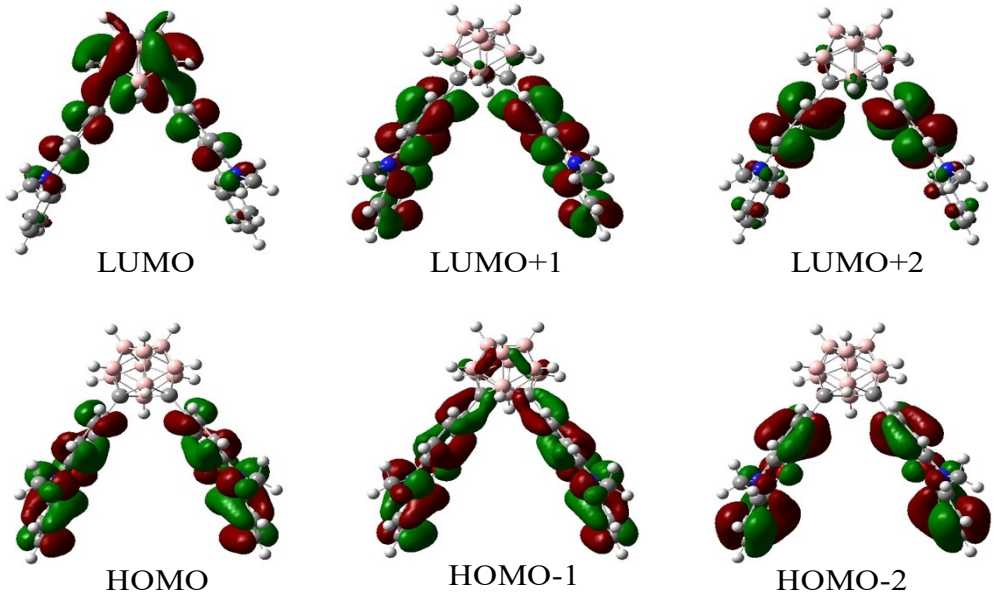

Figure S19. The theoretical calculated singlet state (Fluorescence) frontier orbitals contributions of **CPO** in gas sate estimated by TD-DFT calculation at the B3LYP/6-31G (d, p) level by Gaussian 09.

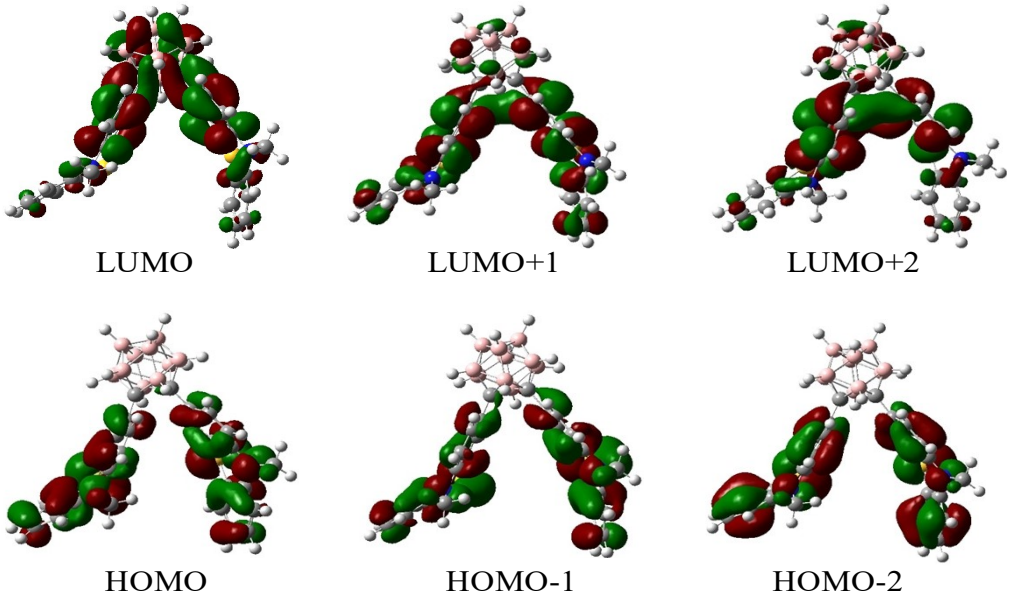

Figure S20. The theoretical calculated ground-state frontier orbitals contributions of **CPS** in gas sate using B3LYP/6-31G (d, p) level by Gaussian 09.

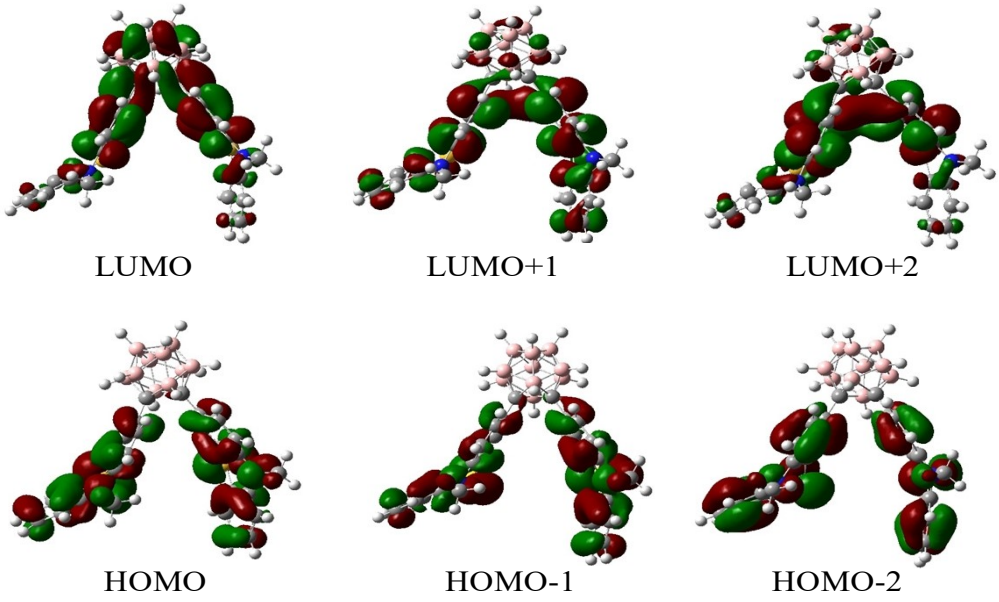

Figure S21. The theoretical calculated UV-Vis absorption frontier orbitals contributions of **CPS** in gas sate estimated by TD-DFT calculation at the B3LYP/6-31G (d, p) level by Gaussian 09.

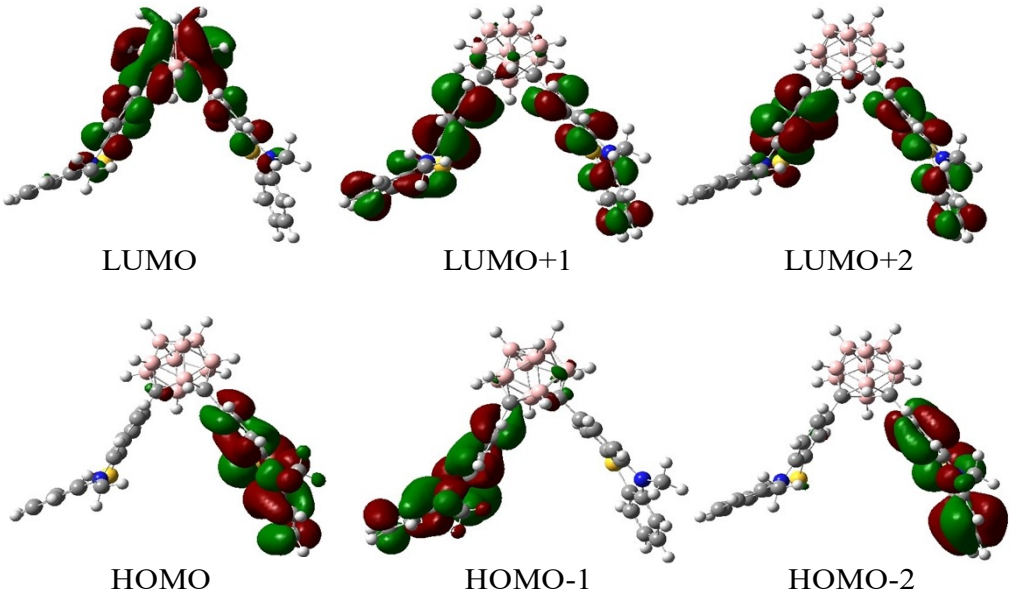

Figure S22. The theoretical calculated singlet state (Fluorescence) frontier orbitals contributions of **CPS** in gas sate estimated by TD-DFT calculation at the B3LYP/6-31G (d, p) level by Gaussian 09.

Table S1. Selected parameters for the UV-vis absorption and Singlet state (Fluorescence) energy of the compounds. Electronic excitation energies (eV), oscillator strengths (*f*), and configurations of the low-lying excited states of **CPO** and **CPS** were calculated using TD-DFT//B3LYP/6-31G(d, p), based on the optimized ground state geometries.

Compound		Transition type	Excitation energy [a]	*f* [b]	Composition [c]	CI [d]
CPO	UV-Vis	$S_0 \rightarrow S_1$	3.2751 eV (379 nm)	0.1088	H→L	0.6843
		$S_0 \rightarrow S_2$	3.3535 eV (370 nm)	0.1483	H−1→L	0.6845
	Fluorescence	$S_0 \rightarrow S_1$	1.7305 eV (716 nm)	0.2198	H→L	0.7063
CPS	UV-Vis	$S_0 \rightarrow S_1$	3.4373 eV (360 nm)	0.0799	H→L	0.6557
		$S_0 \rightarrow S_2$	3.4856 eV (355 nm)	0.0728	H-1→L	0.6464
	Fluorescence	$S_0 \rightarrow S_1$	1.4981 eV (827 nm)	0.1195	H→L	0.7055

[a] Only selected excited states were considered. Numbers in parentheses are the excitation energy in wavelength. [b] Oscillator strength. [c] H stands for the HOMO and L stands for the LUMO. Only the main configurations are presented. [d] Coefficient of the wave function for each excitation. CI coefficients are given in absolute values.