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# Electronic Supplementary Information

## Rotation-Restricted Thermally Activated Delayed Fluorescence Compounds for Efficient Solution-Processed OLEDs with EQE of up to 24.3% and Small Roll-off

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### General information:

All chemicals and reagents were used as received from commercial sources without further purification. 2-(4-bromophenyl)-4,6-diphenyl-1,3,5-triazine,[1] 4-(diphenylamino)phenylboronic acid[2] were prepared according to references. 4-(bis(4-(tert-butyl)phenyl)amino)phenylboronic acid was purchased from Soochiral Chemical Science & Technology. Co., Ltd in Suzhou. Solvents for chemical synthesis were purified according to the standard procedures. NMR spectra were recorded with Bruker Avance 400 NMR or Bruker Avance 500 NMR spectrometersor. MALDI-TOF mass spectra were performed on an AXIMA CFR MS apparatus (COMPACT).

### Optical measurements:

The solution samples ($10^{-5}$ M) were degassed with nitrogen for several minutes prior to use unless otherwise indicated. Thin film samples were deposited on quartz glass substrates by spin-coating. UV-visible (UV-vis) absorption and steady state photoluminescence spectra were measured with a Perkin-Elmer Lambda 35 UV-vis spectrometer and a Perkin-Elmer LS 50B spectrofluorometer, respectively. Fluorescence lifetime and quantum efficiency were carried out with Edinburgh fluorescence spectrometer (FLS980) with an integrating sphere. Lifetime within 20 μs was measured using picosecond pulsed diode laser under the excitation at 375 nm.

### Electrochemical measurements:

Cyclic voltammetry experiments were performed on an EG&G 283 (Princeton Applied Research) potentiostat/galvanostat system. TC, PTC, PAPTC and BPAPTC were tested in dichloromethane using ferrocene as an internal reference and tetra-butyl ammonium hexafluorophosphate as the supporting electrolyte. The HOMO and LUMO energy levels were calculated according to the equation: $E_{HOMO}$ = - [E (onset, ox vs Fc/Fc$^+$) + 4.8] (eV). Or $E_{LUMO}$ = - [E (onset, re vs Fc/Fc$^+$) + 4.8] (eV).

### Crystal structure determination:

The crystals of the compounds were obtained by slow evaporation of tetrahydrofuran/ethanol solution at room temperature. The single crystal X-ray diffraction experiments were carried out using a Bruker Smart APEX diffractometer with CCD detector and graphite monochromator, Mo Kα radiation (λ = 0.71073 Å). The intensity data were recorded with ω scan mode (192 K). Lorentz, polarization factors were made for the intensity data and absorption corrections were performed using SADABS program.[3] The crystal structure was determined using the SHELXTL program and refined using full matrix least squares.[4] All non-hydrogen atoms were assigned with anisotropic displacement parameters, whereas hydrogen atoms were placed at calculated positions theoretically and included in the final cycles of refinement in a riding model along with the attached carbons. The detailed data can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif with CCDC 1960017-1960019 for PTC, PAPTC and BPAPTC.

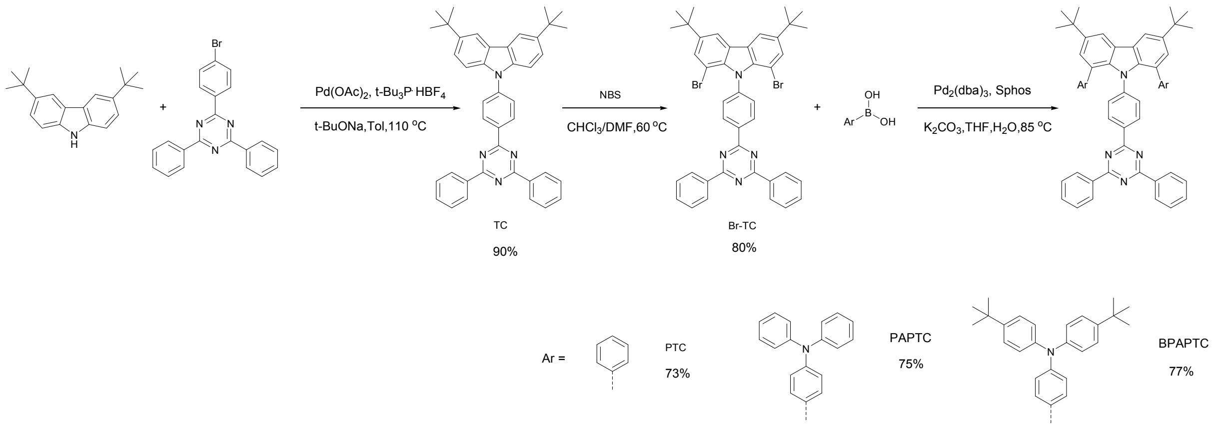
**Theoretical calculation:**

Density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations were performed using the Gaussian 09 program package.[5] The ground state geometries were optimized using DFT, B3LYP/6-31G(d) method, without imposing any symmetry constraints. The computations of the singlet and triplet transition energies were carried out with TD-DFT, BMK /6-31G(d) method based on the crystal structures, which has been successfully predicted for the charge-transfer compounds.[6] Multiwfn and VMD softwares were employed to plot the π-π interaction by Independent Gradient Model.[7]

**Device fabrication and measurements:**

The prepared OLEDs have a configuration of ITO/PEDOT:PSS (40 nm)/SimCP2:emitter (20 wt%) (40 nm)/TmPyPB (60 nm)/LiF (1 nm)/Al (100 nm) (where PEDOT:PSS is poly(ethylenedioxythiophene): poly(styrenesulfonate) and TmPyPB is 1,3,5-tri(m-pyrid-3-ylphenyl)benzene). The PEDOT: PSS layer (AI 4083) was spin-coated onto the pre-cleaned ITO substrate and annealed at 120 °C for 30 min in air condition. And then the device substrates were transferred into nitrogen-filled glovebox to prepare the corresponding emissive layer. Materials were dissolved in fresh chlorobenzene solvent and then stirring at 45 °C for 1 hour before spin-coating them to form ca. 40nm-thick emissive layer. The devices were then annealed at 100°C for 30 min in the glove box. The other layers including TmPyPB (60 nm)/LiF (1 nm)/Al (100 nm) were evaporated in a vacuum chamber at a base pressure less than $2 \times 10^{-7}$ Tor. The J-L-V characteristics were measured by a Keithley source measurement unit (Keithley 2400 and Keithley 2000) with a calibrated silicon photodiode. The EL spectra of the devices were measured by CS2000 spectrophotometer. All measurements were carried out at room temperature under ambient conditions. External quantum efficiencies of the devices were calculated from the luminance, current density and EL spectrum, assuming a Lambertian distribution.

**Synthesis:**



TC: 3,6-di(tert-butyl)-9-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)carbazole

A mixture of 3,6-di(tert-butyl)carbazole (2.64 g, 9.46 mmol), 2-(4-bromophenyl)-4,6-diphenyl-1,3,5-triazine (3.67 g, 9.46 mmol), Pd(OAc)$_2$ (0.0708 g, 0.32 mmol), tri(tert-butyl)phosphine tetrafluoroborate (t-Bu$_3$P·HBF$_4$, 0.183 g, 0.63 mmol) and sodium tert-butoxide (t-BuONa, 1.51 g, 15.76 mmol) were dissolved in toluene (50 mL) under an argon atmosphere. The mixture was heated to 110 °C and stirred for 24 h. After cooled to room temperature, the mixture was diluted with CH$_2$Cl$_2$ (DCM), washed with water and brine, and dried over anhydrous Na$_2$SO$_4$. The solution was filtered and then concentrated in vacuo. The crude product was purified by column chromatography (silica, PE : DCM = 10 : 1) to get white solid. Yield: 4.18 g, 90%. $^1$H NMR (400 MHz, Chloroform-*d*): δ 9.00 (d, *J* = 8.6 Hz, 2H), 8.82 (dd, *J* = 8.0, 1.7 Hz, 4H), 8.16 (d, *J* = 1.3 Hz, 2H), 7.81

(d, *J* = 8.5 Hz, 2H), 7.66-7.57 (m, 6H), 7.50 (d, *J* = 1.2 Hz, 4H), 1.49 (s, 18H). $^{13}$C NMR (101MHz, Chloroform-*d*): δ 171.77, 171.01, 143.42, 142.18, 138.77, 136.19, 134.36, 132.61, 130.56, 129.01, 128.69, 126.23, 123.81, 116.37, 109.41, 76.69, 34.79, 32.01. HRMS [M+H]$^+$ calcd for $C_{53}H_{46}N_4$: 586.3096; found: 586.3082.

Br-TC: 1,8-dibromo-3,6-di(tert-butyl)-9-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)carbazole

TC (0.80 g, 1.36 mmol), NBS (0.50 g, 2.79 mmol), DMF (30 mLl) and $CHCl_3$ (20 mL) were added into a 100 mL flask. The mixture was stirred at 80 °C in the dark for 12 h. After cooled to room temperature, the mixture was poured into 100 mL water, and extracted with DCM three times. The organic layer was washed with water and brine, and dried over anhydrous $Na_2SO_4$. The solution was filtered and concentrated in vacuo. The crude product was purified by column chromatography to give white solid. Yield: 0.81 g, 80%. $^1$H NMR (400 MHz, Chloroform-*d*): δ 8.92 (d, *J* = 8.5 Hz, 2H), 8.82 (dd, *J* = 8.1, 1.7 Hz, 4H), 8.08 (d, *J* = 1.8 Hz, 2H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.66-7.56 (m, 8H), 1.45 (s, 18H). $^{13}$C NMR (126 MHz, Chloroform-*d*): δ 171.80, 171.06, 144.90, 142.38, 137.04, 136.91, 136.14, 132.96, 132.61, 130.19, 129.03, 128.68, 128.49, 125.59, 115.46, 103.82, 34.69, 31.79. HRMS [M+H]$^+$ calcd for $C_{41}H_{36}Br_2N_4$: 742.1307; found: 742.1331.

PTC: 3,6-di(tert-butyl)-9-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-1,8-diphenylcarbazole

A mixture of Br-TC (0.74 g, 1 mmol), phenylboronic (0.48 g, 4 mmol), $Pd_2(dba)_3$ (0.018 g, 0.02 mmol), 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (Sphos, 0.033 g, 0.08 mmol) and $K_3PO_4$ (1.06 g, 4 mmol) were dissolved in a mixture of THF (10 mL) and water (2 mL) under an argon atmosphere. The mixture was heated to 80 °C and stirred for 24 h. After cooled to room temperature, the mixture was diluted with DCM, washed with water and brine, and dried over anhydrous $Na_2SO_4$. The solution was filtered and then concentrated in vacuo. The crude product was purified by column chromatography (silica, PE: DCM = 10:1) to get white solid. Yield: 0.54 g, 73%. $^1$H NMR (400 MHz, Chloroform-*d*): δ 8.76 (dd, *J* = 8.1, 1.7 Hz, 4H), 8.24 (d, *J* = 2.0 Hz, 2H), 7.89 (d, *J* = 8.5 Hz, 2H), 7.67-7.55 (m, 6H), 7.33 (d, *J* = 2.0 Hz, 2H), 6.96-6.89 (m, 4H), 6.86 (dt, *J* = 5.1, 1.8 Hz, 6H), 6.67 (d, *J* = 8.5 Hz, 2H), 1.51 (s, 18H). $^{13}$C NMR (101 MHz, Chloroform-*d*, δ): 171.44, 171.03, 143.61, 142.74, 139.79, 137.26, 136.43, 133.50, 132.43, 129.41, 129.14, 128.94, 128.63, 127.66, 127.38, 127.09, 126.60, 125.86, 124.57, 115.13, 77.33, 34.71, 32.01. HRMS [M+H]$^+$ calcd for $C_{53}H_{46}N_4$: 738.3722; found: 738.3700.

PAPTC: 3,6-di(tert-butyl)-1,8-di(4-(N,N-diphenylaniline)phenyl)-9-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)carbazole

A mixture of Br-TC (0.74 g, 1 mmol) and 4-(diphenylamino)phenylboronic acid (1.16 g, 4 mmol), $Pd_2(dba)_3$ (0.018 g, 0.02 mmol), Sphos (0.033 g, 0.08 mmol) and $K_3PO_4$ (1.06 g, 4 mmol) were dissolved in a mixture of THF (10 mL) and water (2mL) under an argon atmosphere. The mixture was heated to 80 °C and stirred for 24 h. After cooled to room temperature, the mixture was diluted with DCM, washed with water and brine, and dried over anhydrous $Na_2SO_4$. The solution was filtered and then concentrated in vacuo. The crude product was purified by column chromatography (silica, PE : DCM = 10 : 1) to get yellow-green solid. Yield: 0.80 g, 75%. $^1$H NMR (400 MHz, Chloroform-*d*): δ 8.76-8.71 (m, 4H), 8.29 (d, J = 8.5 Hz, 2H), 8.19 (d, J = 2.1 Hz, 2H), 7.65-7.51 (m, 6H), 7.30 (d, J = 2.0 Hz, 2H), 7.00-6.86 (m, 10H), 6.85-6.71 (m, 16H), 6.57 (d, J = 8.1 Hz, 4H), 1.50 (s, 18H). $^{13}$C NMR (101 MHz, Chloroform-*d*): δ 171.78, 171.12, 147.32, 144.67, 142.90, 137.80, 136.20, 133.75, 132.48, 130.00, 129.93, 129.12, 129.03, 128.60, 127.89, 127.54, 126.46, 124.85, 122.84, 120.58, 114.91, 34.70, 32.02. HRMS [M+H]$^+$ calcd for $C_{53}H_{46}N_4$: 1072.5192; found: 1072.5165.

BPAPTC: 3,6-di(tert-butyl)-1,8-di(4-(bis(4-(tert-butyl)phenyl)amino)phenyl)-9-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)carbazole

The compound was prepared from Br-TC (0.52 g, 0.7 mmol) and 4-(bis(4-(tert-butyl)phenyl)amino)phenylboronic acid (0.86 g, 2.1 mmol) by the same procedure of PAPTC. Yellow-green solid. Yield: 0.70 g, 77%. $^1$H NMR (400 MHz, Chloroform-*d*): δ 8.90-8.79 (m, 4H), 8.32 (d, *J* = 8.5 Hz, 2H), 8.19 (s, 2H), 7.65-7.51 (m, 6H), 7.32 (d, *J* = 2.0 Hz, 2H), 6.89 (dd, *J* = 12.7, 8.3 Hz, 10H), 6.79-6.62 (m, 12H), 6.48 (s, 4H), 1.50 (s, 18H), 1.06 (s, 36H). $^{13}$C NMR (101 MHz, Chloroform-*d*): δ 171.57, 171.20, 146.17, 145.96, 144.38, 144.19, 142.61, 137.15, 136.19, 133.32, 132.56, 131.71, 129.89, 129.75, 129.24, 128.69, 127.75, 127.50, 126.48, 125.86, 125.06, 124.50, 118.44, 114.74, 34.68, 34.03, 32.03, 31.18. HRMS [M+H]$^+$ calcd for $C_{93}H_{96}N_6$: 1296.7696; found: 1296.7676.

**Figure:**

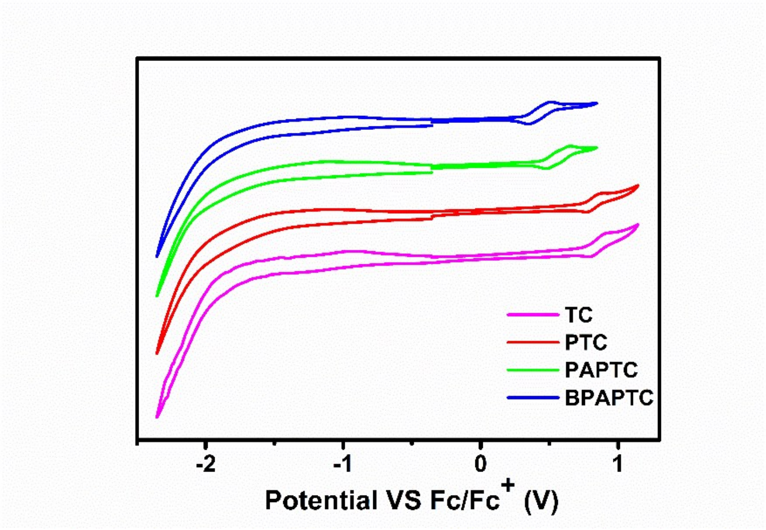


**Figure S1.** Cyclic voltammogram of TC, PTC, PAPTC and BPAPTC.

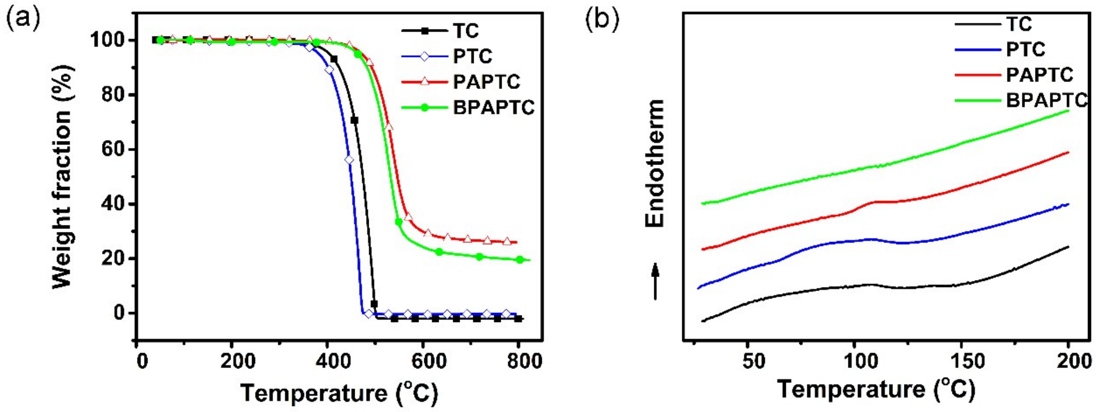


**Figure S2.** a) TGA traces of TC, PTC, PAPTC and BPAPTC recorded at a heating rate of 10 °C min$^{-1}$; b) DSC traces of TC, PTC, PAPTC and BPAPTC recorded at a heating rate of 10 °C min$^{-1}$.

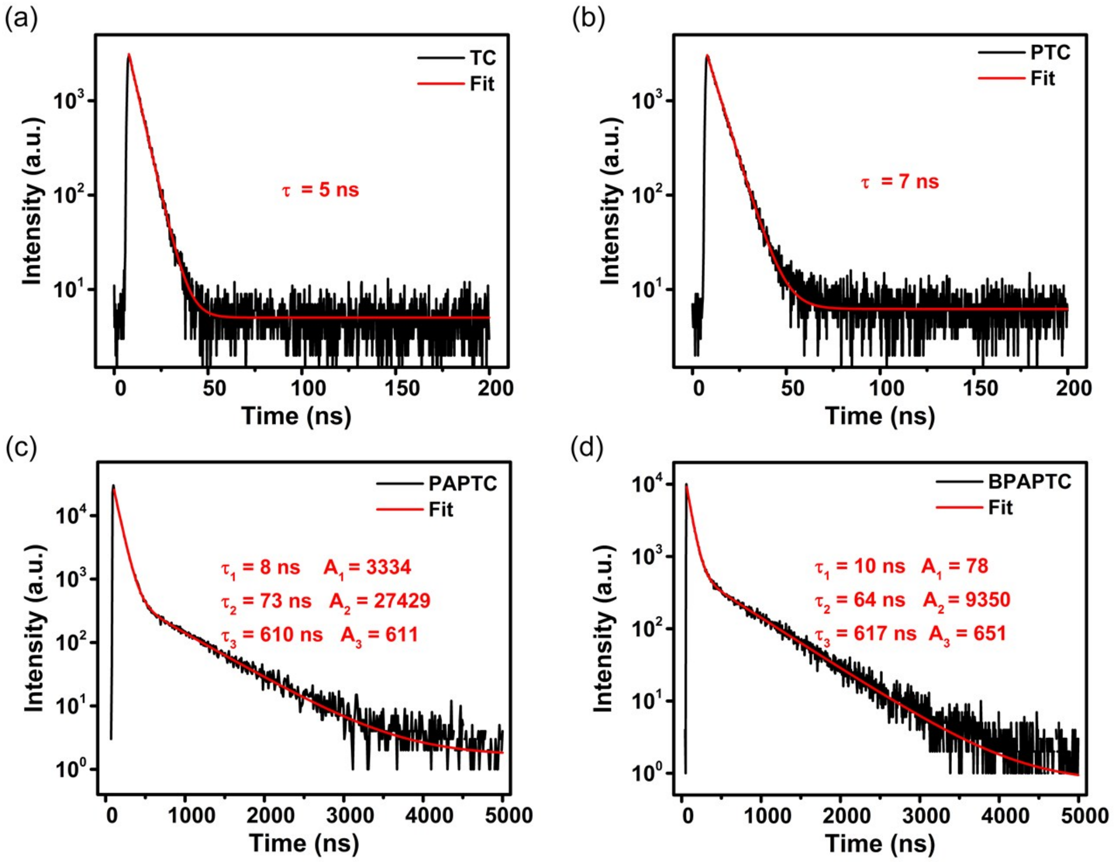


**Figure S3.** Transient decay spectra and exponential fitting curve of the four molecules in toluene.

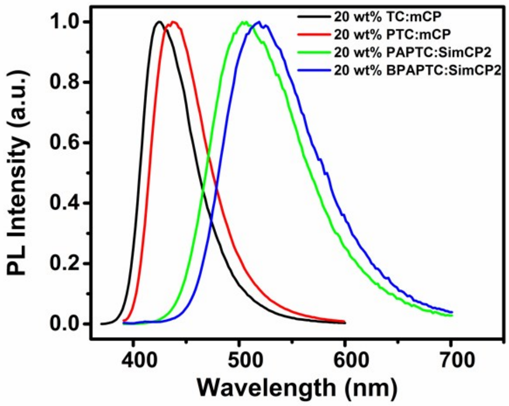


**Figure S4.** PL spectra measured in doped films.

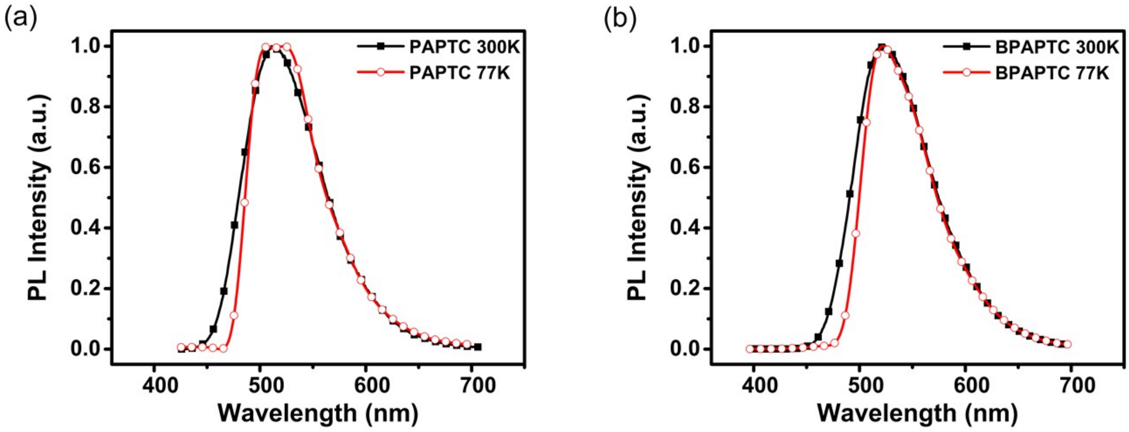


**Figure S5.** PL spectra measured at 300 K and phosphorescence spectra measured at 77 K of PAPTC and BPAPTC in doped films.

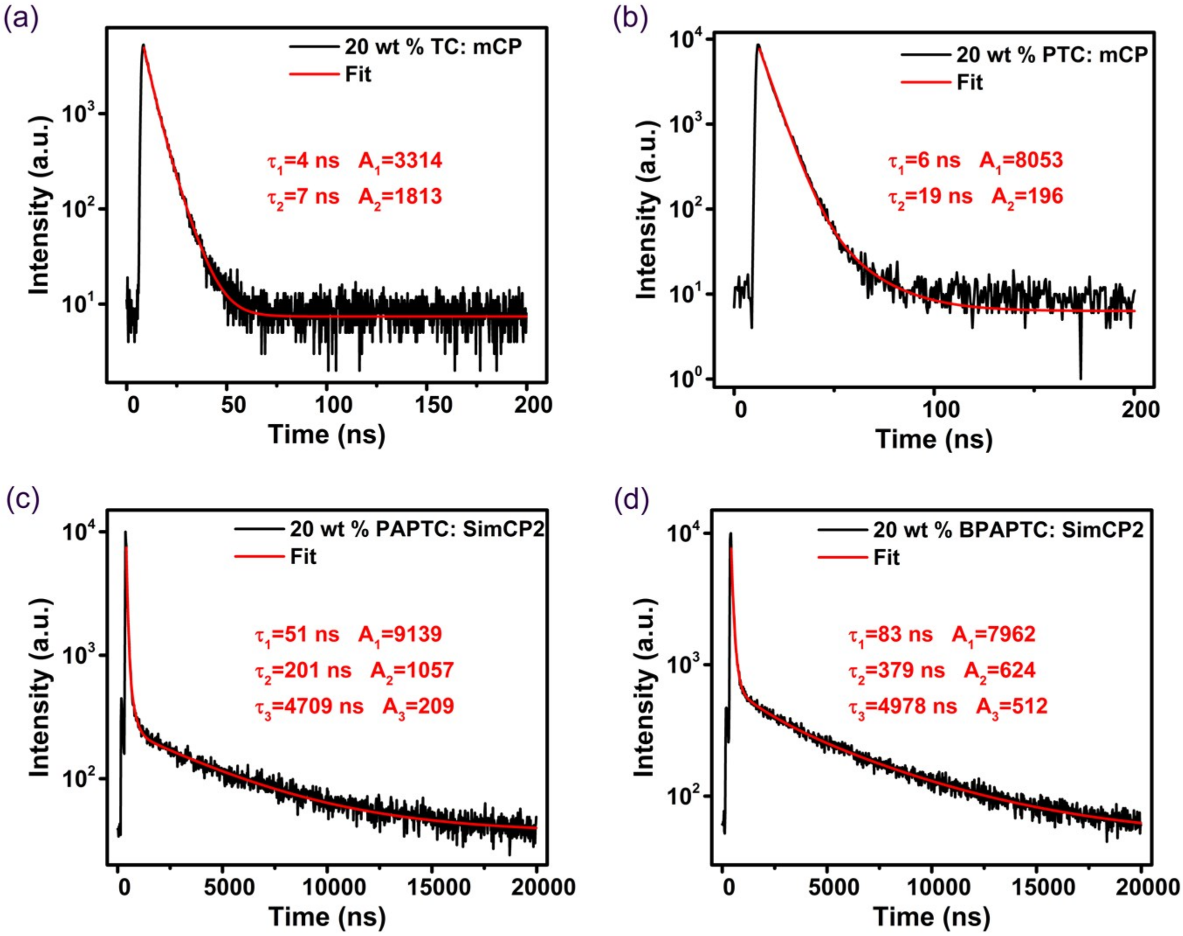


**Figure S6.** Transient decay spectra and exponential fitting curves of the four compounds in doped film at 300 K.

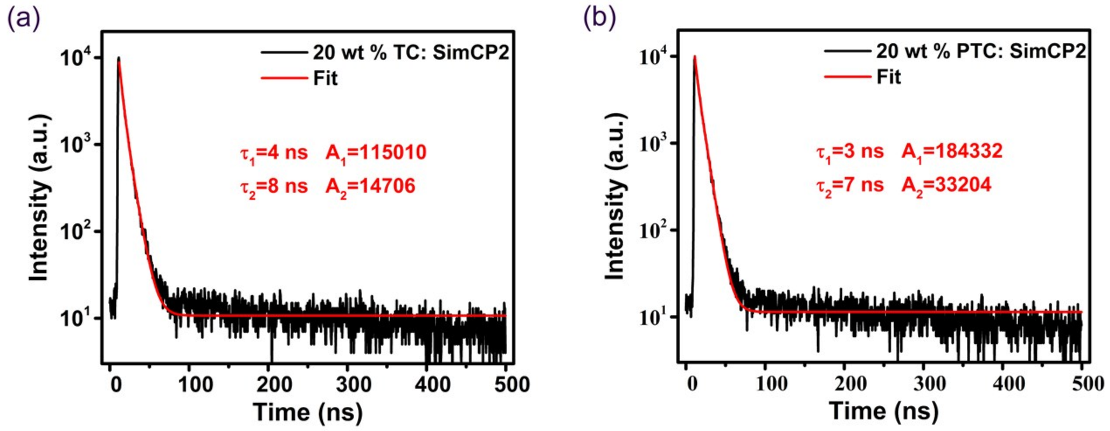


**Figure S7.** Transient decay spectra and exponential fitting curves of TC and PTC in doped film at 300 K.

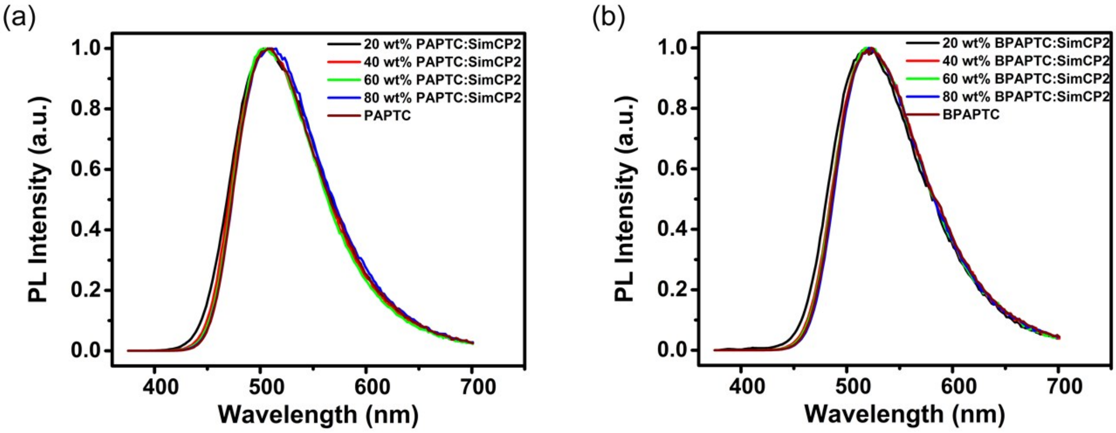


**Figure S8.** PL spectra of (a) PAPTC and (b) BPAPTC doped in SimCP2 with different ratios.

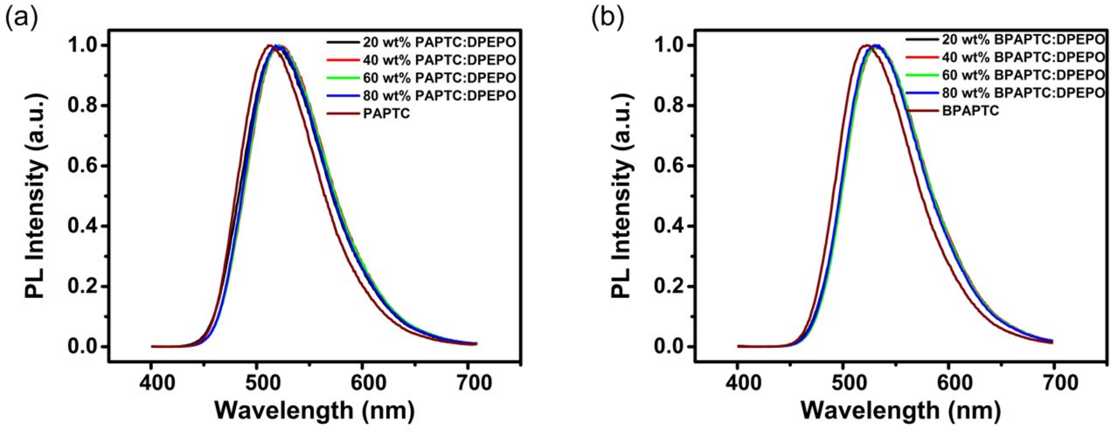


**Figure S9.** PL spectra of (a) PAPTC and (b) BPAPTC doped in DPEPO with different ratios.

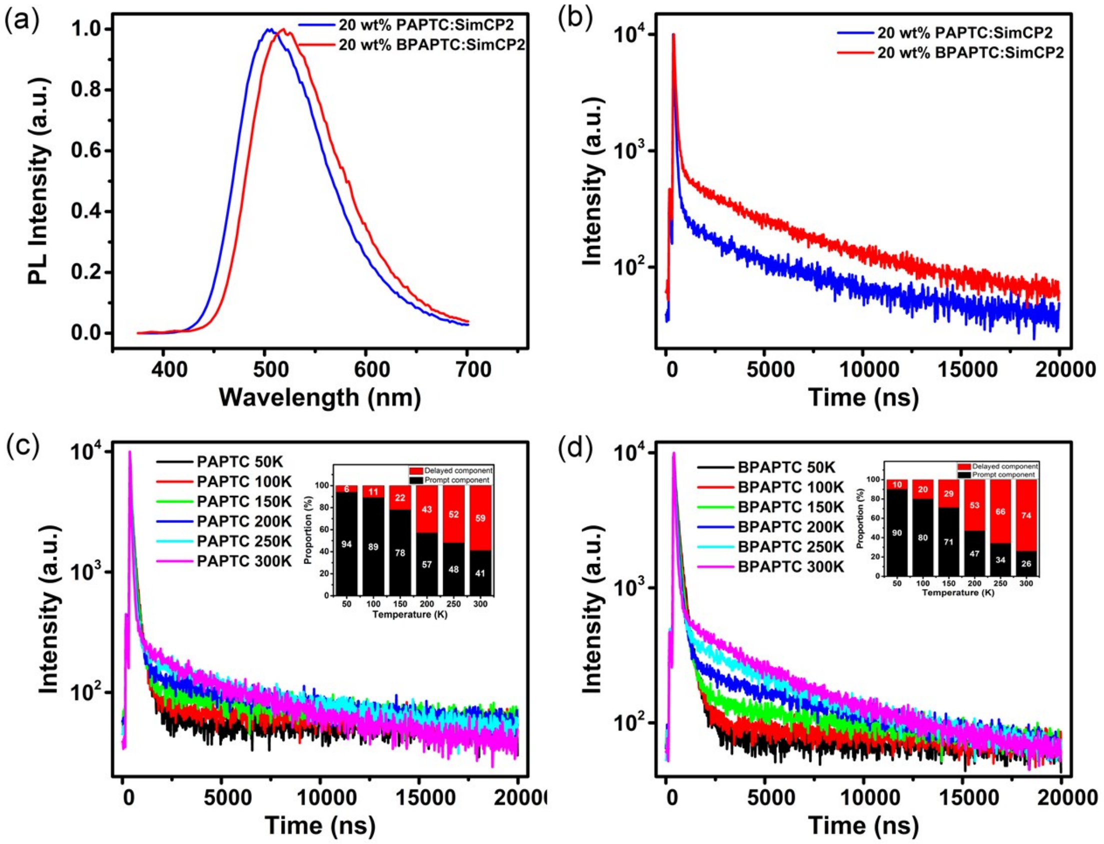


**Figure S10.** a) Steady state emission spectrum of 20 wt% PAPTC:SimCP2 film and 20 wt% BPAPTC:SimCP2 film; b) Transient PL decay characteristics of 20 wt% PAPTC:SimCP2 film and 20 wt% BPAPTC:SimCP2 film; c) Temperature dependent PL transient decay spectra of PAPTC doped film; d) Temperature dependent PL transient decay spectra of BPAPTC doped film.

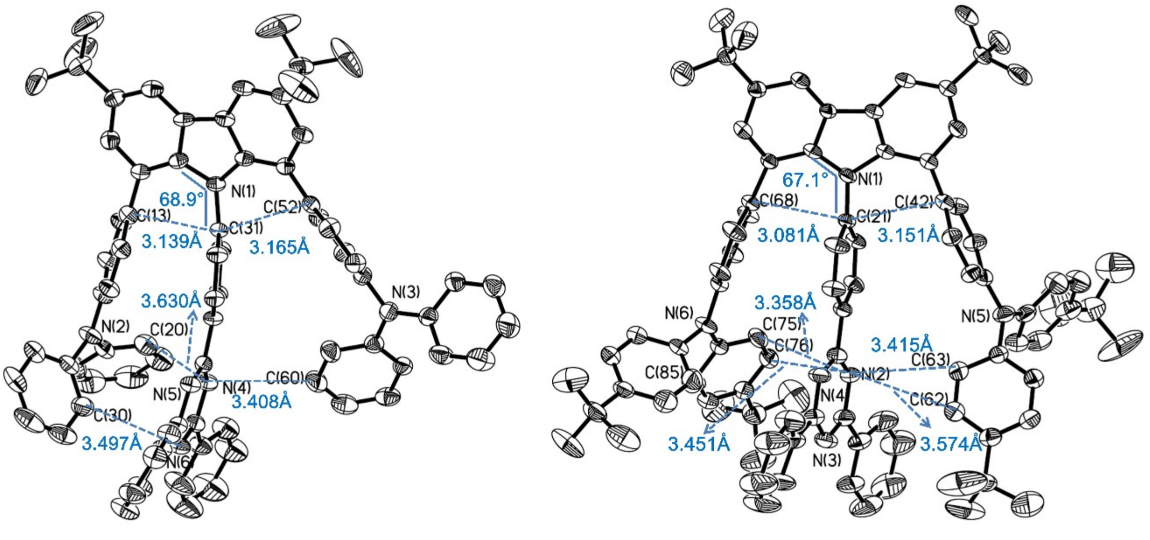


**Figure S11.** Crystal structures of PAPTC and BPAPTC. Hydrogen atoms have been omitted for clarity.

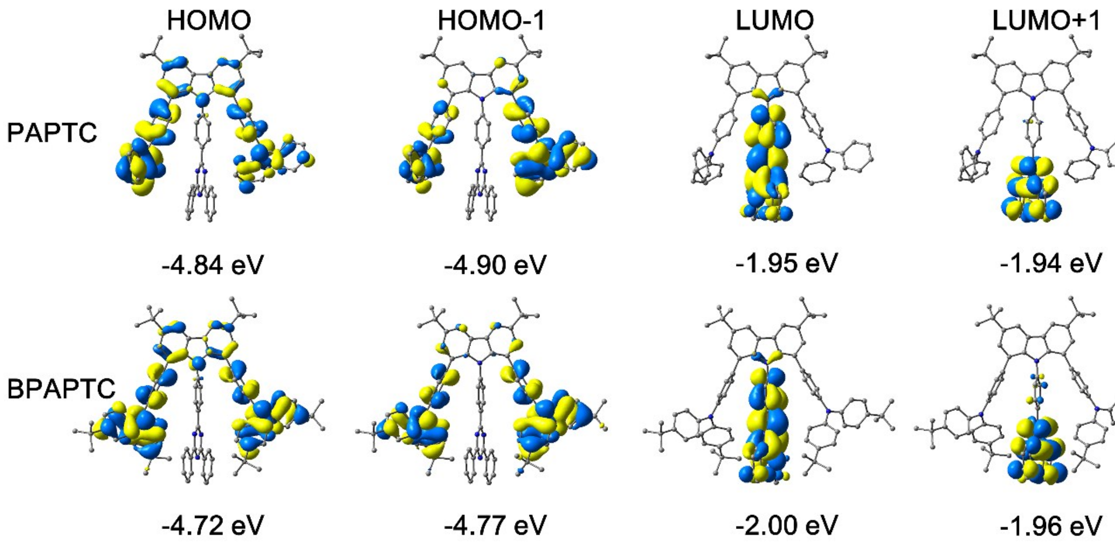


**Figure S12.** The distributions of the HOMOs and LUMOs of PAPTC and BPAPTC obtained from TD-DFT at the B3LYP/6-31G(d) level.

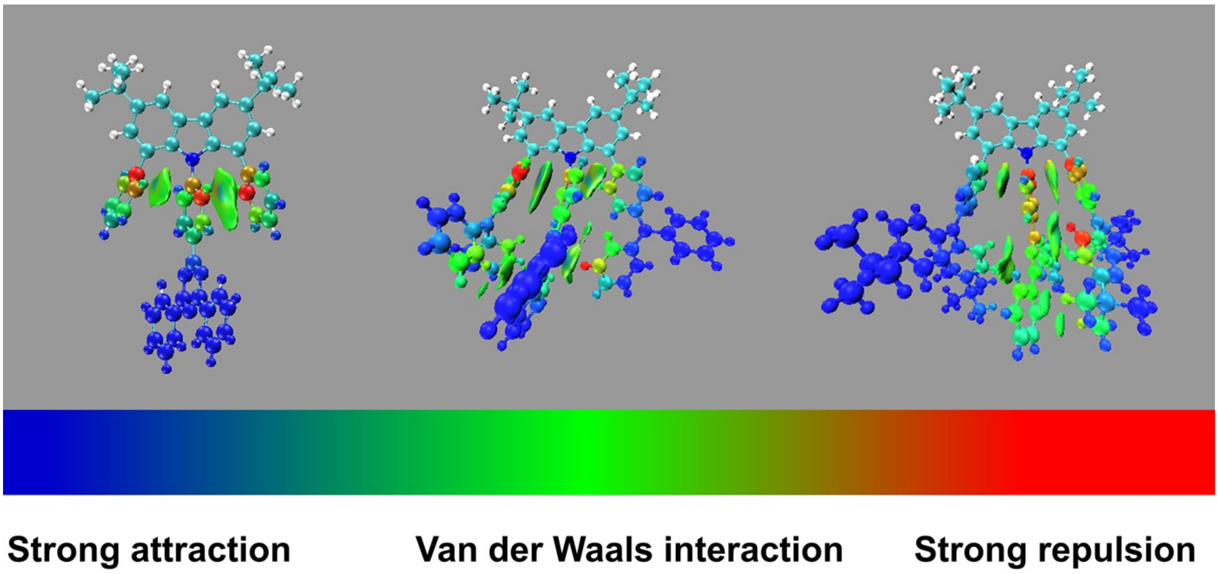


**Figure S13.** Reduced density gradient mapping for PTC, PAPTC and BPAPTC based on their crystal structures. Multiwfn and VMD softwares were employed to plot the π-π interaction by Independent Gradient Model. As shown in Figure S10, there is Van der Waals interaction between peripheral arylamine groups and triphenyltriazine, which further confirms the existence of intramolecular through-space CT. The TD-DFT calculations reveal that both of PAPTC and BPAPTC have degenerate orbit with energy approximation. The HOMO-1 is distributed on the triphenylamine with a small portion on carbazole and the LUMO+1 is only localized on diphenyltriazine for PAPTC and BPAPTC (Figure S9), which is consistent with the results of single crystal analysis and reduced density gradient mapping. At the same time, the HOMO and LUMO have partial overlap on the nitrogen atom of carbazole of PAPTC and BPAPTC, which imply the existence of intramolecular through-bond CT.

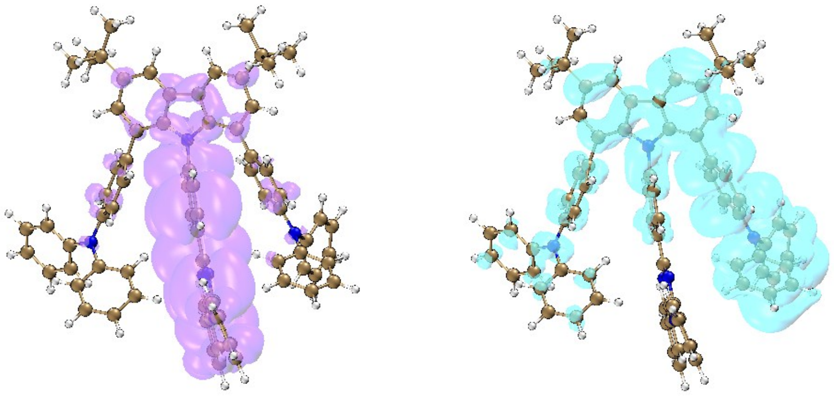


**Figure S14.** The natural transition orbital (NTO) characteristics of the lowest excited triplet state ($T_1$) for PAPTC (Hole, green; Particle, purple).

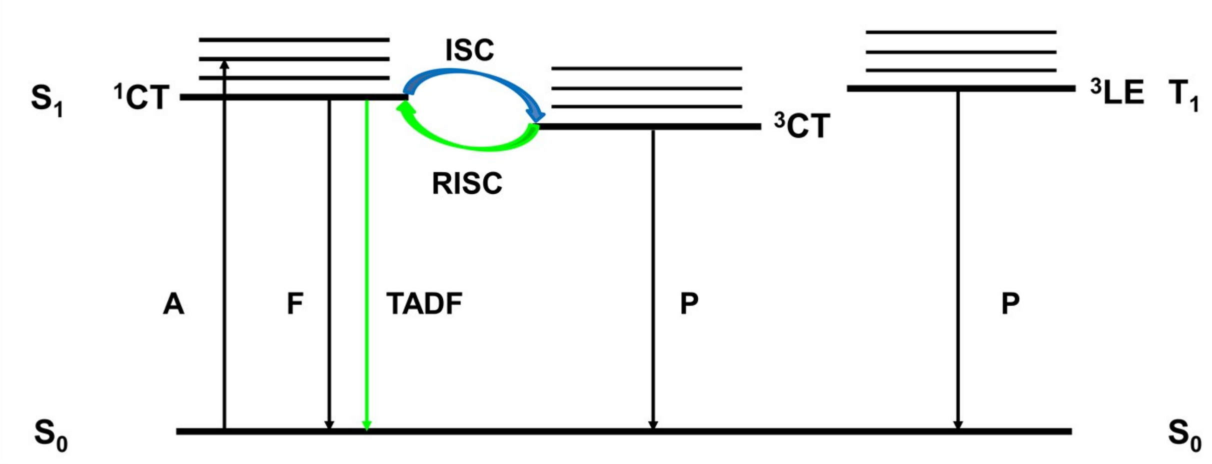


**Figure S15.** Modified Jablonski diagram of PAPTC and BPAPTC.

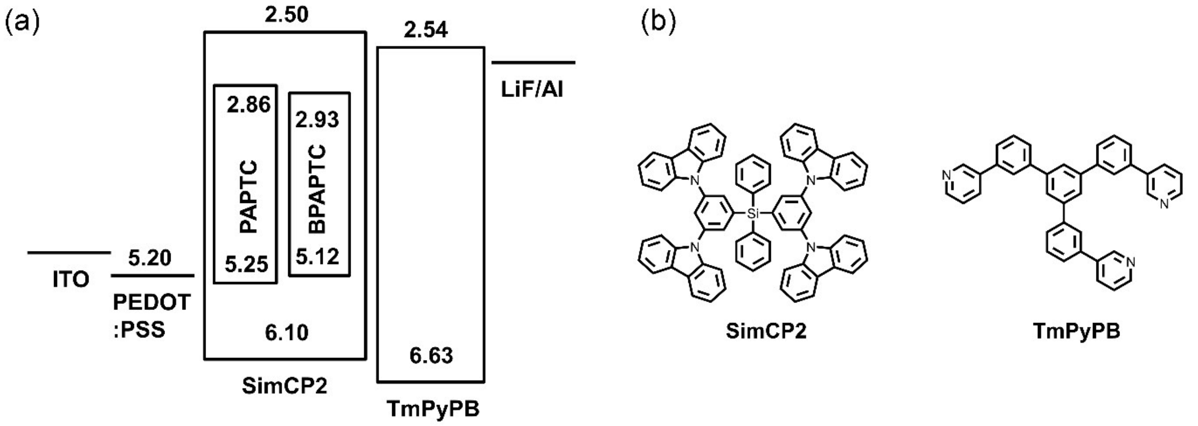


**Figure S16.** a) Energy levels of the EL devices; b) Chemical structure of SimCP2 and TmPyPB.

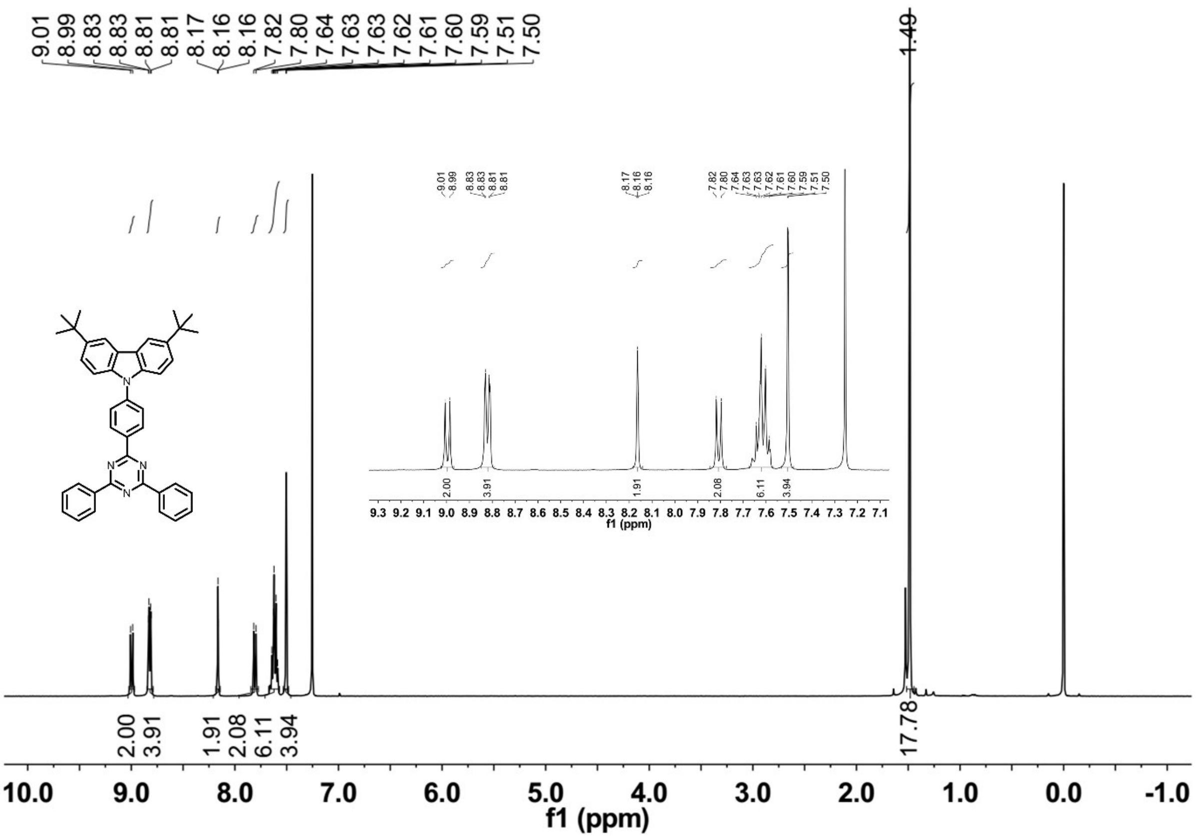


**Figure S17.** $^1H$ NMR spectrum of TC in $CDCl_3$.

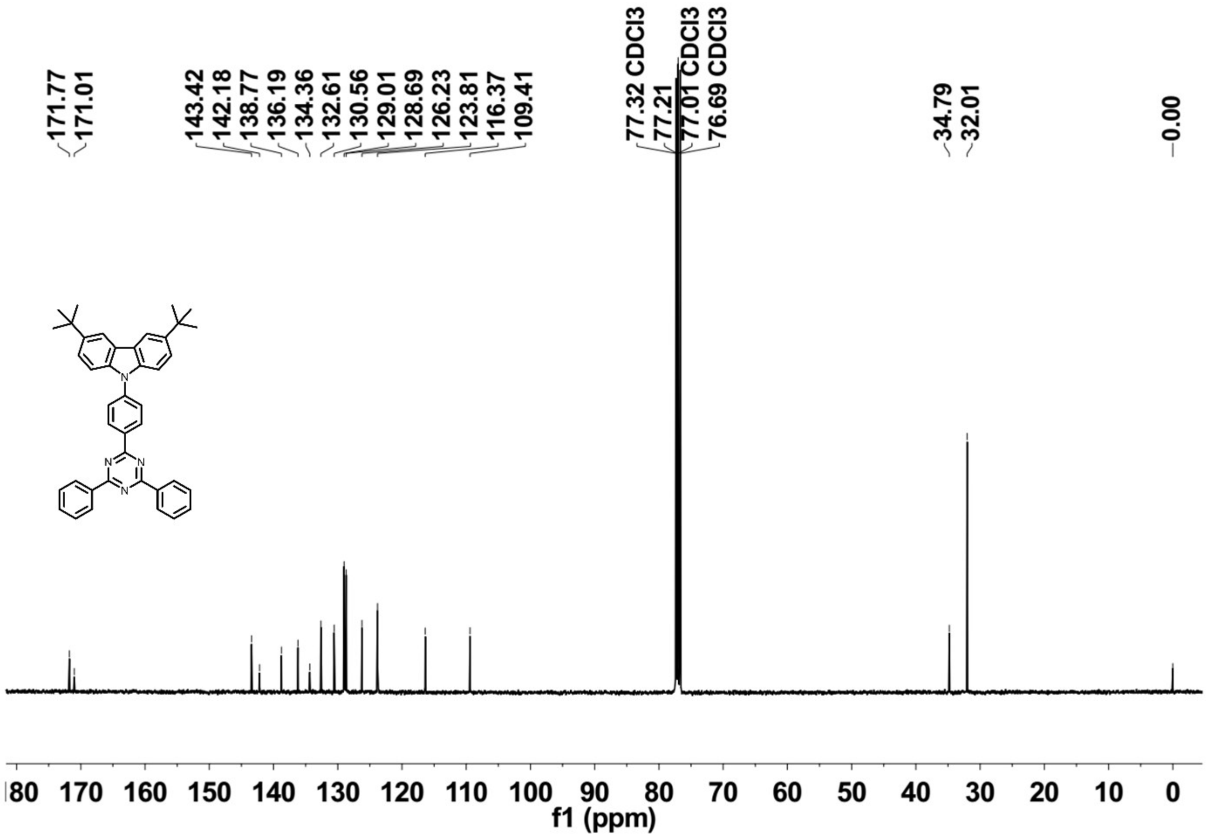


**Figure S18.** $^{13}C$ NMR spectrum of TC in $CDCl_3$.

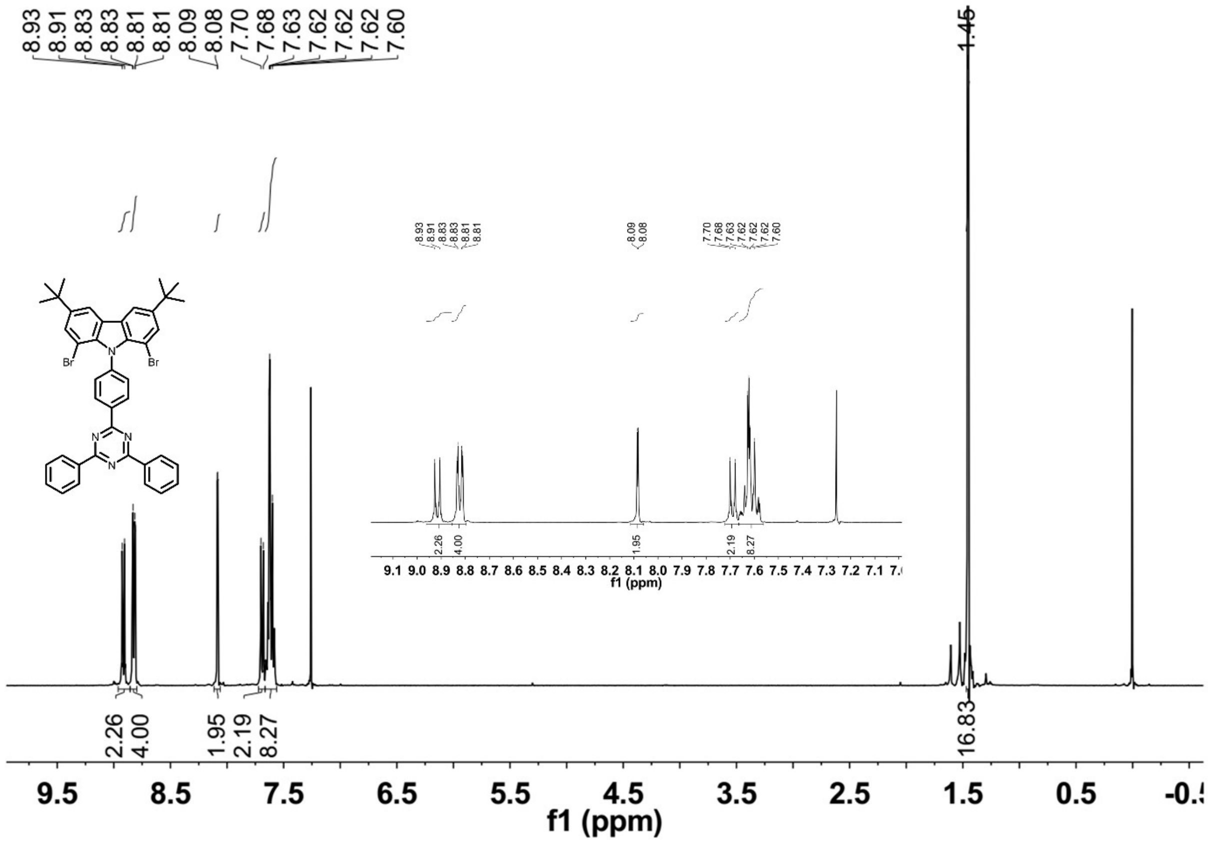


**Figure S19.** $^{1}$H NMR spectrum of Br-TC in $CDCl_3$.

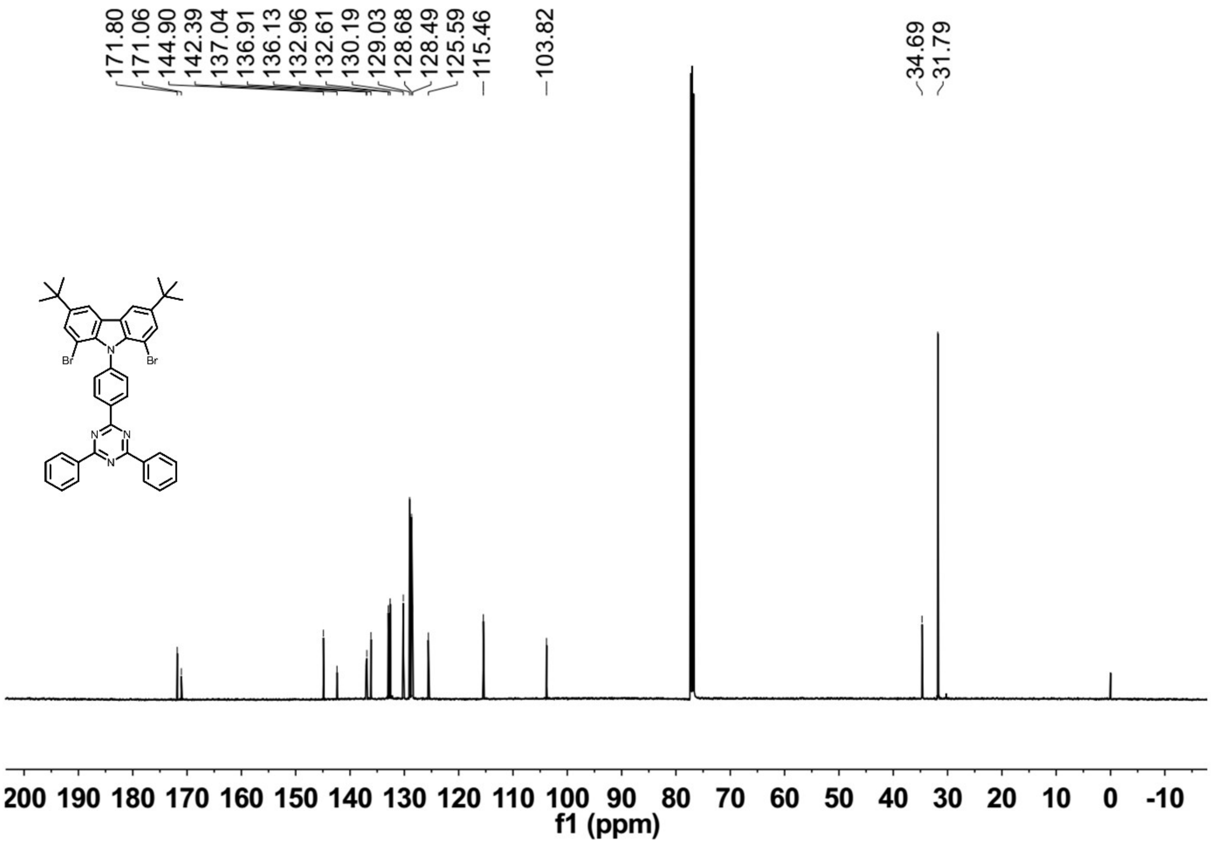


**Figure S20.** $^{13}$C NMR spectrum of Br-TC in $CDCl_3$.

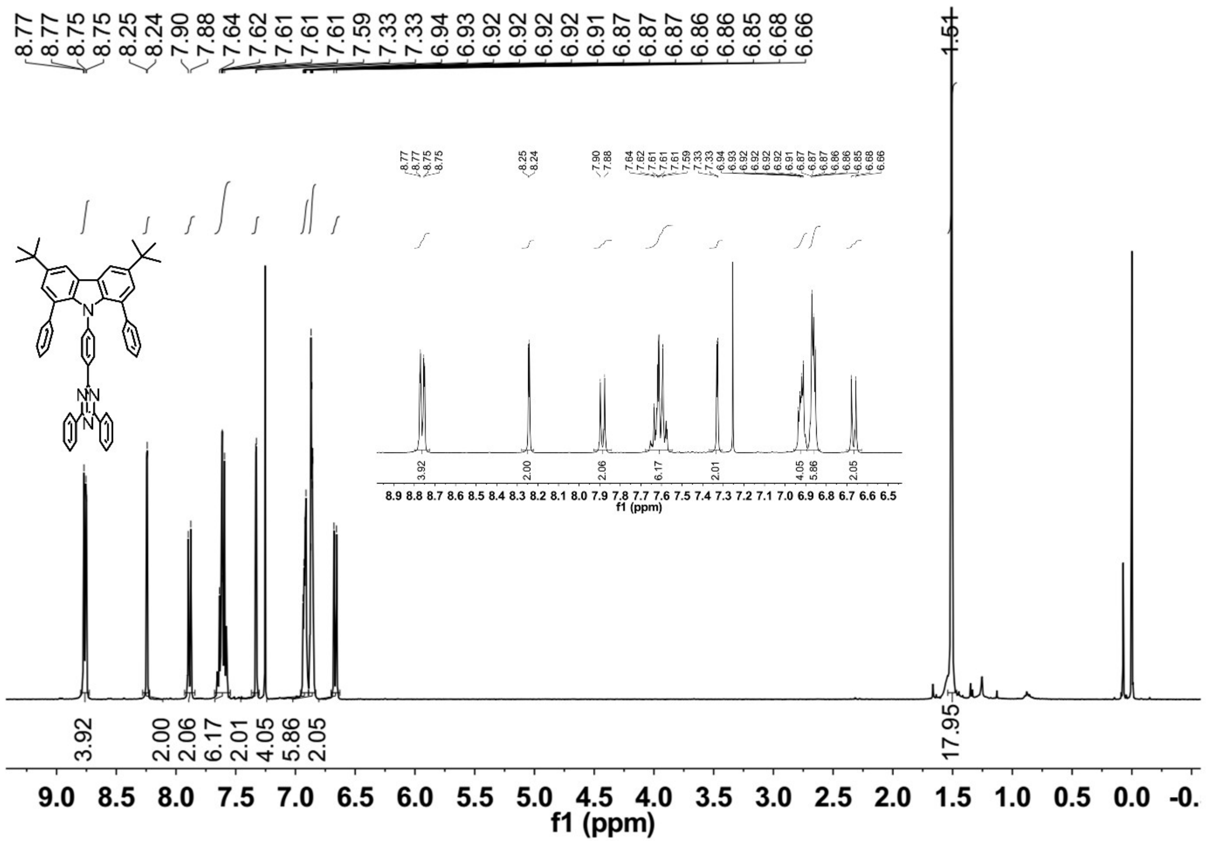


**Figure S21.** $^1H$ NMR spectrum of PTC in $CDCl_3$.

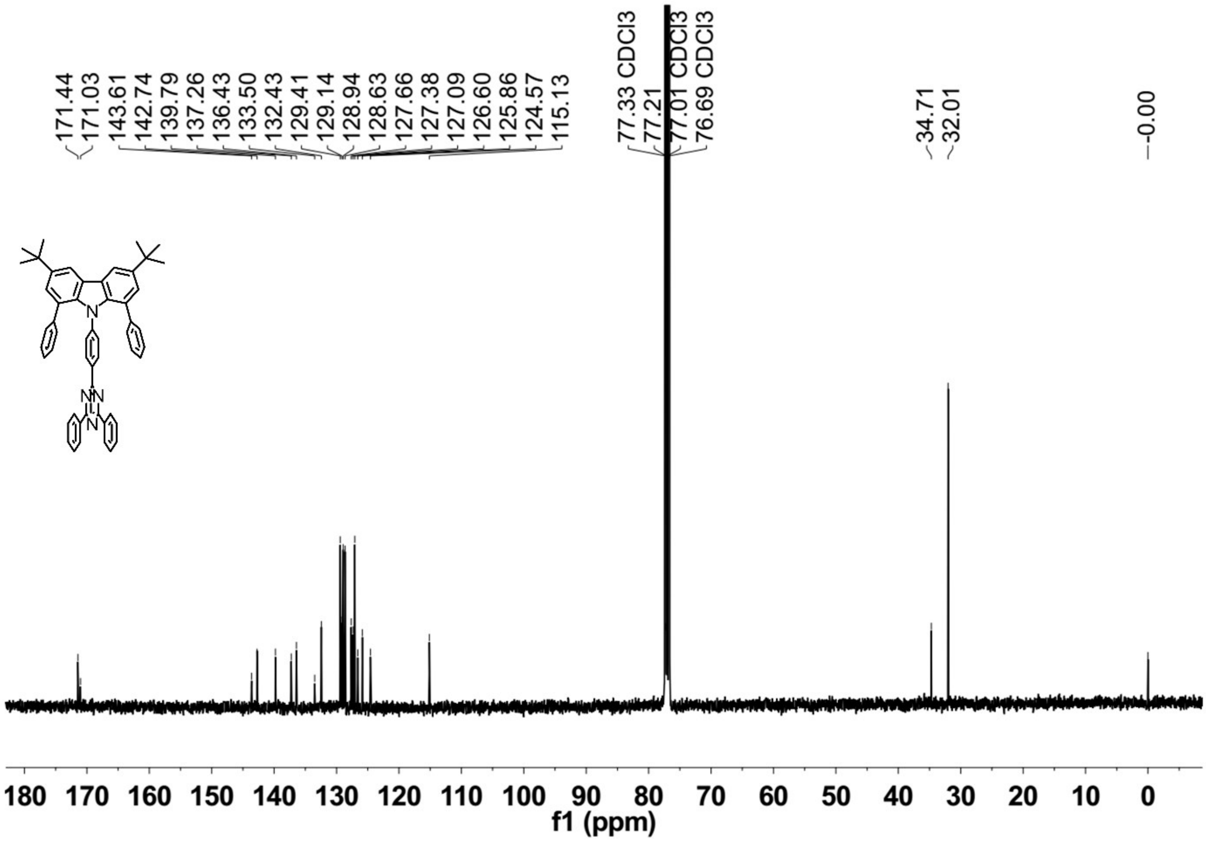


**Figure S22.** $^{13}C$ NMR spectrum of PTC in $CDCl_3$.

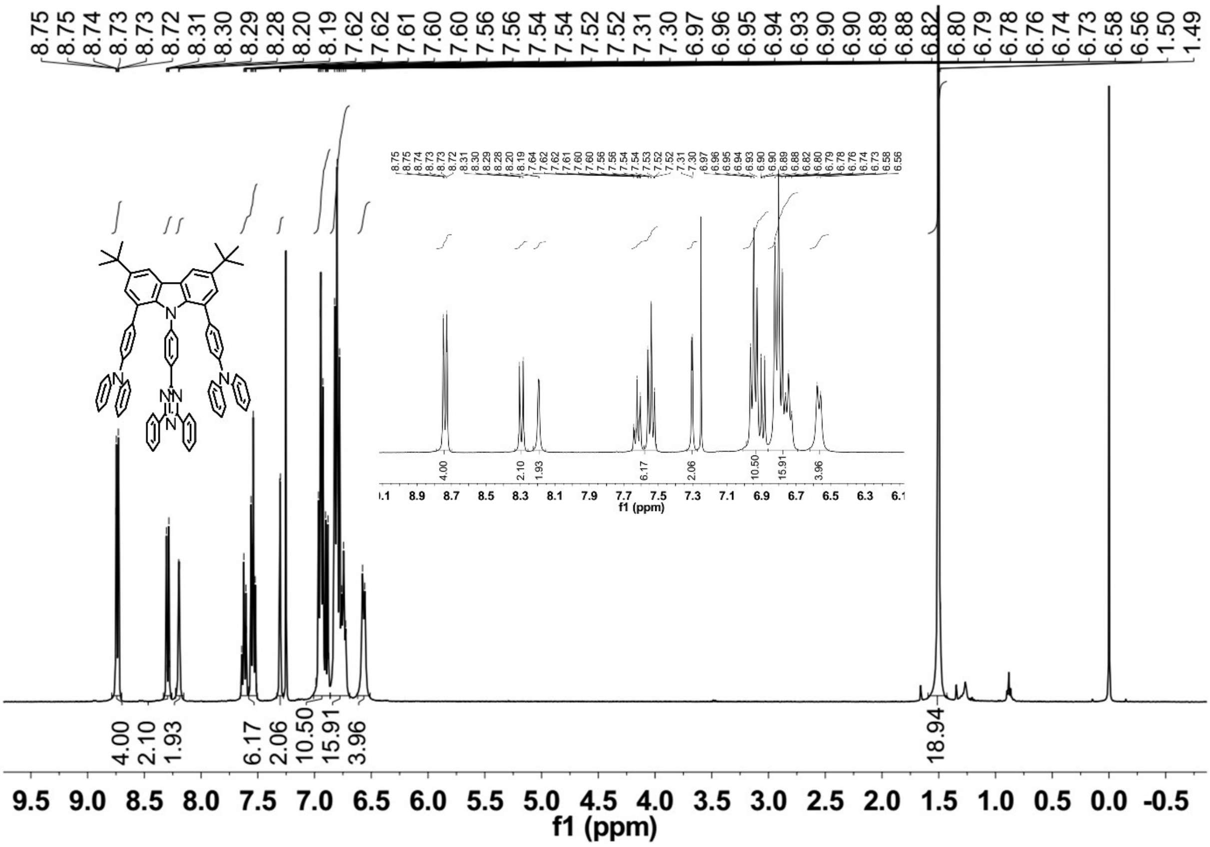


**Figure S23.** $^1H$ NMR spectrum of PAPTC in $CDCl_3$.

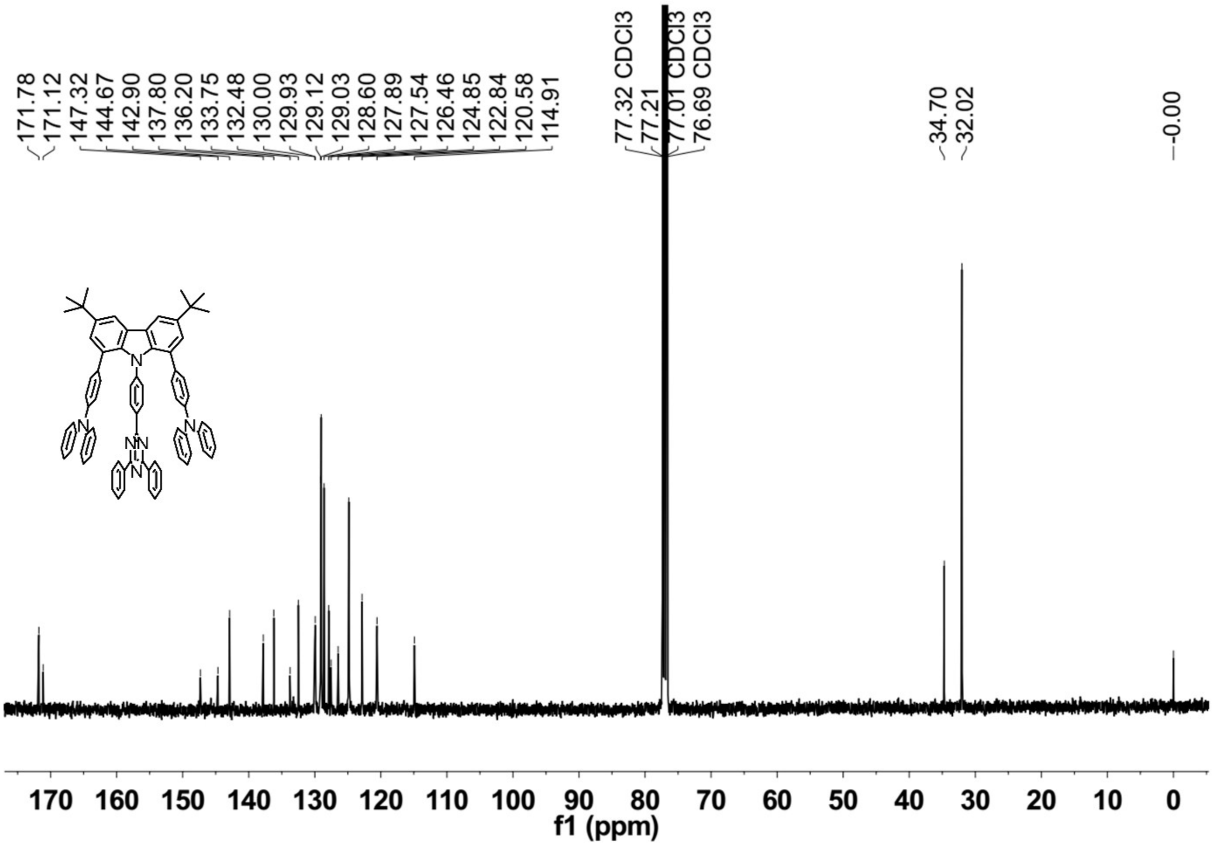


**Figure S24.** $^{13}C$ NMR spectrum of PAPTC in $CDCl_3$.

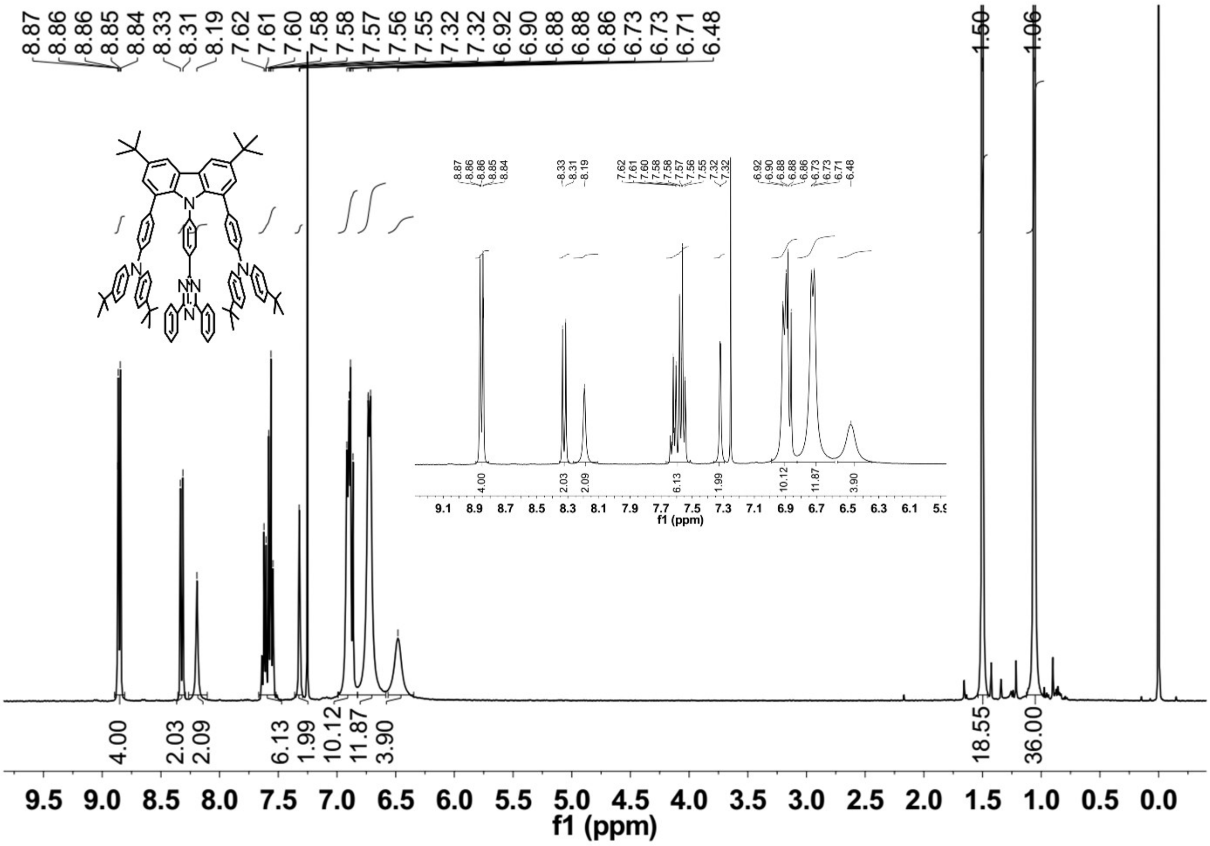


**Figure S25.** $^1$H NMR spectrum of BPAPTC in $CDCl_3$.

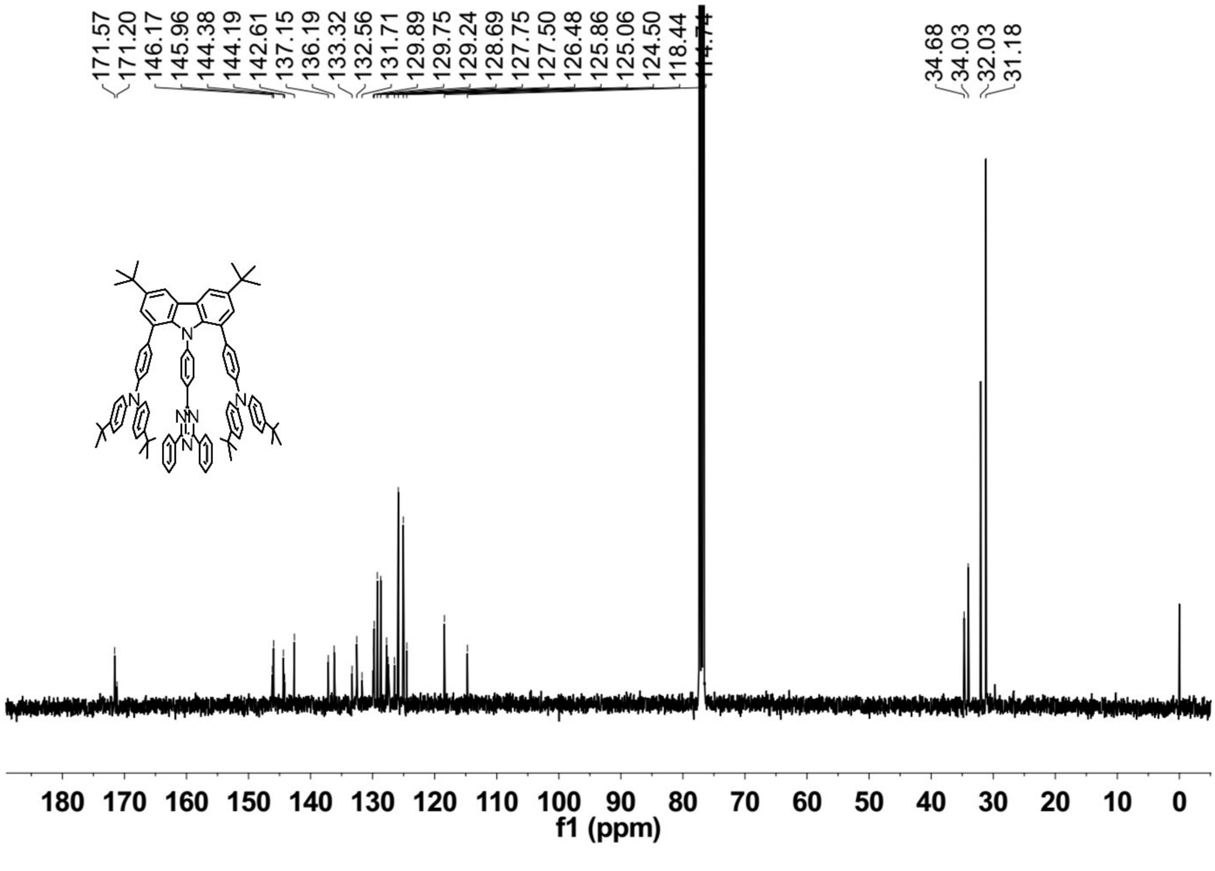


**Figure S26.** $^{13}$C NMR spectrum of BPAPTC in $CDCl_3$.

**Table:**

**Table S1.** Thermal stability properties of TC, PTC, PAPTC and BPAPTC.

| Compound | $T_g$ (°C) a) | $T_d$ (°C) b) |
|---|---|---|
| TC | 403 | 115 |
| PTC | 377 | 115 |
| PAPTC | 472 | 103 |
| BPAPTC | 462 | -- |

a) Measured by TGA recorded at a heating rate of 10 °C min$^{-1}$; b) Measured by DSC recorded at a heating rate of 10 °C min$^{-1}$.

**Table S2.** EL performances of 20 wt% PAPTC and BPAPTC doped film.

| Device | EL [nm] | $V_{on}$ [V] | Max performance | | | | Device performance at 1000/5000/10000 cd m$^{-2}$ | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | L [cd m$^{-2}$] | LE [cd A$^{-1}$] | PE [lm W$^{-1}$] | EQE [%] | $V_d$ [V] | LE [cd A$^{-1}$] | PE [lm W$^{-1}$] | EQE [%] |
| Device I: (PAPTC:SimCP2) | 520 | 3.0 | 17622 | 45.6 | 45.1 | 17.4 | 4.4/5.7/6.8 | 38.1/25.4/15.9 | 26.7/13.6/7.2 | 14.5/9.4/5.9 |
| Device II: (BPAPTC:SimCP2) | 520 | 2.8 | 44927 | 70.5 | 69.8 | 24.3 | 4.1/5.0/5.7 | 65.9/51.1/39.7 | 50.9/31.8/21.7 | 22.6/17.6/13.7 |

**Table S3.** The PLQYs of PAPTC and BPAPTC doped in SimCP2 with different ratio.

| Emitter:SimCP2 | PLQY [%] | | | | |
|---|---|---|---|---|---|
| | 20 wt% | 40 wt% | 60 wt% | 80 wt% | 100 wt% |
| PAPTC | 78 | 79 | 71 | 74 | 65 |
| BPAPTC | 90 | 93 | 92 | 90 | 85 |

**Table S4**. The photophysical properties of PAPTC and BPAPTC in 20 wt% doped film.

| Compound | $\tau_p$ [ns] | $\tau_d$ [ns] | $\Phi_{PL}$ [%] | $\Phi_{PF}$ [%] | $\Phi_{DF}$ [%] | $K_{PF}$ ($10^6$ s$^{-1}$) | $K_{DF}$ ($10^5$ s$^{-1}$) | $K_{ISC}$ ($10^6$ s$^{-1}$) | $K_{RISC}$ ($10^5$ s$^{-1}$) |
|---|---|---|---|---|---|---|---|---|---|
| PAPTC | 51 | 3909 | 78 | 22 | 56 | 4.31 | 1.43 | 3.09 | 5.08 |
| BPAPTC | 83 | 4587 | 90 | 17 | 73 | 2.05 | 1.59 | 1.66 | 8.43 |

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