Supporting Information

Enhancing Stereo Structure via Bulky Peripheral Groups to Improve Resistance to Concentration Quenching in OLEDs

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Characterization:

The intermediates and final compounds were confirmed by ^{1}H NMR or ^{13}C NMR spectra on a Bruker-AF301 AT 400 or 600 MHz spectrometer. Mass spectra were recorded on a high-resolution Fourier-transform mass spectrometer. Differential scanning calorimetry (DSC) was measured under nitrogen on a PE Instruments DSC 2920 unit at a heating rate of 10 °C min^{-1} from 30 to 300 °C. The glass transition temperature (T_g) was determined from the second heating scan. Thermogravimetric analysis (TGA) was undertaken using a PerkinElmer Instruments Pyris1 TGA at a heating rate of 10 °C min^{-1} from 30 to 600 °C under a nitrogen atmosphere. The thermal decomposition temperatures (T_d) corresponded to 5% weight loss temperatures. The UV-vis absorption spectra were measured on a Shimadzu UV-VIS-NIR Spectrophotometer (UV-3600) in the wavelength range of 190-1100 nm. The photoluminescence (PL) spectra were recorded on an Edinburgh Instruments (FLS 920 spectrometer). The absolute photoluminescence quantum yields (PLQY) and time-resolved photoluminescence (TRPL) tests were carried out by using Horiba Fluorolog-QM spectrofluorometer, PLQY test equipped with a calibrated integrating sphere. The lifetime data obtained from TRPL tests were fitted by the single exponential approach. Cyclic voltammetry was recorded on a computer-controlled EG&G Potentiostat/Galvanostat model 283 at room temperature with a conventional three-electrode system, which consisted of a platinum wire counter electrode, Ag/AgNO$_3$ (0.1 M) reference electrode, and a glassy carbon working electrode of 2 mm diameter. A 0.10 M tetrabutylammonium hexafluorophosphate (n-Bu$_4$NPF$_6$) solution in dry dichloromethane and *N*,*N*-dimethylformamide were employed as the supporting electrolyte, and ferrocene was added as a calibrant in the whole measurement. Finally, the dipole orientation was measured by RSQX-01 from Changchun Ruoshui Technology Development Co., Ltd.

Device fabrication and measurements:

The devices used ITO glass substrates, MoO_3, LiF, TAPC, mCBP, PPF, and TmPyPB were commercially available. The devices were fabricated by evaporating organic layers on ITO glass (20 Ω $square^{-1}$), which were precleaned carefully and treated with ozone airflow and ultraviolet light for 20 mins in Mondel UV-O_3 UVO_3 Cleaner. The devices were deposited in the vacuum of 2×10^{-6} Torr. For all of the OLEDs, the emitting areas were determined by the overlap of two electrodes as 0.09 cm^2. The *J-V-L* of the devices was measured using a Keithley 2400 source meter equipped with a calibrated silicon photodiode. The EL spectra were measured using a PR655 spectrometer. All measurements were carried out at room temperature under ambient conditions.

Calculation details:

The density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations were employed to optimize the ground state and excited state geometries and electronic properties, which were carried out with the B3LYP hybrid functional at the basis set level of 6-31G(d). The spin-orbit coupling matrix elements (SOCME) were calculated by the ORCA program and also under the TD-DFT method, and it was carried out with the B3LYP hybrid functional at the basis set level of def2-TZVP.[1]

Specific synthesis steps:

Synthesis of Intermediate DtCz-DBr:

Sequentially take 2,5-dibromo-1,3-difluorobenzene (10 g, 36 mmol), 3,6-di-tert-butyl-9H-carbazole (20 g, 72 mmol), and cesium carbonate (35 g, 108 mmol), and add them to a 250 ml three-neck round-bottom flask. Then, add 100 ml of N,N-dimethylformamide and degas the mixture by purging with nitrogen for eight minutes, replacing the nitrogen five times. Subsequently, heat the mixture to 150 °C under a nitrogen atmosphere, adjust the condenser to maintain an appropriate reflux rate, and stir the reaction for 12 hours. After the reaction is complete, allow the reaction mixture to cool to room temperature. Then, extract the reaction mixture three to five times with ethyl acetate and water. Collect the organic layer and dry it over anhydrous magnesium sulfate. Concentrate the solution under reduced pressure, mix the crude product with an appropriate amount of silica gel, and purify by column chromatography using pure petroleum ether as the eluent to obtain 28 g of white solid with a yield of 90%. ^{1}H NMR (600 MHz, CD_2Cl_2) δ[ppm]: 8.19 (s, 4H), 7.82 (d, J = 1.5 Hz, 2H), 7.55 (d, J = 8.8 Hz, 4H), 7.17 (d, J = 8.5 Hz, 4H), 1.47 (d, J = 1.5 Hz, 36H). HRMS (APCI): Theoretical value: $C_{46}H_{50}Br_2N_2$, 790.7280; Experimental value: 791.7380, [M+H]+.

Synthesis of Intermediate DtCzB-DBr:

Weigh **DtCz-DBr** (10 g, 13 mmol) and add it to a 250 ml three-neck round-bottom flask. Then add 100 ml of m-xylene solution and degas the mixture by purging with nitrogen for eight minutes, replacing the nitrogen five times. Subsequently, place the three-neck flask in a low-temperature reaction bath (-40 °C) and expel the air from the needle. Under a nitrogen atmosphere, withdraw n-butyllithium (n-BuLi) (50 ml, 0.5 mol) and slowly inject it into the flask, stirring thoroughly for 2 hours. Then, allow the mixture to warm to room temperature, degas again, and remove the n-pentane from the n-butyllithium solvent. Next, at -40 °C, slowly add boron tribromide (BBr_3) (50 ml, 13 mmol) and stir at room temperature for 1 hour. After that, add N,N-diisopropylethylamine (100 ml, 1 mol), and heat to 140 °C, adjusting the condenser to maintain an appropriate reflux rate, and continue stirring the reaction for 12 hours. Once the reaction is complete, allow the mixture to cool to room temperature, quench the reaction with ethanol, and concentrate the m-xylene solvent under reduced pressure. Mix the crude product with an appropriate amount of silica gel and purify by column chromatography using pure petroleum ether as the eluent to obtain 7.5 g of yellow solid with a yield of 80%. ^{1}H NMR (600 MHz, CD_2Cl_2) δ[ppm]: 9.01 (s, 2H), 8.43 (d, J = 2.2 Hz, 2H), 8.29 – 8.05 (m, 6H), 7.65 – 7.58 (m, 2H), 1.66 (d, J = 1.8 Hz, 18H), 1.55 (s, 18H). HRMS (APCI): Theoretical value: $C_{46}H_{48}BBrN_2$, 719.6180; Experimental value: 720.6073, [M+H]+.

Synthesis of Intermediate 1:

Take 1,3-dibromo-5-chlorobenzene (8 g, 50 mmol), diphenylamine (8 g, 69 mmol), tris(dibenzylideneacetone)dipalladium (0.6 g, 0.7 mmol), tri-tert-butylphosphonium tetrafluoroborate (0.4 g, 1.4 mmol), and sodium tert-butoxide (14 g, 148 mmol) and add them to a 250 ml three-neck round-bottom flask. Then add 100 ml of anhydrous toluene and degas the mixture by purging with nitrogen for eight minutes, replacing the nitrogen five times. Subsequently, under a nitrogen atmosphere, heat the mixture to 150 °C, adjust the condenser to maintain an appropriate reflux rate, and continue stirring the reaction for 12 hours. Once the reaction is complete, allow the mixture to cool to room temperature, concentrate the toluene solvent under reduced pressure, mix the crude product with an appropriate amount of silica gel, and purify by column chromatography using pure petroleum ether as the eluent to obtain 20 g of yellow solid with a yield of 90%. ^{1}H NMR (600 MHz, CD_2Cl_2) δ[ppm]: 7.26 (dt, J = 28.6, 7.9 Hz, 9H), 7.13 (d, J = 8.0 Hz, 2H), 6.97 (dd, J = 7.8, 4.9 Hz, 12H). HRMS (APCI): Theoretical value: $C_{30}H_{23}ClN_2$, 446.9780; Experimental value: 447.9655, [M+H]+.

Synthesis of Intermediate 2:

Take intermediate 1 (10 g, 23 mmol), dried sodium acetate (5.7 g, 69 mmol), tris(dibenzylideneacetone)dipalladium (1.1 g, 1.2 mmol), 2-(dicyclohexylphosphino)-2',4',6'-triisopropylbiphenyl (1.1 g, 2.4 mmol), and bis(pinacolato)diboron (BPIN) (5.8 g, 23 mmol), and add them to a 250 ml three-neck round-bottom flask. Then add 100 ml of anhydrous dioxane, degas the mixture by purging with nitrogen for eight minutes, and replace the nitrogen five times. Subsequently, under a nitrogen atmosphere, heat the mixture to 110 °C, adjust the condenser to maintain an appropriate reflux rate, and continue stirring the reaction for 12 hours. Once the reaction is complete, allow the mixture to cool to room temperature, concentrate the toluene solvent under reduced pressure, mix the crude product with an appropriate amount of silica gel, and purify by column chromatography using petroleum ether: dichloromethane (30:1) as the eluent to obtain 8 g of white solid with a yield of 65%. ^{1}H NMR (600 MHz, CD_2Cl_2) δ[ppm]: 7.22 (t, J = 7.8 Hz, 8H), 7.04 (dd, J = 14.4, 5.1 Hz, 10H), 6.98 (t, J = 7.4 Hz, 4H), 6.94 (d, J = 2.1 Hz, 1H), 1.26 (s, 12H). HRMS (APCI): Theoretical value: $C_{36}H_{35}BN_2O_2$, 538.4980; Experimental value: 539.4975, [M+H]+.

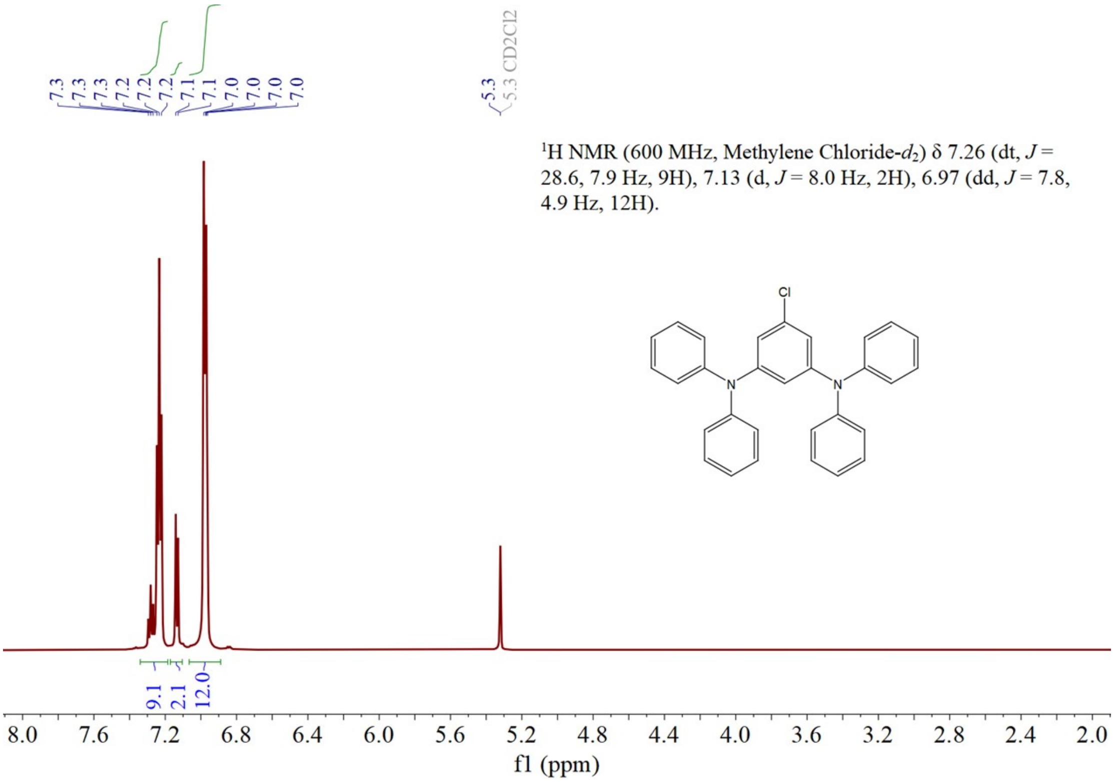
Synthesis of Intermediate 3:

Take 1-bromo-3,5-difluorobenzene (7.8 g, 49.3 mmol) and sodium thiophenolate (8.4 g, 69 mmol), and add them to a 250 ml three-neck round-bottom flask. Then add 100 ml of N-methyl-2-pyrrolidone (NMP), degas the mixture by purging with nitrogen for eight minutes, and replace the nitrogen five times. Subsequently, under a nitrogen atmosphere, heat the mixture to 160 °C, adjust the condenser to maintain an appropriate reflux rate, and continue stirring the reaction for 24 hours. Once the reaction is complete, allow the mixture to cool to room temperature, extract the reaction mixture three to five times with ethyl acetate and water, collect the upper organic phase, and dry it with anhydrous magnesium sulfate. Concentrate the organic phase under reduced pressure, mix the crude product with an appropriate amount of silica gel, and purify by column chromatography using pure petroleum ether as the eluent to obtain 16.5 g of white solid with a yield of 90%. ^{1}H NMR (600 MHz, CD_2Cl_2) δ[ppm]: 7.40 (ddt, J = 13.3, 5.7, 3.8 Hz, 4H), 7.35 (td, J = 5.4, 2.0 Hz, 6H), 7.17 (d, J = 1.8 Hz, 1H), 6.98 (t, J = 1.7 Hz, 1H), 6.70 (dd, J = 9.0, 1.8 Hz, 1H). HRMS (APCI): Theoretical value: $C_{18}H_{13}BrS_2$, 373.3260; Experimental value: 374.3342, [M+H]+.

Synthesis of Intermediate 4:

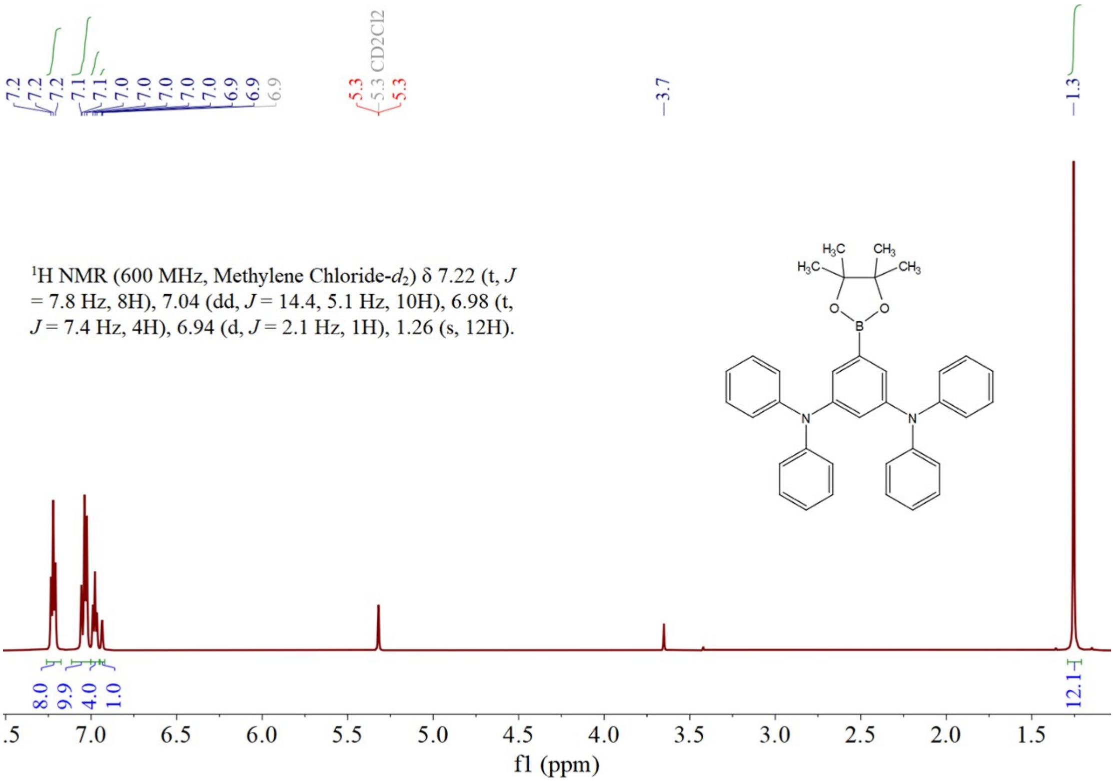
Take intermediate 3 (10 g, 27 mmol), dried potassium acetate (8 g, 81 mmol), [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium (1 g, 1.35 mmol), and BPIN (6.9 g, 27 mmol) sequentially and add them to a 250 ml three-neck round-bottom flask. Then add 100 ml of anhydrous dioxane, and purge with nitrogen for eight minutes, replacing the nitrogen five times. Subsequently, heat under a nitrogen atmosphere to 80 °C, adjust the condenser water to maintain an appropriate reflux rate, and continue stirring for 24 hours. After the reaction is complete, allow the system to return to room temperature, evaporate the toluene solvent, and add an appropriate amount of silica gel to the crude product. Perform column chromatography using petroleum ether: dichloromethane (30:1) as the eluent to obtain 8.4 g of a white solid with a yield of 73%. ^{1}H NMR (600 MHz, CD_2Cl_2) δ[ppm]: δ 7.63 (d, J = 2.0 Hz, 2H), 7.37 – 7.20 (m, 11H), 1.30 (d, J = 1.8 Hz, 12H). HRMS (APCI): Theoretical value: $C_{24}H_{25}BO_2S_2$, 420.3920; Experimental value: 421.3724, [M+H]+.

Figures, tables, and equations:



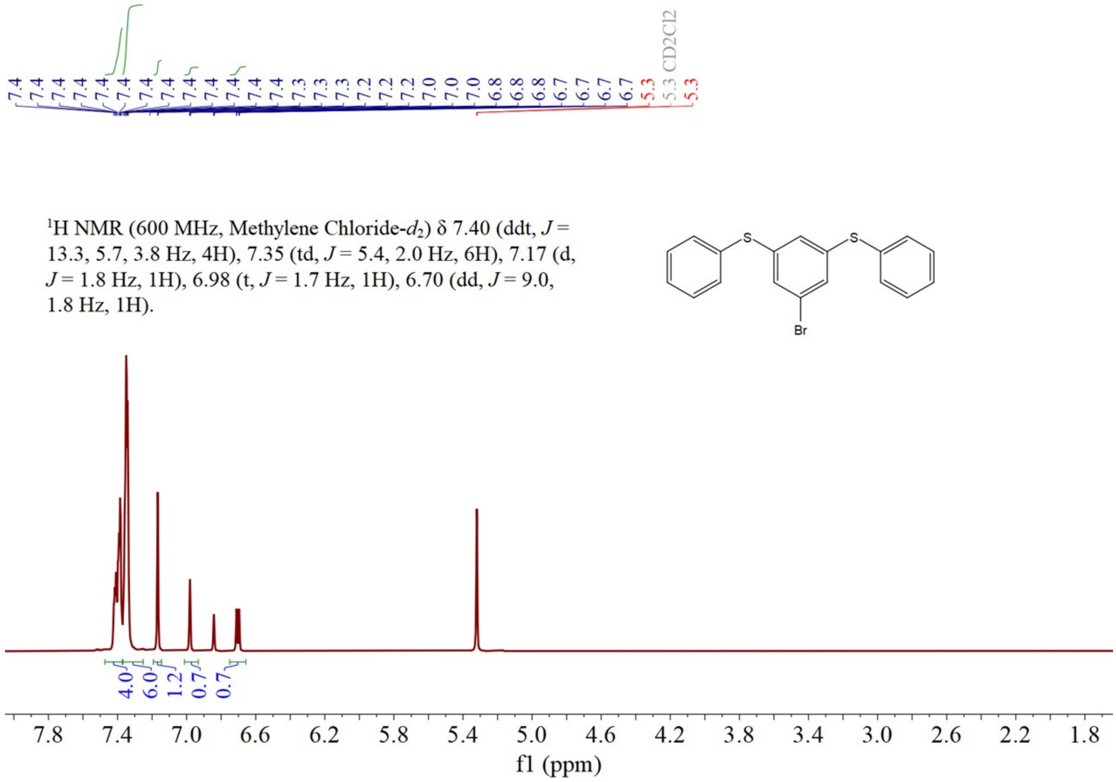
^{1}H NMR (600 MHz, Methylene Chloride-d_2) δ 7.26 (dt, J = 28.6, 7.9 Hz, 9H), 7.13 (d, J = 8.0 Hz, 2H), 6.97 (dd, J = 7.8, 4.9 Hz, 12H).

Fig. S1 ^{1}H NMR spectrum of **Intermediate 1** in CD_2Cl_2.



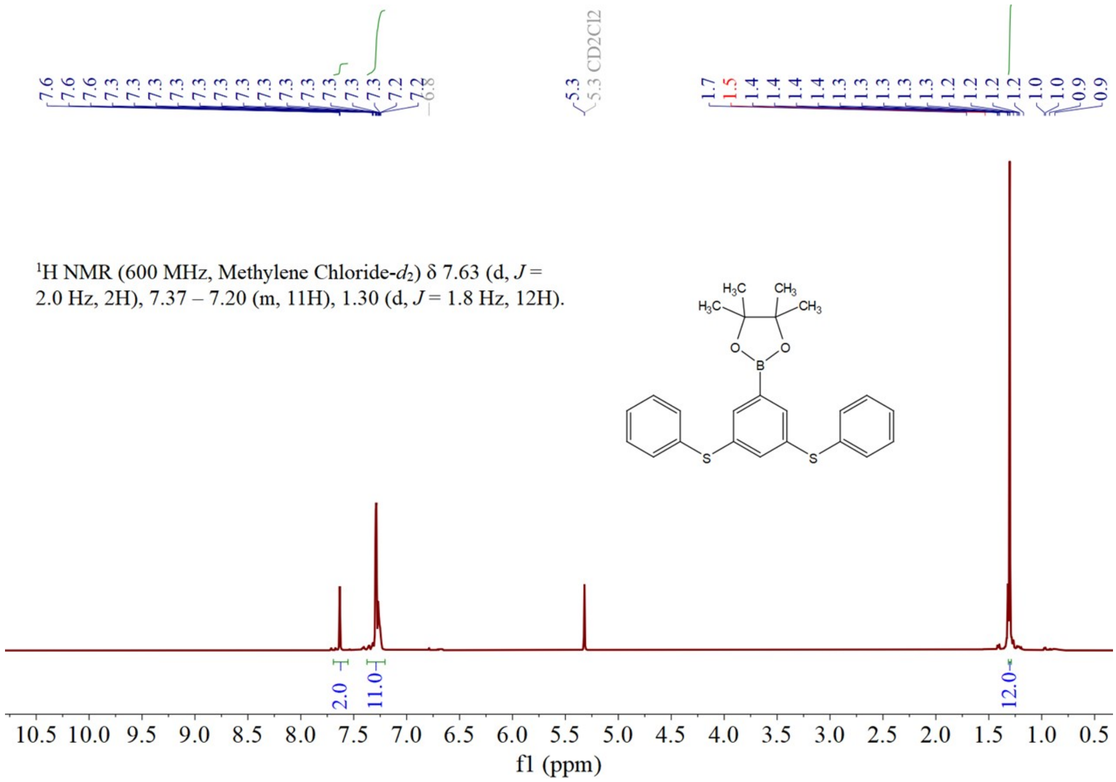
^{1}H NMR (600 MHz, Methylene Chloride-d_2) δ 7.22 (t, J = 7.8 Hz, 8H), 7.04 (dd, J = 14.4, 5.1 Hz, 10H), 6.98 (t, J = 7.4 Hz, 4H), 6.94 (d, J = 2.1 Hz, 1H), 1.26 (s, 12H).

Fig. S2 ^{1}H NMR spectrum of **Intermediate 2** in CD_2Cl_2.



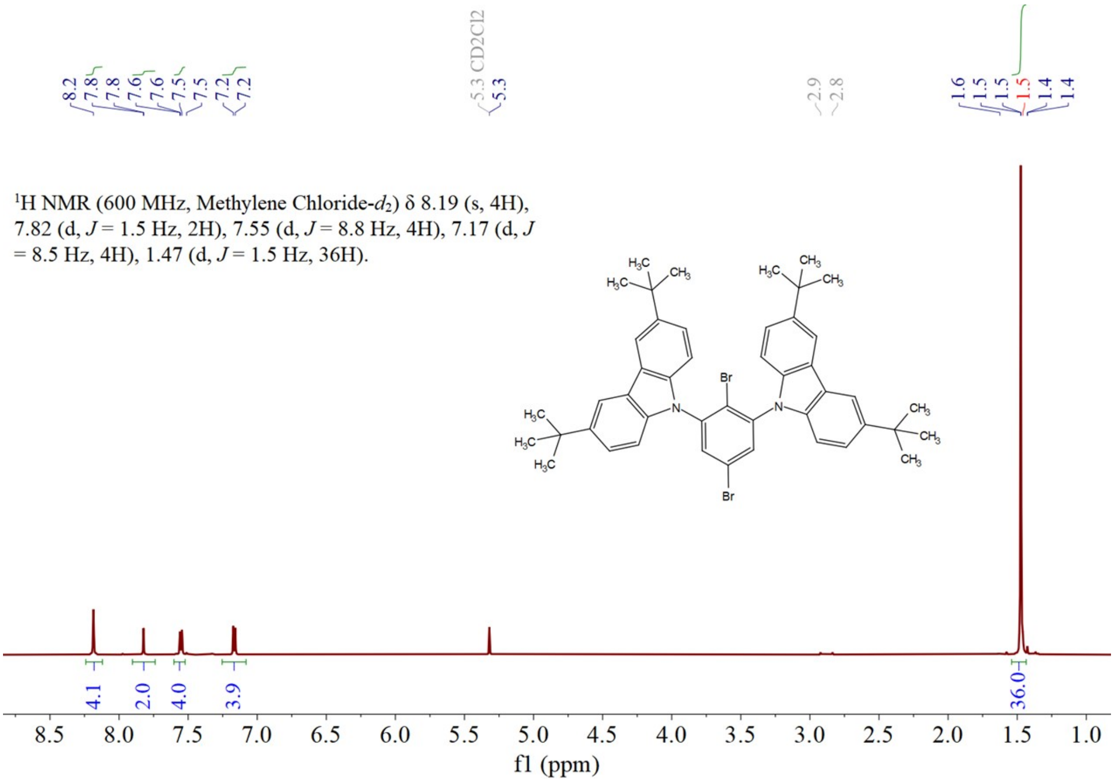
¹H NMR (600 MHz, Methylene Chloride-d_2) δ 7.40 (ddt, J = 13.3, 5.7, 3.8 Hz, 4H), 7.35 (td, J = 5.4, 2.0 Hz, 6H), 7.17 (d, J = 1.8 Hz, 1H), 6.98 (t, J = 1.7 Hz, 1H), 6.70 (dd, J = 9.0, 1.8 Hz, 1H).

Fig. S3 ¹H NMR spectrum of **Intermediate 3** in CD_2Cl_2.



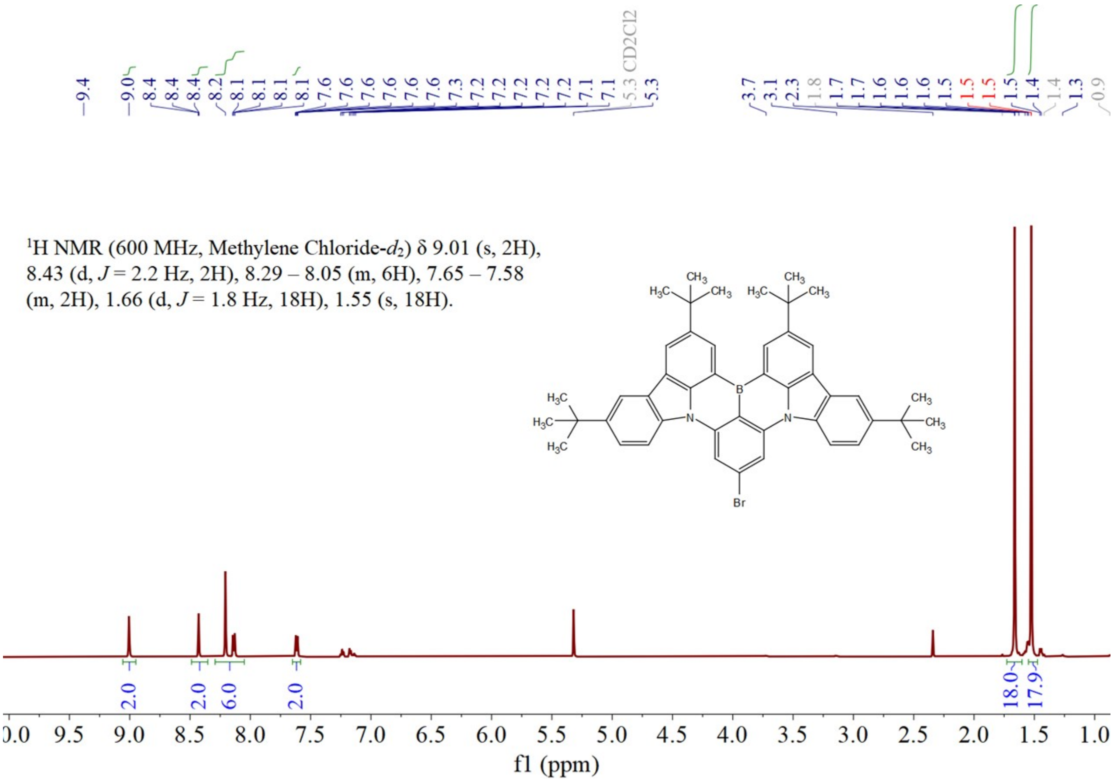
¹H NMR (600 MHz, Methylene Chloride-d_2) δ 7.63 (d, J = 2.0 Hz, 2H), 7.37 – 7.20 (m, 11H), 1.30 (d, J = 1.8 Hz, 12H).

Fig. S4 ¹H NMR spectrum of **Intermediate 4** in CD_2Cl_2.



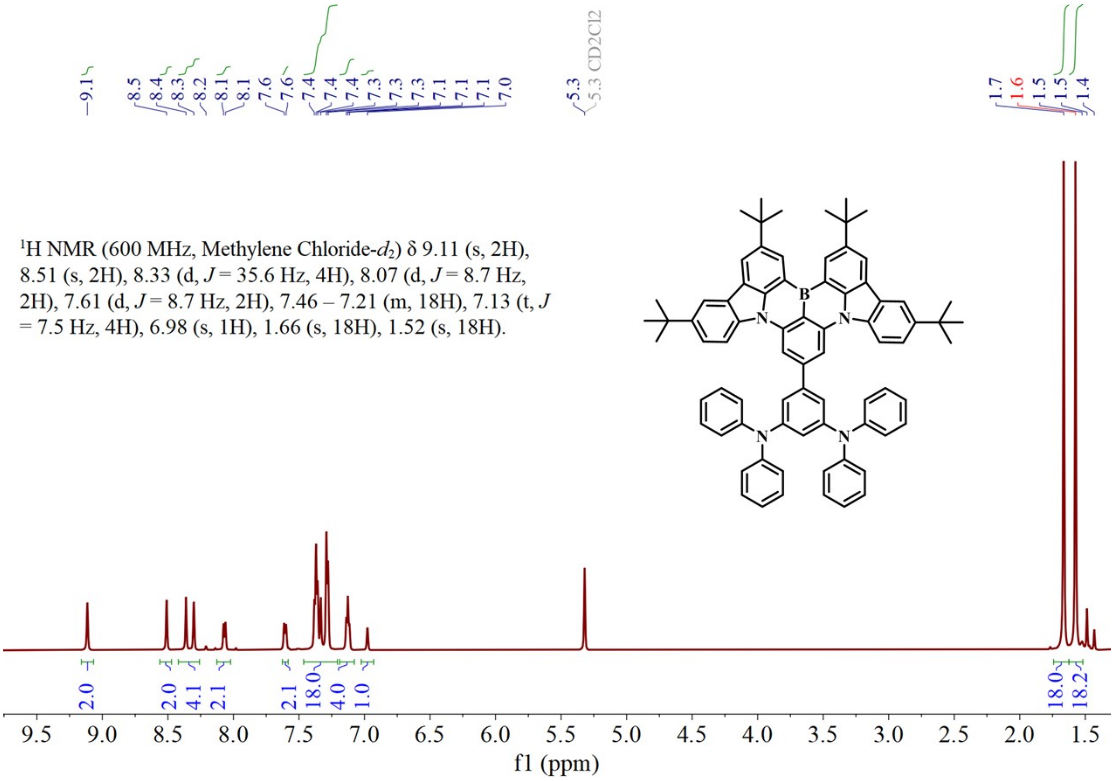
^{1}H NMR (600 MHz, Methylene Chloride-d_2) δ 8.19 (s, 4H), 7.82 (d, J = 1.5 Hz, 2H), 7.55 (d, J = 8.8 Hz, 4H), 7.17 (d, J = 8.5 Hz, 4H), 1.47 (d, J = 1.5 Hz, 36H).

Fig. S5 ^{1}H NMR spectrum of **DtCz-DBr** in CD_2Cl_2.



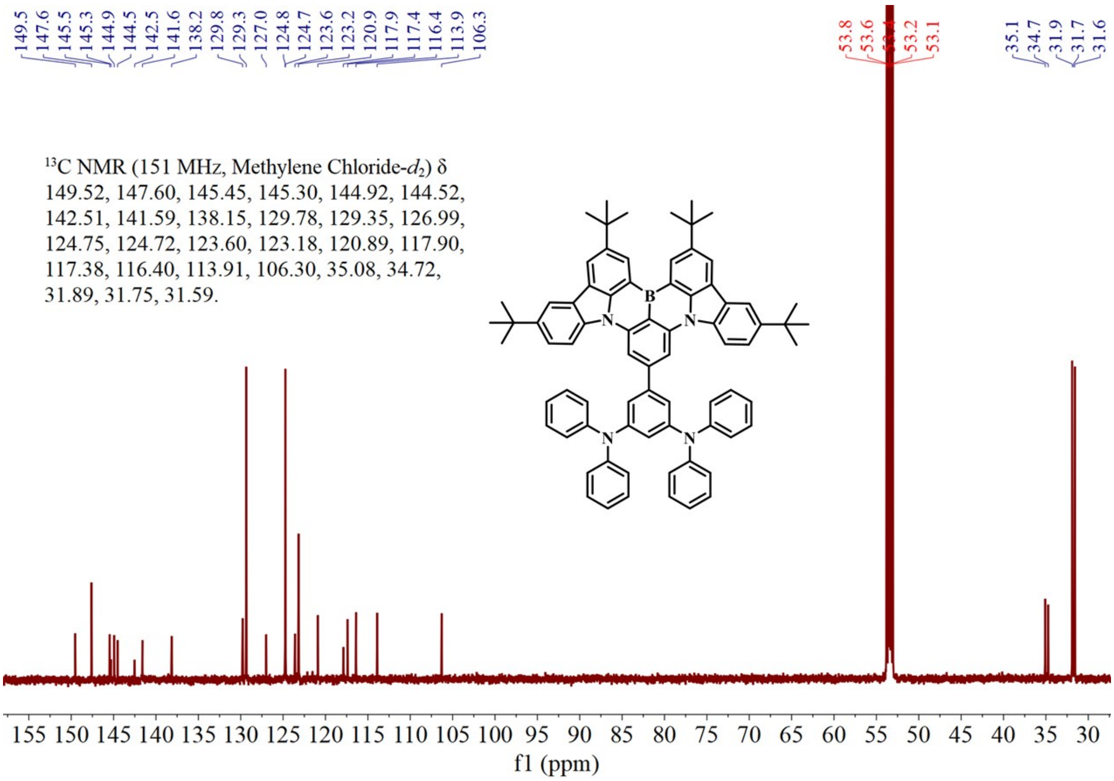
^{1}H NMR (600 MHz, Methylene Chloride-d_2) δ 9.01 (s, 2H), 8.43 (d, J = 2.2 Hz, 2H), 8.29 – 8.05 (m, 6H), 7.65 – 7.58 (m, 2H), 1.66 (d, J = 1.8 Hz, 18H), 1.55 (s, 18H).

Fig. S6 ^{1}H NMR spectrum of **DtCzB-DBr** in CD_2Cl_2.



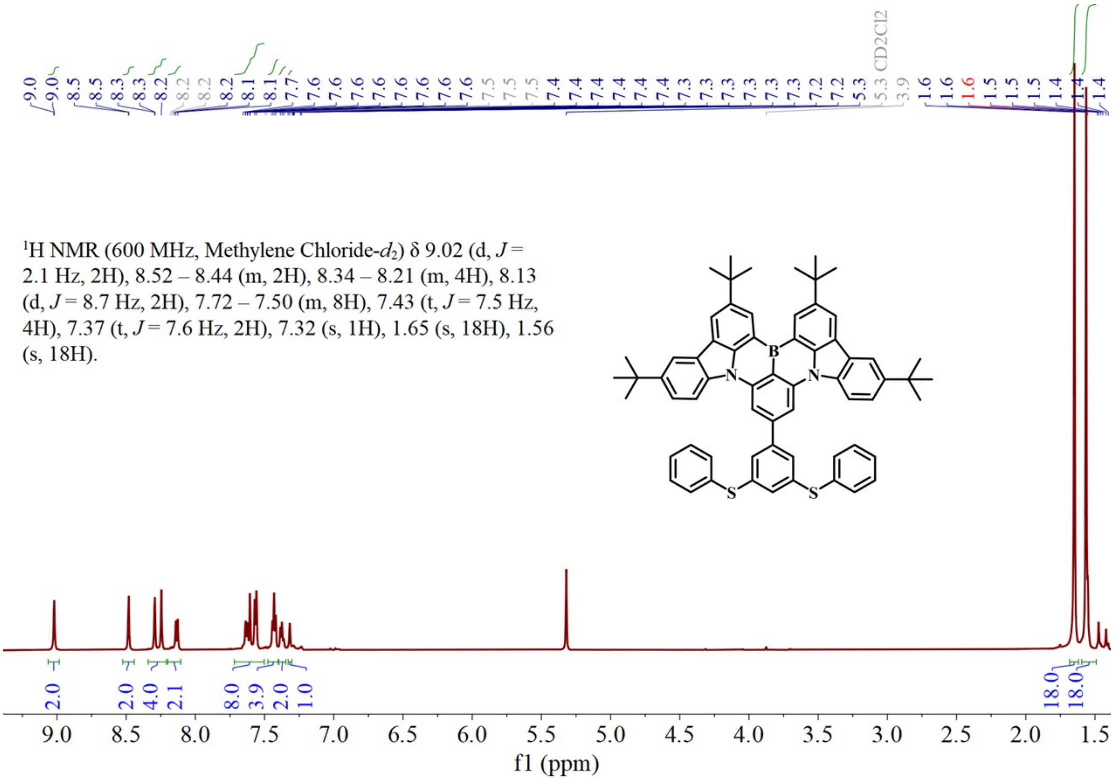
^{1}H NMR (600 MHz, Methylene Chloride-d_2) δ 9.11 (s, 2H), 8.51 (s, 2H), 8.33 (d, J = 35.6 Hz, 4H), 8.07 (d, J = 8.7 Hz, 2H), 7.61 (d, J = 8.7 Hz, 2H), 7.46 – 7.21 (m, 18H), 7.13 (t, J = 7.5 Hz, 4H), 6.98 (s, 1H), 1.66 (s, 18H), 1.52 (s, 18H).

Fig. S7 ^{1}H NMR spectrum of **DtCzB-mDPA** in CD_2Cl_2.



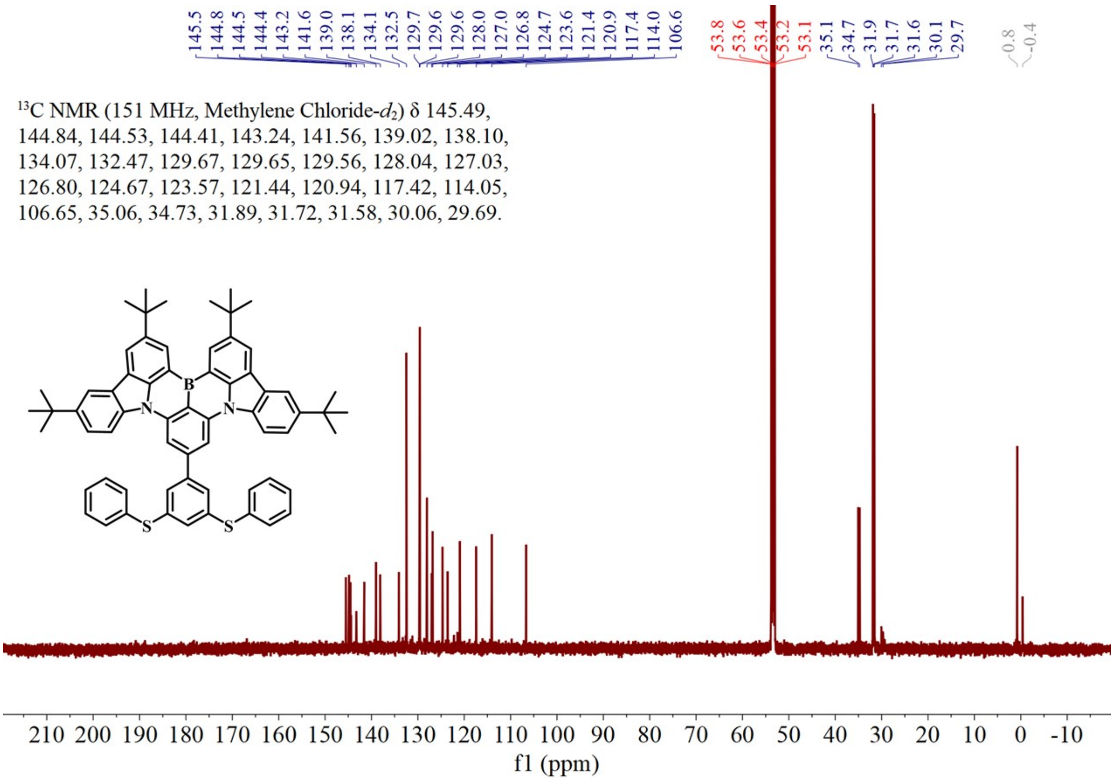
^{13}C NMR (151 MHz, Methylene Chloride-d_2) δ 149.52, 147.60, 145.45, 145.30, 144.92, 144.52, 142.51, 141.59, 138.15, 129.78, 129.35, 126.99, 124.75, 124.72, 123.60, 123.18, 120.89, 117.90, 117.38, 116.40, 113.91, 106.30, 35.08, 34.72, 31.89, 31.75, 31.59.

Fig. S8 ^{13}C NMR spectrum of **DtCzB-mDPA** in CD_2Cl_2.



^{1}H NMR (600 MHz, Methylene Chloride-d_2) δ 9.02 (d, J = 2.1 Hz, 2H), 8.52 – 8.44 (m, 2H), 8.34 – 8.21 (m, 4H), 8.13 (d, J = 8.7 Hz, 2H), 7.72 – 7.50 (m, 8H), 7.43 (t, J = 7.5 Hz, 4H), 7.37 (t, J = 7.6 Hz, 2H), 7.32 (s, 1H), 1.65 (s, 18H), 1.56 (s, 18H).

Fig. S9 ^{1}H NMR spectrum of **DtCzB-mDS** in CD_2Cl_2.



^{13}C NMR (151 MHz, Methylene Chloride-d_2) δ 145.49, 144.84, 144.53, 144.41, 143.24, 141.56, 139.02, 138.10, 134.07, 132.47, 129.67, 129.65, 129.56, 128.04, 127.03, 126.80, 124.67, 123.57, 121.44, 120.94, 117.42, 114.05, 106.65, 35.06, 34.73, 31.89, 31.72, 31.58, 30.06, 29.69.

Fig. S10 ^{13}C NMR spectrum of **DtCzB-mDS** in CD_2Cl_2.

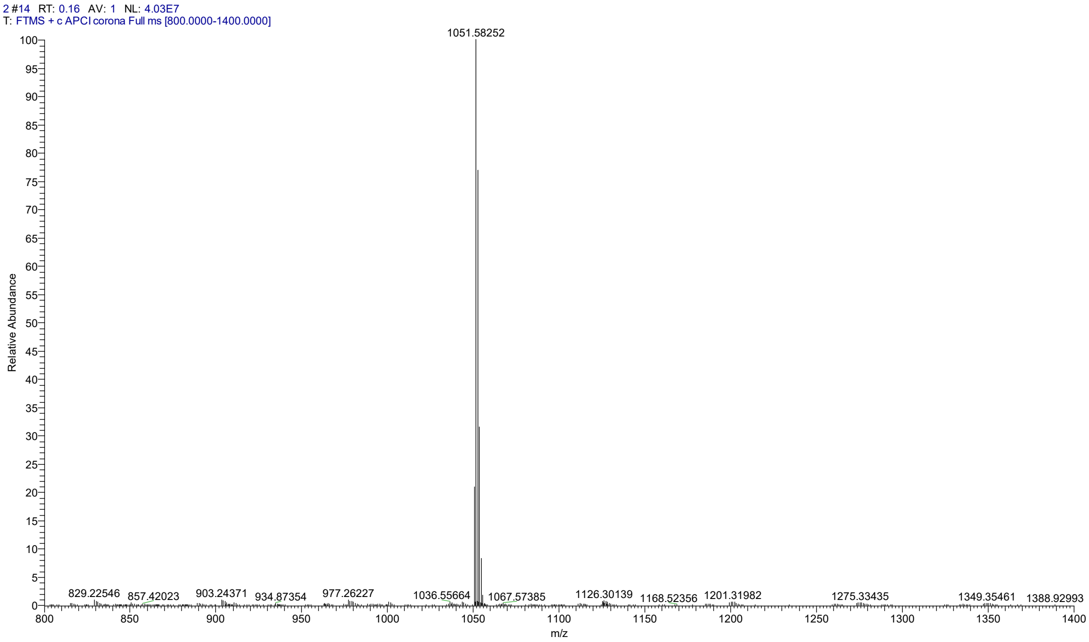


Fig. S11 MS spectrum of **DtCzB-mDPA** in DCM.

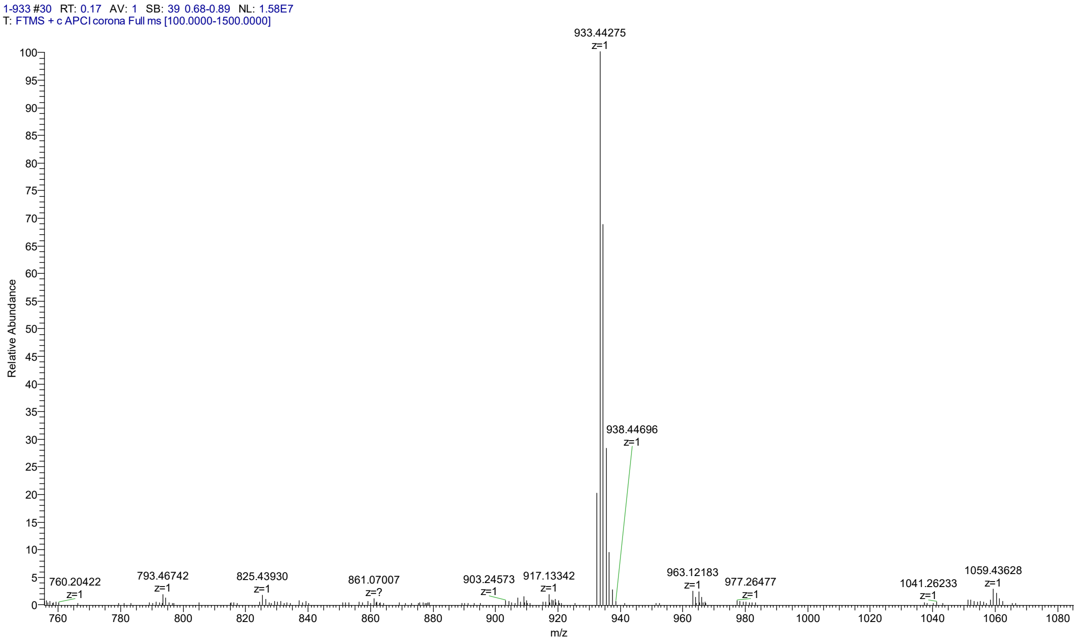


Fig. S12 MS spectrum of **DtCzB-mDS** in DCM.

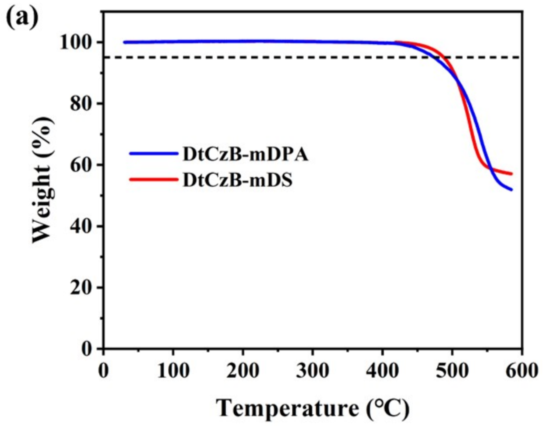


Fig. S13 (a) TGA curves of **DtCzB-mDPA** and **DtCzB-mDS**. (b) DSC analysis curves of **DtCzB-mDPA** and **DtCzB-mDS**.

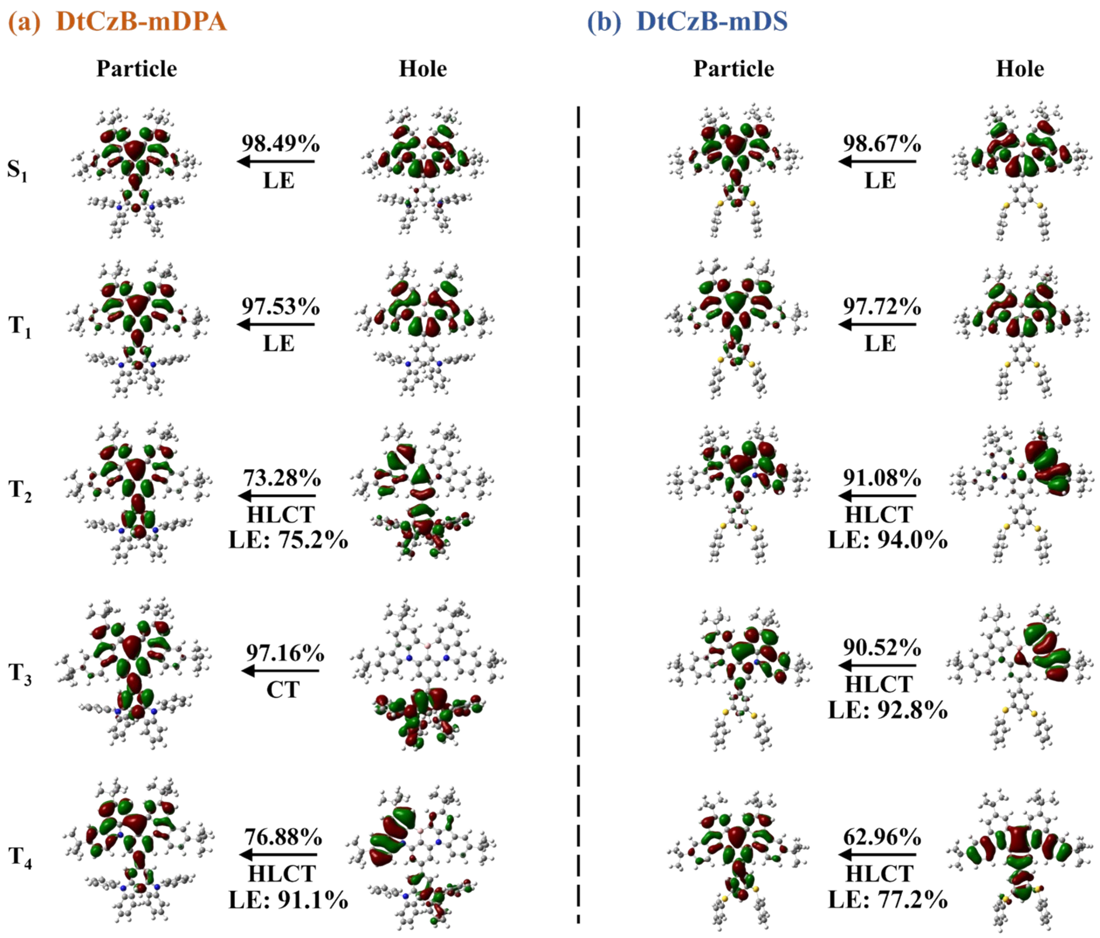


Fig. S14 Diagrams of NTOs for the energy levels of (a) **DtCzB-mDPA** and (b) **DtCzB-mDS**, with both molecular structures optimized.

Table S1 The photophysical data of **DtCzB-mDPA** and **DtCzB-mDS** in different solvents.

Compound	Fluorescence	Cyclohexane	Toluene	Dichloromethane
DtCzB-mDPA	λ_{em} [a] (nm)	482	492	497
	FWHM[b] (nm)	22	22	26
DtCzB-mDS	λ_{em} [a] (nm)	488	494	499
	FWHM[b] (nm)	21	21	22

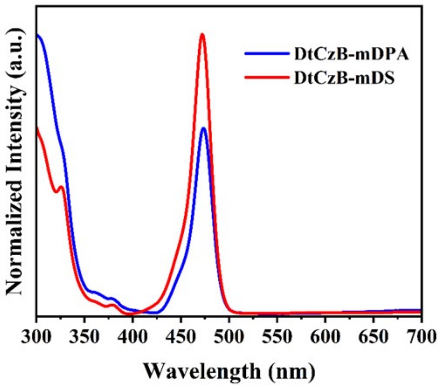


Fig. S15 UV-Vis absorption spectra of **DtCzB-mDPA** and **DtCzB-mDS** in dilute toluene solution.

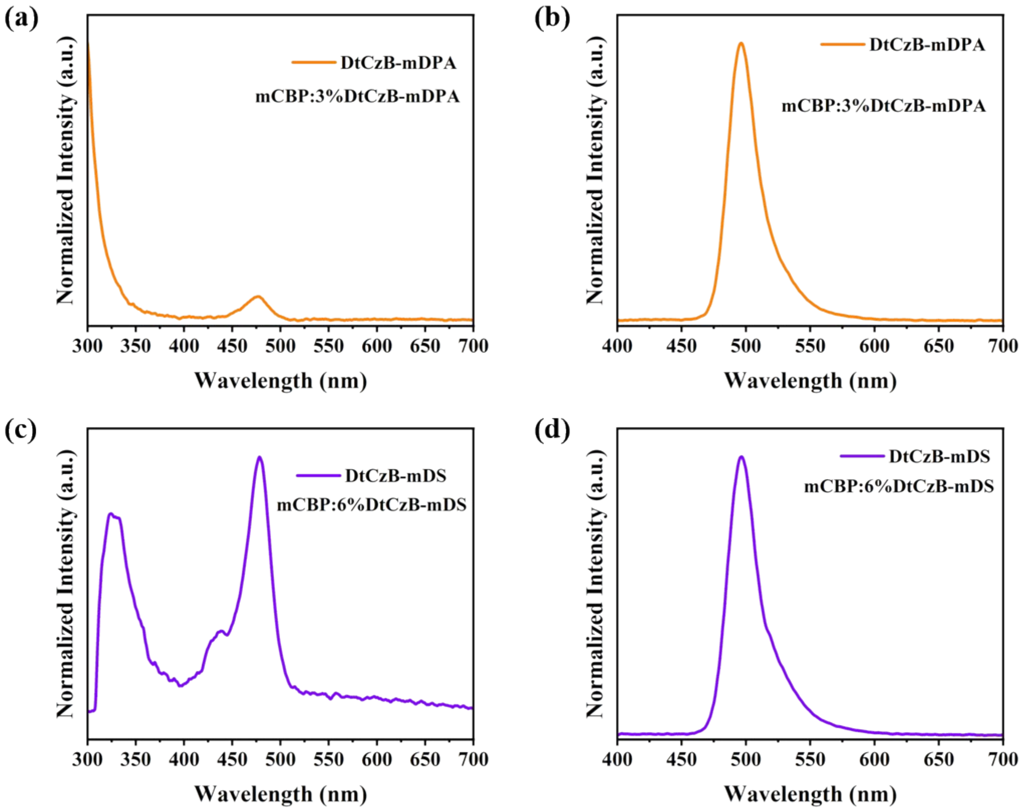


Fig. S16 (a) UV-Vis absorption spectrum of **DtCzB-mDPA** in solid film, (b) fluorescence spectrum of **DtCzB-mDPA** in solid film, (c) UV-Vis absorption spectrum of **DtCzB-mDS** in solid film and (d) fluorescence spectrum of **DtCzB-mDS** in solid film.

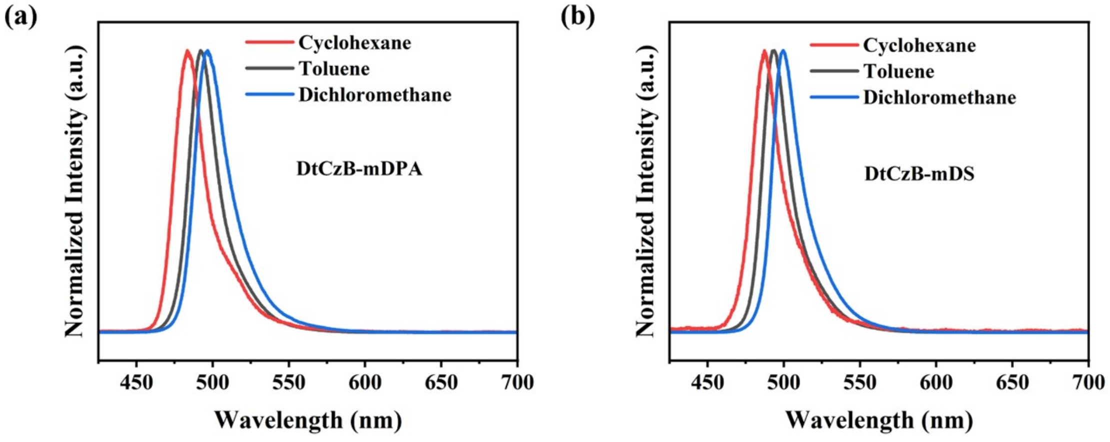


Fig. S17 The fluorescence (Fl, room temperature) spectra of (a) **DtCzB-mDPA** and (b) **DtCzB-mDS** in different solvents (1.0 × 10^{-5} M).

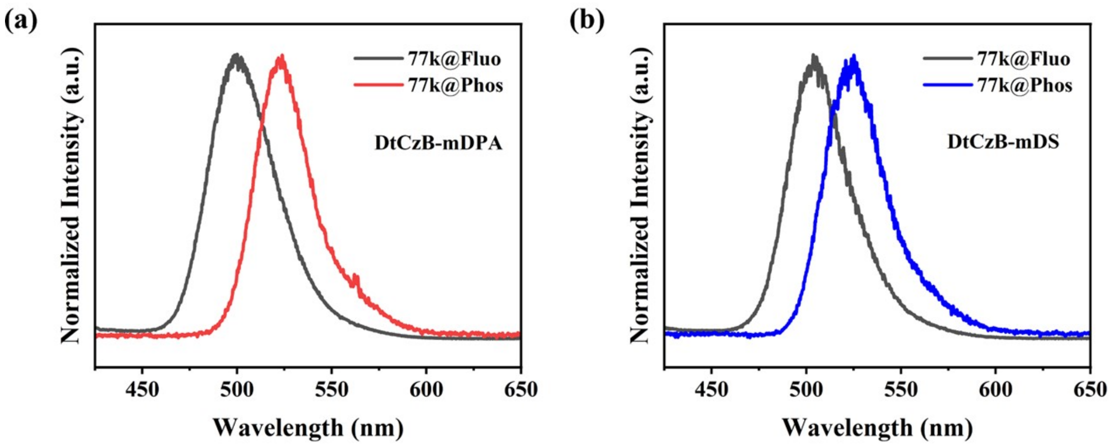


Fig. S18 The low-temperature (77K) fluorescence and phosphorescence spectra of (a) **DtCzB-mDPA** and (b) **DtCzB-mDS** in toluene.

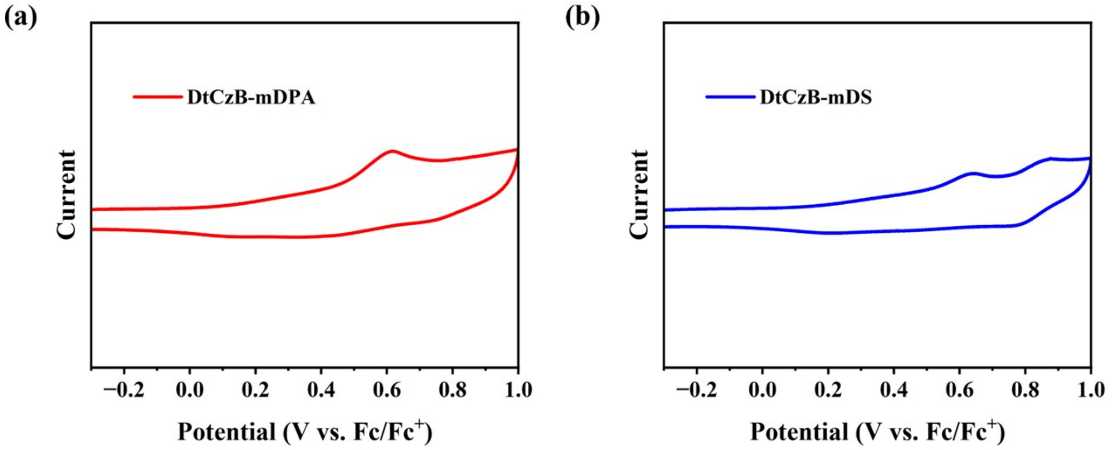


Fig. S19 Cyclic voltammogram of (a) **DtCzB-mDPA** and (b) **DtCzB-mDS**.

Calculation Formulas for the Photophysical Parameters: The evaluations of exciton dynamic rate constants were calculated by equation S1-S6:

$k_{\mathrm{p}} = 1/\tau_{\mathrm{PF}}$ Equation S1

$k_{\mathrm{d}} = 1/\tau_{\mathrm{DF}}$ Equation S2

$k_{\mathrm{F}} = \Phi_{\mathrm{PF}}/\tau_{\mathrm{PF}}$ Equation S3

$\Phi = k_{\mathrm{F}}/(k_{\mathrm{F}} + k_{\mathrm{IC}})$ Equation S4

$\Phi_{\mathrm{PF}} = k_{\mathrm{F}}/(k_{\mathrm{F}} + k_{\mathrm{IC}} + k_{\mathrm{ISC}})$ Equation S5

The total PLQY in the emitter-doped films (mCBP:5% emitter) is sufficiently high. And phosphorescence was not observed at room temperature. Therefore, it is reasonably assumed that 1) $k_r^S \gg k_{nr}^S, k_r^T, k_{nr}^T$ and 2) $k_{RISC} \gg k_r^T, k_{nr}^T$. Where k_r^S and k_{nr}^S

are the rate constants for radiative and non-radiative decay from singlet S_1, k_r^T and k_{nr}^T are the rate constants of radiative and non-radiative decay from triplet T_1, respectively. It is experimentally observed that $k_p \gg k_d$(**Table.S2**), then $k_p \approx k_r + k_{ISC} + k_{RISC}$ and $k_p k_d \approx k_r k_{RISC}$. When $k_{ISC} \gg k_{RISC}$, k_p can be approximately equal to $k_p \approx k_r + k_{ISC}$, and k_{RISC} is gained as:

$$k_{\mathrm{RISC}} = k_{\mathrm{p}}k_{\mathrm{d}}/(k_{\mathrm{p}} - k_{\mathrm{ISC}}) \qquad \text{Equation S6}$$

Table S2 Photophysical parameters of **DtCzB-mDPA** and **DtCzB-mDS** in emitter-doped films (film structure: mCBP:5% emitter).

compound	$\Phi/\Phi_{\mathrm{PF}}/\Phi_{\mathrm{DF}}$ (%)	τ_{PF}(ns)/τ_{DF}(μs)	k_{p} (10^8 s^{-1})	k_{d} (10^4 s^{-1})	k_{F} (10^7 s^{-1})	k_{IC} (10^7 s^{-1})	k_{ISC} (10^7 s^{-1})	k_{RISC} (10^4 s^{-1})
DtCzB-mDPA	82.9/75.1/7.8	9.1/86.3	1.1	1.2	8.2	1.7	1.0	1.3
DtCzB-mDS	92.5/74.8/17.7	9.3/56.7	1.1	1.8	8.1	0.7	2.1	2.2

Table S3 The EL performances of **DtCzB-mDPA** and **DtCzB-mDS** doped in mCBP.

Compound	V_{on} [a] (V)	L_{max} [b] (cd m^{-2})	CE_{max} [b] (cd A^{-1})	PE_{max} [b] (lm W^{-1})	EQE_{max} [b] (%)	λ_{EL} [c]/FWHM [c] (nm)	CIE [d] (x,y)
DtCzB-mDPA(1wt%)	4.1	2794	34.5	23.7	18.1	494/28	(0.101, 0.481)
DtCzB-mDPA(2wt%)	4.1	3036	34.0	20.0	19.2	494/27	(0.095, 0.491)
DtCzB-mDPA(3wt%)	4.1	3144	39.9	27.4	23.4	495/27	(0.104, 0.526)
DtCzB-mDPA(6wt%)	4.0	2091	34.3	20.4	16.6	495/27	(0.112, 0.565)
DtCzB-mDPA(9wt%)	3.8	1804	32.3	20.2	14.7	496/27	(0.119, 0.575)
DtCzB-mDS(3wt%)	4.0	1937	38.2	27.2	24.8	496/27	(0.113, 0.539)
DtCzB-mDS(6wt%)	3.8	1764	42.9	33.4	25.4	496/27	(0.117, 0.540)

DtCzB-mDS(9wt%)	3.5	1828	45.9	36.0	23.9	496/32	(0.142, 0.576)

[a] Voltage at 1 cd m^{-2} (V).

[b] Maximum Luminance (cd m^{-2}), maximum Current efficiency (cd A^{-1}), maximum Power efficiency (lm W^{-1}), and maximum External quantum efficiency (%).

[c] The peak of the EL spectrum; Full width at half maxima of EL spectrum.

[d] Commission Internationale de l'Eclairage coordinates.

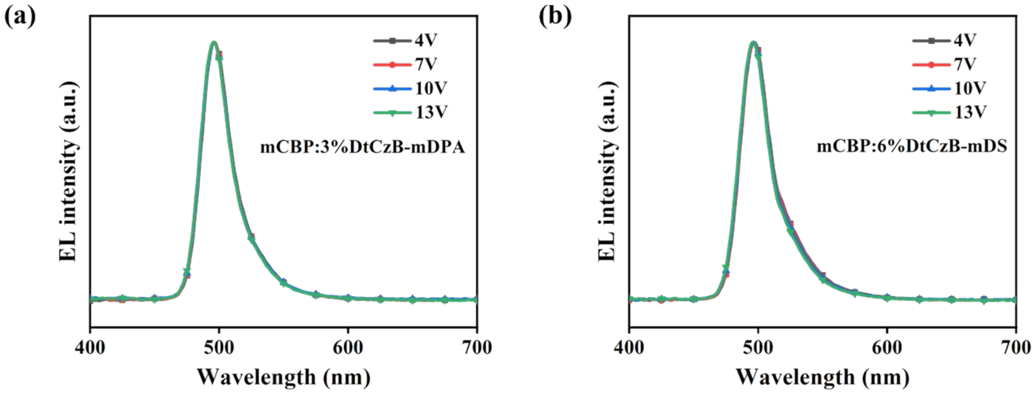


Fig. S20 The electroluminescence spectra of (a) **DtCzB-mDPA** and (b) **DtCzB-mDS** from 4 V to 13 V at optimal doping ratios.

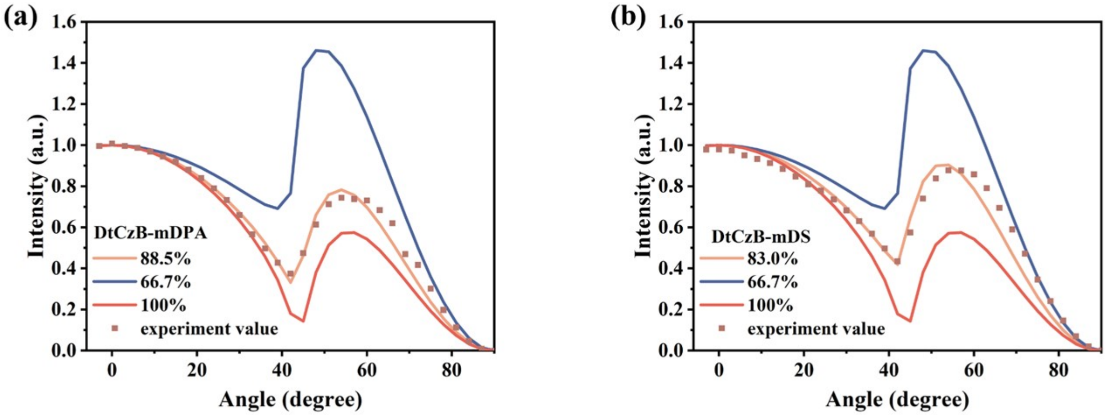


Fig. S21 The horizontal dipole orientation (Θ//) intensity plots of (a) **DtCzB-mDPA** and (b) **DtCzB-mDS** thin films, film structure: mCBP: 6wt% dopant.

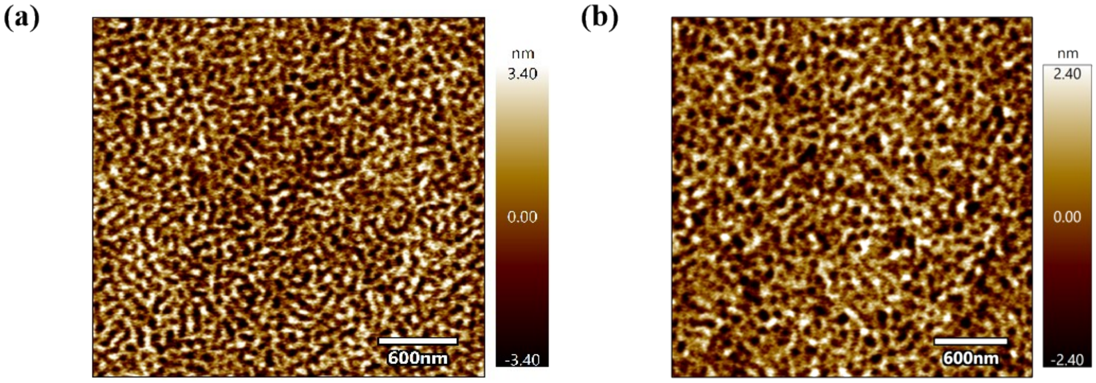


Fig. S22 The morphology of EML films at the optimal doping concentration of (a) **DtCzB-mDPA** and (b) **DtCzB-mDS**.

References

1 F. Neese, *WIREs Comput. Mol. Sci.*, 2012, **2**, 73-78.