Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Title: Perceived the Influence of Phenyl-carbazole Isomers on Sulfone/Thioxanthone-based D-A-D Hosts: Realizing Efficient Red-Phosphorescent OLEDs

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Contents

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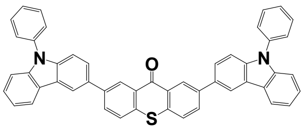
1. Experimental

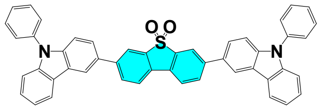
All reactions and manipulations were performed under a nitrogen atmosphere unless specified, and solvents were freshly distilled according to standard procedures. The ^{1}H and ^{13}C NMR were recorded on a Bruker AVIII HD 400. The ^{1}H and ^{13}C NMR chemical shifts were reported on δ scale downfield from $(CH_3)_4Si$. The coupling constants (J) were given in hertz. Absorption spectra were recorded on a Shimadzu UV-1800 spectrophotometer, and emission spectra were obtained using a Hitachi F-4500 spectrofluorimeter. Emission spectra in solutions were measured using a spectral grade solvent and right-angle detection. Fourier-transform infrared spectroscopy (FTIR) spectra were obtained using a PerkinElmer sp100. Redox potentials were measured using cyclic voltammetry on a Zahner Ennium analyser. All measurements were performed in CH_2Cl_2 solution containing 0.1 M tetrabutylammonium hexaflourophosphate as supporting electrolyte under ambient conditions after purging the solution with N_2 for 10 min. The conventional three-electrode configuration was employed that consists of a glassy carbon working electrode, a platinum counter electrode, and an Ag/Ag^+ reference electrode calibrated with ferrocene/ ferrocenium (Fc/Fc^+) as an internal reference. Mass spectra were recorded on a Jeol JMS-700 double-focusing mass spectrometer. Analytical thin layer chromatography (TLC) was performed on Silica gel 60 F 254 Merck. Column chromatography was performed using the silica gel from Merck (Kieselgel Si 60; 40–63 μm). Solvent THF was distilled with sodium benzophenone ketyl. Toluene and dichloromethane were distilled with CaH_2. Other solvents and reagents were reagent grade, purchased from Acros, Alfa, Merck, Lancaster, TCI, Sigma-Aldrich, and Showa, which were directly used without purification.

Fabrication and Characterization of OLEDs: Indium tin oxide (ITO)-coated glass and commercial organic materials were purchased from Lumtec and Shine Materials Technology.

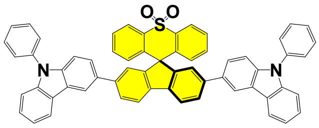
Organic materials were subjected to temperature-gradient sublimation in a high vacuum before use. The ITO substrate was washed in sequence with deionized water and acetone, followed by treatment with plasma for 5 minutes. The bottom-emitting OLEDs were fabricated using ITO as the anode, followed by the deposition of multiple organic layers, topped by a metal cathode layer. The organic and metal layers were deposited by thermal evaporation in a vacuum chamber with a base pressure of $< 10^{-6}$ Torr. Device fabrication was completed in a single cycle without breaking the vacuum. The deposition rates of organic materials and aluminum were respectively kept at around 0.1 and 0.5 nm s^{-1}. The active area was defined by the shadow mask (2×2 mm^2). Current density-voltage-luminance characterization was done using two Keysight B2901A current source-measure units equipped with a calibrated Si-photodiode. The electroluminescent spectra of the devices were recorded using an Ocean Optics spectrometer (Ocean Optics 2000).



TXO-CzP



DBTS-CzP
(TC-3)



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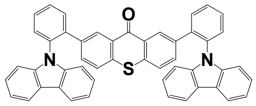

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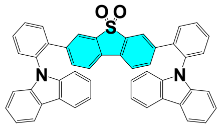

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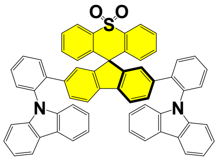

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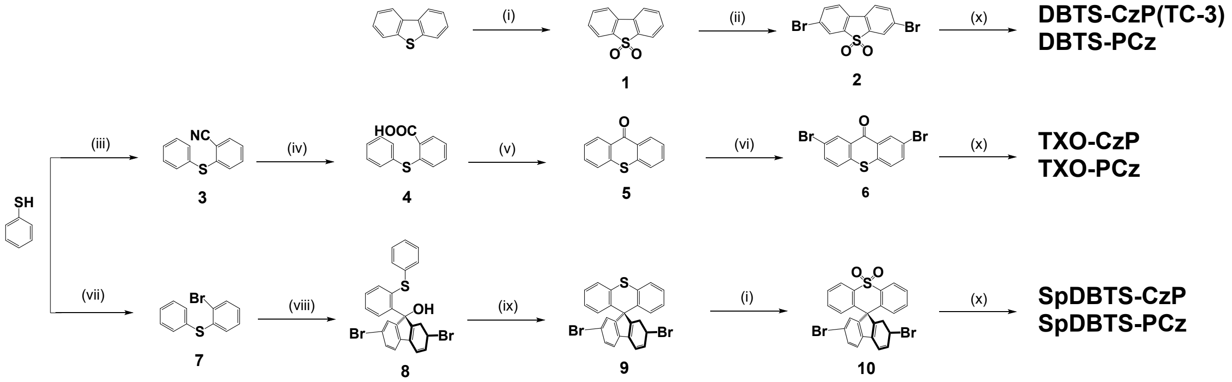

Synthetic conditions of organic OLED hosts: (i) 30% H_2O_2, HOAc, THF, 110 °C, 20 h; (ii) NBS, H_2SO_4, 0 °C, 2 h; (iii) K_2CO_3, DMF, 80 °C, 14 h; (iv) (a)KOH, EtOH, H_2O, 110°C, 12 h. (b) then 3M HCl, rt, 2 h; (v) Polyphosphoric acid (PPA), 150°C, 48 h; (vi) Br_2, HOAc, 90 °C, 5 h; (vii) *o*-Bromoiodobenzene, CuI, L-Proline, K_2CO_3, DME, 80°C, 16 h (viii) (a) 2,7-Dibromofluoren-9-one, *n*-BuLi, THF, -78°C, 1 h. (b) then 2,7-Dibromofluorenone, THF, -78°C to rt, 8 h. (c) then 3M HCl, rt, 1 h. (ix) CF_3SO_3H, CH_2Cl_2, rt, 12 h. (x) 2 or 6 or 10, $Pd(PPh_3)_2Cl_2$, 2M K_2CO_3(aq), THF, toluene, 90°C, 18 hr.

Intermediates **1~6** and **DBTS-CzP(TC-3)** can be found in our previous report.[1]

(o-Bromophenyl)(phenyl)sulfane (7). Bromoiodobenzene (16.05 g, 56.73 mmol), benzenethiol (5 g, 45.38 mmol), CuI (0.86 g, 4.54 mmol), *L*-Proline (1.05 g, 9.08 mmol) and K_2CO_3 (12.54 g, 90.77 mmol) were mixed in DMF (30 mL) at 80°C. After 16 hrs, the mixture was extracted using methylene chloride and the organic layer was dried over anhydrous $MgSO_4$ and evaporated under vacuum. The crude product was purifies by silica gel column chromatograph eluted with hexane, yielding a colorless liquid (**7)** was obtained in a 90% yield (10.83 g, 40.842 mmol). δ_H (400 MHz, $CDCl_3$) 7.61 (d, 1H, J = 7.84 Hz), 7.50-7.52 (m, 2H), 7.41-7.45 (m, 3H), 7.17 (t, 1H), 6.99-7.07 (m, 2H). δ_C (100 MHz, $CDCl_3$) 138.5, 133.2, 132.8, 132.6, 129.5, 129.4, 128.2, 127.6, 127.0, 122.8.

2,7-Dibromo-9-(*o*-(phenylthio)phenyl)-9*H*-fluoren-9-ol (8). In a three-necked round-bottom flask, compound **7** (1.08 g, 4.06 mmol) was placed in 15 mL of dry THF at -78°C. *n*-Butyllithium (2.79 mL, 4.47 mmol; 1.6M in hexane) was added dropwise. After 1 hour, 2,7-dibromo-9H-fluoren-9-one (1.65 g, 4.87 mmol) was dissolved in 50 mL of dry THF and added dropwise. After 8 hours, the mixture was quenched with 3M HCl (100 mL), and the resulting solution was extracted using methylene chloride. The organic layer was then dried with anhydrous MgSO4 and evaporated under vacuum. The crude product, obtained without further purification, yielded a yellow solid (**8**).

2,7-Dibromospiro[fluorene-9,9'-thioxanthene] (9). To a three-necked round-bottom flask containing crude **8** in methylene chloride (20 mL), and added CF_3SO_3H (several drops) was stirred at r.t. for 12 h. The mixture was extracted using methylene chloride and the organic layer was dried over anhydrous $MgSO_4$ and evaporated under vacuum. The crude product was purifies by silica gel column chromatograph eluted with hexane, yielding a white solid (**9)** was obtained in a 74% yield (1.52 g, 3.0 mmol). δ_H (400 MHz, $CDCl_3$) 7.71 (d, 2H, *J* = 1.0 Hz), 7.62 (d, 2H, *J* = 8.2 Hz), 7.52 (dd, 2H, *J* = 9.5 Hz, 1.4 Hz), 7.44 (d, 2H, 7.7 Hz), 7.19 (t, 2H), 6.93 (t, 2H), 6.54 (d, 2H, *J* = 7.8 Hz). δ_C (100 MHz, $CDCl_3$) 155.7, 137.5, 135.5, 131.6, 130.9, 128.8, 128.0, 127.7, 126.4, 122.3, 121.5, 60.3.

2,7-Dibromospiro[fluorene-9,9'-thioxanthene] 10',10'-dioxide (10) . To a three-necked round-bottom flask containing compound **9** (1 g, 1.98 mmol) in THF/AcOH (v/v=1/1, 24 mL) and 30% H_2O_2 (0.81 mL, 7.90 mmol) with dropwsie at 110 °C. After 20 h, the product was extracted with methylene chloride and the organic layer dried over anhydrous $MgSO_4$. The crude product was dried under vacuum, and was purifies by silica gel column chromatograph eluted with CH_2Cl_2/hexane (3/1). The white solid of **10** was obtained in 86.3% yield (0.92 g, 1.71 mmol). δ_H (400 MHz, $CDCl_3$) 8.25 (1H, dd, *J* = 8.9 Hz, 1.0 Hz), 7.68 (d, 1H, *J* = 8.2 Hz), 7.57-7.50 (m, 2H) , 7.46 (d, 1H, *J* = 1.6 Hz), 7.30-7.34 (m, 1H), 6.56 (d, 1H, *J* = 8.2 Hz). δ_C (100 MHz, $CDCl_3$) 153.7, 138.3, 138.2, 136.7, 133.0, 132.1, 129.1, 128.8, 128.7, 123.6, 122.9, 121.7.

3,7-Bis(*o*-(9*H*-carbazol-9-yl)phenyl)dibenzo[*b*,*d*]thiophene 5,5-dioxide (DBTS-PCz). To a three-necked round-bottom flask containing **2** (0.5 g, 1.34 mmol) and 9-(2-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-9*H*-carbazole (1.73 g, 4.68 mmol), $Pd(PPh_3)_2Cl_2$ (141 mg, 0.201 mmol) and 2M $K_2CO_{3\ (aq)}$ (2.00 mL, 4.68 mmol) in THF/toluene (v/v=2/1, 45mL) was heated to 90°C for 18 hr. After cooling, the products were extracted with methylene chloride and the organic layer dried over anhydrous $MgSO_4$. The crude product was dried under vacuum, and was purifies by silica gel column chromatograph eluted with CH_2Cl_2/hexane (2/1). The yellow solid of **DBTS-PCz** was obtained in 74.2% yield (0.7 g, 1.0 mmol). δ_H (400 MHz, $CDCl_3$) 8.00 (d, 2H, *J* = 7.7 Hz), 7.59-7.67 (m, 4H), 7.50-7.53 (m, 1H), 7.25-7.29 (m, 2H), 7.14-7.17 (m, 2H), 7.01 (d, 2H, *J* = 8.0 Hz), 6.81-6.86 (m, 2H). δ_C (100 MHz, $CDCl_3$) 141.0, 140.8, 138.5, 137.9, 134.8, 132.7, 131.1, 130.1, 130.0, 129.8, 129.2, 126.0, 123.1, 121.4, 121.1, 120.2, 119.9, 109.9. MS (FAB, 70 eV): m/z (relative intensity) 699 ($(M+H)^+$, 100); HRMS calcd for $C_{48}H_{31}N_2O_2S$: 699.2101, found 699.2112.

2,7-Bis(9-phenyl-9*H*-carbazol-3-yl)-9*H*-thioxanthen-9-one (TXO-CzP). Compound **TXO-CzP** was synthesized according to the same procedure as that of **DBTS-PCz**. Yellow solid of **TXO-CzP** was obtained in 72.5% yield. δ_H (400 MHz, $CDCl_3$) 9.05 (s, 1H), 8.51 (s, 1H), 8.25(d, 1H, *J* = 7.7 Hz), 7.72-7.81 (m, 2H), 7.60-7.67 (m, 4H), 7.52 (d, 2H, *J* = 8.4 Hz), 7.44 (s, 2H), 7.34 (s, 1H). δ_C (100 MHz, $CDCl_3$) 178.2, 141.4, 140.7, 140.2, 137.5, 135.3, 131.7, 131.3, 129.9, 129.5, 127.8, 127.6, 127.1, 126.6, 126.3, 125.3, 124.1, 123.4, 120.5, 120.2, 118.9, 110.3, 110.0. MS (FAB, 70 eV): m/z (relative intensity) 695 ($[M+H]^+$, 100); HRMS calcd. for $[C_{49}H_{31}N_2OS]$: 695.2152, found 695.2158.

2,7-Bis(*o*-(9*H*-carbazol-9-yl)phenyl)-9*H*-thioxanthen-9-one (TXO-PCz). Compound **TXO-PCz** was synthesized according to the same procedure as that of **DBTS-PCz**.

Yellow solid of **TXO-PCz** was obtained in 73.9% yield. δ_H (400 MHz, $CDCl_3$) 8.66 (d, 1H, *J* = 1.3 Hz), 8.03 (d, 2H, *J* = 7.7 Hz), 7.78 (dd, 1H, *J* = 9.2 Hz, 1.6 Hz), 7.58-7.67 (m, 2H), 7.51 (dd, 1H, *J* = 9.0 Hz, 1.3 Hz), 7.25-7.29 (m, 2H), 7.15-7.19 (m, 2H), 7.08 (d, 2H, *J* = 8.1 Hz), 6.83-6.88 (m, 2H). δ_C (100 MHz, $CDCl_3$) 179.3, 141.0, 139.3, 137.1, 136.1, 134.8, 131.7, 131.2, 129.9, 129.4, 129.1, 129.0, 125.9, 125.6, 123.1, 120.1, 119.7, 109.8. MS (FAB, 70 eV): m/z (relative intensity) 695 ($[M+H]^+$, 100); HRMS calcd. for [$C_{49}H_{31}N_2OS$]: 695.2152, found 695.2153.

2,7-Bis(9-phenyl-9*H*-carbazol-3-yl)spiro[fluorene-9,9'-thioxanthene] 10',10'-dioxide (SpDBTS-CzP). Compound **SpDBTS-CzP** was synthesized according to the same procedure as that of **DBTS-PCz**. White solid of **SpDBTS-CzP** was obtained in 71.9% yield. δ_H (400 MHz, $CDCl_3$) 8.30 (d, 2H, *J* = 6.6 Hz), 8.16 (d, 1H, *J* = 7.8 Hz), 7.98 (d, 1H, *J* = 8.0 Hz), 7.78 (s, 1H), 7.44-7.62 (m, 7H), 7.38-7.40 (m, 3H), 7.27-7.34 (m, 2H), 6.82 (d, 1H, *J* = 7.8 Hz). δ_C (100 MHz, $CDCl_3$) 153.3, 142.3, 141.3, 140.4, 140.2, 138.7, 137.5, 136.9, 132.9, 132.3, 129.8, 129.1, 128.3, 127.5, 127.4, 127.0, 126.1, 125.1, 124.3, 123.9, 123.4, 123.4, 120.6, 120.5, 120.0, 118.5, 110.1, 109.8, 58.2. MS (FAB, 70 eV): m/z (relative intensity) 863 ($[M+H]^+$, 100); HRMS calcd. for [$C_{61}H_{39}N_2O_2S$]: 863.2727, found 863.2726.

2,7-Bis(*o*-(9*H*-carbazol-9-yl)phenyl)spiro[fluorene-9,9'-thioxanthene] 10',10'-dioxide (SpDBTS-PCz). Compound **SpDBTS-PCz** was synthesized according to the same procedure as that of **DBTS-PCz**. White solid of **SpDBTS-PCz** was obtained in 74.9% yield. δ_H (400 MHz, $CDCl_3$) 8.66 (d, 1H, *J* = 1.3 Hz), 8.03 (d, 2H, *J* = 7.7 Hz), 8.10 (dd, 1H, *J* = 9.0 Hz, 1.1 Hz), 7.91 (dd, 2H, *J* = 7.9 Hz, 0.8 Hz), 7.35-7.49 (m, 5H), 7.03-7.14 (m, 7H), 6.86 (d, 2H, *J* = 7.8 Hz), 6.78 (dd, 1H, *J* = 9.4 Hz, 1.5 Hz), 5.95 (d, 1H, *J* = 7.7 Hz). δ_C (100 MHz, $CDCl_3$) 152.6, 140.7, 140.3, 139.6, 139.0, 138.7, 136.2, 134.6, 132.6, 131.3, 129.4, 128.9, 128.6, 128.5, 127.9, 127.9, 125.5, 125.1, 123.1, 122.8, 119.9, 119.9, 129.2, 109.7, 57.4. MS (FAB, 70 eV): m/z (relative intensity) 863 ($[M+H]^+$, 100); HRMS calcd. for [$C_{61}H_{39}N_2O_2S$]: 863.2727, found 863.2730.

2. ^{1}H and ^{13}C NMR spectra

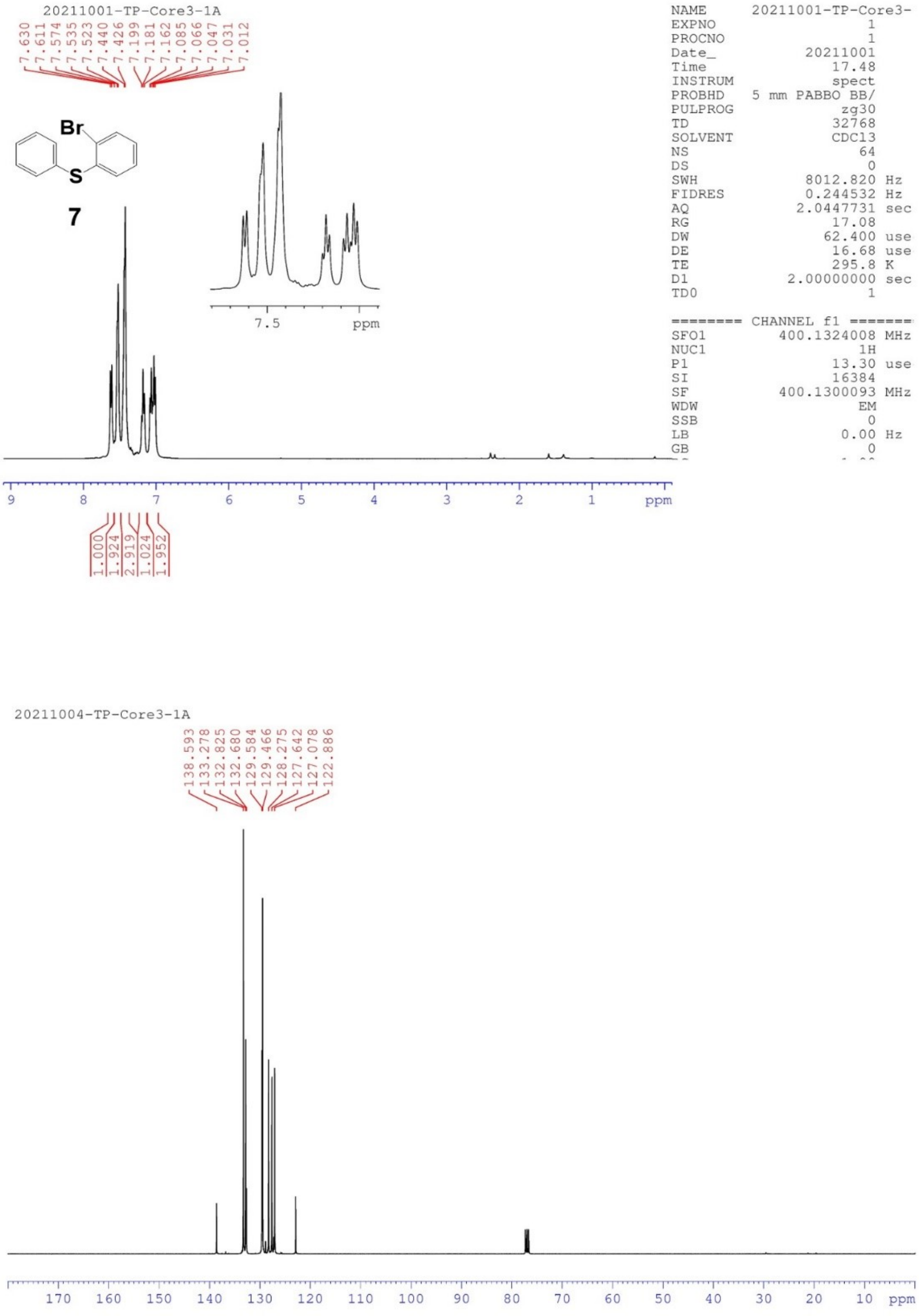

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Fig. S1 ^{1}H NMR (upper) and ^{13}C NMR (lower) spectra of **7**.

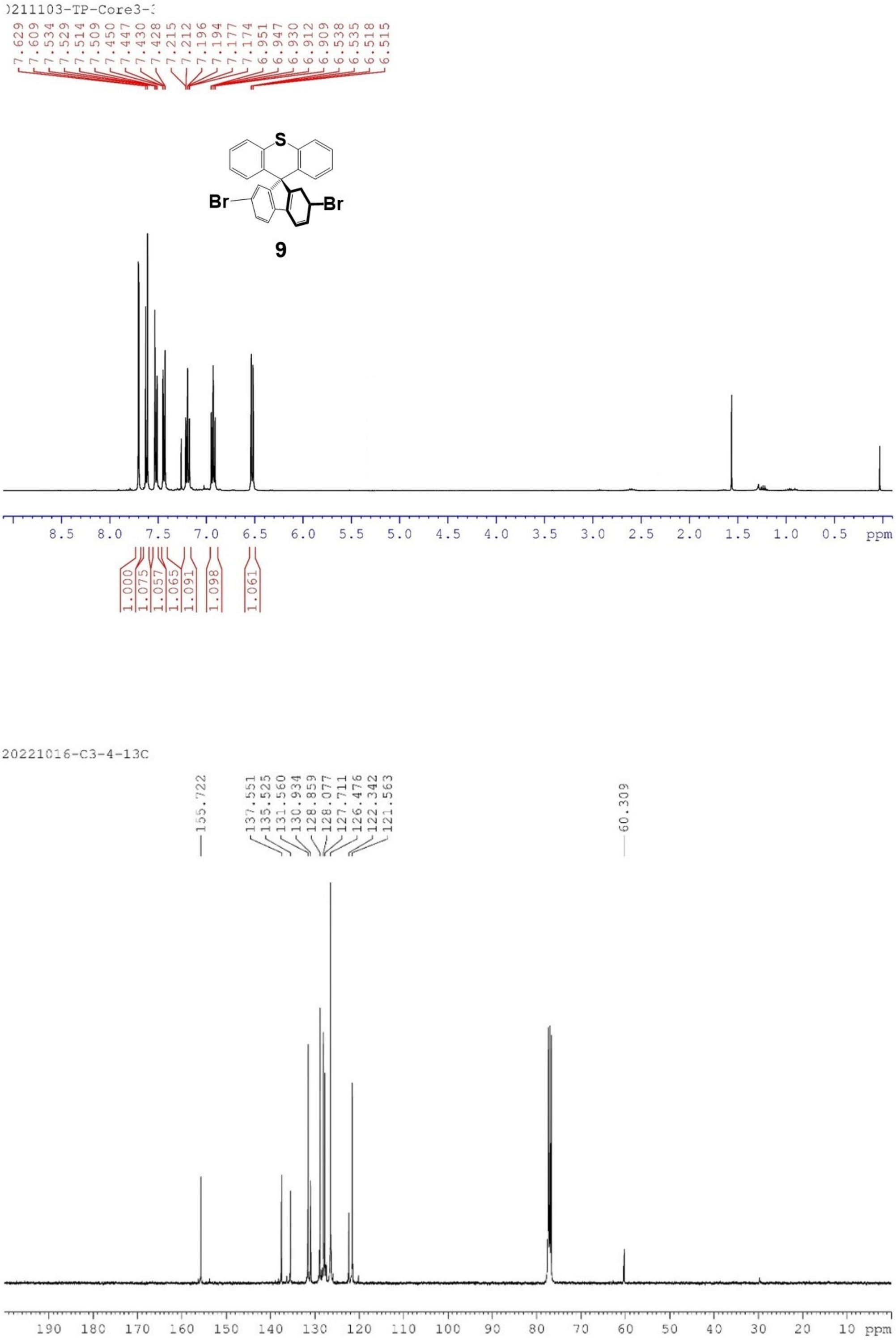

Fig. S2 ^{1}H NMR (upper) and ^{13}C NMR (lower) spectra of **9**.

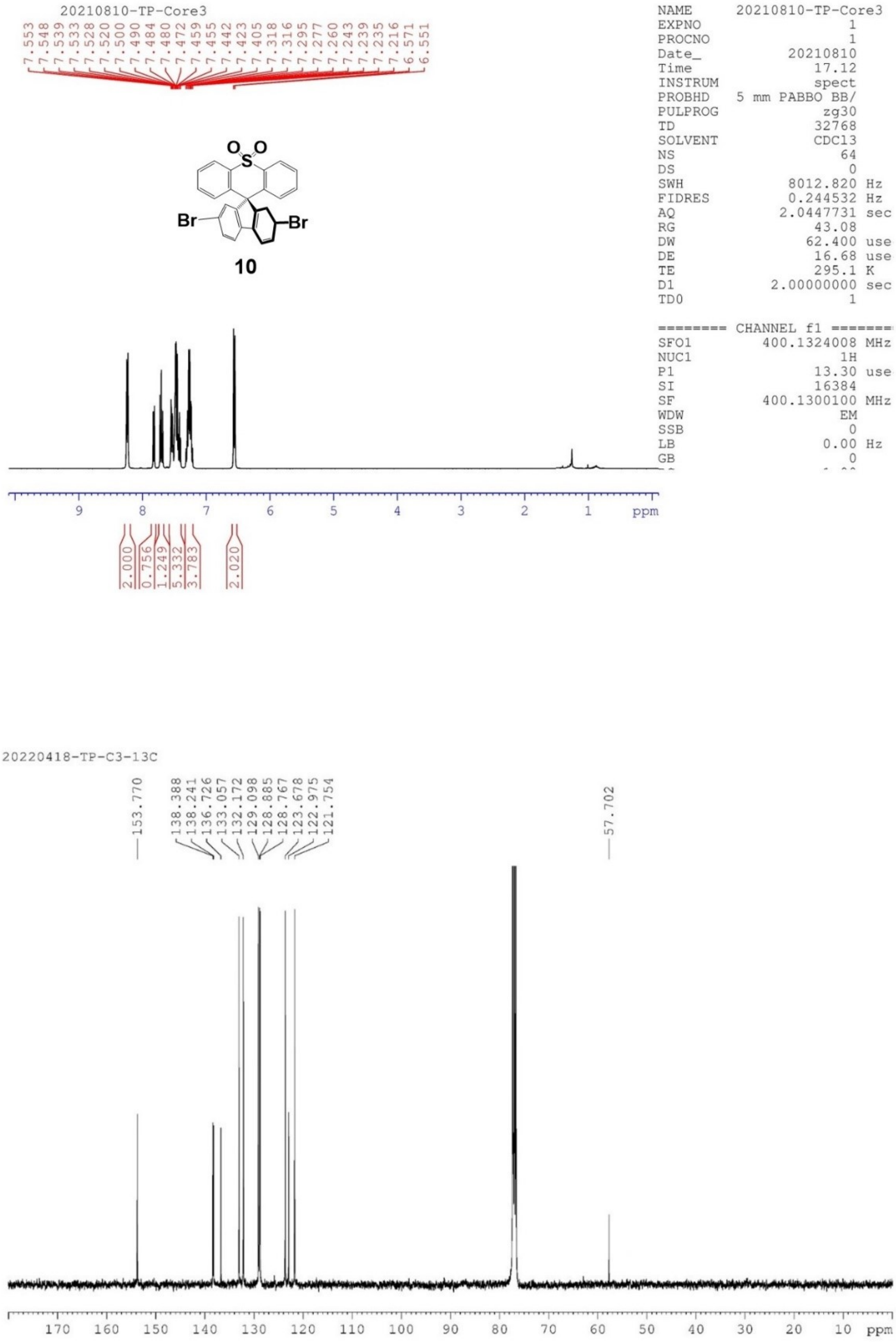

Fig. S3 ^{1}H NMR (upper) and ^{13}C NMR (lower) spectra of **10**.

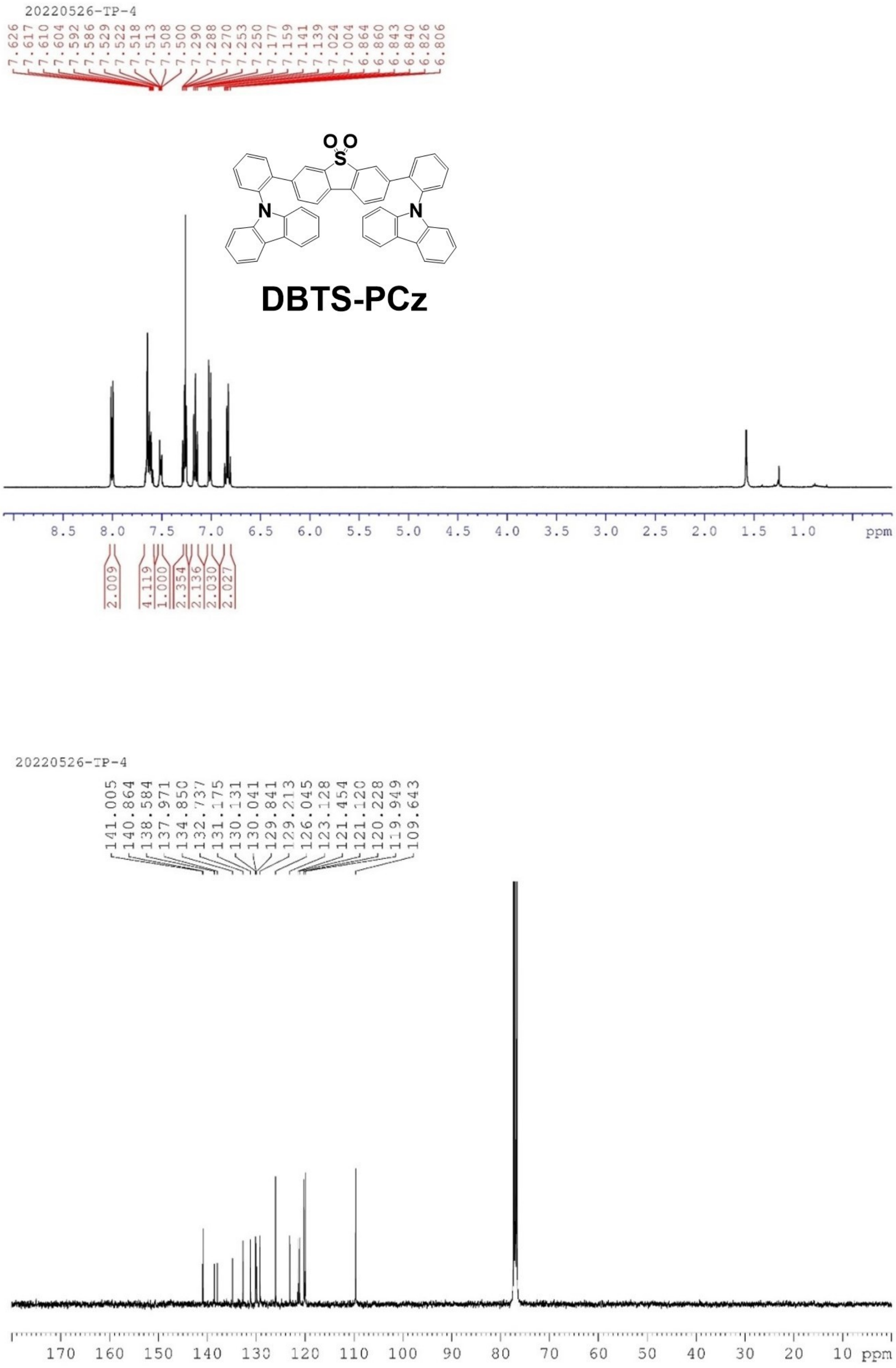

Fig. S4 ^{1}H NMR (upper) and ^{13}C NMR (lower) spectra of **DBTS-PCz**.

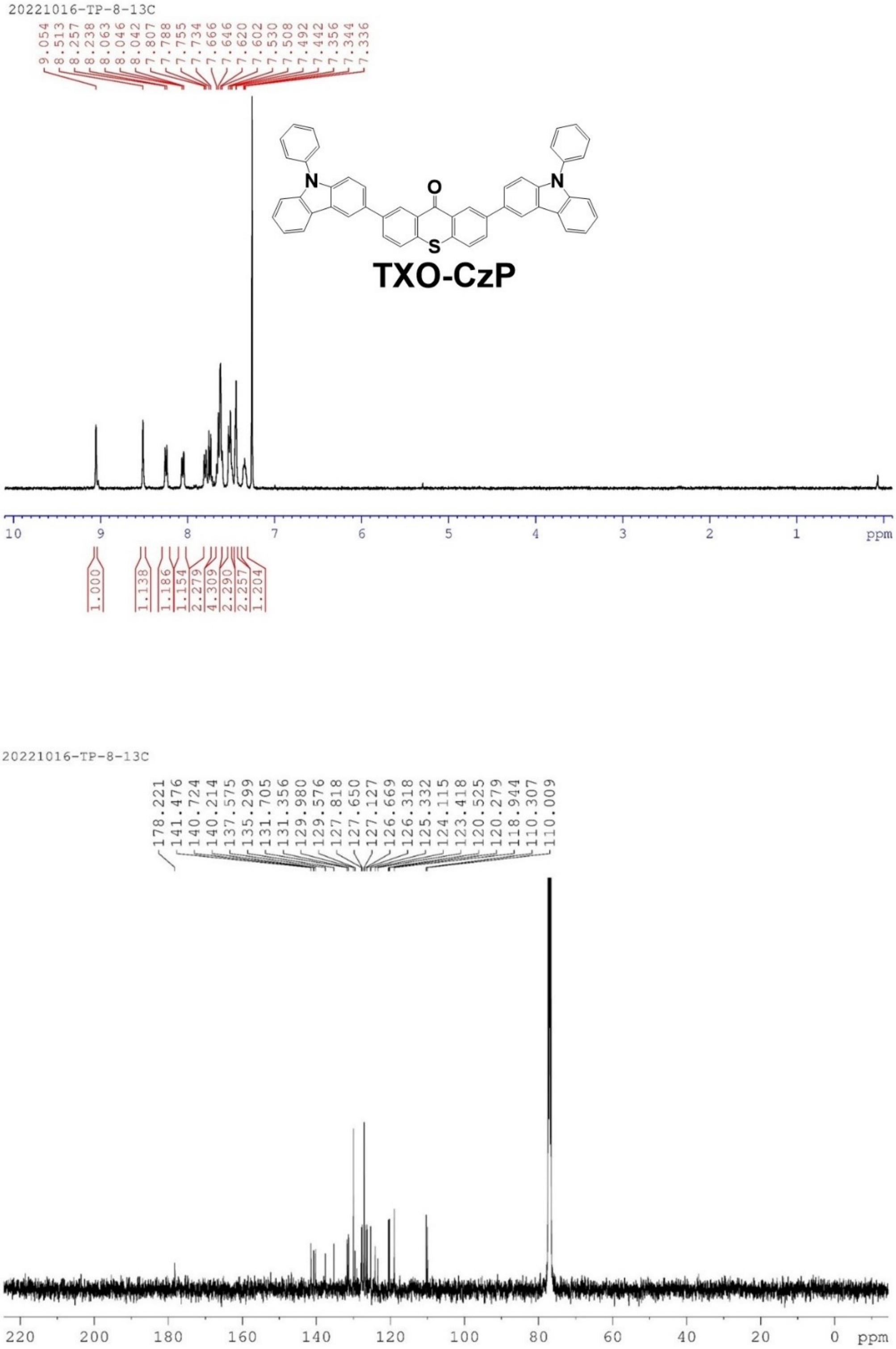

Fig. S5 ^{1}H NMR (upper) and ^{13}C NMR (lower) spectra of **TXO-CzP**.

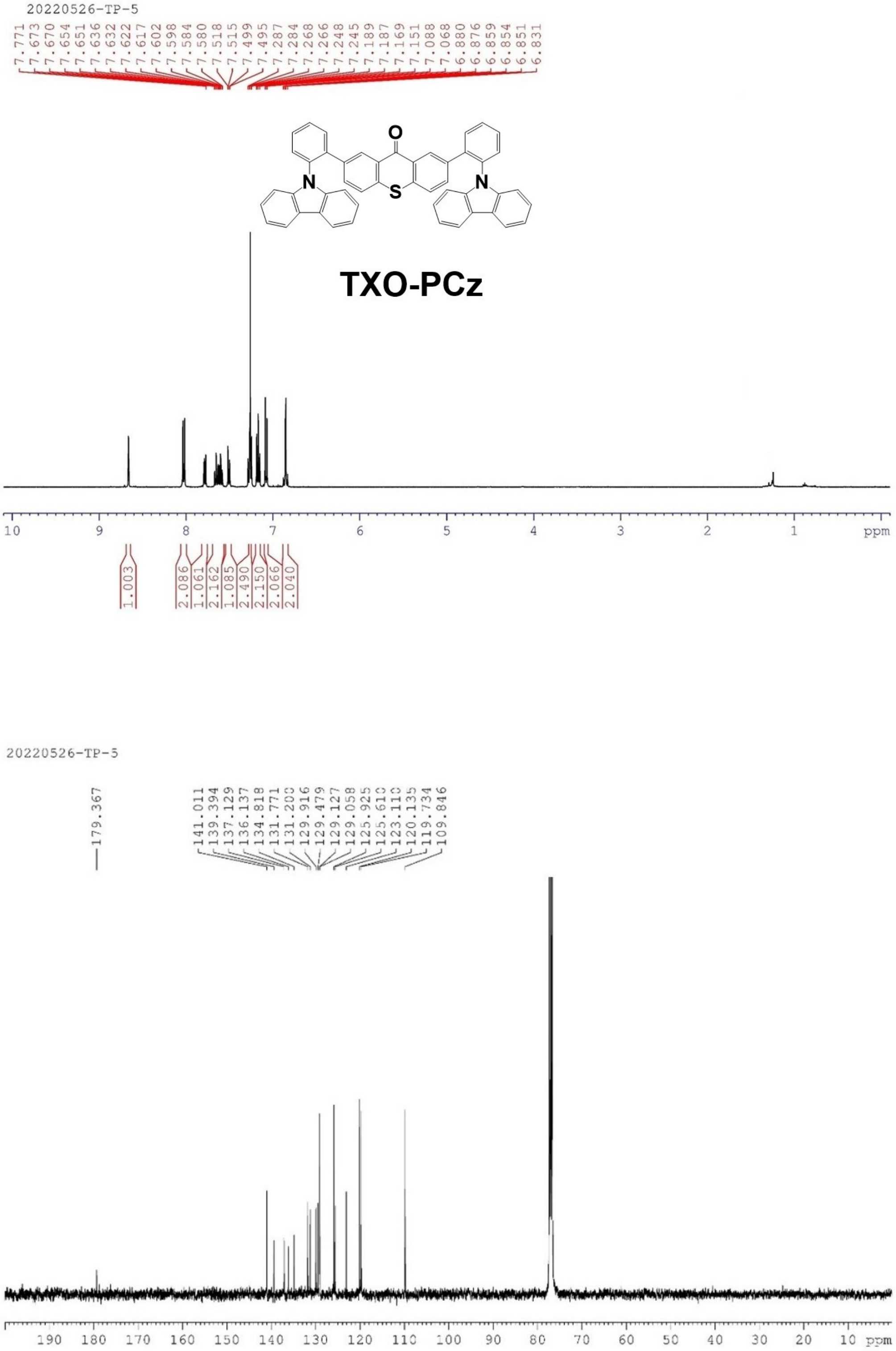

Fig. S6 ^{1}H NMR (upper) and ^{13}C NMR (lower) spectra of **TXO-PCz**.

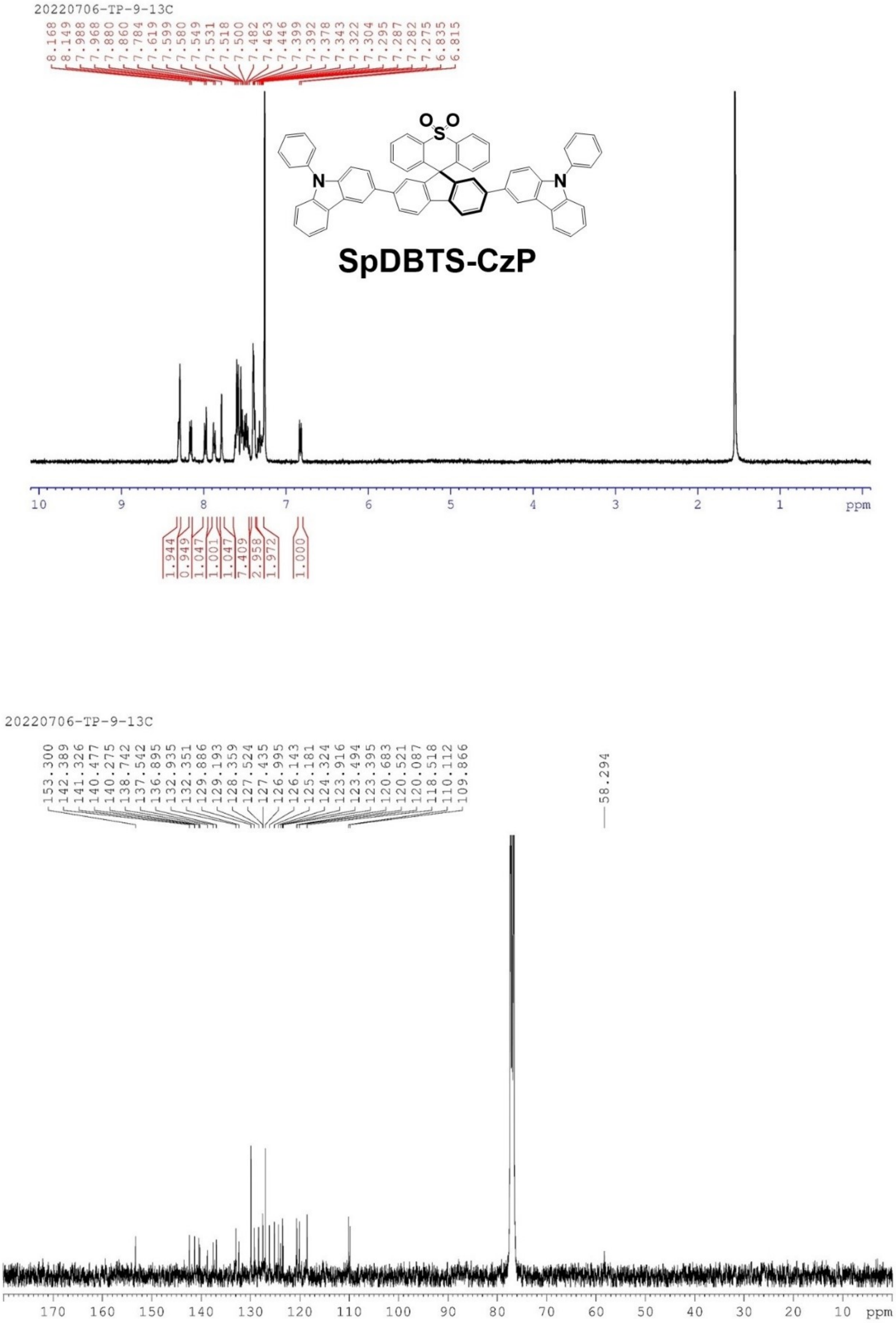

Fig. S7 ^{1}H NMR (upper) and ^{13}C NMR (lower) spectra of **SpDBTS-CzP**.

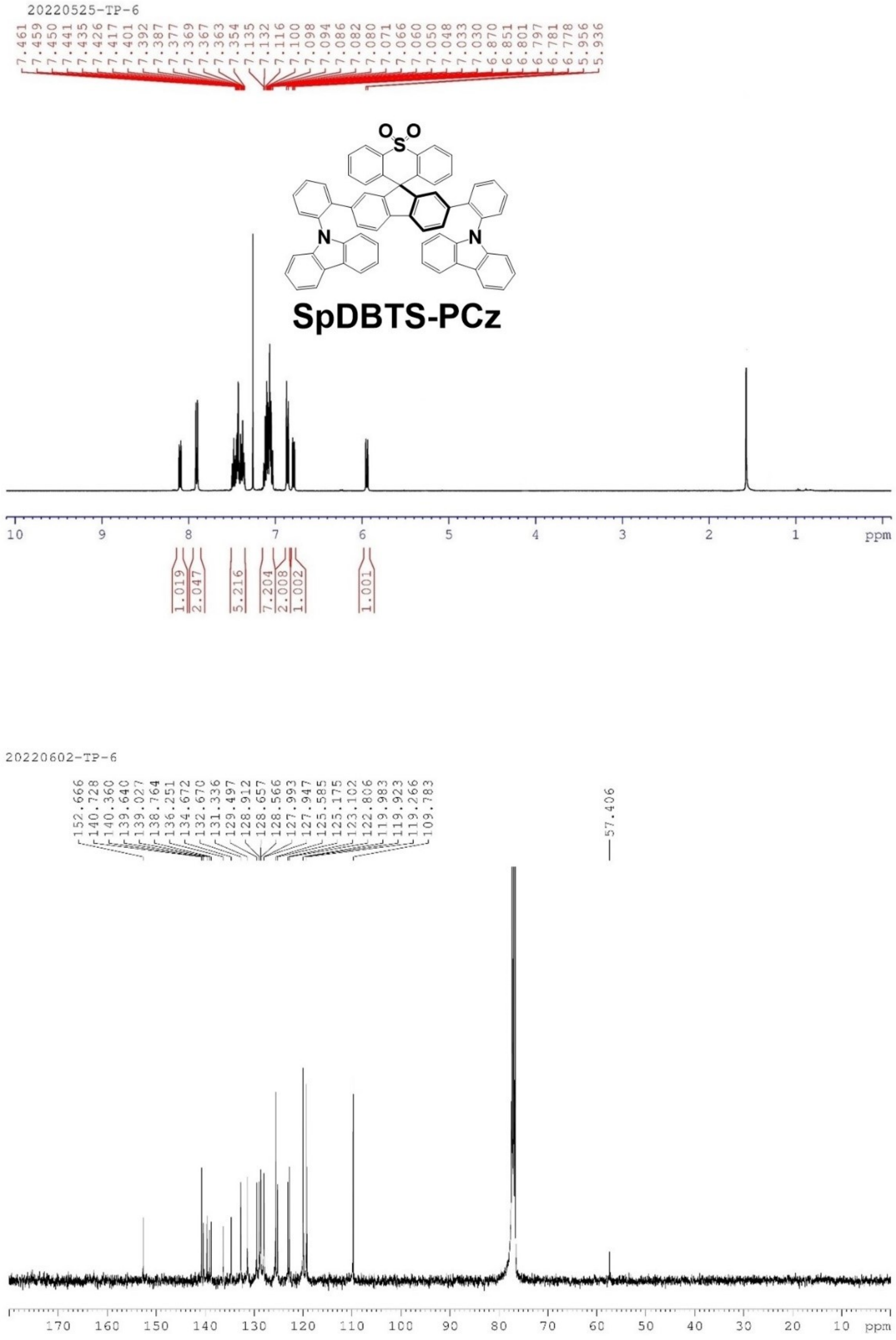

Fig. S8 ^{1}H NMR (upper) and ^{13}C NMR (lower) spectra of **SpDBTS-PCz**.

3. Single crystals X-ray diffraction Analysis

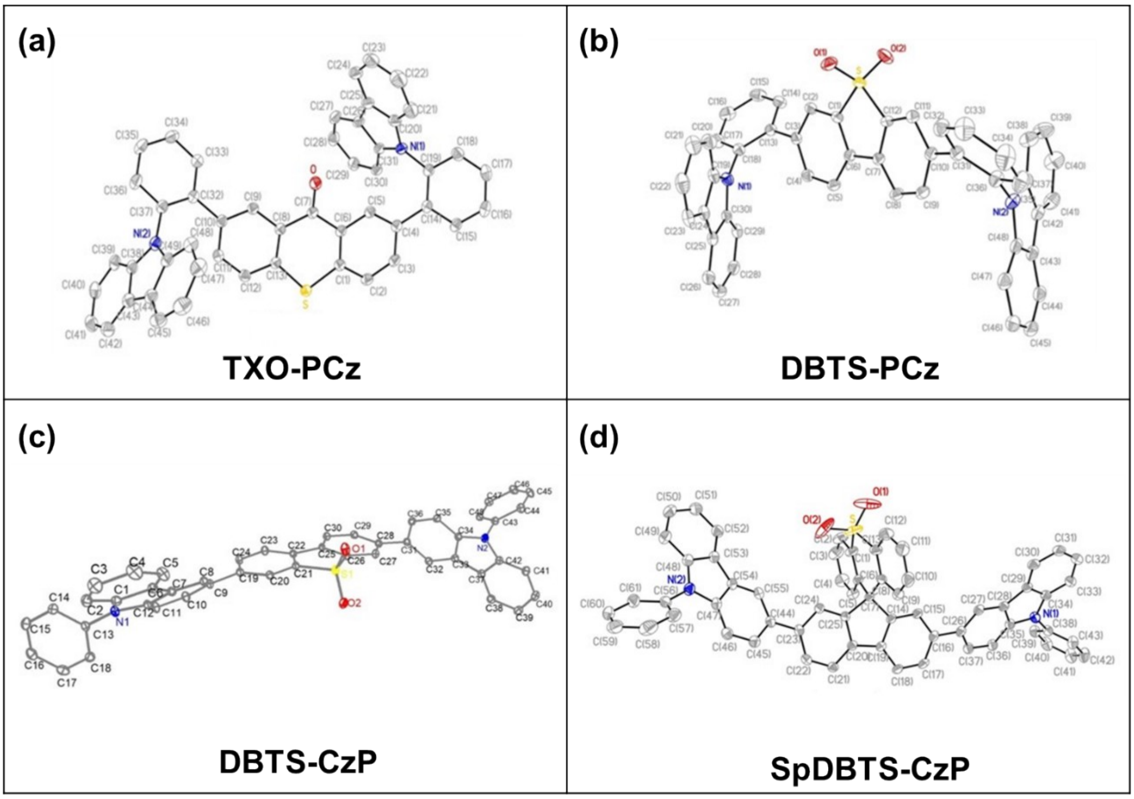

Fig. S9 Single crystal structures of (a) **TXO-PCz**, (b) **DBTS-PCz**, (c) **DBTS-CzP**, and (d) **SpDBTS-CzP**.

Table S1 Crystal data and structure refinement for OLED hosts materials.

Indentifcation Code	**TXO-PCz**	**DBTS-CzP (TC-3)**	**DBTS-PCz**	**SpDBTS-CzP**
Empirical formula	$C_{50}H_{32}Cl_2N_2O_2S$	$C_{48}H_{30}N_2O_2S$	$C_{48}H_{30}N_2O_2S$	$C_{61}H_{38}N_2O_2S$
Formula weight	779.73	698.80	698.80	862.99
Temperature	150(2) K	150(2) K	150(2) K	150(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic	Orthorhombic	Triclinic
Space group	P-1	P-1	Pbcn	P-1
Unit cell dimensions	a = 11.0108(6) Å	a = 11.0378(5) Å	a = 32.7909(16) Å	a =12.3715(8) Å

	α= 68.1102(18)°.	α= 67.5033(13)°.	α= 90°.	α= 71.3232(19)°.
	b = 13.1764(6) Å	b = 12.7509(5) Å	b = 9.3220(4) Å	b = 13.7395(8) Å
	β= 81.136(2)°.	β= 74.5113(14)°.	β= 90°.	β= 79.068(2)°.
	c = 15.4240(8) Å γ = 66.3689(18)°.	c = 14.5837(6) Å γ = 87.8279(14)°.	c = 26.2401(12) Å γ = 90°.	c = 15.9996(8) Å γ = 71.866(2)°.
Volume	1902.27(17) Å^3	1822.71(13) Å^3	8021.0(6) Å^3	2436.1(2) Å^3
Z	2	2	8	2
Density (calculated)	1.361 mg/m^3	1.273 mg/m^3	1.157 mg/m^3	1.176 mg/m^3
Absorption coefficient	0.269 mm^{-1}	0.132 mm^{-1}	0.120 mm^{-1}	0.112 mm^{-1}
F(000)	808	728	2912	900
Crystal size	0.280 x 0.230 x 0.130 mm^3	0.300 x 0.240 x 0.100 mm^3	0.330 x 0.290 x 0.120 mm^3	0.360 x 0.340 x 0.270 mm^3
Theta range for data collection	3.381 to 27.900°	2.678 to 27.905°	2.400 to 27.897°	2.837 to 27.921°
Index ranges	-14<=h<=14, -17<=k<=16, -20<=l<=20	-14<=h<=14, -14<=k<=16, -19<=l<=19	-43<=h<=43, -12<=k<=12, -34<=l<=34	-16<=h<=16, -18<=k<=18, -21<=l<=19
Reflections collected	41880	37489	147581	53620
Independent reflections	9066 [R(int) = 0.0359]	8638 [R(int) = 0.0544]	9583 [R(int) = 0.0601]	11597 [R(int) = 0.0351]
Completeness to theta = 25.242°	99.7 %	99.1 %	99.8 %	99.7 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmitttion	0.7456 and 0.6877	0.7456 and 0.6652	0.7456 and 0.6448	0.7456 and 0.6904
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2

Data / restraints / parameters	9066 / 0 / 505	8638 / 0 / 478	9583 / 0 / 478	11597 / 0 / 595
Goodness-of-fit on F^2	1.009	1.010	1.068	1.006
Final R indices [I>2sigma(I)]	R1 = 0.0421, wR2 = 0.1190	R1 = 0.0448, wR2 = 0.1274	R1 = 0.0475, wR2 = 0.1249	R1 = 0.0565, wR2 = 0.1698
R indices (all data)	R1 = 0.0530, wR2 = 0.1301	R1 = 0.0579, wR2 = 0.1392	R1 = 0.0560, wR2 = 0.1307	R1 = 0.0694, wR2 = 0.1840
Extinction coefficient	n/a	n/a	n/a	n/a
Largest diff. peak and hole	0.879 and -1.014 e. Å^{-3}	0.370 and -0.399 e. Å^{-3}	0.301 and -0.522 e. Å^{-3}	0.873 and -0.605 e. Å^{-3}

4. Cyclic voltammetry analysis

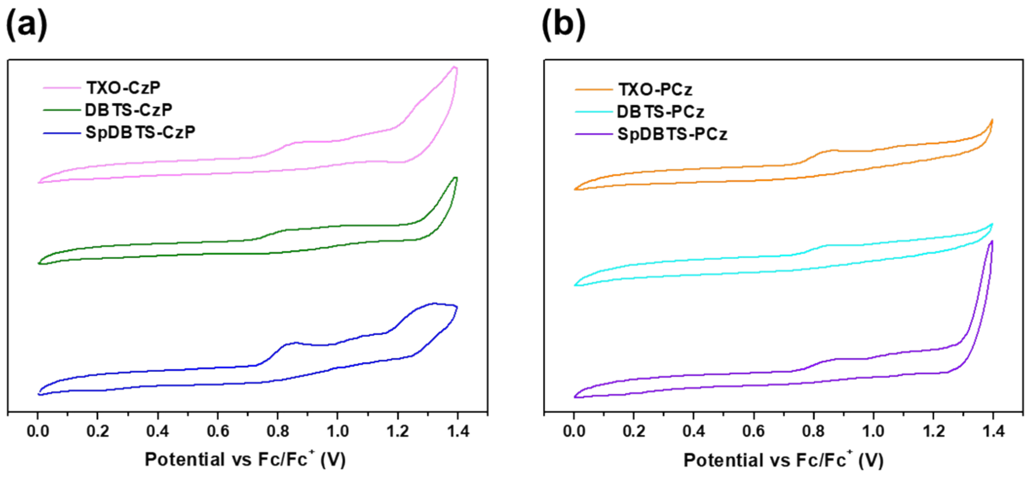

Fig. S10 Oxidative voltammograms of (a) **TXO-CzP**, **DBTS-CzP**, **SpDBTS-CzP** and (b) **TXO-PCz**, **DBTS-PCz**, **SpDBTS-PCz**.

5. Thermal stability of host materials

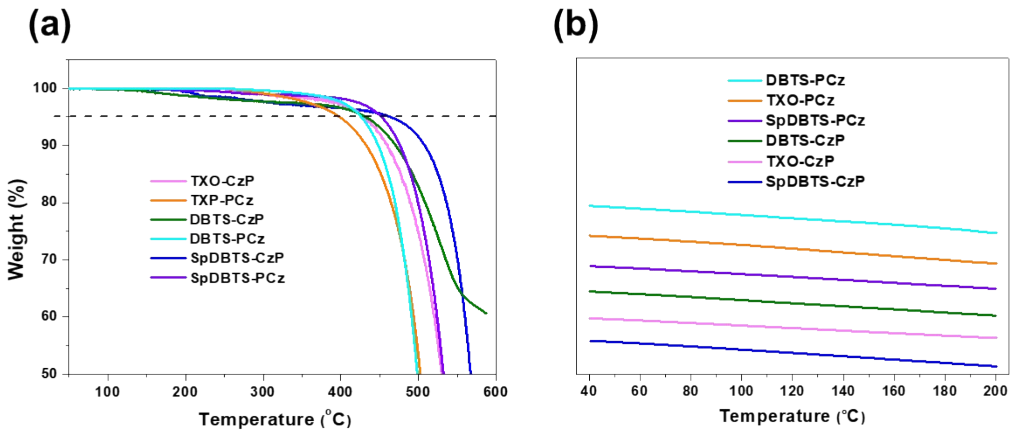

Fig. S11 (a) Thermogravimetric analysis curves and (b) differential scanning calorimetry curves of OLED host materials.

6. Theoretical calculation

Table S2 Theoretically calculated energy level of first excited triplet state (T_1), HOMO-LUMO energy gap (E_g), and singlet-triplet energy difference (ΔE_{ST}) of host materials.

Host	**S_0 (eV)**	**S_1 (eV)**	**T_1 (eV)**	**E_g (eV)**	**ΔE_{ST} (eV)**	**S_0-T_1 Energy Gap (eV)**
TXO-CzP	-5.214	-1.808	-3.008	3.406	1.200	2.206
TXO-PCz	-5.410	-1.938	-3.008	3.472	1.017	2.402
DBTS-CzP	-5.464	-2.295	-3.013	3.169	0.718	2.451
DBTS-PCz	-5.515	-2.078	-3.015	3.437	0.937	2.500
SpDBTS-CzP	-4.955	-1.402	-3.015	3.553	1.613	1.940
SpDBTS-PCz	-5.256	-1.559	-3.017	3.697	1.458	2.239

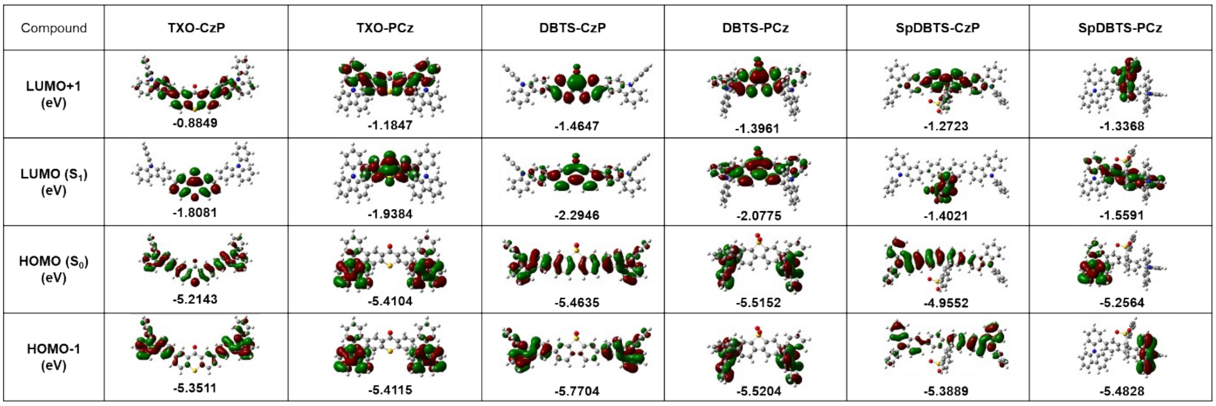

Fig. S12 Frontier molecule orbital density distribution and energy levels of host materials.

7. Space-charge-limited current (SCLC)□

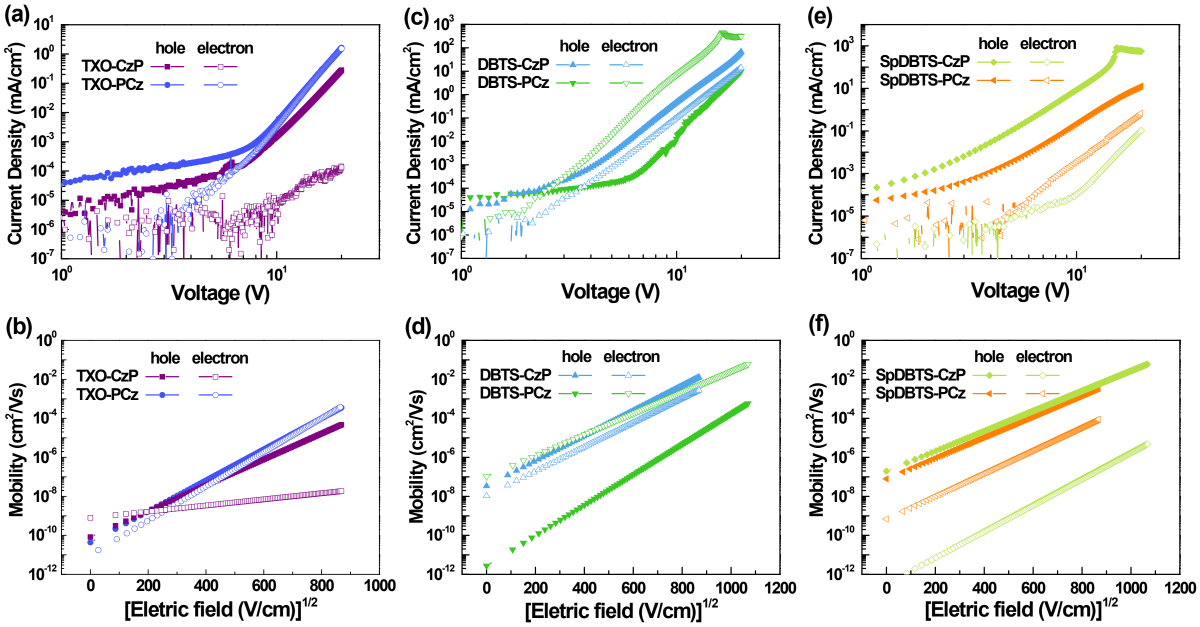

Fig. S13 Current density–voltage (*J*–*V*) characteristics of the hole-only and electron-only devices: (a) **TXO-CzP** and **TXO-PCz**; (c) **DBTS-CzP** and **DBTS-PCz**; (e) **SpDBTS-CzP** and **SpDBTS-PCz**. Comparative field dependence mobility: (b) **TXO-CzP** and **TXO-PCz**; (d) **DBTS-CzP** and **DBTS-PCz**; (f) **SpDBTS-CzP** and **SpDBTS-PCz**.

Table S3 Hole/electron mobility values determined at a field of 0.25 MV/cm

Mobility	**BXO-CzP**	**BZO-PCz**	**DBTS-CzP**	**DBTS-PCz**	**SpDBTS-CzP**	**SpDBTS-PCz**
Hole (cm^2/V s)	1.7×10^{-7}	4.2×10^{-7}	5.6×10^{-5}	2.2×10^{-8}	7.3×10^{-5}	3.8×10^{-5}
Electron (cm^2/V s)	4.9×10^{-9}	2.4×10^{-7}	1.4×10^{-5}	5.1×10^{-5}	7.4×10^{-10}	6.1×10^{-7}

8. Fast screen exciplex host experiments

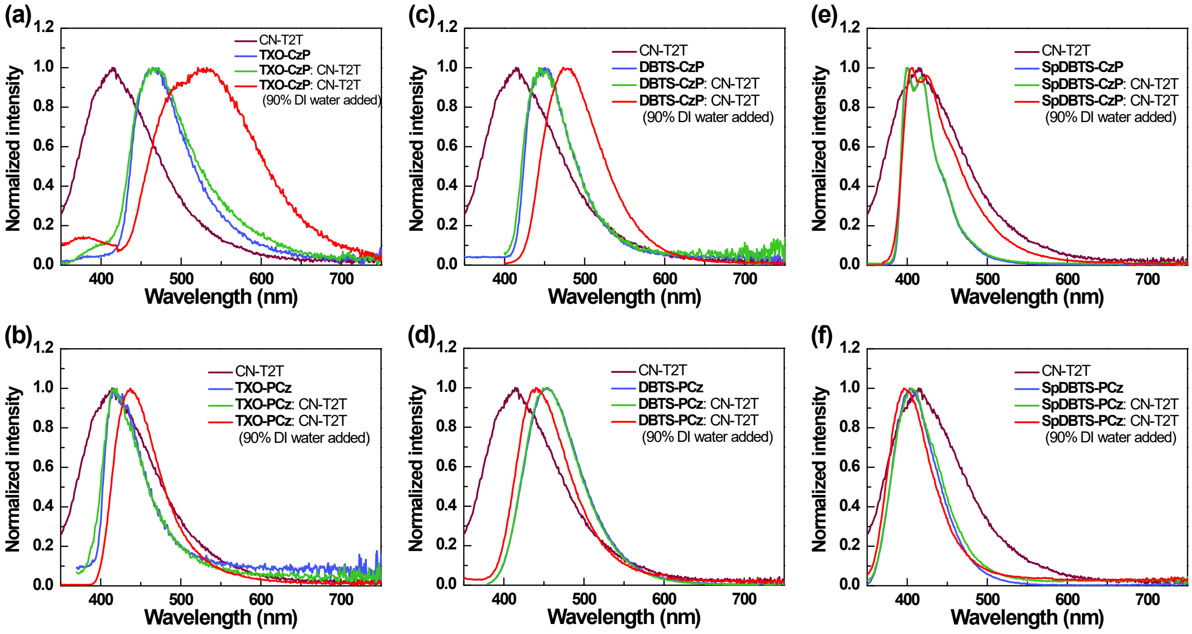

Fig. S14 Normalized PL spectra of CN-T2T, the six synthesized materials, and their mixtures, in pure THF and with 90% water added. (a) **TXO-CzP**; (b) **TXO-PCz**; (c) **DBTS-CzP**; (d) **DBTS-PCz**; (e) **SpDBTS-CzP**; and (f) **SpDBTS-PCz**.

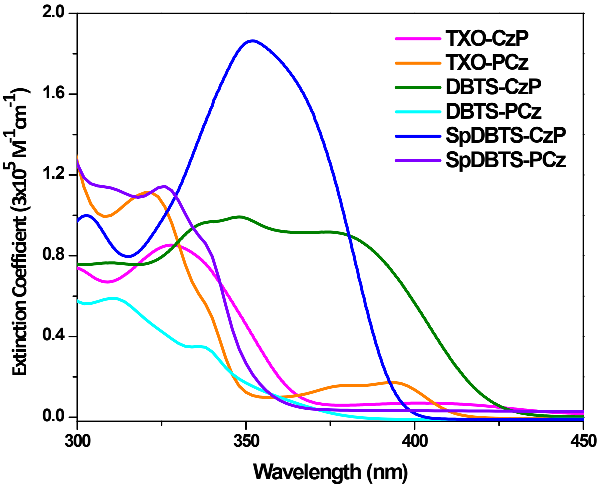

Fig. S15 The UV-Visible absorption spectrum with molar extinction coefficient (ε) vs wavelength at the concentration of 3×10^{-5} M toluene solution.

Reference

[1] T. C. Yiu, P. Gnanasekaran, W.-L. Chen, W.-H. Lin, M.-J. Lin, D.-Y. Wang, C.-W. Lu, C.-H. Chang and Y. J. Chang, *ACS Appl. Mater. Interfaces* **2023**, *15*, 1748-1761.