Supplementary Information for

BN-Benzo[*b*]fluoranthenes: facile synthesis, characterization, and optoelectronic properties

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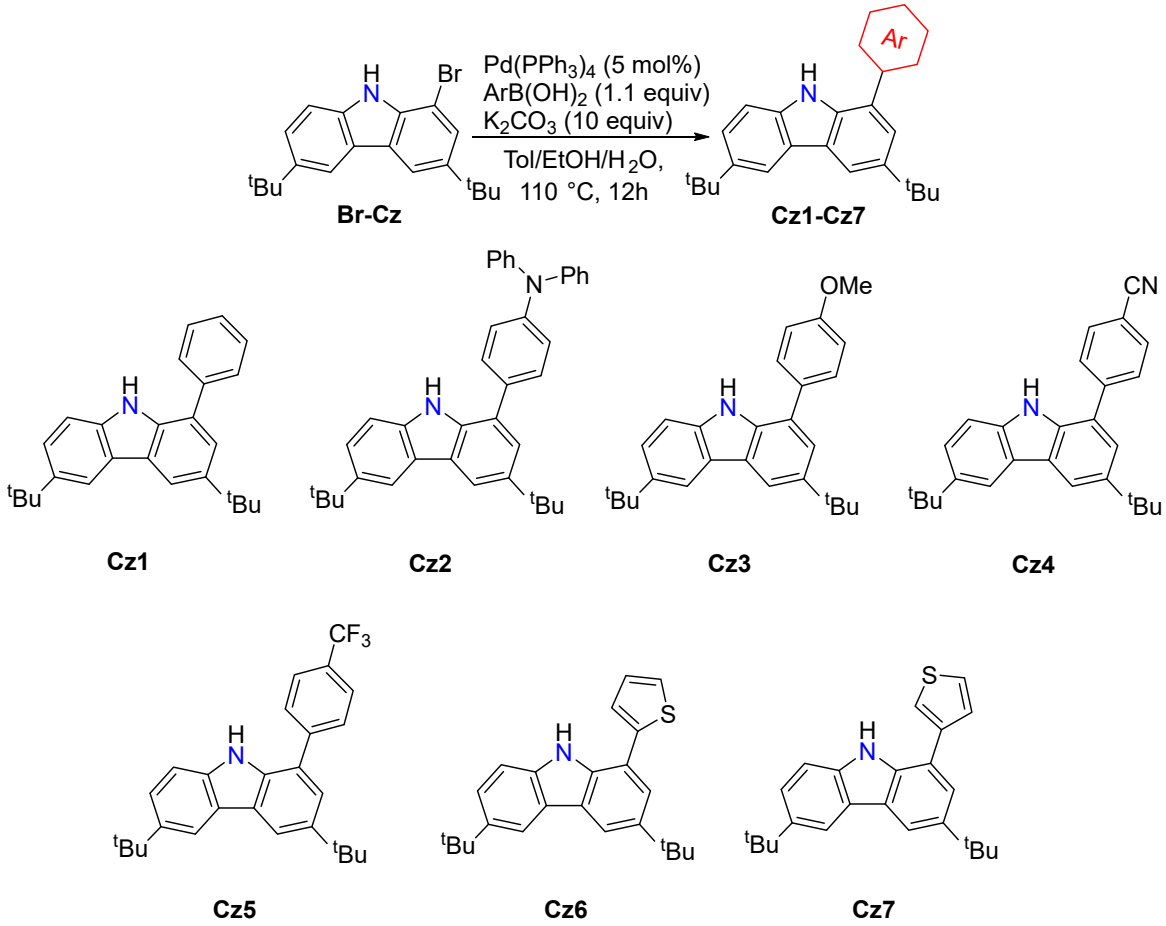
1. Synthetic procedures

General considerations: All oxygen- and moisture-sensitive manipulations were carried out under dry nitrogen using standard Schlenk techniques or in a Vigor inert atmosphere dry-box containing an atmosphere of purified nitrogen. Solvents were dried by standard methods and freshly distilled prior to use. The NMR spectra were recorded with a JEOL-400 MHz spectrometer, referenced to residual solvent signals as internal standards (^{1}H and $^{13}C\{^{1}H\}$) or with an external reference ($BF_3{\cdot}OEt_2$ for ^{11}B). Abbreviations: s = singlet; d = doublet; t = triplet; m = multiplet; br = broad. The UV-Vis absorption spectra of the compounds were recorded on a Perkin-Elmer Lambda-950 Spectrophotometer. The photoluminescence (PL) spectra, related emission lifetimes, and the absolute fluorescence quantum yields of the compounds were studied with Edinburgh Instruments Ltd (FLSP980) fluorescence spectrophotometer. The mass spectra (MS) were characterized on an Agilent 6540 electrospray ionization quadrupole time-of-flight mass spectrometer or the WATERS I-Class VION IMS Qtof mass spectroscopy.



Scheme S1 Synthesis of **Cz1**-**Cz7**.

Typical procedures: A sealed tube containing 1-bromo-3,6-di-tert-butyl-9H-carbazole (2.56 g, 7.2 mmol, 1.0 equiv), $Pd(PPh_3)_4$ (0.42 g, 0.36 mmol, 0.05 equiv), arylboronic acid (7.9 mmol, 1.1 equiv) and K_2CO_3 (9.95 g, 72.0 mmol, 10.0 equiv) was pumped and then refilled with nitrogen three times. A mixed solvent (Toluene/EtOH/H_2O = 5/1/1, 140 mL) was added to the above mixture by syringe. The reaction mixture was heated to 110 ℃ and stirred for 12 hours. After cooling to room temperature, the solvent was extracted three times with dichloromethane, dried over anhydrous magnesium sulfate, and filtered. The solvent was removed under vacuum to produce the crude product. The crude product was purified by column chromatography on silica gel to give the

corresponding coupling compounds **Cz1-Cz7**.

Cz1: R_f = 0.75 (PE:DCM = 2:1), m.p. 182-183 ℃, white solid (2.05 g, yield = 80 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (d, *J* = 8.4 Hz, 2H, Ar), 8.18 (s, 1H, NH), 7.81 (d, *J* = 7.7 Hz, 2H, Ar), 7.69 - 7.60 (m, 3H, Ar), 7.59 - 7.49 (m, 2H, Ar), 7.38 (d, *J* = 8.5 Hz, 1H, Ar), 1.62 (s, 9H, CH_3), 1.58 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.88, 142.44, 139.82, 138.13, 135.97, 129.31, 128.54, 127.48, 124.38, 123.88, 123.82, 123.74, 123.62, 116.44, 115.62, 110.23, 34.93, 34.84, 32.24, 32.19.

Cz2: R_f = 0.60 (PE:DCM = 2:1), m.p. 214-216 ℃, white solid (2.18 g, yield = 58 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (s, 1H, Ar), 8.11 (s, 1H, Ar), 8.06 (s, 1H, Ar), 7.58 (d, *J* = 8.5 Hz, 2H, Ar), 7.50 - 7.44 (m, 2H, Ar), 7.37 - 7.28 (m, 5H, Ar), 7.22 (t, *J* = 8.6 Hz, 5H, Ar), 7.07 (t, *J* = 7.3 Hz, 2H, Ar), 1.50 (s, 9H, CH_3), 1.47 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.82, 147.27, 142.90, 142.43, 138.13, 135.97, 133.67, 129.50, 129.18, 124.66, 124.29, 124.04, 123.85, 123.77, 123.68, 123.53, 123.21, 116.44, 115.30, 110.22, 34.94, 34.86, 32.25, 32.19. HRMS (ESI) m/z calcd for ($C_{38}H_{38}N_2$) $[M+H]^+$, 523.31087, found: 523.30941.

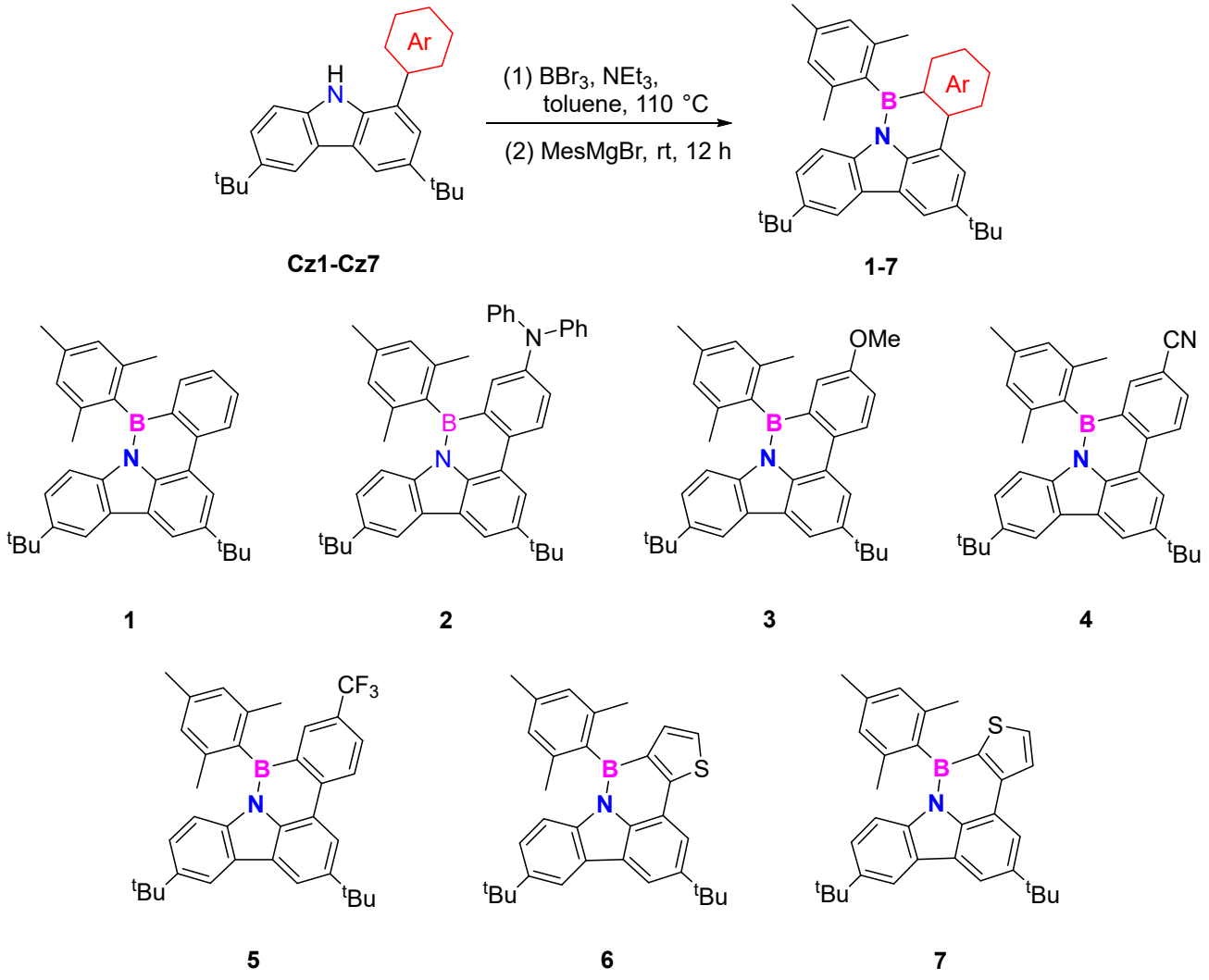
Cz3: R_f = 0.20 (PE:DCM = 2:1), m.p. 185-186 ℃, white solid (1.66 g, yield = 60 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14-8.03 (m, 3H, Ar), 7.64 (d, *J* = 8.7 Hz, 2H, Ar), 7.50-7.43 (m, 2H, Ar), 7.32 (d, *J* = 8.5 Hz, 1H, Ar), 7.10 (d, *J* = 8.5 Hz, 2H, Ar), 3.91 (s, 3H, OCH_3), 1.50 (s, 9H, CH_3), 1.47 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.11, 142.87, 142.40, 138.16, 136.09, 132.17, 129.60, 124.12, 123.78, 123.74, 123.70, 123.56, 116.44, 115.17, 114.72, 110.21, 55.51, 34.92, 34.85, 32.25, 32.19. HRMS (ESI) m/z calcd for ($C_{27}H_{31}NO$) $[M+H]^+$, 386.24784, found: 386.24812.

Cz4: R_f = 0.30 (PE:DCM = 1:1), m.p. 290-291 ℃, white solid (1.37 g, yield = 50 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (s, 1H, Ar), 8.11 (s, 1H, Ar), 8.06 (s, 1H, NH), 7.83 (s, 4H, Ar), 7.50 (d, *J* = 6.7 Hz, 1H, Ar), 7.45 (s, 1H, Ar), 7.35 (d, *J* = 8.5 Hz, 1H, Ar), 1.49 (s, 9H, CH_3), 1.46 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.72, 143.19, 142.94, 138.20, 135.59, 133.09, 129.15, 124.48, 124.28, 123.61, 123.38, 122.33, 119.07, 117.05, 116.49, 110.92, 110.41, 34.94, 34.87, 32.17, 32.13. HRMS (ESI) m/z calcd for ($C_{27}H_{28}N_2$) $[M+H]^+$, 381.23253, found: 381.23320.

Cz5: R_f = 0.40 (PE:DCM = 6:1), m.p. 210-211 ℃, white solid (1.46 g, yield = 48 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (s), 8.11 (s), 8.05 (s, 1H, NH), 7.82 (s, 4H, Ar), 7.51-7.44 (m, 2H, Ar), 7.34 (d, *J* = 8.5 Hz, 1H, Ar), 1.50 (s, 9H, CH_3), 1.46 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): 143.53, 143.12, 142.82, 138.17, 135.79, 129.70 (q, $J_{C–F}$ = 32.6 Hz), 128.83, 126.24 (q, $J_{C–F}$ = 3.7 Hz), 124.37 (q, $J_{C–F}$ = 271.9 Hz), 124.26, 124.15, 123.70, 123.50, 122.89, 116.55, 116.52, 110.34, 34.95, 34.88, 32.20, 32.16. HRMS (ESI) m/z calcd for ($C_{27}H_{28}F_3N$) $[M+H]^+$, 424.22466, found: 424.22528.

Cz6: R_f = 0.55 (PE:DCM = 2:1), m.p. 149-150 ℃, white solid (1.38 g, yield = 52 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 (s, 1H, NH), 8.11 (s, 1H, Ar), 8.09 (s, 1H, Ar), 7.61 (s, 1H, Ar), 7.50 (d, *J* = 6.8 Hz, 1H, Ar), 7.43 (t, *J* = 4.5 Hz, 2H, Ar), 7.38 (d, *J* = 8.5 Hz, 1H, Ar), 7.23 (dd, *J* = 5.1, 3.6 Hz, 1H, Ar), 1.50 (s, 9H, CH_3), 1.47 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.83, 142.74, 141.91, 138.16, 135.62, 128.10, 124.95, 124.71, 124.27, 124.05, 123.56, 123.46, 117.24, 116.47, 116.25, 110.43, 34.89, 32.18. HRMS (ESI) m/z calcd for ($C_{24}H_{27}NS$) $[M+H]^+$, 362.19370, found: 362.19387.

Cz7: R_f = 0.55 (PE:DCM = 2:1), m.p. 170-171 ℃, white solid (1.35 g, yield = 52 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (s, 1H, NH), 8.11 (s, 1H, Ar), 8.07 (s, 1H, Ar), 7.57-7.59 (m, 1H, Ar), 7.56-7.52 (m, 2H, Ar), 7.51-7.46 (m, 2H, Ar), 7.35 (d, *J* = 8.5 Hz, 1H, Ar), 1.49 (s, 9H, CH_3), 1.47 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.79, 142.59, 140.41, 138.18, 136.09, 127.87, 126.79, 124.02, 123.89, 123.68, 123.23, 121.66, 119.36, 116.47, 115.66, 110.32, 34.90, 34.87, 32.23, 32.18. HRMS (ESI) m/z calcd for ($C_{24}H_{27}NS$) $[M+H]^+$, 362.19370, found: 362.19468.



Scheme S2 Synthesis of **1**-**7**.

Typical procedures: A mixture of 3,6-di-tert-butyl-1-aryl-9H-carbazole (0.5 mmol, 1.0 equiv), triethylamine (0.21 mL, 1.5 mmol, 3 equiv) in toluene (15 mL) was stirred at room temperature in 10 minutes. Then boron tribromide (1.0 M in heptane, 0.55 mL, 0.55 mmol, 1.1 equiv) was dropwise added to the reaction mixture. After stirring at room temperature for 10 minutes, the reaction mixture was heated up to 110 ℃ for 12 hours. After cooling to room temperature, mesitylmagnesium bromide (1.0 M in THF, 2.0 mL, 2.0 mmol, 4.0 equiv) was added under a nitrogen atmosphere and stirred for 12 h at room temperature. Then the mixture was quenched with water. The solvent was removed by vacuum. The mixture was extracted with dichloromethane and washed with water. The combined organic layer was dried over $MgSO_4$ and filtered. After the removal of the solvents, the residue was purified by column chromatography on silica gel to give the corresponding target product **1-7**.

1: R_f = 0.80 (PE:DCM = 2:1), m.p. 215-216 ℃, white solid (169.2 mg, yield = 70 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298K): δ 8.59 (d, *J* = 8.0 Hz, 1H, Ar), 8.52 (s, 1H, Ar), 8.23 (s, 1H, Ar), 8.10 (s, 1H, Ar), 7.86 (d, *J* = 7.5 Hz, 1H, Ar), 7.80 (t, *J* = 7.5 Hz, 1H, Ar), 7.44 (t, *J* = 7.4 Hz, 1H, Ar), 7.28 (d, *J* = 1.9 Hz, 1H, Ar), 7.01 (s, 2H, Ar), 6.85 (d, *J* = 8.6 Hz, 1H, Ar), 2.46 (s, 3H, CH_3), 2.04 (s, 6H, CH_3), 1.61 (s, 9H, CH_3), 1.42 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, 298K): δ 146.90, 146.37, 142.31, 139.84, 138.14, 138.05, 137.64, 136.34, 131.78, 128.85, 127.61, 127.16, 126.79, 124.97, 122.10, 121.63, 117.97, 116.86, 116.76, 114.94, 35.52, 34.98, 32.39, 31.94, 22.60, 21.64 (B-aryl carbons were not observed). ^{11}B NMR (128 MHz, $CDCl_3$, 298K): δ 43.63. HRMS (ESI) m/z calcd for ($C_{35}H_{38}BN$) $[M+H]^+$, 484.31701, found: 484.31704.

2: R_f = 0.50 (PE:DCM = 8:1), m.p. 178-179 ℃, pale yellow solid (227.7 mg, yield = 70 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298K): δ 8.46 (d, *J* = 8.6 Hz, 1H, Ar), 8.41 (s, 1H, Ar), 8.18 (s, 1H, Ar), 8.09 (s, 1H, Ar), 7.57 (s, 1H, Ar), 7.52 (d, *J* = 8.6 Hz, 1H, Ar), 7.21 (t, *J* = 8.0 Hz, 5H, Ar), 7.09 (d, *J* = 8.1 Hz, 4H, Ar), 6.98 (t, *J* = 7.2 Hz, 2H, Ar), 6.86 (s, 2H, Ar), 6.79 (d, *J* = 8.6 Hz, 1H, Ar), 2.35 (s, 3H, CH_3), 1.98 (s, 3H, CH_3), 1.59 (s, 3H, CH_3), 1.42 (s, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, 298K): δ 147.74, 146.88, 146.46, 146.37, 142.27, 139.53, 137.85, 136.08, 133.20, 132.67, 129.24, 128.97, 128.62, 127.52, 127.02, 124.84, 123.83, 123.31, 122.71, 121.53, 117.60, 116.81, 116.01, 115.01, 35.48, 34.97, 32.37, 31.93, 22.51, 21.51 (B-aryl carbons were not observed). ^{11}B NMR (128 MHz, $CDCl_3$, 298K): δ 42.68. HRMS (ESI) m/z calcd for ($C_{47}H_{47}BN_2$) $[M+H]^+$, 651.39051, found: 651.38822.

3: R_f = 0.45 (PE:DCM = 8:1), m.p. 183-184 ℃, white solid (130.9 mg, yield = 51 %) ^{1}H NMR (400 MHz, $CDCl_3$, 298K): δ 8.54 (d, *J* = 8.8 Hz, 1H, Ar), 8.44 (s, 1H, Ar), 8.18 (s, 1H, Ar), 8.10 (s, 1H, Ar), 7.39 (d, *J* = 8.7 Hz, 1H, Ar), 7.33 (s, 1H, Ar), 7.28 (s, 1H, Ar), 7.00 (s, 2H, Ar), 6.84 (d, *J* = 8.6 Hz, 1H, Ar), 3.82 (s), 2.45 (s, 3H, CH_3), 2.05 (s, 6H, CH_3), 1.61 (s, 9H, CH_3), 1.43 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, 298K): δ 158.53, 146.88, 146.43, 142.30, 139.71, 137.97, 135.73, 131.60, 129.02, 127.64, 127.03, 124.85, 123.73, 121.64, 120.15, 119.15, 117.42, 116.85, 115.71, 114.95, 55.54, 35.49, 34.97, 32.39, 31.93, 22.53, 21.62 (B-aryl carbons were not observed). ^{11}B NMR (128 MHz, $CDCl_3$, 298K): δ 42.68. HRMS (ESI) m/z calcd for ($C_{36}H_{40}BNO$) $[M+H]^+$, 514.32757, found: 514.32420.

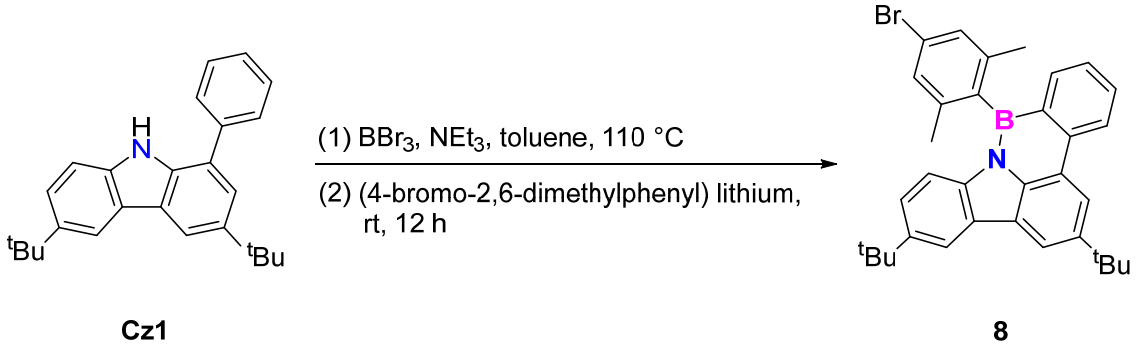
4: R_f = 0.55 (PE : DCM = 2:1), m.p. 288-289 ℃, pale solid (83.9 mg, yield = 33 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298K): δ 8.66 (d, *J* = 8.4 Hz, 1H, Ar), 8.50 (s, 1H, Ar), 8.32 (s, 1H, Ar), 8.15 (s, 1H, Ar), 8.11 (s, 1H, Ar), 8.01 (d, *J* = 8.3 Hz, 1H, Ar), 7.31 (d, *J* = 8.6 Hz, 1H, Ar), 7.04 (s, 2H, Ar), 6.89 (d, *J* = 8.6 Hz, 1H, Ar), 2.47 (s, 3H, CH_3), 2.02 (s, 6H, CH_3), 1.61 (s, 9H, CH_3), 1.43 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, 298K): δ 147.68, 147.08, 142.06, 142.02, 141.69, 139.66, 138.75, 136.90, 133.92, 128.66, 127.95, 127.67, 125.48, 122.98, 120.20, 119.64, 118.77, 118.57, 117.05, 115.15, 110.02, 35.57, 35.04, 32.29, 31.88, 22.60, 21.61 (B-aryl carbons were not observed). ^{11}B NMR (128 MHz, $CDCl_3$, 298K): δ 42.68. HRMS (ESI) m/z calcd for ($C_{36}H_{37}BN_2$) $[M+H]^+$, 509.31226, found: 509.30724.

5: R_f = 0.70 (PE), m.p. 110-112 ℃, white solid (124.1 mg, yield = 45 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298K): δ 8.69 (d, *J* = 8.4 Hz, 1H, Ar), 8.53 (s, 1H, Ar), 8.30 (s, 1H, Ar), 8.11 (s, 2H, Ar), 8.01 (d, *J* = 8.4 Hz, 1H, Ar), 7.30 (d, *J* = 6.7 Hz, 1H, Ar), 7.03 (s, 2H, Ar), 6.83 (d, *J* = 8.7 Hz, 1H, Ar), 2.47 (s, 3H, CH_3), 2.03 (s, 6H, CH_3), 1.62 (s, 9H, CH_3), 1.43 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, 298K): δ 147.43, 146.85, 142.19, 141.12, 139.72, 138.48, 136.76, 134.27 (q, $J_{C–F}$ = 3.4 Hz), 128.77, 128.47 (q, $J_{C–F}$ = 32.1 Hz), 128.04 (q, $J_{C–F}$ = 3.3 Hz), 127.90, 127.52, 125.32, 124.64 (q, $J_{C–F}$ = 271.9 Hz), 122.70, 120.53, 118.42, 118.08, 116.98, 115.16, 35.57, 35.02, 32.34, 31.90, 22.60, 21.63 (B-aryl carbons were not observed). ^{11}B NMR (128 MHz, $CDCl_3$, 298K): δ 41.48. HRMS (ESI) m/z calcd for ($C_{36}H_{37}BF_3N$) $[M+H]^+$, 552.30439, found: 552.30601.

6: R_f = 0.70 (PE:DCM = 2:1), m.p. 213-214 ℃, pale solid (159.1 mg, yield = 65 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298K): δ 8.21 (s, 1H, Ar), 8.10 (s, 1H, Ar), 8.08 (s, 1H, Ar),

7.39 (d, J = 5.0 Hz, 1H, Ar), 7.32 (d, J = 5.0 Hz, 1H, Ar), 7.28 (d, J = 2.0 Hz, 1H, Ar), 6.99 (s, 2H, Ar), 6.89 (d, J = 8.6 Hz, 1H, Ar), 2.44 (s, 3H, CH_3), 2.08 (s, 6H, CH_3), 1.59 (s, 9H, CH_3), 1.42 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, 298K): δ 150.06, 146.91, 146.73, 142.80, 139.67, 138.00, 135.96, 132.90, 128.80, 127.59, 127.14, 125.10, 124.28, 119.43, 118.77, 117.07, 116.91, 114.91, 35.43, 34.97, 32.32, 31.92, 22.60, 21.60 (B-aryl carbons were not observed). ^{11}B NMR (128 MHz, $CDCl_3$, 298K): δ 40.37. HRMS (ESI) m/z calcd for ($C_{33}H_{36}BNS$) $[M+H]^+$, 490.27343, found: 490.27194.

7: R_f = 0.70 (PE:DCM = 2:1), m.p. 222-223 °C, pale solid (159.1 mg, yield = 65 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298K): δ 8.25 (d, J = 6.3 Hz, 2H, Ar), 8.14-8.08 (m, 2H, Ar), 7.96 (d, J = 4.8 Hz, 1H, Ar), 7.28 (d, J = 7.0 Hz, 1H, Ar), 7.01 (s, 2H, Ar), 6.90 (d, J = 8.6 Hz, 1H, Ar), 2.45 (s, 3H, CH_3), 2.12 (s, 6H, CH_3), 1.60 (s, 9H, CH_3), 1.42 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, 298K): δ 146.86, 146.45, 145.97, 142.67, 139.81, 138.35, 136.49, 135.67, 129.03, 127.70, 126.91, 124.99, 123.25, 119.60, 119.07, 117.05, 116.43, 114.85, 35.45, 34.98, 32.37, 31.93, 22.54, 21.66 (B-aryl carbons were not observed). ^{11}B NMR (128 MHz, $CDCl_3$, 298K): δ 38.74. HRMS (ESI) m/z calcd for ($C_{33}H_{36}BNS$) $[M+H]^+$, 490.27343, found: 490.27127.



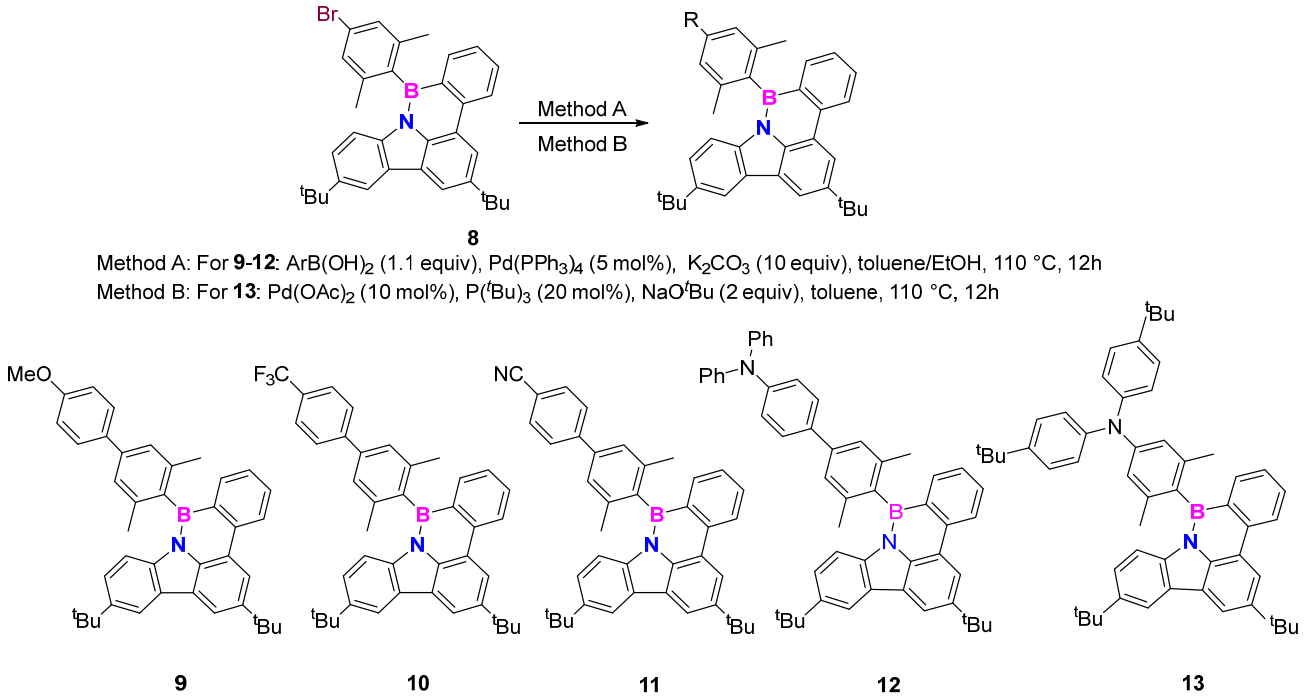
Cz1 **8**

Scheme S4 Synthesis of **8**.

A mixture of 3,6-di-tert-butyl-1-phenyl-9H-carbazole (177.8 mg, 0.50 mmol, 1.0

equiv), triethylamine (0.21 mL, 1.50 mmol, 3 equiv) in toluene (10 mL) was stirred at room temperature in 10 minutes. Then boron tribromide (1.0 M in heptane, 0.55 mL, 0.55 mmol, 1.1 equiv) was dropwise added to the reaction mixture. After stirring at room temperature for 10 minutes, the reaction mixture was heated up to 110 ℃ for 12 hours. After cooling to room temperature, (4-bromo-2,6-dimethylphenyl)lithium which was prepared from 5-bromo-2-iodo-1,3-dimethylbenzene and n-BuLi (in THF, 2.0 mmol, 4.0 equiv) was added under a nitrogen atmosphere and stirred for 12 h at room temperature. Then the mixture was quenched with water. The solvent was removed by vacuum. The mixture was extracted with dichloromethane and washed with water. The combined organic layer was dried over $MgSO_4$ and filtered. After the removal of the solvents, the residue was purified by column chromatography on silica gel to give the target product **8**.

8: R_f = 0.30 (PE), m.p. 198-199 ℃, white solid (208.4 mg, yield = 76 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298K): δ 8.60 (d, *J* = 7.9 Hz, 1H, Ar), 8.53 (s, 1H, Ar), 8.24 (s, 1H, Ar), 8.11 (s, 1H, Ar), 7.88-7.72 (m, 2H, Ar), 7.46 (t, *J* = 7.4 Hz, 1H, Ar), 7.36 (s, 2H, Ar), 7.30 (d, *J* = 8.6 Hz, 1H, Ar), 6.85 (d, *J* = 8.6 Hz, 1H, Ar), 2.05 (s, 6H, CH_3), 1.61 (s, 9H, CH_3), 1.43 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, 298K): δ 147.25, 146.66, 142.13, 142.01, 138.23, 137.25, 136.17, 132.04, 129.64, 128.96, 127.22, 126.93, 125.10, 122.73, 122.25, 121.62, 118.08, 117.06, 116.95, 114.69, 35.53, 34.99, 32.37, 31.91, 22.42 (B-aryl carbons were not observed). ^{11}B NMR (128 MHz, $CDCl_3$, 298K): δ 42.21. HRMS (ESI) m/z calcd for ($C_{34}H_{35}BBrN$) $[M+Na]^+$, 570.19381, found: 570.19498.



Scheme S5 Synthesis of **9-13**.

Typical procedures: A sealed tube containing **8** (106.0 mg, 0.19 mmol, 1.0 equiv), $Pd(PPh_3)_4$ (11.17 mg, 0.0097 mmol, 0.05 equiv), arylboronic acid (0.21 mmol, 1.1 equiv) and K_2CO_3 (262.60 mg, 1.9 mmol, 10.0 equiv) was pumped and then refilled with nitrogen three times. A mixed solvent (Toluene/EtOH/H_2O = 5/1/1, 12 mL) was added to the above mixture by syringe. The reaction mixture was heated to 110℃ and stirred for 12 hours. After cooling to room temperature, the solvent was extracted three times with dichloromethane, dried over anhydrous magnesium sulfate, and filtered. The solvent was removed under vacuum to produce the crude product. The crude product was purified by column chromatography on silica gel to give the corresponding coupling compounds **9-12**.

A sealed tube containing 8 (111.0 mg, 0.20 mmol, 1.0 equiv), $Pd(OAc)_2$ (4.50 mg, 0.02 mmol, 0.10 equiv), bis(4-(tert-butyl)phenyl)amine (61.90 mg, 0.22 mmol, 1.1 equiv) and t-BuONa (38.44 mg, 0.40 mmol, 2.0 equiv) was pumped and then refilled

with nitrogen three times. Then $(t\text{-}Bu)_3P$ (0.1mL, 0.04 mmol, 0.2 equiv) and dry toluene (15 mL) were added in sequence by syringe. The reaction mixture was heated to 110 ℃ and stirred for 12 hours. After cooling to room temperature, the solvent was extracted three times with dichloromethane, dried over anhydrous magnesium sulfate, and filtered. The solvent was removed under vacuum to produce the crude product. The crude product was purified by column chromatography on silica gel to give the target compound **13**.

9: R_f = 0.35 (PE:DCM = 4:1), m.p. 257-258 ℃, white solid (71.1 mg, yield = 65 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298K): δ 8.62 (d, *J* = 8.0 Hz, 1H, Ar), 8.55 (s, 1H, Ar), 8.25 (s, 1H, Ar), 8.12 (s, 1H, Ar), 7.92 (d, *J* = 7.4 Hz, 1H, Ar), 7.82 (t, *J* = 7.6 Hz, 1H, Ar), 7.73 (d, *J* = 8.6 Hz, 2H, Ar), 7.47 (t, *J* = 7.3 Hz, 1H, Ar), 7.41 (s, 2H, Ar), 7.28 (d, *J* = 8.7 Hz, 1H, Ar), 7.05 (d, *J* = 8.7 Hz, 2H, Ar), 6.93 (d, *J* = 8.6 Hz, 1H, Ar), 3.90 (s, 3H, CH_3), 2.14 (s, 6H, CH_3), 1.62 (s, 9H, CH_3), 1.42 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, 298K): δ 159.22, 147.03, 146.48, 142.27, 140.73, 140.40, 138.19, 137.64, 136.32, 134.10, 131.86, 128.90, 128.22, 127.20, 126.85, 125.04, 122.15, 121.66, 118.01, 116.91, 116.81, 114.95, 114.32, 55.53, 35.53, 34.99, 32.38, 31.92, 22.84 (B-aryl carbons were not observed). ^{11}B NMR (128 MHz, $CDCl_3$, 298K): δ 38.73. HRMS (ESI) m/z calcd for ($C_{41}H_{42}BNO$) $[M+H]^+$, 576.34322, found: 576.33999.

10: R_f = 0.65 (PE:DCM = 8:1), m.p. 274-275 ℃, white solid (58.3 mg, yield = 50 %). ^{1}H NMR (400 MHz, $CDCl_3$, 298K): δ 8.65 (d, *J* = 8.1 Hz, 1H, Ar), 8.58 (s, 1H, Ar), 8.29 (s, 1H, Ar), 8.15 (s, 1H, Ar), 7.91 (d, *J* = 8.2 Hz, 3H, Ar), 7.85 (t, *J* = 7.6 Hz, 1H, Ar), 7.78 (d, *J* = 8.2 Hz, 2H, Ar), 7.55-7.44 (m, 3H, Ar), 7.30 (d, *J* = 8.6 Hz, 1H, Ar),

6.93 (d, J = 8.6 Hz, 1H, Ar), 2.19 (s, 6H, CH_3), 1.65 (s, 9H, CH_3), 1.45 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, 298K): δ 147.19, 146.64, 145.15, 142.17, 140.80, 139.74, 138.26, 137.45, 136.28, 131.99, 129.27 (q, $J_{C–F}$ = 32.1 Hz), 128.99, 127.50, 127.23, 126.91, 125.82 (q, $J_{C–F}$ = 3.5 Hz), 125.59, 125.02, 124.59 (q, $J_{C–F}$ = 271.6 Hz), 122.25, 121.67, 118.09, 117.04, 116.91, 114.77, 35.55, 35.01, 32.38, 31.91, 22.82 (B-aryl carbons were not observed). ^{11}B NMR (128 MHz, $CDCl_3$, 298K): δ 44.66. HRMS (ESI) m/z calcd for ($C_{41}H_{39}BF_3N$) $[M+H]^+$, 614.32004, found: 614.31706.

11: R_f = 0.35 (PE:DCM = 2:1), m.p. 319-320 ℃, white solid (56.4 mg, yield = 52 %). ^1H NMR (400 MHz, $CDCl_3$, 298K): δ 8.65 (d, J = 8.0 Hz, 1H, Ar), 8.58 (s, 1H, Ar), 8.29 (s, 1H, Ar), 8.16 (s, 1H, Ar), 7.92-7.77 (m, 6H, Ar), 7.52-7.42 (m, 3H, Ar), 7.29 (d, J = 8.6 Hz, 1H, Ar), 6.91 (d, J = 8.6 Hz, 1H, Ar), 2.19 (s, 6H, CH_3), 1.64 (s, 9H, CH_3), 1.44 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, 298K): δ 147.22, 146.68, 146.11, 142.10, 140.97, 139.14, 138.26, 137.34, 136.22, 132.72, 132.02, 128.99, 127.79, 127.20, 126.90, 125.51, 124.98, 122.27, 121.64, 119.31, 118.11, 117.08, 116.94, 114.66, 110.75, 35.54, 35.00, 32.36, 31.90, 22.80 (B-aryl carbons were not observed). ^{11}B NMR (128 MHz, $CDCl_3$, 298K): δ 41.73. HRMS (ESI) m/z calcd for ($C_{41}H_{39}BN_2$) $[M+H]^+$, 571.32791, found: 571.32599.

12: R_f = 0.50 (PE:DCM = 8:1), m.p. 284-285 ℃, white solid (94.8 mg, yield = 70 %). ^1H NMR (400 MHz, $CDCl_3$, 298K): δ 8.61 (d, J = 8.0 Hz, 1H, Ar), 8.54 (s, 1H, Ar), 8.25 (s, 1H, Ar), 8.11 (s, 1H, Ar), 7.91 (d, J = 7.5 Hz, 1H, Ar), 7.82 (t, J = 7.0 Hz, 1H, Ar), 7.68 (d, J = 8.5 Hz, 2H, Ar), 7.47 (t, J = 7.3 Hz, 1H, Ar), 7.43 (s, 2H, Ar), 7.34-7.27 (m, 5H, Ar), 7.24-7.15 (m, 6H, Ar), 7.05 (t, J = 7.3 Hz, 2H, Ar), 6.91 (d, J = 8.6

Hz, 1H, Ar), 2.14 (s, 6H, CH_3), 1.62 (s, 9H, CH_3), 1.42 (s, 9H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, 298K): δ 147.93, 147.20, 147.02, 146.48, 142.25, 140.57, 140.44, 138.19, 137.61, 136.31, 135.69, 131.88, 129.41, 128.90, 127.90, 127.20, 126.86, 125.01, 124.43, 124.41, 122.93, 122.16, 121.66, 118.02, 116.92, 116.82, 114.93, 35.52, 34.98, 32.38, 31.92, 22.84 (B-aryl carbons were not observed). ^{11}B NMR (128 MHz, $CDCl_3$, 298K): δ 40.12. HRMS (ESI) m/z calcd for ($C_{52}H_{49}BN_2$) $[M+H]^+$, 713.40616, found: 713.40229.

13: R_f = 0.65 (PE:DCM = 4:1), m.p. 168-169℃, white solid (92.9 mg, yield = 62 %). ^1H NMR (400 MHz, $CDCl_3$, 298K): δ 8.60 (d, *J* = 8.1 Hz, 1H, Ar), 8.53 (s, 1H, Ar), 8.25 (s, 1H, Ar), 8.13 (s, 1H, Ar), 7.99 (d, *J* = 6.5 Hz, 1H, Ar), 7.82 (t, *J* = 7.6 Hz, 1H, Ar), 7.51 (t, *J* = 7.3 Hz, 1H, Ar), 7.39-7.31 (m, 5H, Ar), 7.17 (d, *J* = 8.7 Hz, 4H, Ar), 7.02 (d, *J* = 8.6 Hz, 1H, Ar), 6.93 (s, 2H, Ar), 1.98 (s, 6H, CH_3), 1.61 (s, 9H, CH_3), 1.47 (s, 9H, CH_3), 1.36 (s, 18H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$, 298K): δ 148.33, 146.94, 146.39, 145.56, 145.27, 142.34, 140.91, 138.17, 137.79, 136.39, 131.80, 128.94, 127.15, 126.81, 126.13, 124.84, 123.94, 122.11, 121.95, 121.66, 117.99, 116.97, 116.75, 115.08, 35.53, 35.02, 34.45, 32.40, 31.99, 31.66, 22.77 (B-aryl carbons were not observed). ^{11}B NMR (128 MHz, $CDCl_3$, 298K): δ 42.62. HRMS (ESI) m/z calcd for ($C_{54}H_{61}BN_2$) $[M+H]^+$, 749.50006, found: 749.49994.

2. Crystal structural parameters

Single-Crystal X-ray Structure Determinations: Crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold N_2 flow. The data of all compounds were collected on a Bruker D8-VENTURE diffractometer. The structures were solved by direct methods and refined on F^2 with the SHELX-97[S1] and X-Seed software packages.[S2] The positions of the H atoms were calculated and considered isotropically according to a riding model. CCDC: 2323362-2323367 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from the Cambridge Crystallography Data Center via www.ccdc.cam.ac.uk/data_request/cif.

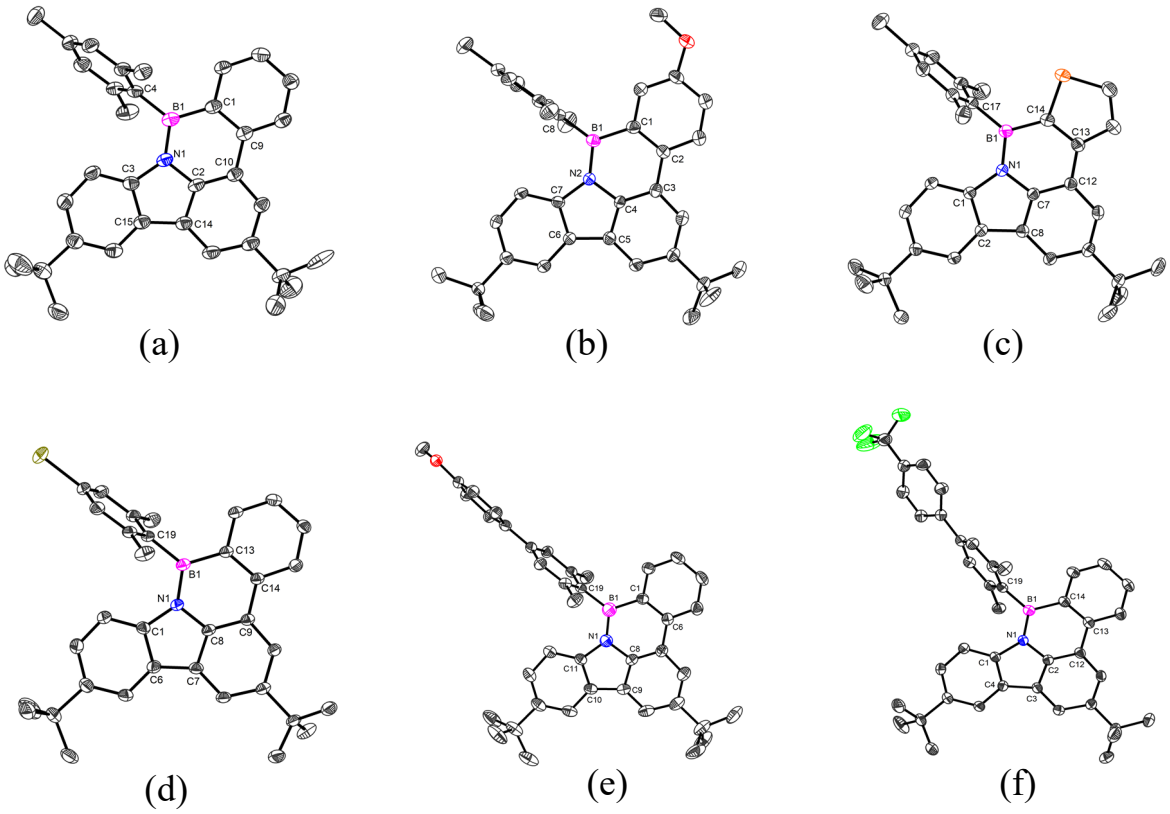


Fig. S1 Molecular structures of **1** (a), **3** (b), **7** (c), **8** (d), **9** (e), and **10** (f). H atoms are omitted for clarity.

Table S1 Crystal data and structure refinement for **1**.

Empirical formula	C35 H38 B N	
Formula weight	483.47	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 18.9886(11) Å	α= 90°.
	b = 11.5022(6) Å	β= 110.398(2)°.
	c = 14.0085(6) Å	γ = 90°.
Volume	2867.8(3) $Å^3$	
Z	4	
Density (calculated)	1.120 Mg/m^3	
Absorption coefficient	0.063 mm^{-1}	
F(000)	1040	
Crystal size	0.300 x 0.240 x 0.150 mm^3	
Theta range for data collection	2.108 to 27.515°.	
Index ranges	-22<=h<=24, -14<=k<=14, -17<=l<=18	
Reflections collected	30803	
Independent reflections	6578 [R(int) = 0.1233]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6578 / 46 / 378	
Goodness-of-fit on F^2	1.011	
Final R indices [I>2sigma(I)]	R1 = 0.0608, wR2 = 0.1245	
R indices (all data)	R1 = 0.1329, wR2 = 0.1628	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.293 and -0.264 $e.Å^{-3}$	

Table S2 Crystal data and structure refinement for **3**.

Identification code	C:_0530ome_0m_a_sq	
Empirical formula	C41 H42 B N O	
Formula weight	575.56	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 14.8622(9) Å	α= 90°.
	b = 10.8648(7) Å	β= 93.551(2)°.
	c = 21.9339(10) Å	γ = 90°.
Volume	3535.0(4) $Å^3$	
Z	4	
Density (calculated)	1.081 Mg/m^3	
Absorption coefficient	0.063 mm^{-1}	
F(000)	1232	
Crystal size	0.230 x 0.120 x 0.100 mm^3	
Theta range for data collection	2.093 to 24.760°.	
Index ranges	-17<=h<=17, -12<=k<=12, -23<=l<=25	
Reflections collected	53077	
Independent reflections	6022 [R(int) = 0.1423]	
Completeness to theta = 24.760°	99.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6022 / 15 / 424	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0536, wR2 = 0.1204	
R indices (all data)	R1 = 0.0888, wR2 = 0.1483	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.297 and -0.228 e.$Å^{-3}$	

Table S3 Crystal data and structure refinement for **7**.

Empirical formula	C33 H34 B N S	
Formula weight	487.48	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 10.7821(6) Å	α= 90°.
	b = 22.6036(10) Å	β= 90°.
	c = 22.7200(13) Å	γ = 90°.
Volume	5537.2(5) $Å^3$	
Z	8	
Density (calculated)	1.170 Mg/m^3	
Absorption coefficient	0.139 mm^{-1}	
F(000)	2080	
Crystal size	0.180 x 0.140 x 0.100 mm^3	
Theta range for data collection	2.013 to 25.378°.	
Index ranges	-12<=h<=12, -27<=k<=26, -27<=l<=27	
Reflections collected	189664	
Independent reflections	5060 [R(int) = 0.0944]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5060 / 0 / 334	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I)]	R1 = 0.0478, wR2 = 0.1251	
R indices (all data)	R1 = 0.0554, wR2 = 0.1341	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.686 and -0.340 $e.Å^{-3}$	

Table S4 Crystal data and structure refinement for **8**.

Empirical formula	C34 H35 B Br N	
Formula weight	548.35	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 18.6908(5) Å	α= 90°.
	b = 11.6182(3) Å	β= 109.9070(10)°.
	c = 14.1142(4) Å	γ = 90°.
Volume	2881.81(14) $Å^3$	
Z	4	
Density (calculated)	1.264 Mg/m^3	
Absorption coefficient	1.449 mm^{-1}	
F(000)	1144	
Crystal size	0.250 x 0.160 x 0.140 mm^3	
Theta range for data collection	2.101 to 27.503°.	
Index ranges	-24<=h<=24, -13<=k<=15, -18<=l<=18	
Reflections collected	54434	
Independent reflections	6606 [R(int) = 0.0674]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6606 / 0 / 342	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R1 = 0.0394, wR2 = 0.0960	
R indices (all data)	R1 = 0.0480, wR2 = 0.1018	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.834 and -0.256 $e.Å^{-3}$	

Table S5 Crystal data and structure refinement for **9**.

Empirical formula	C41 H42 B N O	
Formula weight	575.56	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 14.8622(9) Å	α= 90°.
	b = 10.8648(7) Å	β= 93.551(2)°.
	c = 21.9339(10) Å	γ = 90°.
Volume	3535.0(4) $Å^3$	
Z	4	
Density (calculated)	1.081 Mg/m^3	
Absorption coefficient	0.063 mm^{-1}	
F(000)	1232	
Crystal size	0.230 x 0.120 x 0.100 mm^3	
Theta range for data collection	2.093 to 24.760°.	
Index ranges	-17<=h<=17, -12<=k<=12, -23<=l<=25	
Reflections collected	53077	
Independent reflections	6022 [R(int) = 0.1423]	
Completeness to theta = 24.760°	99.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6022 / 15 / 424	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0536, wR2 = 0.1204	
R indices (all data)	R1 = 0.0888, wR2 = 0.1483	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.297 and -0.228 $e.Å^{-3}$	

Table S6 Crystal data and structure refinement for **10**.

Empirical formula	C41 H39 B F3 N	
Formula weight	613.54	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 15.7996(5) Å	α= 90°.
	b = 11.0848(3) Å	β= 103.4970(10)°.
	c = 19.6140(6) Å	γ = 90°.
Volume	3340.23(17) $Å^3$	
Z	4	
Density (calculated)	1.220 Mg/m^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	1296	
Crystal size	0.250 x 0.170 x 0.070 mm^3	
Theta range for data collection	1.886 to 27.492°.	
Index ranges	-20<=h<=20, -14<=k<=12, -25<=l<=25	
Reflections collected	63998	
Independent reflections	7658 [R(int) = 0.0879]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7658 / 51 / 459	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0559, wR2 = 0.1374	
R indices (all data)	R1 = 0.0761, wR2 = 0.1571	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.414 and -0.435 $e.Å^{-3}$	

3. Photophysical properties

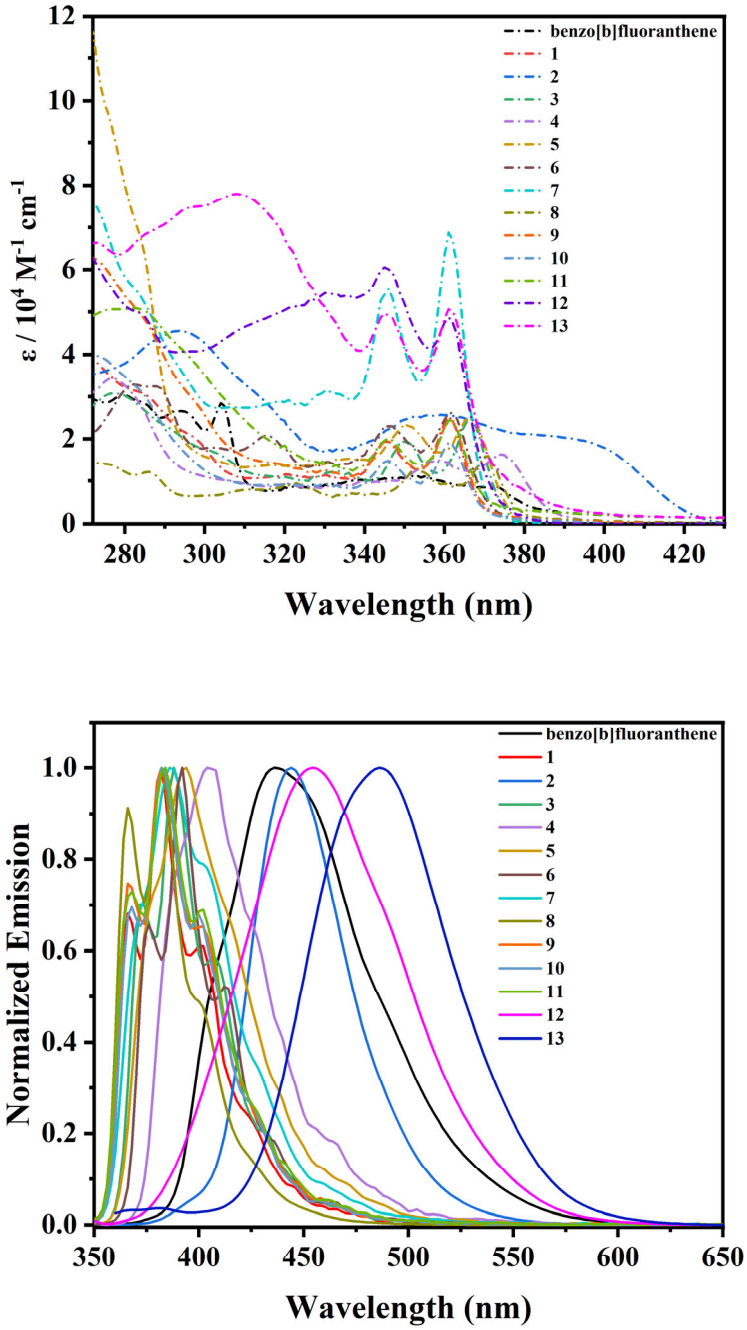


Fig. S2 UV-Vis absorption (top) and fluorescence (bottom) spectra of "*parental*" benzo[*b*]fluoranthene and **1**-**13** in dichloromethane at the concentration of 1×10^{-5} M.

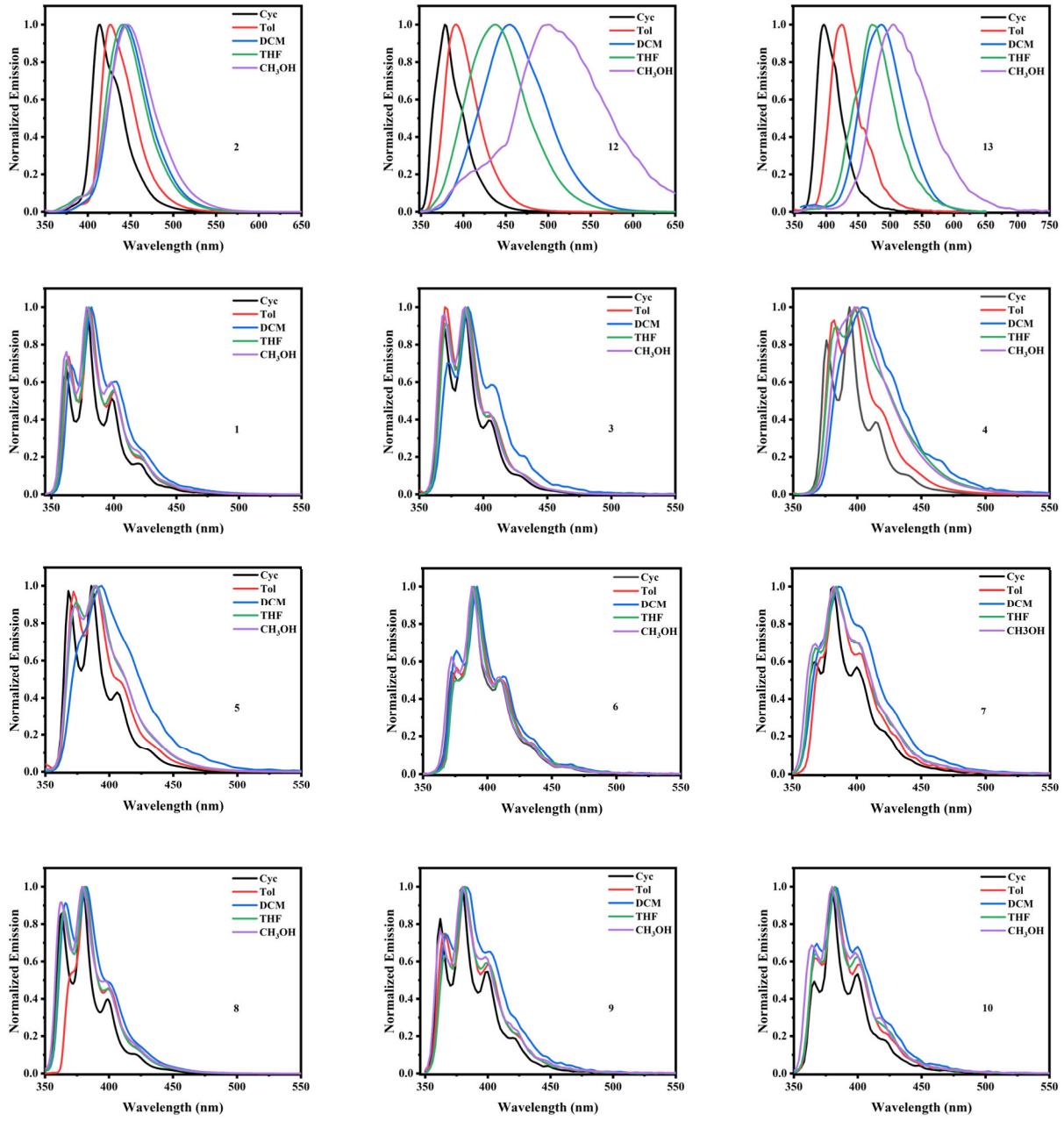


Fig. S3 Fluorescence spectra of **1-13** in various solvents at the concentration of 1×10^{-5} M. **2**, **12**, and **13** show noticeable solvatochromism and **1** and **3-13** show neglectable solvatochromism.

Table S7 Photophysical data for compounds **1**−**13**

Comp	λ_{abs}[a] nm	ε (M^{-1} cm^{-1})[b]	λ_{em} (λ_{ex})[c] nm	Lifetime[d] τ (ns)	Φ_{pl}[d] %
1	346, 361	25241 (361)	366, 382, 402 (343)	3.18	60.48
2	359, 391	20206 (391)	444 (347)	4.81	52.37
3	350, 366	24660 (366)	373, 388, 406 (347)	3.02	52.71
4	358, 374	16289 (374)	404 (346)	3.65	44.87
5	350, 366	24716 (366)	394 (346)	3.29	49.93
6	353, 371	15730 (371)	376, 392, 412 (346)	1.83	31.28
7	346, 361	25992 (361)	386, 402 (344)	1.64	25.51
8	346, 361	68761 (361)	366, 382 (343)	2.90	53.92
9	346, 361	24810 (361)	366, 382, 402 (343)	2.95	54.51
10	346, 361	19143 (361)	368, 382, 400 (343)	3.02	56.34
11	346, 361	24280 (361)	368, 384, 402 (343)	2.95	58.04
12	346, 361	48672 (361)	454 (343)	9.05	43.86
13	345, 361	50561 (361)	486 (343)	16.94	22.48

[a]Absorption (λ_{abs}) maxima measured in DCM. [b]Molar Absorption Coefficient ε = A/bc. [c]Emission maxima (λ_{em}) measured in DCM. [d]Measured in DCM at the concentration of 1×10^{-5} M.

4. Device performance

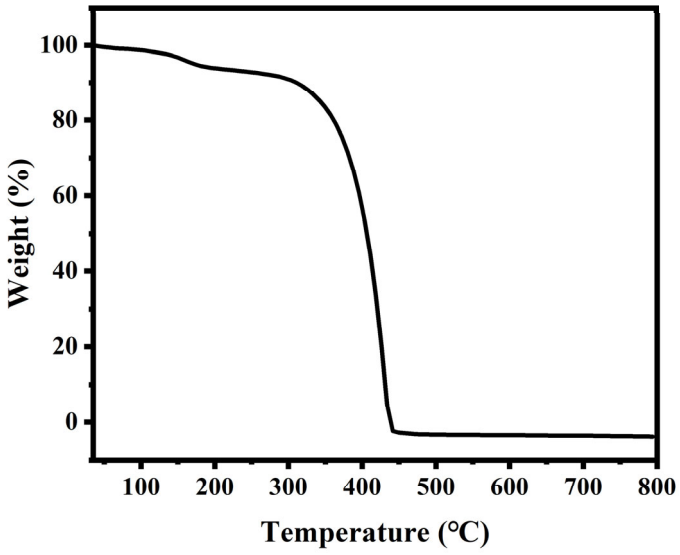


Fig. S4 The TG curve of **2**.

Table S8 EL performance of the OLEDs.

Device	Dopant	$V_{turn-on}$ (V)	Luminance L_{max}[a] (cd m-2)	η_{ext} (%)	η_L (cd A^{-1})	η_P (lm W^{-1})	λ_{max}[c] (nm)
A1	**2** (4.0 wt%)	4.5	964 (14)	1 (4.5)[a]	1.28 (4.5)	0.89 (4.5)	448
				0.94[b]	0.93	0.32	(0.19,0.12)
A2	**2** (6.0 wt%)	4	958 (14.5)	1.02 (4)[a]	1.76 (4)	1.39 (4)	448
				0.88[b]	0.95	0.33	(0.20,0.14)
A3	**2** (8.0 wt%)	4	950 (14)	0.86 (4)[a]	1.68 (4)	1.32 (4)	448
				0.74[b]	0.88	0.32	(0.23,0.16)

[a]Maximum values of the devices. Values in the parentheses are the voltage at which they were obtained. [b]Values were collected at *ca.* 100cd m^{-2}. [c]Values were collected at 8 V and CIE coordinates (x,y) are shown in parentheses.

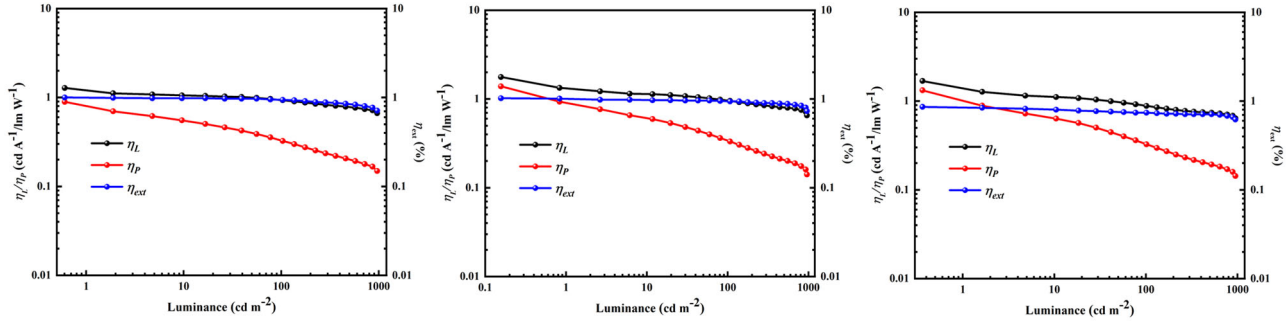


Fig. S5 Relationship between EL efficiencies and luminance for the devices with doping levels of 4 wt% (left), 6 wt% (middle), and 8 wt% (right).

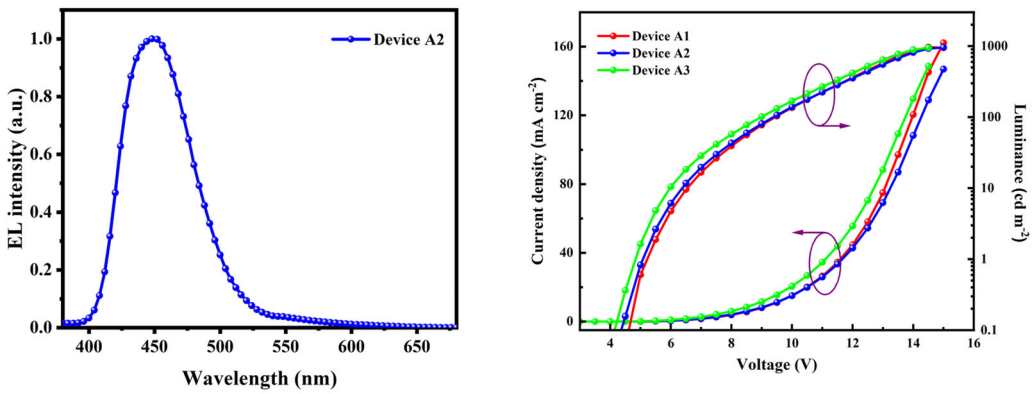


Fig. S6 EL spectrum for the device A2 and current density-voltage-luminance (*J-V-L*) characteristics for the OLEDs.

5. Computational details

All quantum chemical calculations were carried out using Gaussian 09.[S3] The geometries of all compounds were optimized by using the hybrid functional B3LYP with the 6-31G(d) basis set. In addition, frequency calculations are carried out at the same level of theory to confirm the stationary points are minima with no imaginary frequencies. Nucleus-independent chemical shifts (NICS) were calculated using the gauge invariant atomic orbital (GIAO) approach at the same level of theory. For excited singlet states, we employed time-dependent density functional theory (TD-DFT) at the same level of theory to predict absorption and emission frequencies in dichloromethane.

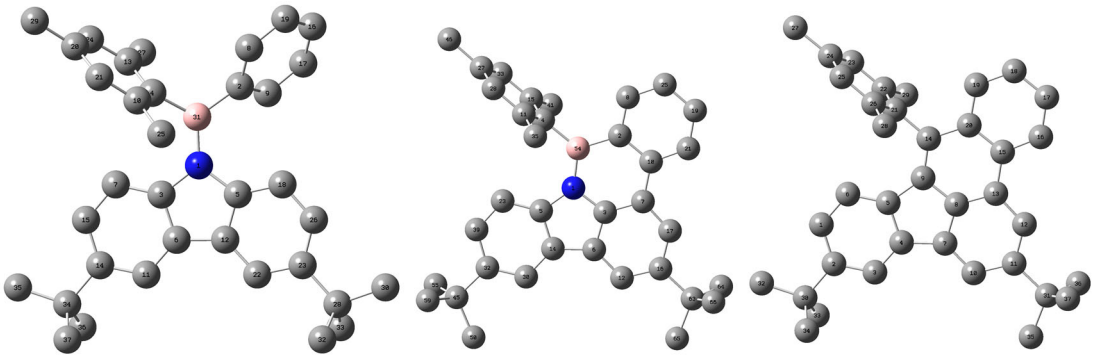


Fig. S7 Optimized structure of **1'** (left), **1** (middle), and **C-1** (right). (Hydrogen atoms were omitted for clarity)

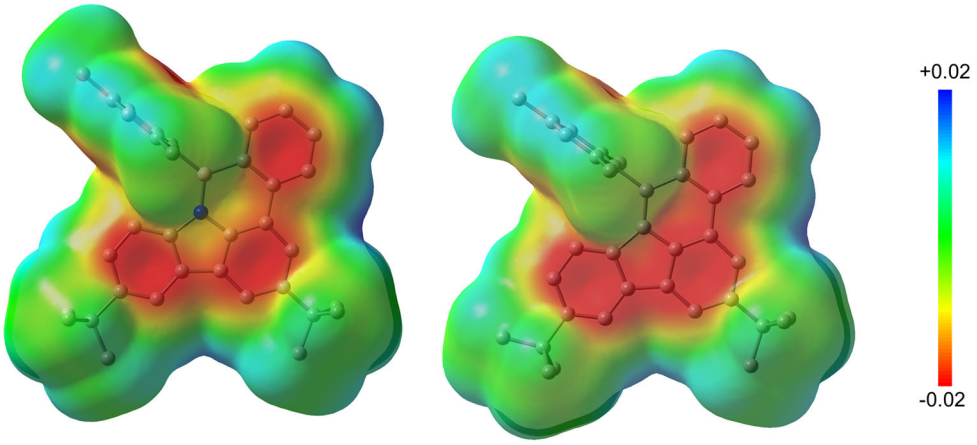


Fig. S8 Calculated electrostatic potential (ESP) distribution maps of **1** and **C-1**. Red colour being the electron-rich region and blue being the electron-deficient region.

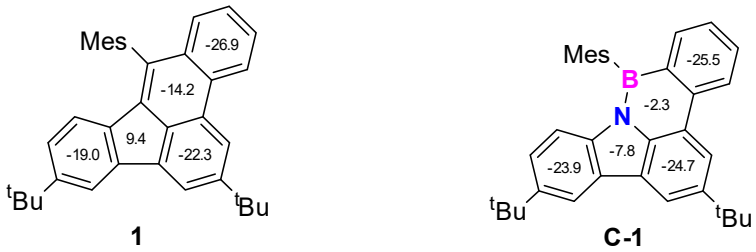


Fig. S9 Calculated NICS(1)$_{zz}$ values for **1** and **C-1**.

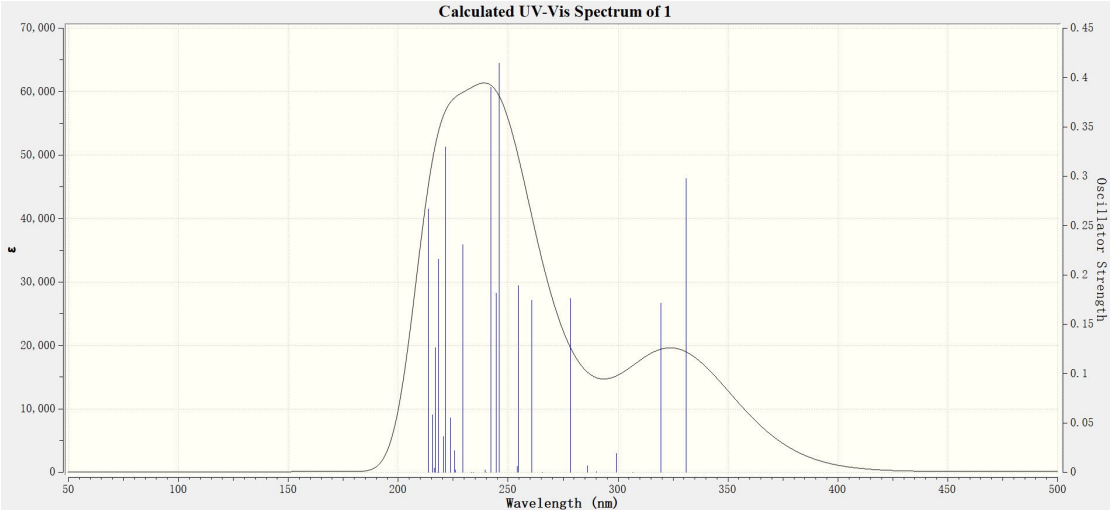


Fig. S10 Calculated UV-Vis spectrum of **1** at B_3LYP/6-31 G(d) level of theory. The solvent effect of DCM is accounted for by the CPCM solvation model.

Table S9 TDDFT description of first 5 electronically excited states in **1**

Excitation energies and oscillator strengths of the excited states with high oscillator strengths are marked in bold. The highest occupied molecular orbital of **1** is MO 130.

Excited State 1:	**Singlet-A**	**3.7472 eV**	**330.87 nm**	**f=0.2977**	**<S**2>=0.000**
129 ->131	**0.44302**				
130 ->131	**0.52473**				
Excited State 2:	**Singlet-A**	**3.8800 eV**	**319.54 nm**	**f=0.1714**	**<S**2>=0.000**
127 ->131	**-0.16181**				
129 ->131	**0.50650**				
130 ->131	**-0.43309**				
Excited State 3:	Singlet-A	4.0406 eV	306.85 nm	f=0.0000	<S**2>=0.000
128 ->131	0.69053				
128 ->132	-0.14177				
Excited State 4:	Singlet-A	4.1432 eV	299.25 nm	f=0.0192	<S**2>=0.000
126 ->131	-0.14530				
127 ->131	0.58425				
129 ->131	0.10642				
129 ->132	-0.31900				
Excited State 5:	Singlet-A	4.2698 eV	290.38 nm	f=0.0004	<S**2>=0.000
126 ->131	0.66636				
126 ->132	-0.10220				
127 ->131	0.19875				

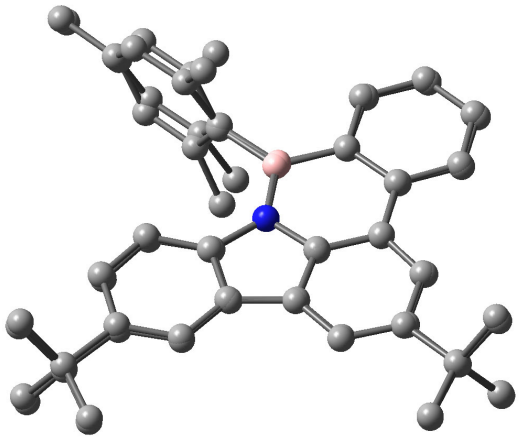


Fig. S11 The comparison of the optimized S_0 and S_1 structures for **1**, and the twisted angles between the mesityl groups and the B/N involved-rings are 101.8° (S_1) and 90.74° (S_0).

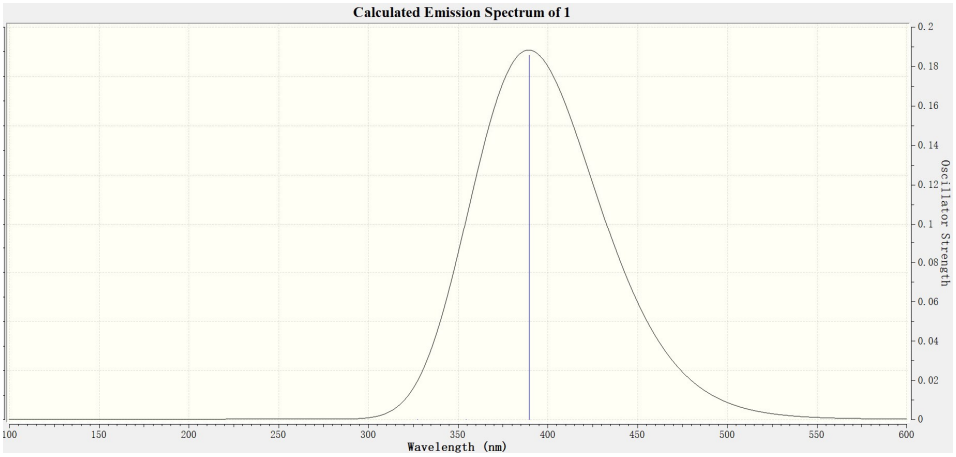


Fig. S12 Calculated emission spectrum from TDDFT excitations for **1**

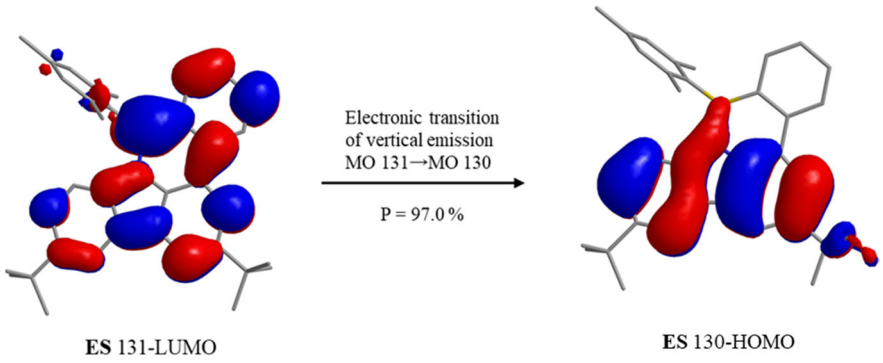


Fig. S13 The calculated orbitals HOMO and LUMO of the excited state (ES) most likely involved in the vertical transition of emission for compound **1** in DCM.

Output for TDDFT excitations for emission of **1**

The highest occupied molecular orbital of **1** is MO 130.

Excitation energies and oscillator strengths:

Excited State	**1:**	**Singlet-A**	**3.1832 eV**	**389.50 nm**	**f=0.1858**	**<S**2>=0.000**
130 ->131		**-0.69626**				
Excited State	2:	Singlet-A	3.4985 eV	354.39 nm	f=0.4821	<S**2>=0.000
129 ->131		-0.68907				
Excited State	3:	Singlet-A	3.7871 eV	327.38 nm	f=0.0345	<S**2>=0.000
128 ->131		0.69632				

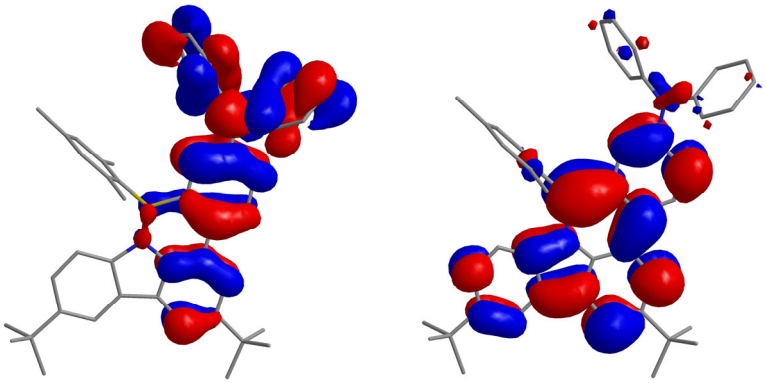


Fig. S14 The HOMO and LUMO orbitals for **2**.

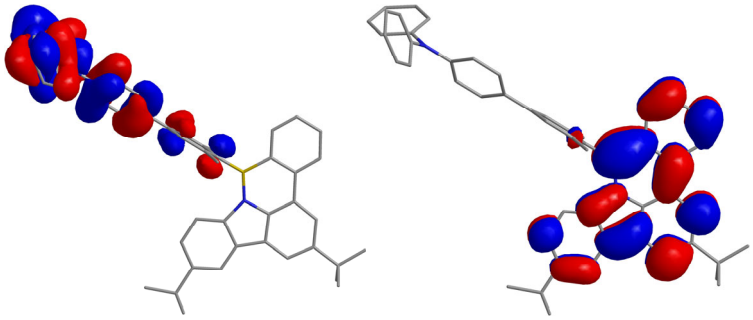


Fig. S15 The HOMO and LUMO orbitals for **12**.

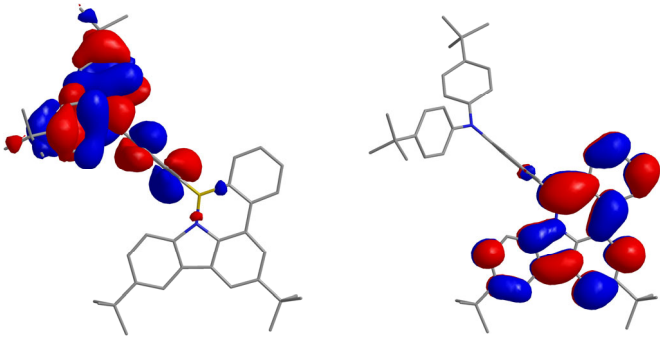


Fig. S16 The HOMO and LUMO orbitals for **13**.

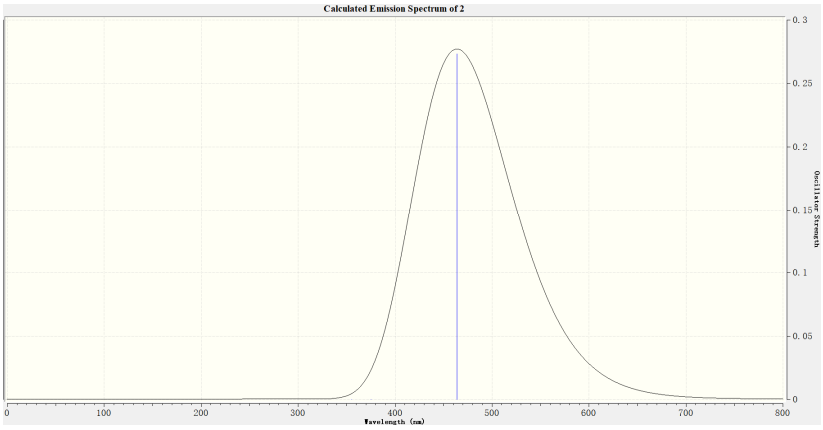


Fig. S17 Calculated emission spectrum from TDDFT excitations for **2**.

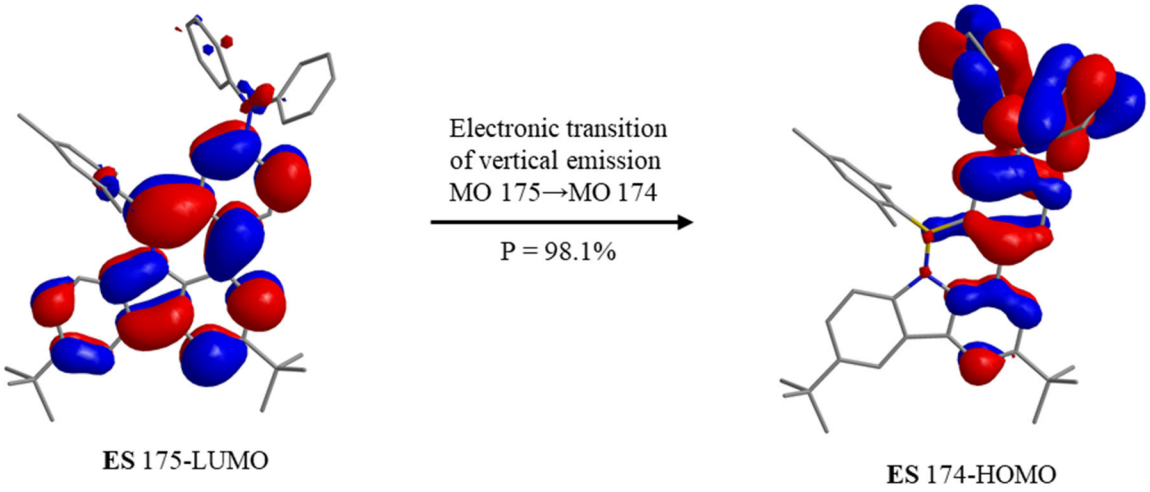


Fig. S18 The calculated orbitals HOMO and LUMO of the excited state (ES) most likely involved in the vertical transition of emission for compound **2** in DCM.

Output for TDDFT excitations for emission of **2**

The highest occupied molecular orbital of **2** is MO 174.

Excitation energies and oscillator strengths:

Excited State	**1:**	**Singlet-A**	**2.6717 eV**	**464.06 nm**	**f=0.2734**	**<S**2>=0.000**
174 ->175		**0.70021**				
Excited State	2:	Singlet-A	3.3062 eV	375.01 nm	f=0.2689	<S**2>=0.000
174 ->176		0.68817				
Excited State	3:	Singlet-A	3.4961 eV	354.63 nm	f=0.1201	<S**2>=0.000

172 ->175 -0.43271
173 ->175 0.53611

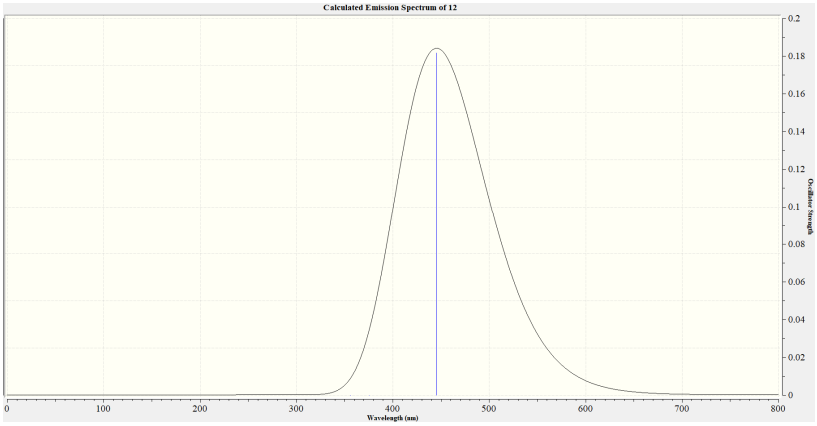


Fig. S19 Calculated emission spectrum from TDDFT excitations for **12**.

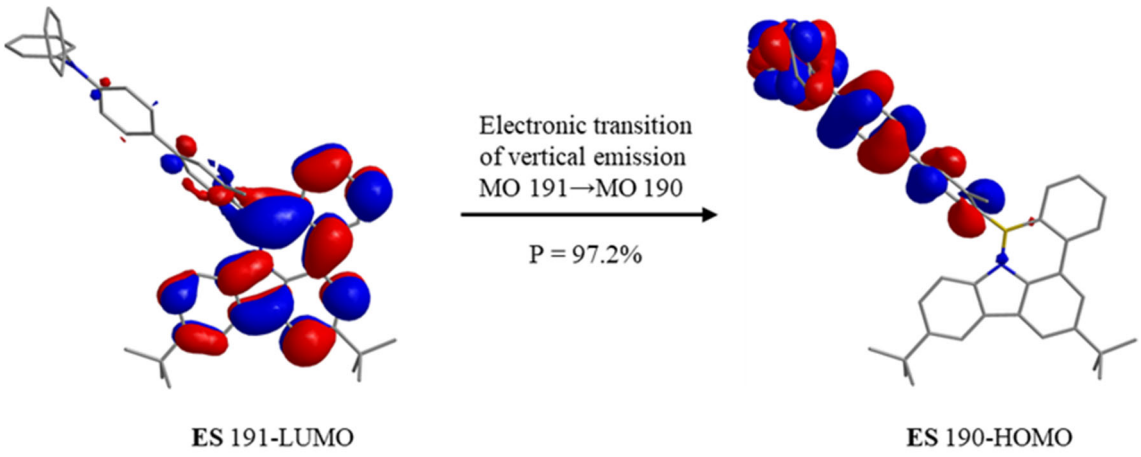


Fig. S20 The calculated orbitals HOMO and LUMO of the excited state (ES) most likely involved in the vertical transition of emission for compound **12** in DCM.

Output for TDDFT excitations for emission of **12**

The highest occupied molecular orbital of **12** is MO 190.

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.7819 eV 445.68 nm f=0.1817 <S2>=0.000**
190 ->191 -0.69696
Excited State 2: Singlet-A 3.2973 eV 376.02 nm f=1.1148 <S**2>=0.000
189 ->191 -0.11113

190 ->192	0.61703					
190 ->193	-0.30460					
Excited State 3:	Singlet-A	3.4856 eV	355.70 nm	f=0.4558	<S**2>=0.000	
188 ->191	-0.29779					
189 ->191	-0.61756					
190 ->192	-0.10751					

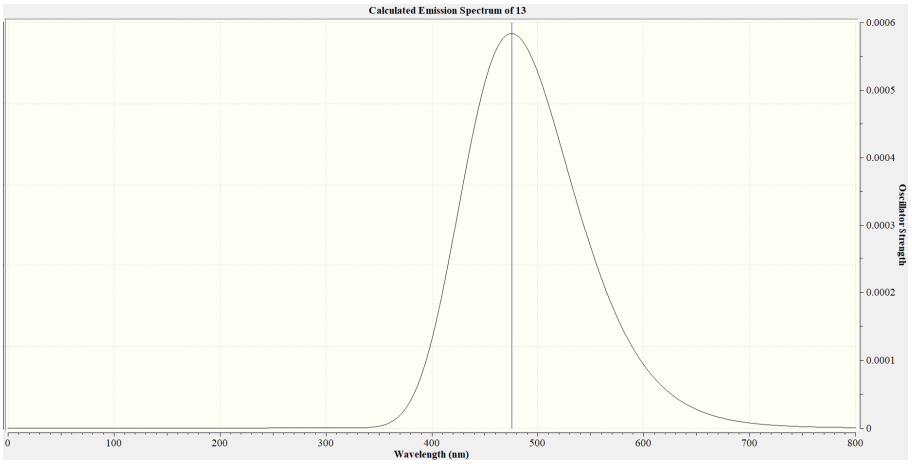


Fig. S21 The Calculated emission spectrum from TDDFT excitations for **13**.

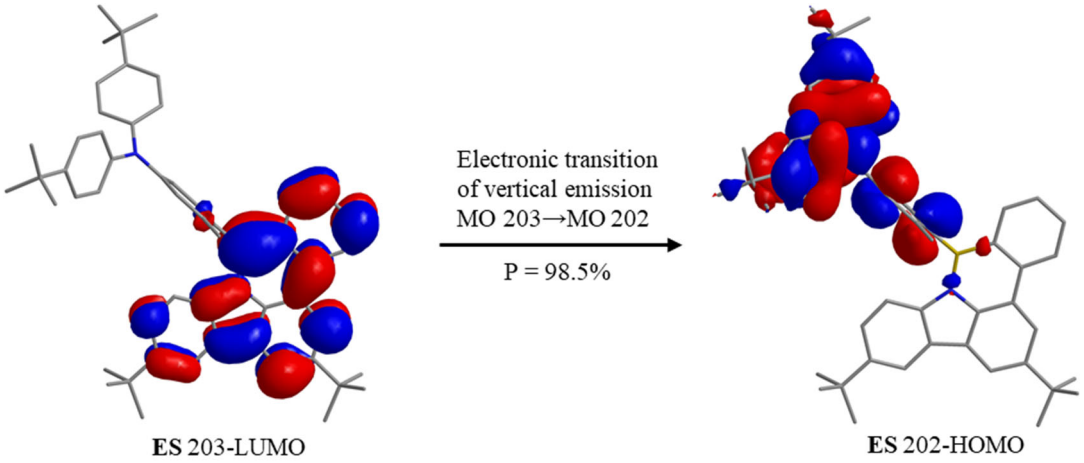


Fig. S22 The calculated orbitals HOMO and LUMO of excited state (ES) most likely involved in the vertical transition of emission for compound **13** in DCM.

Output for TDDFT excitations for emission of **13**

The highest occupied molecular orbital of **13** is MO 203.

Excited State 1:	**Singlet-A**	**2.6080 eV**	**475.40 nm**	**f=0.0006**	**<S**2>=0.000**
202 ->203	**0.70177**				
Excited State 2:	Singlet-A	3.3902 eV	365.71 nm	f=0.0027	<S**2>=0.000
202 ->204	0.70062				
Excited State 3:	Singlet-A	3.5057 eV	353.66 nm	f=0.3671	<S**2>=0.000
200 ->203	-0.67927				
201 ->203	0.10064				

Table S10 Cartesian Coordinates for **1'**-S_0 (ground state)

N	0.264025	-0.403595	-0.118980	C	-6.010346	-1.705064	-0.605676
C	1.708790	-2.546078	-0.612647	C	-1.581617	5.047742	-0.632021
C	0.011151	0.996241	-0.233890	C	-0.481114	6.105529	-0.840944
C	2.864856	-0.277502	0.294988	C	-2.539950	5.107507	-1.845299
C	-1.013594	-1.015745	0.061875	C	-2.361255	5.415404	0.652913
C	-1.377459	1.244446	-0.172136	H	1.960600	1.904999	-0.508818
C	0.891475	2.057023	-0.444406	H	3.232043	-3.026363	0.839872
C	2.648563	-3.397665	0.000965	H	0.276842	-2.421855	-2.227435
C	1.003968	-3.053823	-1.723854	H	-2.951538	2.698802	-0.250631
C	3.038584	0.079122	1.653799	H	1.072087	4.155892	-0.719437
C	-1.877578	2.540223	-0.301256	H	2.304132	-6.193004	-1.908967
C	-2.028943	-0.035608	0.028765	H	0.674519	-4.708697	-3.061876
C	3.913764	-0.003084	-0.616360	H	-0.592983	-3.111290	0.427276
C	-1.010620	3.623032	-0.496633	H	3.568931	-5.345559	0.057809
C	0.368041	3.346278	-0.564748	H	4.352184	0.942764	3.119043
C	2.139448	-5.180488	-1.549026	H	-4.124897	0.391626	0.183081
C	1.221981	-4.347370	-2.194982	H	5.869838	0.842349	-0.886375
C	-1.346836	-2.339637	0.346266	H	1.556636	-1.188800	2.635096
C	2.849671	-4.704321	-0.445413	H	2.330384	-0.006872	3.696447
C	5.265882	0.964620	1.174318	H	1.101665	0.510928	2.535233
C	4.231620	0.681813	2.068884	H	-2.925946	-3.704567	0.742933
C	-3.366361	-0.385880	0.217211	H	4.643026	0.020192	-2.654371
C	-3.727471	-1.716417	0.463337	H	3.701317	-1.422550	-2.246774
C	5.081373	0.621219	-0.168760	H	2.882507	0.112172	-2.528775
C	1.951303	-0.166863	2.681952	H	6.404482	2.180266	2.560019
C	-2.691328	-2.667477	0.531860	H	7.315227	0.836204	1.864670
C	3.779208	-0.341233	-2.087272	H	6.976077	2.263423	0.883761
C	-5.210273	-2.084487	0.663147	H	-6.480829	-3.800920	1.051424
C	6.554476	1.597587	1.644911	H	-5.054283	-4.199933	0.086080
C	-5.413195	-3.589531	0.922578	H	-4.899749	-3.920111	1.832633
B	1.557167	-1.049696	-0.147593	H	-6.836190	-1.555742	2.027080
C	-5.777984	-1.308819	1.875614	H	-5.705926	-0.225051	1.736183

H	-5.234433	-1.563711	2.792549	H	-2.961407	6.114882	-1.951589
H	-5.636469	-2.248257	-1.481129	H	-3.374887	4.406833	-1.739797
H	-7.071448	-1.953259	-0.478432	H	-2.012263	4.859769	-2.773414
H	-5.942574	-0.634189	-0.824457	H	-1.704390	5.390166	1.529897
H	-0.936275	7.098557	-0.929656	H	-2.781066	6.425721	0.570717
H	0.219398	6.137588	0.001268	H	-3.190365	4.724323	0.837975
H	0.092627	5.922738	-1.756653				

Table S11 Cartesian Coordinates for **1**-S_0 (ground state)

N	-0.237543	-0.320070	-0.000005	C	-4.840118	-0.896866	1.198151
C	-0.541251	-2.827625	-0.000021	H	-5.375815	-0.824538	2.143381
C	1.139793	-0.570559	-0.000016	C	-2.725377	-1.153409	-2.542527
C	-2.738916	-1.170004	0.000016	H	-3.427540	-1.150807	-3.382429
C	-0.384036	1.093766	0.000018	H	-2.116416	-2.062621	-2.618149
C	1.874007	0.626797	0.000007	H	-2.046220	-0.301464	-2.676504
C	1.739481	-1.834068	-0.000030	C	-1.389793	3.260989	0.000023
C	-1.368211	-3.970971	-0.000027	H	-2.292584	3.864889	0.000030
H	-2.446047	-3.831508	-0.000011	C	-2.725545	-1.154275	2.542544
C	0.872931	-3.019095	-0.000043	H	-2.045273	-0.303191	2.676278
C	-3.453125	-1.078179	-1.216070	H	-2.117764	-2.064265	2.618404
C	3.267518	0.578387	0.000020	H	-3.427693	-1.150545	3.382454
H	3.834549	1.502279	0.000045	C	-0.062590	5.440112	0.000059
C	0.891363	1.701255	0.000028	C	-7.057146	-0.644275	-0.000073
C	-3.453208	-1.078506	1.216070	H	-7.563490	-1.619170	-0.001000
C	3.922779	-0.664785	0.000001	H	-7.402338	-0.100287	-0.886049
C	3.145776	-1.837455	-0.000022	H	-7.402545	-0.101839	0.886767
H	3.659539	-2.792611	-0.000030	C	1.386763	5.962191	0.000058
C	0.546648	-5.430134	-0.000087	H	1.938768	5.633676	0.888103
H	0.970676	-6.431242	-0.000114	H	1.384306	7.058067	0.000046
C	1.391252	-4.327628	-0.000079	H	1.938772	5.633650	-0.887976
H	2.464667	-4.489394	-0.000102	B	-1.176987	-1.405051	0.000009
C	-1.538416	1.875503	0.000018	C	-0.769545	5.989198	1.262260
H	-2.524530	1.427755	0.000028	H	-1.821886	5.689498	1.303814
C	-0.843035	-5.256746	-0.000059	H	-0.734604	7.085645	1.273586
H	-1.502218	-6.120717	-0.000065	H	-0.282503	5.623843	2.173591
C	-5.554587	-0.806053	-0.000032	C	-0.769564	5.989287	-1.262089
C	-4.840037	-0.896550	-1.198194	H	-0.282556	5.623975	-2.173455
H	-5.375672	-0.823983	-2.143444	H	-0.734591	7.085734	-1.273350
C	1.011495	3.094431	0.000032	H	-1.821918	5.689631	-1.303640
H	2.001713	3.536639	0.000035	C	5.460993	-0.783776	0.000001
C	-0.130939	3.901191	0.000026	C	5.922610	-1.550321	1.262380

C	6.155196	0.591804	0.000065	H	5.896900	1.179771	0.888188
C	5.922604	-1.550210	-1.262450	H	5.896933	1.179839	-0.888022
H	7.015561	-1.644117	-1.274409	H	7.015568	-1.644224	1.274323
H	5.616401	-1.023827	-2.173665	H	5.502032	-2.560474	1.304351
H	5.502017	-2.560356	-1.304505	H	5.616413	-1.024021	2.173645
H	7.242522	0.455531	0.000078				

Table S12 Cartesian Coordinates for **1**-S_1 (first excited state)

N	-0.227257	-0.328238	0.020453	C	-2.556481	-0.642148	-2.516040
C	-0.582146	-2.840643	0.051599	H	-3.195222	-0.519318	-3.396946
C	1.116710	-0.584533	-0.000558	H	-1.909637	-1.512146	-2.680903
C	-2.763998	-1.172746	-0.033989	H	-1.898698	0.235546	-2.461899
C	-0.364841	1.071410	0.049075	C	-1.334585	3.257642	0.146261
C	1.885748	0.645219	-0.009886	H	-2.233787	3.863383	0.199212
C	1.719601	-1.871633	0.000502	C	-2.994489	-1.700804	2.450576
C	-1.389053	-4.022181	0.066710	H	-2.138549	-1.068673	2.716443
H	-2.470203	-3.903107	0.059385	H	-2.628554	-2.734682	2.439236
C	0.856020	-3.048139	0.038427	H	-3.737317	-1.617744	3.251156
C	-3.380830	-0.800363	-1.255206	C	-0.005048	5.442531	0.140726
C	3.298889	0.596129	-0.037034	C	-7.066654	-0.480612	-0.262295
H	3.868191	1.516443	-0.044472	H	-7.595232	-1.411929	-0.507802
C	0.932491	1.686125	0.021791	H	-7.322380	0.248799	-1.038620
C	-3.586293	-1.306897	1.112165	H	-7.472426	-0.121700	0.689875
C	3.917529	-0.643516	-0.051589	C	1.443444	5.963552	0.092811
C	3.112673	-1.846300	-0.031285	H	2.030402	5.616580	0.950948
H	3.641645	-2.791777	-0.038756	H	1.439718	7.058686	0.116487
C	0.554740	-5.470428	0.082290	H	1.958179	5.654493	-0.824171
H	0.984360	-6.467975	0.096479	B	-1.210852	-1.465913	0.027814
C	1.379885	-4.354051	0.054787	C	-0.662132	5.958181	1.443693
H	2.456581	-4.505228	0.047130	H	-1.710928	5.652881	1.523491
C	-1.500229	1.863970	0.120328	H	-0.632302	7.053813	1.473485
H	-2.492443	1.432488	0.158212	H	-0.133141	5.579173	2.325625
C	-0.851720	-5.292497	0.086598	C	-0.766086	6.014743	-1.079466
H	-1.506383	-6.161044	0.101716	H	-0.312933	5.675457	-2.017996
C	-5.573630	-0.701470	-0.179572	H	-0.735443	7.110646	-1.063292
C	-4.760428	-0.571278	-1.310190	H	-1.818859	5.712659	-1.085613
H	-5.212809	-0.288869	-2.259863	C	5.441847	-0.803058	-0.085559
C	1.060089	3.099598	0.047182	C	5.905075	-1.584740	1.170474
H	2.054119	3.531145	0.020759	C	6.174089	0.551627	-0.104962
C	-0.068252	3.905852	0.108828	C	5.846949	-1.589509	-1.358583
C	-4.963302	-1.067634	1.024327	H	6.935838	-1.713952	-1.385085
H	-5.575185	-1.165122	1.920048	H	5.543072	-1.051280	-2.263354

H	5.397437	-2.586923	-1.391896	H	6.994166	-1.708252	1.147848
H	7.255734	0.381578	-0.130969	H	5.458507	-2.582361	1.227632
H	5.953578	1.146497	0.788338	H	5.642167	-1.043575	2.086260
H	5.910299	1.144242	-0.987984				

Table S13 Cartesian Coordinates for **C-1**-S_0 (ground state)

C	-3.670090	1.748045	-3.075971	C	2.173450	-5.169722	-2.293523
C	-4.134407	3.177932	-2.832327	H	-4.534909	3.266557	-1.797671
C	-4.846724	0.796602	-2.903296	H	-4.932231	3.438032	-3.563486
C	-3.121240	1.626987	-4.491470	H	-3.275203	3.874117	-2.958280
C	0.773262	-4.932691	-1.743234	H	-5.247039	0.885851	-1.868622
C	-0.237342	-5.001787	-2.880527	H	-5.644361	1.057325	-3.634437
C	0.445623	-6.000948	-0.708339	H	-4.508451	-0.248725	-3.081150
C	-2.188240	2.349147	-1.150480	H	-3.713580	0.872219	-5.055587
C	-2.596900	1.396820	-2.093163	H	-2.055765	1.307952	-4.449651
C	-2.018954	0.122438	-2.131894	H	-3.192986	2.612694	-5.003333
C	-1.022163	-0.172277	-1.202471	H	-1.260523	-4.827926	-2.478479
C	-0.611945	0.787967	-0.253557	H	-0.190755	-6.006571	-3.356981
C	-1.188308	2.056223	-0.216607	H	0.001213	-4.221445	-3.637446
C	-0.242046	-1.391743	-0.991907	H	-0.577737	-5.826825	-0.306861
C	0.628057	-1.136482	0.089295	H	0.492031	-7.005470	-1.185362
C	0.435598	0.197004	0.577378	H	1.183644	-5.951312	0.123305
C	-0.207731	-2.630960	-1.604294	H	-2.660736	3.342480	-1.144365
C	0.711694	-3.581655	-1.101424	H	-2.341349	-0.623776	-2.872992
C	1.561318	-3.309010	-0.032713	H	-0.867144	2.803760	0.523692
C	1.543978	-2.045141	0.611061	H	-0.869811	-2.868606	-2.449973
C	1.182052	0.646644	1.624916	H	2.256845	-4.085751	0.317880
C	1.021867	1.886749	2.098253	H	3.469590	-3.419578	1.993678
C	2.343428	-1.571600	1.730312	H	4.811088	-2.580434	3.895109
C	3.312441	-2.393617	2.357967	H	4.473465	-0.244748	4.745431
C	4.064092	-1.926249	3.421781	H	2.791593	1.229344	3.681553
C	3.874948	-0.614852	3.899972	H	2.820155	4.704606	2.787676
C	2.935397	0.206094	3.304355	H	-1.409603	3.970372	3.279898
C	2.154610	-0.253819	2.213428	H	4.169106	2.311031	2.666936
C	2.120716	2.738859	2.207482	H	3.866907	2.916028	0.979326
C	1.953578	4.032590	2.701424	H	3.411949	1.215471	1.430221
C	0.687623	4.474149	3.085979	H	0.100968	5.814817	4.650742
C	-0.411229	3.622093	2.976667	H	-0.199981	6.419903	2.962941
C	-0.244088	2.328308	2.482808	H	1.490754	6.385492	3.628085
C	3.479384	2.264963	1.794623	H	-1.253554	0.507738	2.989307
C	0.508290	5.862625	3.616057	H	-1.555115	1.113577	1.301886
C	-1.423408	1.413727	2.365527	H	-2.338449	1.940334	2.717882

H	2.117493	-5.335727	-3.392650	H	2.616966	-6.066162	-1.805201
H	2.808922	-4.280055	-2.085107				

Table S14 Cartesian Coordinates for **2**-S_0 (ground state)

N	1.609564	-0.150797	0.033904	H	4.846382	-3.489025	0.381974
C	-0.852418	0.410969	-0.051547	C	-0.054433	-2.472399	-2.285602
C	1.843919	1.223768	-0.097791	H	0.950587	-2.064105	-2.452052
C	-0.036809	-2.204865	0.242620	H	-0.765858	-1.656921	-2.466032
C	2.889419	-0.765785	0.105157	H	-0.229532	-3.240998	-3.045214
C	3.218925	1.506530	-0.111408	C	7.086146	-1.932778	0.251632
C	0.859013	2.211705	-0.201382	C	-0.984345	-6.423909	0.714672
C	-2.203276	0.016451	-0.024273	H	-2.072423	-6.574841	0.717452
H	-2.438992	-1.037823	0.083545	H	-0.599415	-6.826116	1.658078
C	-0.546430	1.798436	-0.178798	H	-0.576727	-7.028330	-0.103106
C	-0.177670	-2.771482	1.529549	C	8.069827	-0.752345	0.141673
C	3.648100	2.828013	-0.232774	H	7.953881	-0.211547	-0.804559
H	4.709725	3.046817	-0.242993	H	9.099595	-1.124754	0.184735
C	3.894534	0.223208	0.018481	H	7.942991	-0.037668	0.962886
C	-0.202146	-3.036874	-0.887760	B	0.270508	-0.664916	0.074803
C	2.701598	3.861275	-0.339132	C	7.371729	-2.904595	-0.918193
C	1.334380	3.530265	-0.320570	H	6.732736	-3.792808	-0.876580
H	0.610697	4.334195	-0.401496	H	8.414919	-3.242893	-0.888162
C	-2.928556	2.301436	-0.265173	H	7.200409	-2.415423	-1.883901
H	-3.727838	3.030093	-0.358602	C	7.352910	-2.655411	1.593654
C	-1.607619	2.717975	-0.278919	H	7.167907	-1.986323	2.441781
H	-1.403329	3.778813	-0.386309	H	8.395902	-2.991561	1.646241
C	3.232211	-2.110768	0.236575	H	6.713044	-3.535279	1.717676
H	2.476068	-2.883147	0.303144	C	3.113072	5.342131	-0.474167
C	-3.249366	0.935841	-0.134169	C	2.560398	5.916029	-1.800608
C	-0.634373	-4.962938	0.551462	C	4.642708	5.527436	-0.478191
C	-0.470299	-4.132779	1.663964	C	2.538514	6.151159	0.713084
H	-0.572687	-4.555210	2.662323	H	2.821662	7.207697	0.628692
C	5.245437	-0.134895	0.064073	H	2.921655	5.771428	1.667119
H	5.997802	0.643127	-0.004621	H	1.445238	6.102207	0.750497
C	5.615732	-1.477142	0.195755	H	4.884555	6.591764	-0.576252
C	-0.492427	-4.394403	-0.717806	H	5.115468	5.003483	-1.316730
H	-0.612847	-5.023272	-1.598486	H	5.099919	5.170000	0.451523
C	0.007382	-1.920514	2.769058	H	2.844197	6.970202	-1.908971
H	-0.227229	-2.484650	3.677466	H	1.467817	5.859803	-1.846976
H	-0.638005	-1.033727	2.749968	H	2.958921	5.366279	-2.660918
H	1.041091	-1.562374	2.859744	N	-4.604847	0.512549	-0.123373
C	4.585654	-2.439609	0.279467	C	-5.573456	1.248961	0.610467

C	-6.854898	1.471530	0.079534	C	-5.875704	-1.581805	-0.276468
C	-5.264159	1.768916	1.878196	C	-4.494162	-0.885623	-2.136710
C	-7.802370	2.189515	0.806317	C	-6.259825	-2.714006	-0.992551
H	-7.100613	1.079123	-0.902047	H	-6.257671	-1.411296	0.725040
C	-6.212877	2.501643	2.589038	C	-4.869664	-2.029899	-2.837633
H	-4.279934	1.593240	2.300627	H	-3.816335	-0.166185	-2.585223
C	-7.488543	2.713727	2.062264	C	-5.757451	-2.948877	-2.274051
H	-8.788617	2.351556	0.379001	H	-6.945376	-3.423961	-0.537105
H	-5.955028	2.895675	3.568721	H	-4.475767	-2.194784	-3.837173
H	-8.227832	3.279008	2.622487	H	-6.053280	-3.836453	-2.826038
C	-4.990565	-0.651670	-0.844169				

Table S15 Cartesian Coordinates for **2**-S_1 (first excited state)

N	1.600701	-0.169612	0.033479	C	5.234468	-0.145070	0.059683
C	-0.855884	0.367623	-0.048880	H	5.988214	0.632327	-0.011400
C	1.828334	1.205174	-0.103179	C	5.604607	-1.483925	0.192018
C	-0.069739	-2.238293	0.256223	C	-0.553542	-4.440676	-0.681788
C	2.865719	-0.774461	0.104796	H	-0.695268	-5.073503	-1.556920
C	3.207359	1.492747	-0.117368	C	0.058002	-1.962858	2.782160
C	0.834412	2.201291	-0.212343	H	-0.164426	-2.522432	3.696957
C	-2.230746	0.009529	-0.029167	H	-0.565343	-1.061017	2.772491
H	-2.496039	-1.037775	0.088820	H	1.100447	-1.624334	2.844905
C	-0.554827	1.791771	-0.186117	C	4.570157	-2.452460	0.277830
C	-0.171251	-2.809884	1.547037	H	4.832477	-3.501790	0.380432
C	3.639970	2.827847	-0.243888	C	-0.153790	-2.531227	-2.270009
H	4.701828	3.045190	-0.254759	H	0.839390	-2.102393	-2.453677
C	3.879150	0.221383	0.014742	H	-0.880200	-1.729037	-2.447139
C	-0.266924	-3.081866	-0.862791	H	-0.323785	-3.312820	-3.018175
C	2.691988	3.854073	-0.353465	C	7.074435	-1.941919	0.247449
C	1.320156	3.528214	-0.336734	C	-1.002151	-6.468663	0.770957
H	0.599905	4.334420	-0.422365	H	-2.088892	-6.621919	0.823125
C	-2.942848	2.342098	-0.255883	H	-0.575548	-6.870730	1.696398
H	-3.741406	3.065543	-0.374953	H	-0.631880	-7.072374	-0.064893
C	-1.614722	2.721563	-0.291956	C	8.060860	-0.763945	0.135214
H	-1.389726	3.776655	-0.417880	H	7.943893	-0.223729	-0.811241
C	3.219483	-2.122503	0.236409	H	9.090027	-1.138689	0.178120
H	2.464057	-2.896455	0.303605	H	7.934552	-0.047467	0.954945
C	-3.241122	0.948796	-0.133788	B	0.228900	-0.688996	0.075562
C	-0.659361	-5.006984	0.592581	C	7.360445	-2.917017	-0.919919
C	-0.461078	-4.171806	1.696559	H	6.717807	-3.802775	-0.877938
H	-0.531183	-4.591700	2.699161	H	8.402616	-3.258878	-0.887225

H	7.193768	-2.427632	-1.886720	C	-5.065310	1.675826	1.972315
C	7.343628	-2.664436	1.589404	C	-7.738962	2.017521	1.203200
H	7.165247	-1.992360	2.437045	H	-7.201262	1.016955	-0.622816
H	8.385491	-3.005208	1.639177	C	-5.955198	2.328843	2.815471
H	6.699686	-3.541124	1.716234	H	-4.036268	1.514321	2.269559
C	3.103278	5.335593	-0.492373	C	-7.291681	2.503249	2.438879
C	2.552131	5.907915	-1.820288	H	-8.769683	2.169369	0.898862
C	4.632547	5.524718	-0.494999	H	-5.607700	2.696753	3.775705
C	2.526471	6.149573	0.690645	H	-7.980213	3.018787	3.100916
H	2.808781	7.206315	0.602491	C	-5.018001	-0.514262	-0.972871
H	2.911053	5.774160	1.646272	C	-5.981353	-1.452286	-0.541352
H	1.433345	6.097651	0.726799	C	-4.440318	-0.641637	-2.255018
H	4.872221	6.589602	-0.595500	C	-6.360276	-2.488198	-1.386101
H	5.106580	4.997682	-1.330821	H	-6.390681	-1.381734	0.459963
H	5.088528	5.168536	0.435742	C	-4.838191	-1.677104	-3.089516
H	2.834323	6.962744	-1.929290	H	-3.712638	0.089378	-2.586751
H	1.459882	5.847767	-1.868212	C	-5.796193	-2.605133	-2.661328
H	2.955592	5.358349	-2.678961	H	-7.086246	-3.218223	-1.042262
N	-4.611156	0.531270	-0.125989	H	-4.405967	-1.758894	-4.081735
C	-5.517227	1.173459	0.731236	H	-6.096417	-3.417364	-3.315794
C	-6.865280	1.358343	0.349558				

Table S16 Cartesian Coordinates for **12**-S_0 (ground state)

N	-3.415944	-0.330798	0.009462	C	-4.677962	3.074370	-0.080589
C	1.189706	-0.924571	-1.175270	H	-5.669394	3.519002	-0.093720
H	1.725640	-0.910267	-2.121171	C	-6.795748	-1.866956	0.043956
C	1.908981	-0.798756	0.022427	H	-7.296492	-2.825974	0.067741
C	-4.513450	-3.032149	0.078208	C	3.379095	-0.606466	0.017416
C	-5.533960	0.606845	-0.017856	C	-7.574952	-0.702193	0.012429
C	-5.384678	-1.852082	0.046067	C	-4.555823	1.686611	-0.044357
C	-4.792146	-0.588683	0.014297	C	-6.922361	0.547541	-0.018671
C	-3.275110	1.084177	-0.026811	H	-7.501587	1.466100	-0.043439
C	-5.025864	-4.343044	0.112469	C	1.189705	-0.863347	1.224948
H	-6.098445	-4.509860	0.115917	H	1.717749	-0.741098	2.167504
C	-2.127685	1.869746	-0.045068	C	-3.099639	-2.834965	0.074491
H	-1.139080	1.427763	-0.031766	C	-4.176411	-5.441103	0.142408
C	-0.195690	-1.106121	-1.186145	H	-4.596011	-6.443732	0.168579
C	-0.910552	-1.167935	0.031837	C	5.391759	0.348808	-0.981790
C	-2.278801	3.259186	-0.081412	H	5.850660	0.963669	-1.749488
H	-1.376186	3.859069	-0.095243	C	-0.195367	-1.046367	1.245126

C	-3.536578	3.890429	-0.100066	C	-4.478176	5.893370	1.108965
C	4.014407	0.157825	-0.976856	C	-4.475980	5.827178	-1.414076
H	3.414064	0.646372	-1.739306	C	-2.340869	6.155646	-0.158470
C	-2.267673	-3.974559	0.105533	H	-4.605957	6.982831	1.092419
H	-1.190345	-3.830992	0.102910	H	-3.944220	5.627416	2.028375
C	4.196510	-1.180438	1.006722	H	-5.474752	5.442307	1.160115
H	3.747525	-1.806836	1.772485	H	-2.508159	7.238305	-0.187332
C	6.197971	-0.237090	0.007772	H	-1.744727	5.890572	-1.039031
C	-2.787219	-5.261906	0.139052	H	-1.746398	5.937622	0.736006
H	-2.124383	-6.122731	0.162488	H	-4.604198	6.915957	-1.454692
C	-0.922110	-1.229792	-2.509641	H	-5.472312	5.373615	-1.443522
H	-1.610024	-0.389223	-2.668061	H	-3.940170	5.513820	-2.317336
H	-1.521479	-2.147110	-2.557411	N	7.605278	-0.052628	0.003161
H	-0.219956	-1.244849	-3.349316	C	8.299394	0.162084	1.225591
C	5.576566	-1.010098	1.002143	C	7.767513	1.012676	2.208428
H	6.183557	-1.485483	1.766062	C	9.528427	-0.472522	1.468532
C	-9.116781	-0.743288	0.010547	C	8.447760	1.213049	3.408038
C	-0.923893	-1.086164	2.572670	H	6.821690	1.512493	2.025150
H	-0.222916	-1.051361	3.412737	C	10.209981	-0.251425	2.663770
H	-1.524769	-1.998091	2.675089	H	9.942904	-1.136503	0.716640
H	-1.610626	-0.236549	2.678895	C	9.674092	0.587608	3.643104
C	-3.695917	5.422802	-0.140400	H	8.020938	1.875060	4.157084
C	-9.672185	-2.179857	0.046332	H	11.159964	-0.751335	2.834414
H	10.767618	-2.150580	0.043563	H	10.204819	0.751858	4.576561
H	-9.359776	-2.716770	0.949298	C	8.323534	-0.081228	-1.223799
H	-9.356541	-2.762212	-0.826858	C	9.346265	0.848415	-1.473026
B	-2.471750	-1.410612	0.037824	C	8.022355	-1.039890	-2.204952
C	-9.653963	0.006646	1.252983	C	10.054173	0.810464	-2.672776
H	10.750842	-0.006435	1.262930	H	9.580583	1.596592	-0.722483
H	-9.334264	1.053868	1.268373	C	8.723639	-1.058102	-3.409044
H	-9.299650	-0.463592	2.177372	H	7.238385	-1.766525	-2.016891
C	-9.649099	-0.058055	-1.270735	C	9.746125	-0.138006	-3.650402
H	-9.291490	-0.575155	-2.168447	H	10.842389	1.538084	-2.848244
H	-9.328927	0.986941	-1.338642	H	8.476907	-1.807573	-4.156649
H	10.745939	-0.071430	-1.284119	H	10.295367	-0.159905	-4.587335

Table S17 Cartesian Coordinates for **12**-S_1 (first excited state)

N	3.418999	-0.320703	-0.082018	H	-1.611587	-0.189641	2.034454
C	-1.140144	-0.511388	1.110564	C	-1.939492	-0.791760	-0.020950

C	4.498211	-3.029398	0.107136	C	-5.611610	-1.113092	-0.871302
C	5.546792	0.603969	0.010541	H	-6.240134	-1.689972	-1.539092
C	5.371439	-1.864976	0.125145	C	9.115778	-0.769719	0.336492
C	4.792689	-0.587987	0.025895	C	0.730913	-1.925474	-2.508834
C	3.296127	1.071223	-0.192984	H	0.007263	-1.933706	-3.330591
C	5.002881	-4.345245	0.198475	H	1.132288	-2.939572	-2.400623
H	6.075833	-4.501960	0.277313	H	1.572334	-1.284943	-2.796741
C	2.164906	1.873168	-0.369168	C	3.763551	5.414456	-0.477579
H	1.174319	1.439114	-0.443574	C	9.654592	-2.208654	0.454205
C	0.237525	-0.696178	1.096650	H	10.747996	-2.187235	0.531998
C	0.893228	-1.168582	-0.077482	H	9.396453	-2.813863	-0.422217
C	2.325114	3.256115	-0.458260	H	9.268694	-2.717083	1.345077
H	1.433207	3.857539	-0.594399	B	2.460397	-1.433935	-0.078323
C	4.715978	3.067515	-0.220811	C	9.752208	-0.127775	-0.919418
H	5.708353	3.509548	-0.168180	H	10.847504	-0.154653	-0.852899
C	6.788354	-1.878354	0.228851	H	9.449771	0.917789	-1.038673
H	7.281979	-2.837496	0.313190	H	9.454119	-0.667422	-1.826184
C	-3.385657	-0.599697	0.006948	C	9.573907	0.010926	1.591582
C	7.575971	-0.711206	0.224013	H	9.148490	-0.429517	2.501165
C	4.590098	1.675298	-0.129831	H	9.264037	1.060392	1.552540
C	6.949618	0.539459	0.110966	H	10.667534	-0.012927	1.682340
H	7.534875	1.454413	0.096990	C	4.662119	5.764504	-1.687769
C	-1.285384	-1.264451	-1.180413	C	4.427642	5.944465	0.815731
H	-1.860795	-1.447163	-2.083062	C	2.420824	6.149273	-0.656133
C	3.060959	-2.823659	0.000350	H	4.800409	6.850654	-1.763332
C	4.171750	-5.454397	0.190405	H	4.210997	5.413723	-2.623481
H	4.593180	-6.453879	0.260635	H	5.653449	5.307023	-1.602857
C	-5.365237	0.472594	0.966504	H	2.596515	7.229696	-0.715721
H	-5.795578	1.190139	1.654708	H	1.742720	5.970003	0.186161
C	0.093297	-1.447106	-1.222591	H	1.908897	5.845977	-1.576636
C	3.591574	3.884557	-0.382586	H	4.565563	7.031881	0.760314
C	-4.001317	0.287821	0.931462	H	5.410626	5.491161	0.981872
H	-3.384311	0.878489	1.598159	H	3.805937	5.725273	1.691862
C	2.245856	-3.999861	0.014888	N	-7.582782	-0.040554	0.087268
H	1.165517	-3.877807	-0.037086	C	-8.365177	-0.205737	-1.095180
C	-4.246522	-1.291358	-0.888706	C	-7.942015	0.373031	-2.302566
H	-3.831114	-2.019714	-1.575040	C	-9.565976	-0.930666	-1.038380
C	-6.208452	-0.224216	0.061304	C	-8.717000	0.214101	-3.448449
C	2.767498	-5.272951	0.097860	H	-7.028633	0.957644	-2.330674
H	2.106814	-6.137396	0.099529	C	-10.330486	-1.081828	-2.191407
C	1.034277	-0.406005	2.348170	H	-9.880130	-1.382221	-0.103591
H	1.696976	0.455581	2.202841	C	-9.909888	-0.512558	-3.397752
H	1.673648	-1.256475	2.611959	H	-8.393897	0.670397	-4.378876
H	0.378753	-0.187566	3.197248	H	-11.252977	-1.652446	-2.149563

H	-10.511484	-0.632143	-4.293440	C	-8.612220	-0.006440	3.663716
C	-8.250145	0.318186	1.296967	H	-7.219393	-1.159950	2.487834
C	-9.220780	1.332229	1.280946	C	-9.574625	1.007095	3.653456
C	-7.948607	-0.356804	2.490809	H	-10.618026	2.464686	2.450153
C	-9.875985	1.672459	2.460671	H	-8.385529	-0.535834	4.583854
H	-9.440073	1.854939	0.356207	H	-10.090640	1.275472	4.570085

Table S18 Cartesian Coordinates for **13**-S_0 (ground state)

N	-3.016524	-0.369548	0.092018	C	-3.399753	3.387631	-1.797008
C	-2.549848	-2.585701	1.209982	C	1.647067	-1.115965	-0.756361
C	-4.374321	-0.685672	0.220299	H	2.202908	-1.430842	-1.634487
C	-0.464929	-0.956164	0.452450	C	-0.537176	0.188919	2.721243
C	-2.963196	0.901015	-0.542622	H	0.144147	0.600052	3.472759
C	-5.185287	0.333542	-0.305287	H	-1.100301	-0.627766	3.189079
C	-4.890141	-1.853422	0.791555	H	-1.261929	0.973179	2.466977
C	-1.650468	-3.550232	1.711844	C	-2.101837	2.900006	-1.528342
H	-0.584353	-3.351982	1.639391	H	-1.240868	3.498093	-1.812589
C	-3.948153	-2.852834	1.309993	C	-0.411081	-2.081425	-1.826439
C	0.214954	-0.284037	1.494095	H	-1.148064	-1.429908	-2.313328
C	-6.572395	0.197341	-0.266237	H	-0.949586	-2.974018	-1.484988
H	-7.198489	0.984078	-0.671427	H	0.308236	-2.395919	-2.589094
C	-4.275360	1.357810	-0.797925	C	-3.569203	4.755557	-2.484715
C	0.277004	-1.375039	-0.676251	C	-5.049644	5.125696	-2.695552
C	-7.144891	-0.955860	0.296932	H	-5.564824	4.399321	-3.334469
C	-6.292961	-1.950533	0.810421	H	-5.119506	6.103527	-3.185354
H	-6.743080	-2.837266	1.243238	H	-5.592528	5.192933	-1.745813
C	-3.465343	-4.983378	2.381118	B	-2.007490	-1.272664	0.568629
H	-3.822988	-5.906040	2.831442	C	-2.880449	4.727134	-3.870105
C	-4.379851	-4.056406	1.898216	H	-1.809996	4.511118	-3.789639
H	-5.440175	-4.273816	1.980862	H	-2.987931	5.697559	-4.370370
C	-1.862951	1.674580	-0.909521	H	-3.327761	3.961146	-4.513816
H	-0.850138	1.339237	-0.723322	C	-2.919709	5.856834	-1.613055
C	-2.090299	-4.733884	2.290196	H	-3.395364	5.906687	-0.626911
H	-1.376269	-5.460263	2.669044	H	-3.027426	6.837404	-2.093077
C	2.321029	-0.456679	0.280819	H	-1.850532	5.677816	-1.458673
C	1.589072	-0.049054	1.404199	C	-8.671799	-1.164461	0.369611
H	2.102210	0.453850	2.218417	C	-9.059284	-2.442092	-0.412512
C	-4.486553	2.592206	-1.419947	C	-9.453993	0.017420	-0.234980
H	-5.503514	2.920549	-1.604450	C	-9.105440	-1.316561	1.847142

H	-10.189989	-1.467639	1.913699	H	3.607224	4.354733	0.620069
H	-8.850793	-0.420149	2.423985	H	6.899315	2.241653	2.406370
H	-8.620846	-2.171644	2.329934	C	5.889899	4.845081	2.068085
H	-10.529954	-0.176345	-0.160200	C	4.852309	5.528402	2.990488
H	-9.218560	0.163540	-1.295363	C	7.204602	4.693762	2.856561
H	-9.250609	0.955348	0.294279	C	6.163791	5.755085	0.846827
H	-10.143438	-2.603713	-0.367842	H	3.902039	5.703407	2.475116
H	-8.573413	-3.334645	-0.004657	H	4.644967	4.910451	3.871607
H	-8.770967	-2.358240	-1.466547	H	5.227836	6.499515	3.336319
N	3.717610	-0.209902	0.195278	H	7.995694	4.241285	2.247756
C	4.586386	-1.203390	-0.332760	H	7.558571	5.679983	3.177742
C	5.634813	-0.854937	-1.199359	H	7.072546	4.081445	3.755924
C	4.424054	-2.555225	-0.005067	H	6.549848	6.728765	1.173332
C	6.486961	-1.830400	-1.704925	H	6.905392	5.301551	0.179304
H	5.778050	0.185758	-1.472990	H	5.255641	5.936288	0.262241
C	5.276144	-3.524355	-0.535157	C	7.296679	-4.235709	-1.986870
H	3.624248	-2.849544	0.667233	C	6.964827	-5.667503	-1.525490
C	6.333047	-3.192906	-1.393768	C	7.213525	-4.197021	-3.531563
H	7.284756	-1.515702	-2.372554	C	8.744147	-3.912172	-1.545847
H	5.107382	-4.557323	-0.250690	H	7.035858	-5.771893	-0.436773
C	4.255035	1.020116	0.661759	H	5.958138	-5.972322	-1.833483
C	3.609703	2.237559	0.390927	H	7.674457	-6.373462	-1.971726
C	5.445500	1.055787	1.398609	H	7.477622	-3.211399	-3.929166
C	4.140005	3.436603	0.853449	H	7.902415	-4.929204	-3.970914
H	2.688975	2.237155	-0.184028	H	6.200189	-4.434677	-3.874924
C	5.974619	2.268884	1.840162	H	9.445555	-4.643039	-1.967215
H	5.961280	0.128057	1.625891	H	9.058938	-2.917865	-1.879800
C	5.338317	3.491520	1.587116	H	8.836562	-3.942204	-0.454135

Table S19 Cartesian Coordinates for **13**-S_1 (first excited state)

N	3.011945	-0.318552	-0.125304	C	3.977020	-2.705516	-1.503816
C	2.544050	-2.451294	-1.399165	C	-0.249117	-0.230765	-1.575033
C	4.376993	-0.620960	-0.259073	C	6.585051	0.239290	0.320255
C	0.455391	-0.919393	-0.546929	H	7.199863	0.999419	0.788132
C	2.943451	0.889192	0.582855	C	4.262722	1.338265	0.892277
C	5.176610	0.365741	0.349143	C	-0.271322	-1.372129	0.590876
C	4.901814	-1.754163	-0.911057	C	7.156391	-0.867669	-0.314232
C	1.675541	-3.419760	-1.998114	C	6.318390	-1.836190	-0.912710
H	0.600465	-3.257890	-1.933770	H	6.783358	-2.686721	-1.399338

C	3.539625	-4.773682	-2.740740	H	10.225747	-1.262484	-1.927808
H	3.916255	-5.656513	-3.250939	H	8.893680	-0.177452	-2.375102
C	4.420963	-3.866531	-2.176084	H	8.657979	-1.931183	-2.410974
H	5.487918	-4.060307	-2.256901	H	10.540638	-0.122593	0.234329
C	1.837198	1.645619	0.987351	H	9.213516	0.135581	1.376364
H	0.824641	1.329804	0.761765	H	9.261867	1.038844	-0.149996
C	2.140208	-4.541658	-2.647878	H	10.156553	-2.556777	0.259008
H	1.442055	-5.250132	-3.088756	H	8.586877	-3.258748	-0.167019
C	-2.325370	-0.467058	-0.336681	H	8.776113	-2.388612	1.362490
C	-1.615574	-0.005577	-1.464637	N	-3.706041	-0.243557	-0.233563
H	-2.153241	0.489079	-2.266196	C	-4.544073	-1.204874	0.383470
C	4.446965	2.536551	1.604764	C	-5.589439	-0.794698	1.231106
H	5.459123	2.857755	1.829139	C	-4.344985	-2.574649	0.148726
C	3.353969	3.298812	2.016433	C	-6.401559	-1.744753	1.829923
C	-1.639706	-1.153344	0.687240	H	-5.737694	0.259794	1.435981
H	-2.182305	-1.471801	1.570683	C	-5.175726	-3.510660	0.755368
C	0.483411	0.253837	-2.805127	H	-3.562327	-2.898644	-0.528216
H	-0.194090	0.758807	-3.500459	C	-6.221461	-3.126477	1.611217
H	0.963434	-0.579287	-3.328999	H	-7.187982	-1.400394	2.493309
H	1.278982	0.956933	-2.532090	H	-5.003183	-4.557869	0.539760
C	2.053965	2.826164	1.690802	C	-4.279114	0.946276	-0.748424
H	1.185615	3.402129	1.998727	C	-3.630721	2.181945	-0.569115
C	0.448268	-2.073280	1.719815	C	-5.501938	0.903446	-1.435811
H	1.185982	-1.408693	2.184613	C	-4.203131	3.338748	-1.075273
H	0.996482	-2.945880	1.348875	H	-2.701473	2.228924	-0.012181
H	-0.249210	-2.403266	2.495667	C	-6.055077	2.075072	-1.940712
C	3.502517	4.616322	2.801069	H	-5.998203	-0.047033	-1.598050
C	4.976047	4.979749	3.065575	C	-5.425833	3.321087	-1.776640
H	5.484290	4.211490	3.659396	H	-3.688565	4.279238	-0.908455
H	5.030262	5.921173	3.624564	H	-6.990347	2.003269	-2.482176
H	5.535476	5.114894	2.132851	C	-6.014780	4.630090	-2.322799
B	2.014818	-1.227962	-0.692228	C	-5.008498	5.265764	-3.313081
C	2.789396	4.491108	4.168999	C	-7.348508	4.409616	-3.060976
H	1.722861	4.270609	4.053201	C	-6.264834	5.605455	-1.146388
H	2.877555	5.426638	4.735896	H	-4.048631	5.489352	-2.836237
H	3.234084	3.687818	4.768158	H	-4.817778	4.599048	-4.161616
C	2.862117	5.775739	2.000407	H	-5.414087	6.206072	-3.703737
H	3.358799	5.900771	1.031013	H	-8.115397	3.985910	-2.402730
H	2.951774	6.719914	2.552503	H	-7.723714	5.370510	-3.428568
H	1.797788	5.600334	1.810628	H	-7.232449	3.747806	-3.926643
C	8.685949	-1.068733	-0.384245	H	-6.680866	6.546048	-1.525165
C	9.071382	-2.398703	0.306504	H	-6.977835	5.182465	-0.429640
C	9.463250	0.065423	0.311535	H	-5.342435	5.842714	-0.606491
C	9.139969	-1.115166	-1.862825	C	-7.150711	-4.137904	2.298095

C	-6.804650	-5.593784	1.933419	H	-7.306749	-2.972652	4.165519
C	-7.028164	-3.978112	3.833533	H	-7.692101	-4.691139	4.335557
C	-8.611995	-3.861351	1.867542	H	-6.003296	-4.173718	4.168469
H	-6.901292	-5.780308	0.857905	H	-9.285541	-4.573798	2.357466
H	-5.787432	-5.861889	2.240264	H	-8.937258	-2.852662	2.142427
H	-7.493788	-6.271120	2.448738	H	-8.730204	-3.971852	0.783653

6. References

[S1] Barbour LJ. X-Seed–A software tool for supramolecular crystallography. Elsevier; 2001.

[S2] Sheldrick G. SHELXS-97, program for crystal structure solution. University of Göttingen Germany; 1997.

[S3] Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

7. NMR Spectra Collection

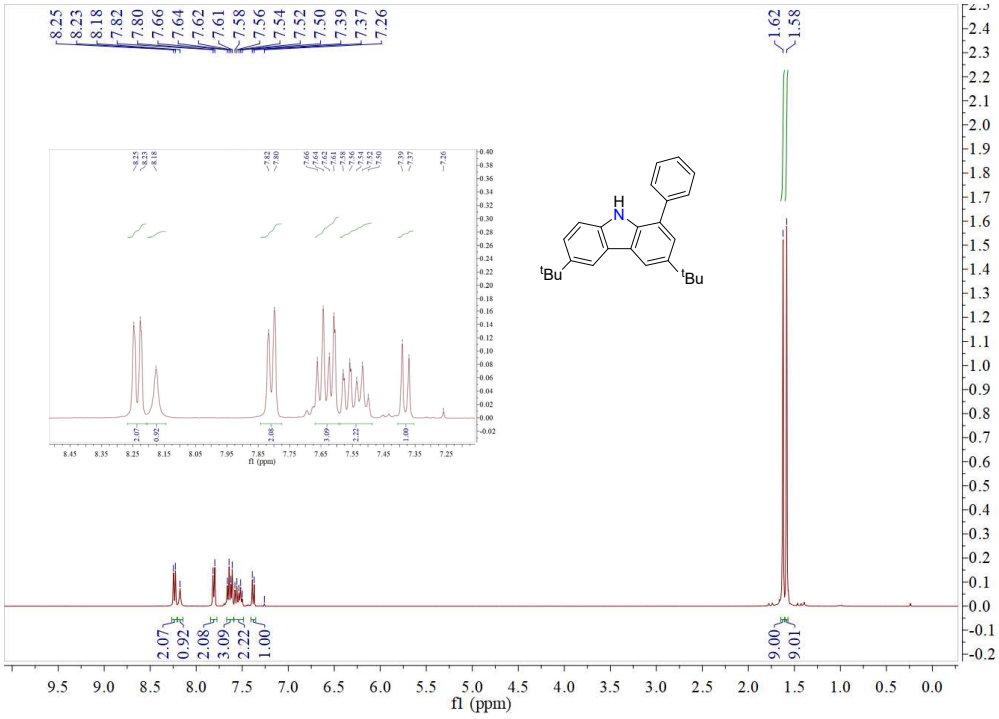


Fig. S23 ^{1}H NMR Spectra of **Cz1** (400 MHz, $CDCl_3$)

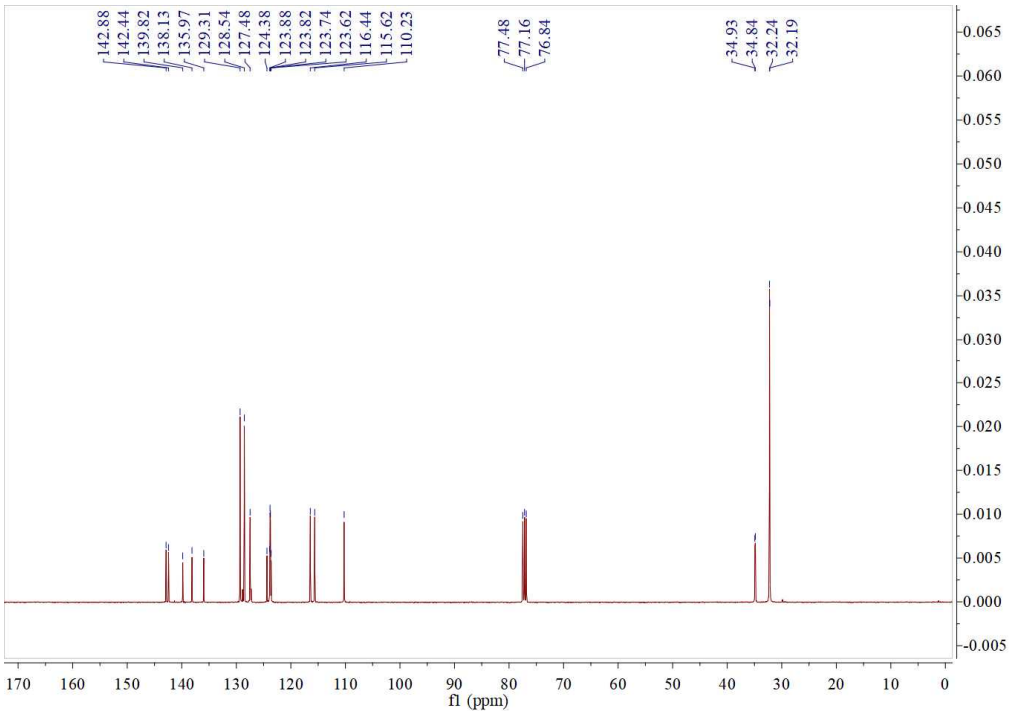


Fig. S24 ^{13}C NMR Spectra of **Cz1** (100 MHz, $CDCl_3$)

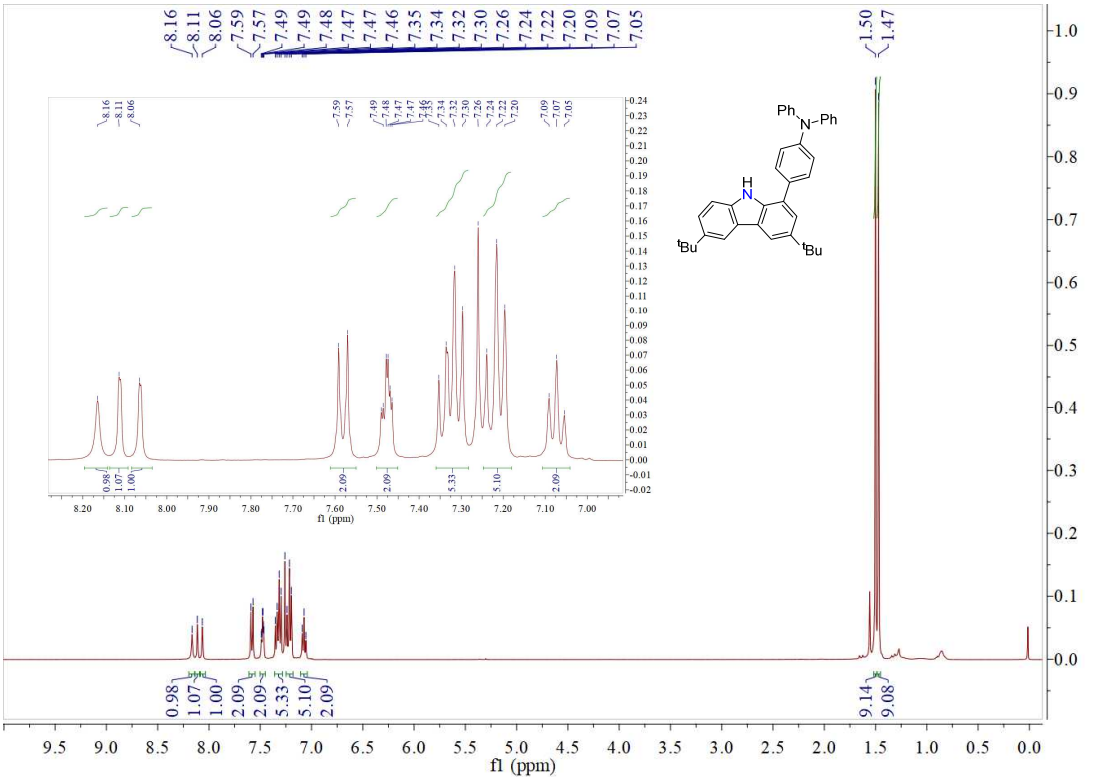


Fig. S25 ^{1}H NMR Spectra of **Cz2** (400 MHz, $CDCl_3$)

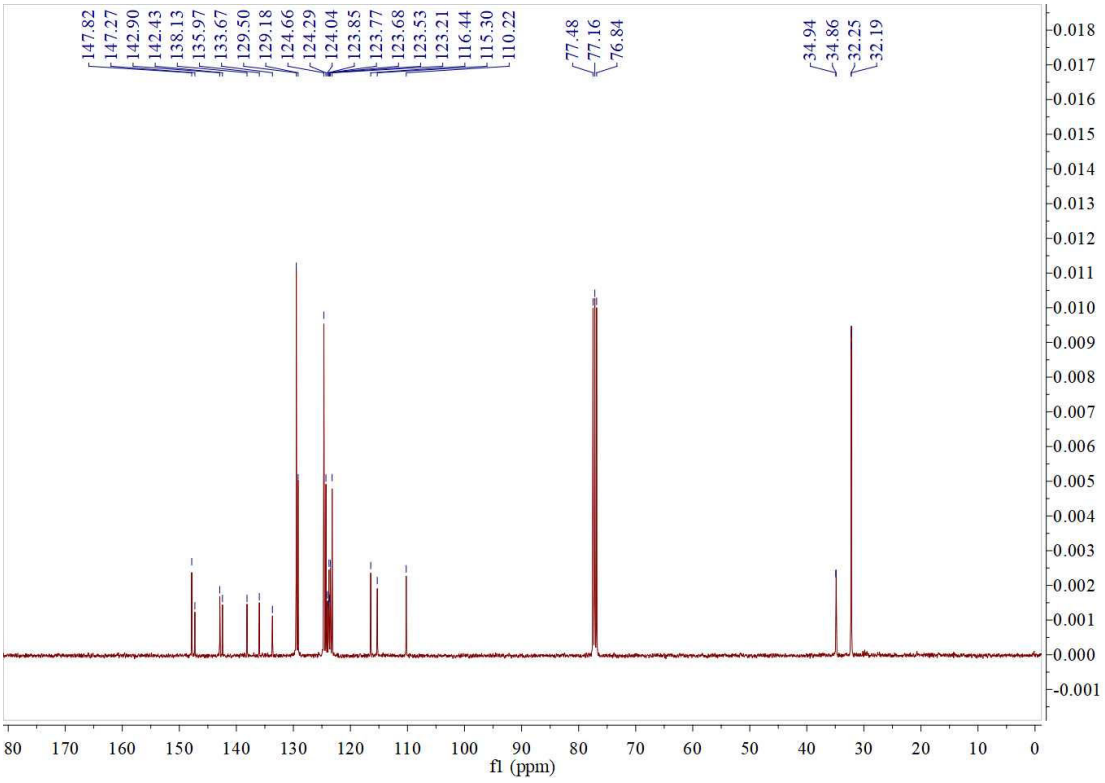


Fig. S26 ^{13}C NMR Spectra of **Cz2** (100 MHz, $CDCl_3$)

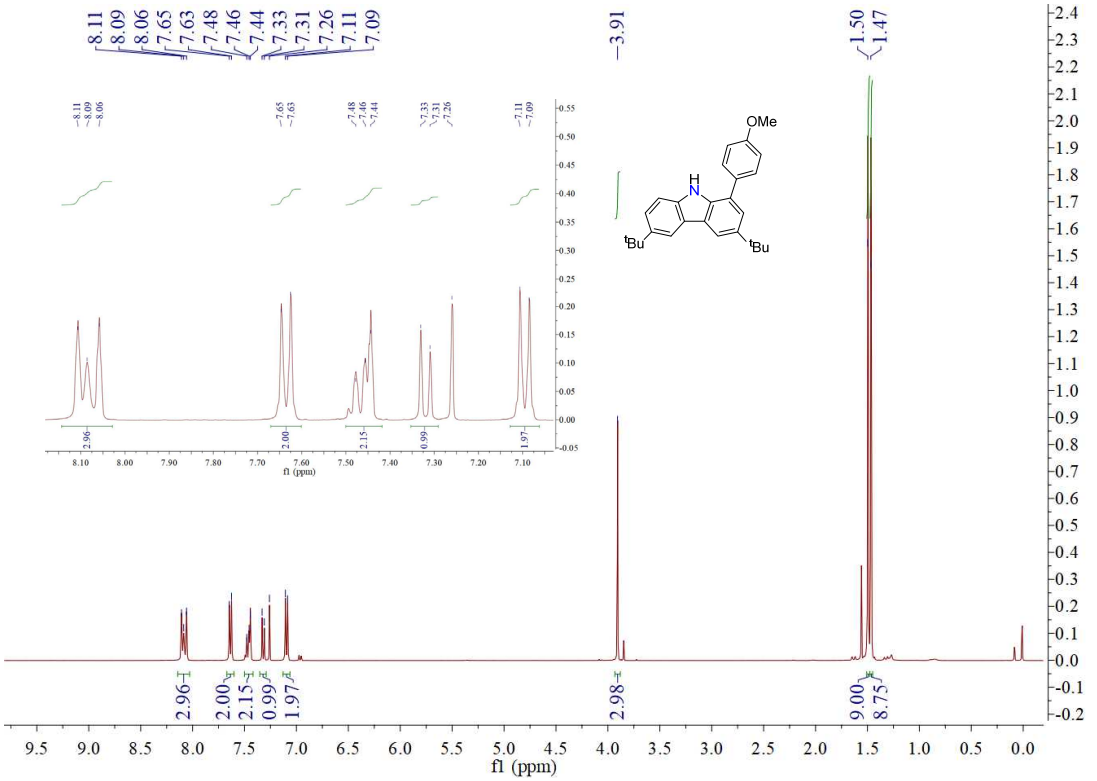


Fig. S27 ^{1}H NMR Spectra of **Cz3** (400 MHz, $CDCl_3$)

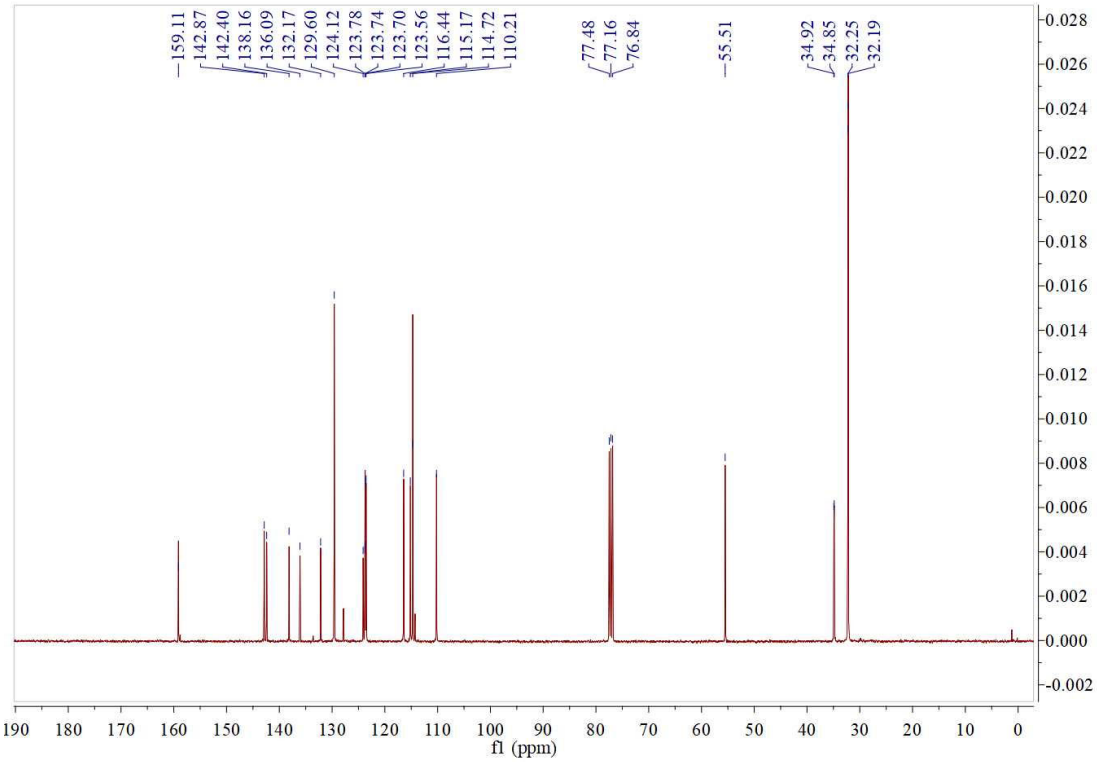


Fig. S28 ^{13}C NMR Spectra of **Cz3** (100 MHz, $CDCl_3$)

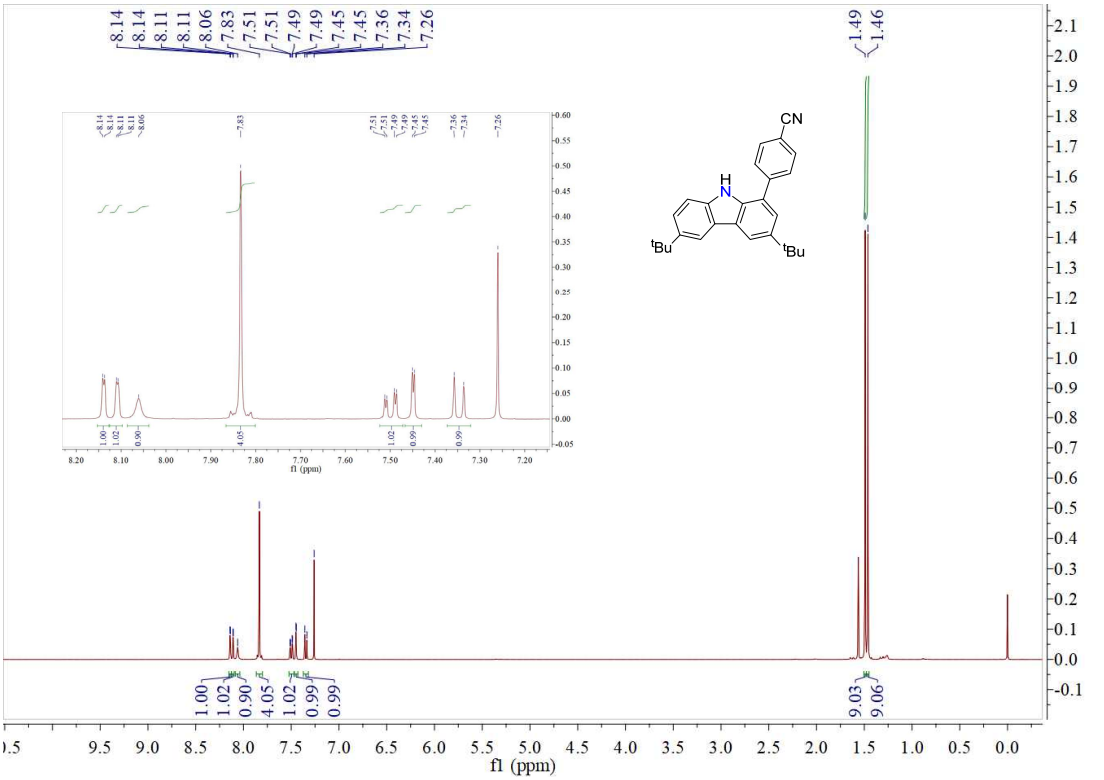


Fig. S29 ^{1}H NMR Spectra of **Cz4** (400 MHz, $CDCl_3$)

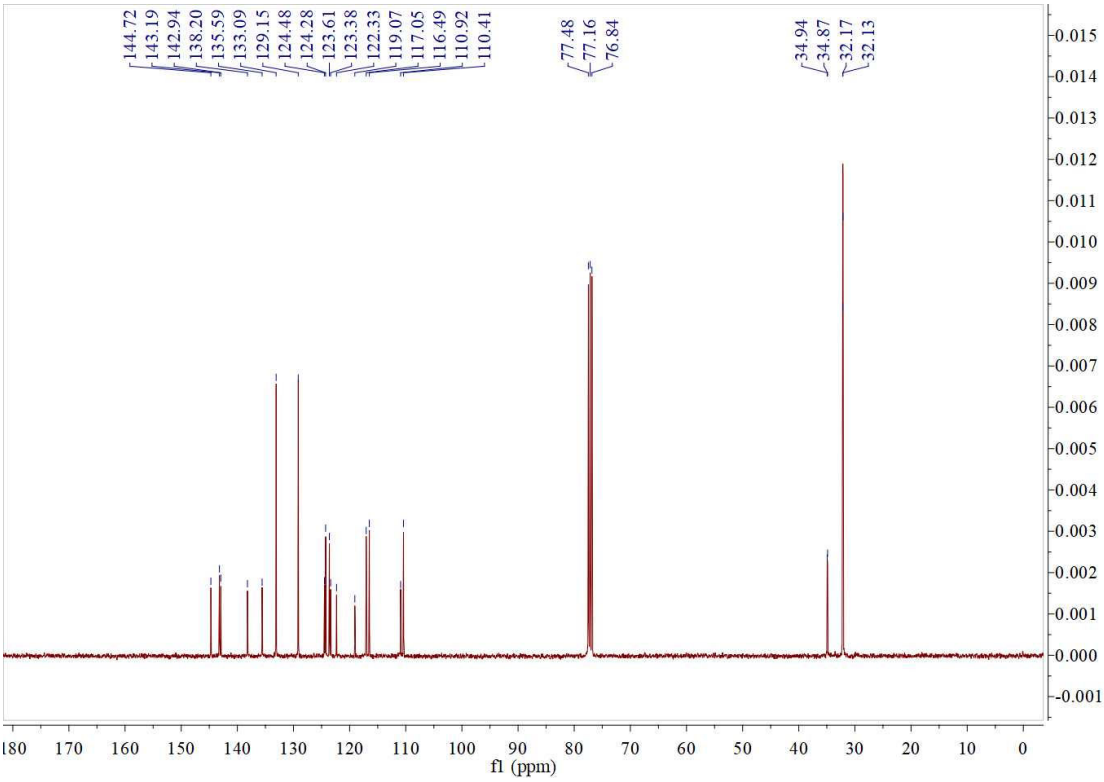


Fig. S30 ^{13}C NMR Spectra of **Cz4** (100 MHz, $CDCl_3$)

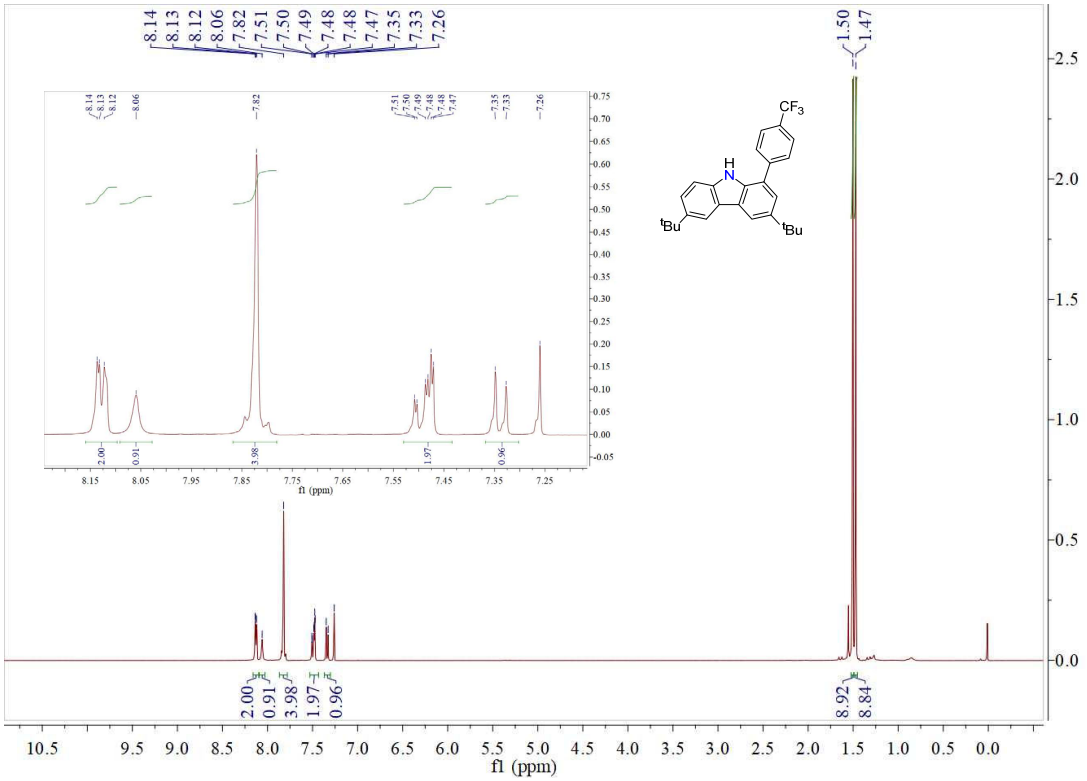


Fig. S31 ^{1}H NMR Spectra of **Cz5** (400 MHz, $CDCl_3$)

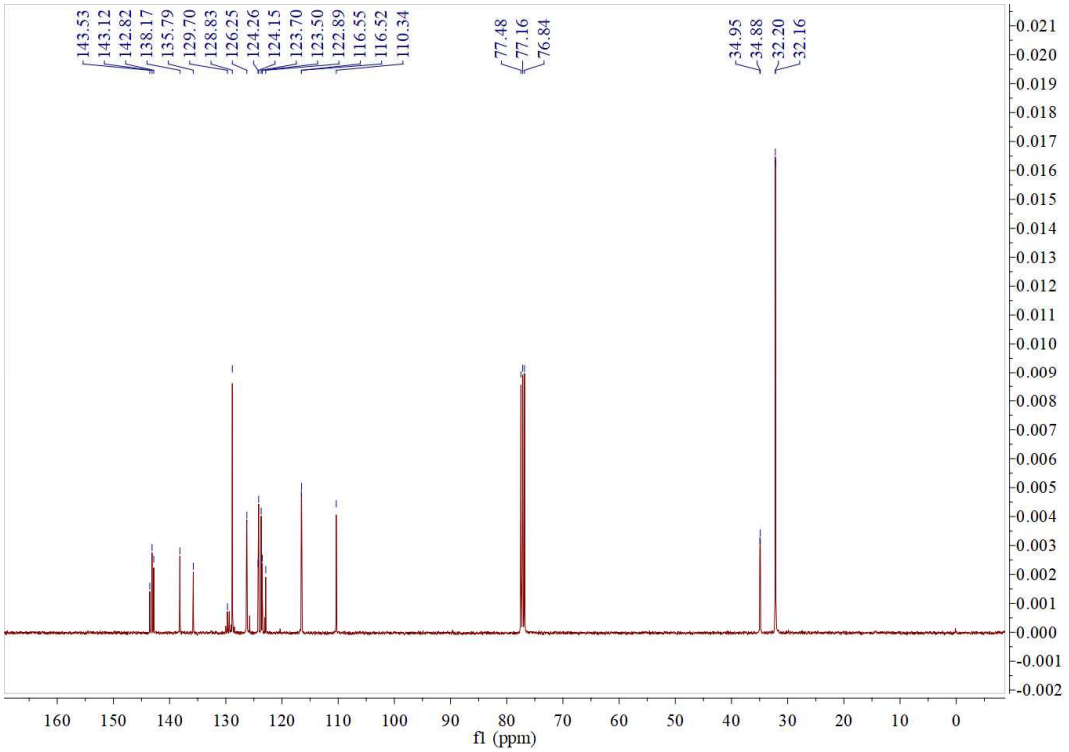


Fig. S32 ^{13}C NMR Spectra of **Cz5** (100 MHz, $CDCl_3$)

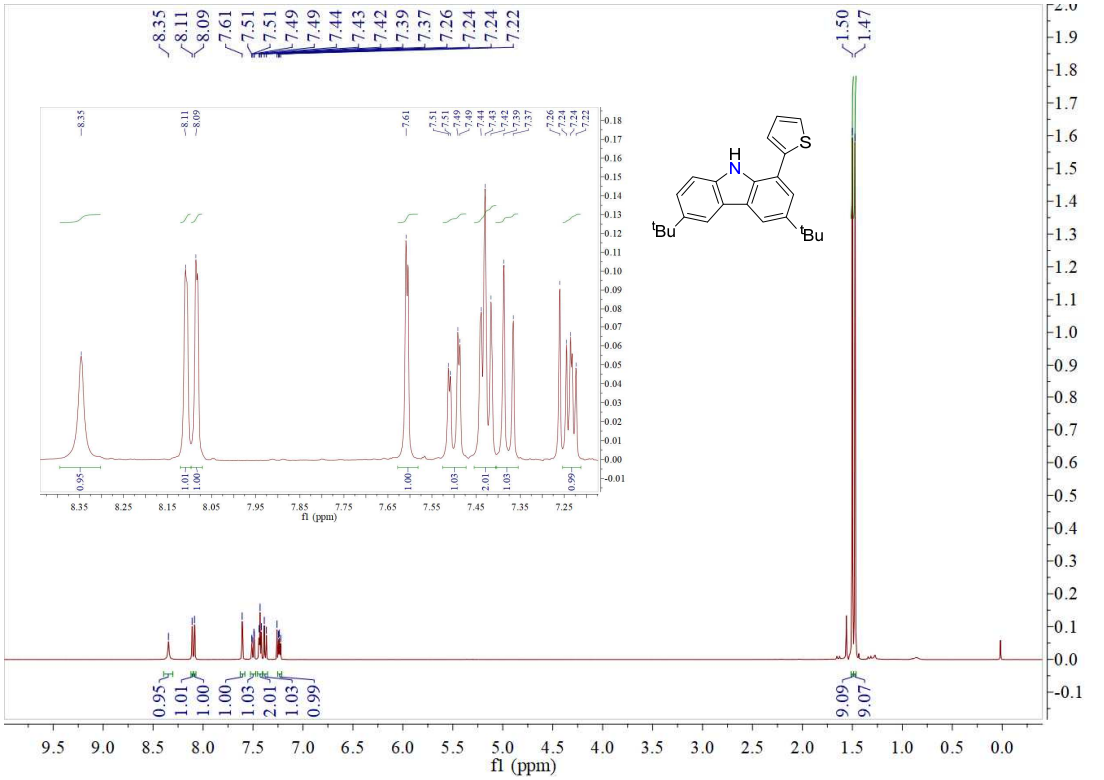


Fig. S33 ^{1}H NMR Spectra of **Cz6** (400 MHz, $CDCl_3$)

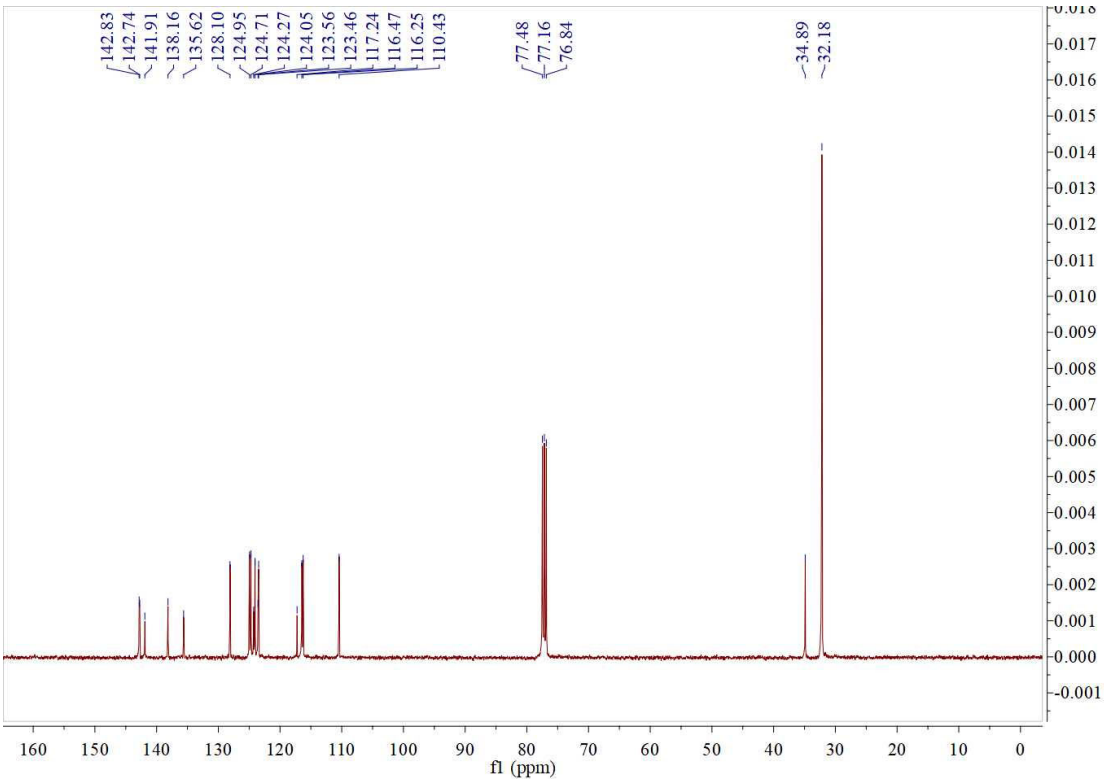


Fig. S34 ^{13}C NMR Spectra of **Cz6** (100 MHz, $CDCl_3$)

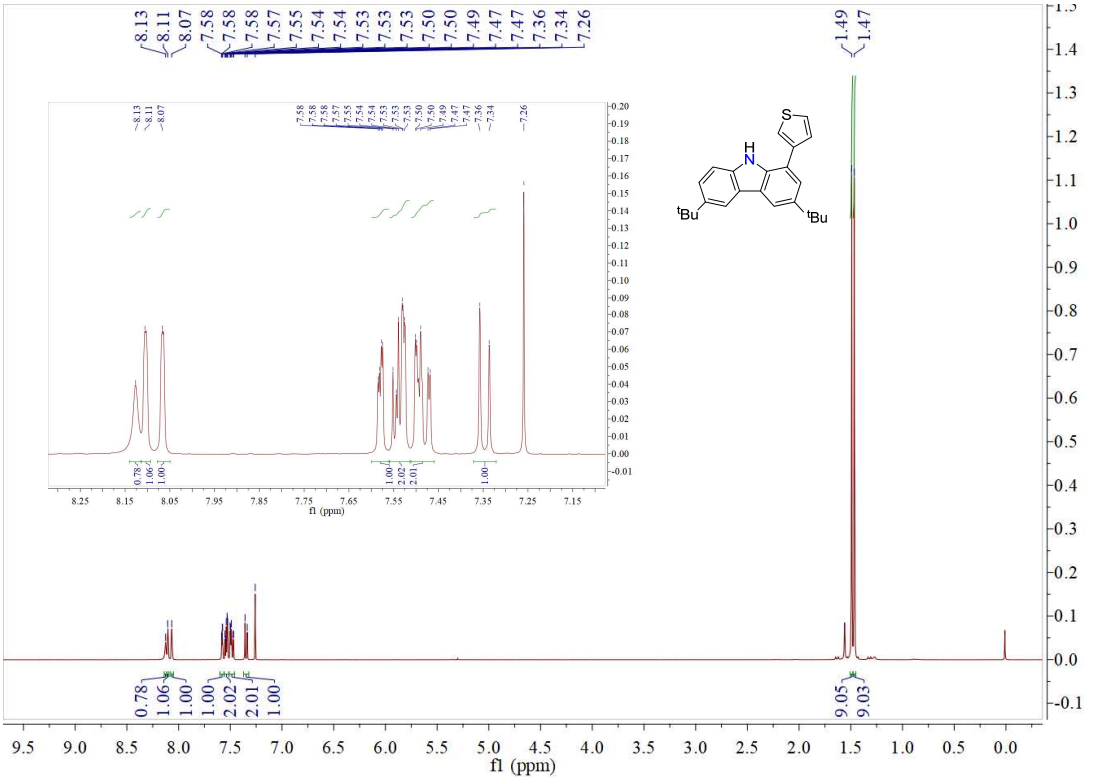


Fig. S35 ^{1}H NMR Spectra of **Cz7** (400 MHz, $CDCl_3$)

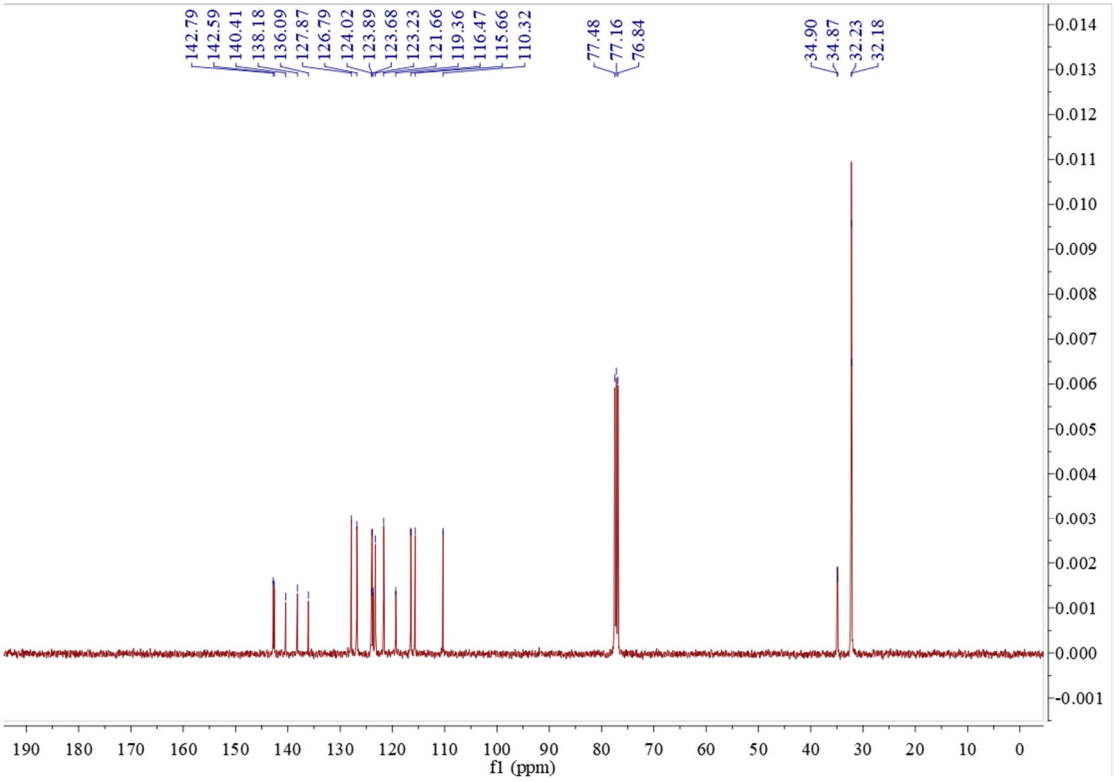


Fig. S36 ^{13}C NMR Spectra of **Cz7** (100 MHz, $CDCl_3$)

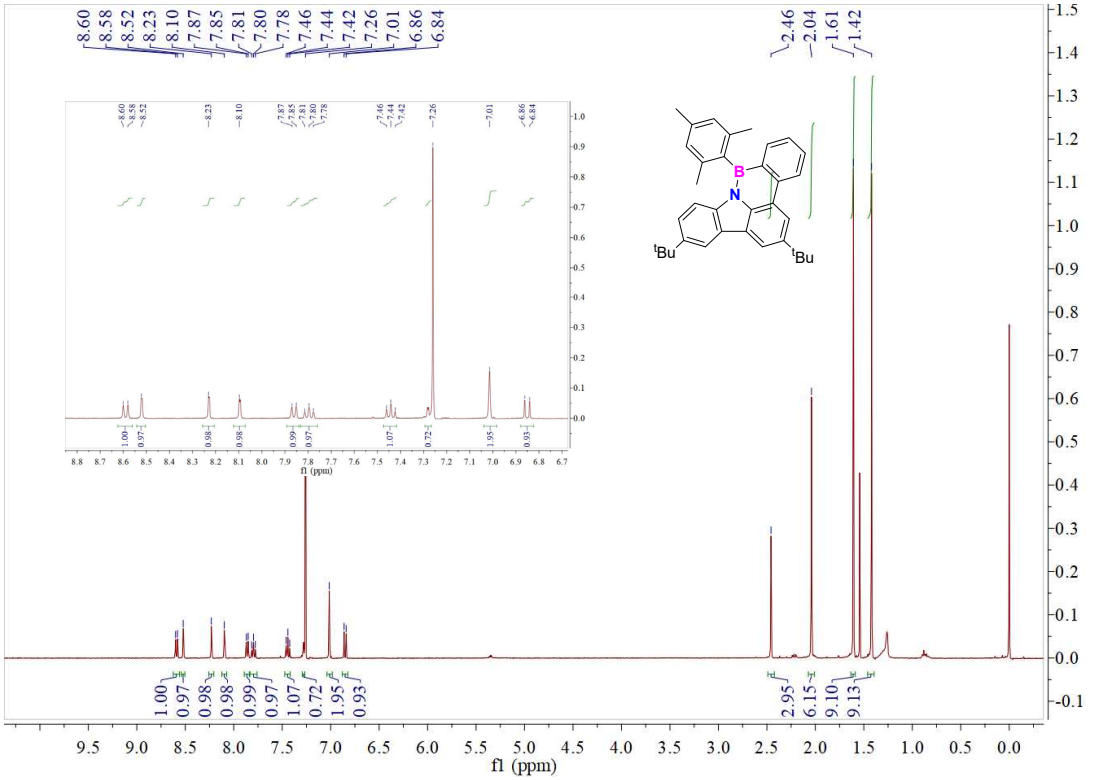


Fig. S37 ^{1}H NMR Spectra of **1** (400 MHz, $CDCl_3$)

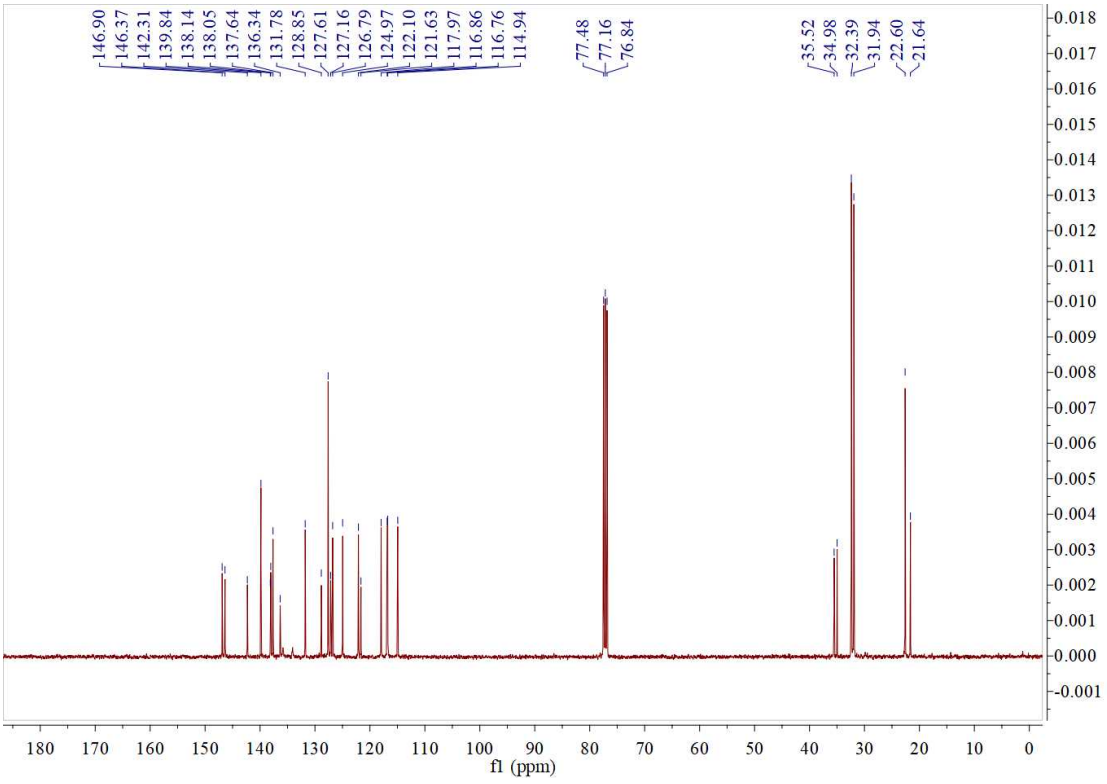


Fig. S38 ^{13}C NMR Spectra of **1** (100 MHz, $CDCl_3$)

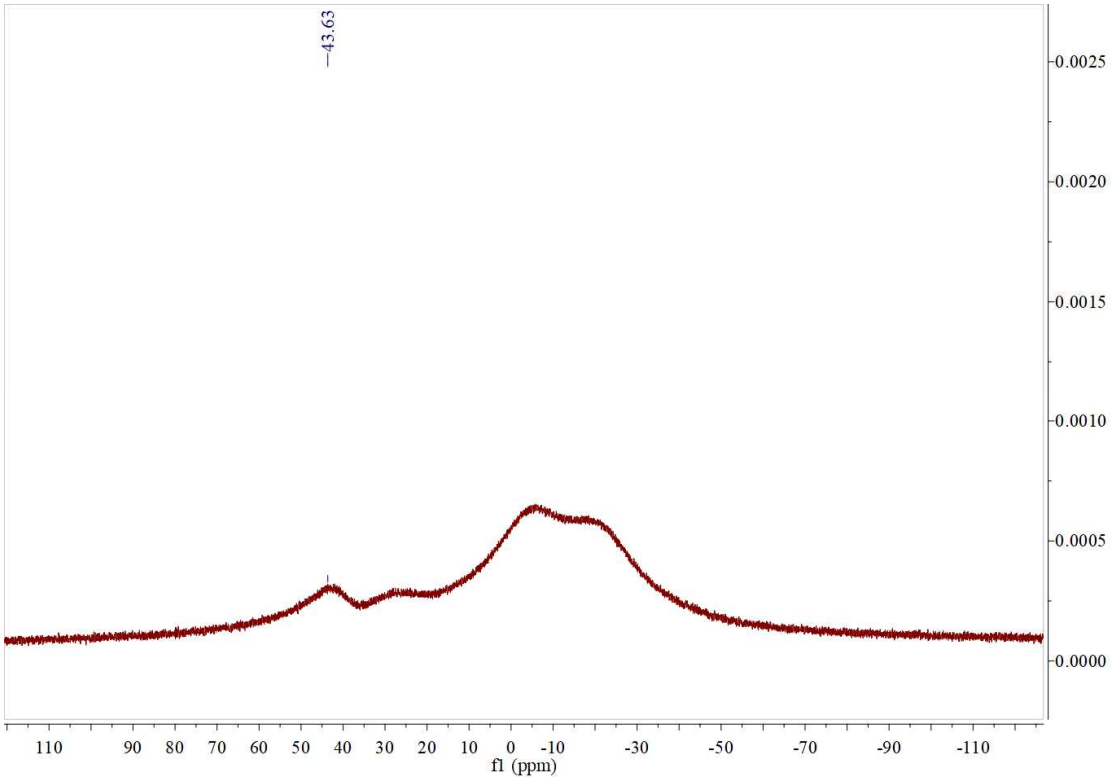


Fig. S39 ^{11}B NMR Spectra of **1** (128 MHz, $CDCl_3$)

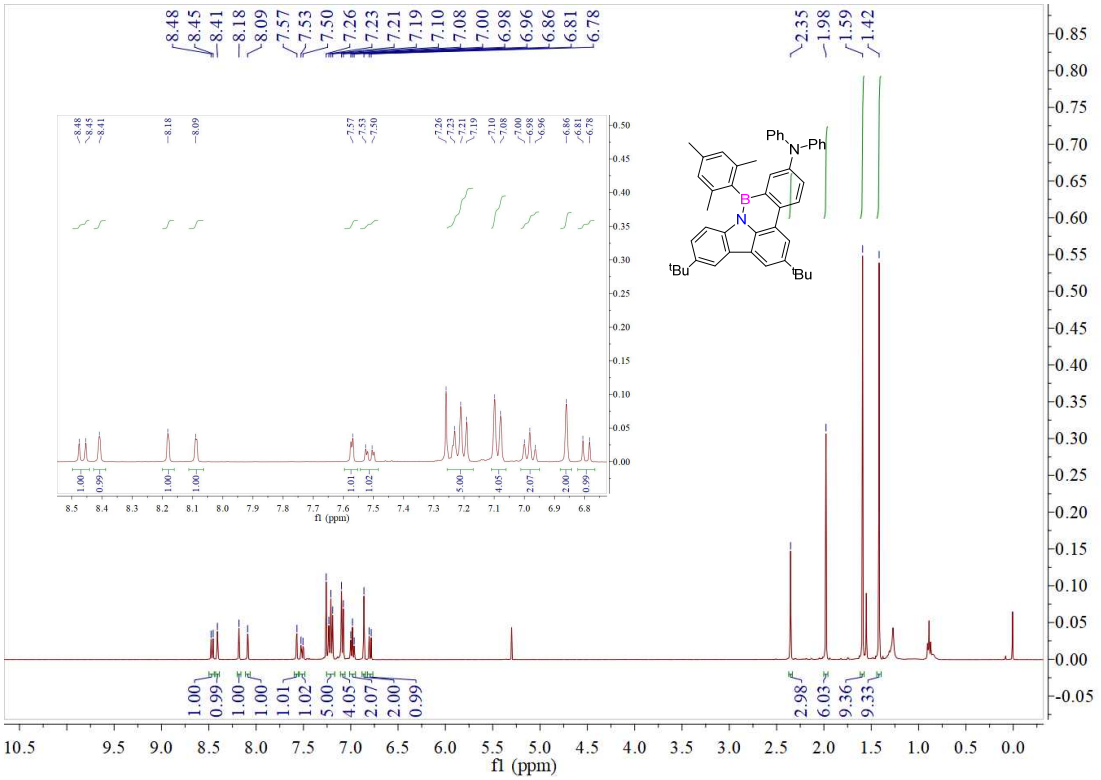


Fig. S40 ^{1}H NMR Spectra of **2** (400 MHz, $CDCl_3$)

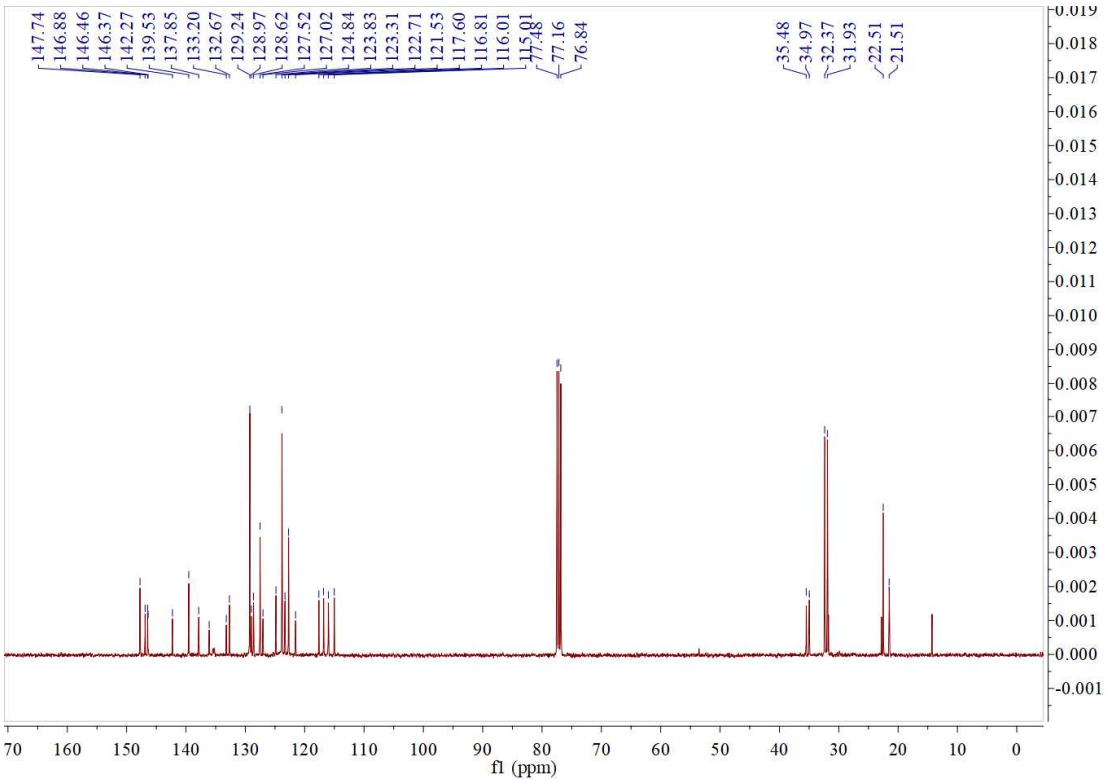


Fig. S41 ^{13}C NMR Spectra of **2** (100 MHz, $CDCl_3$)

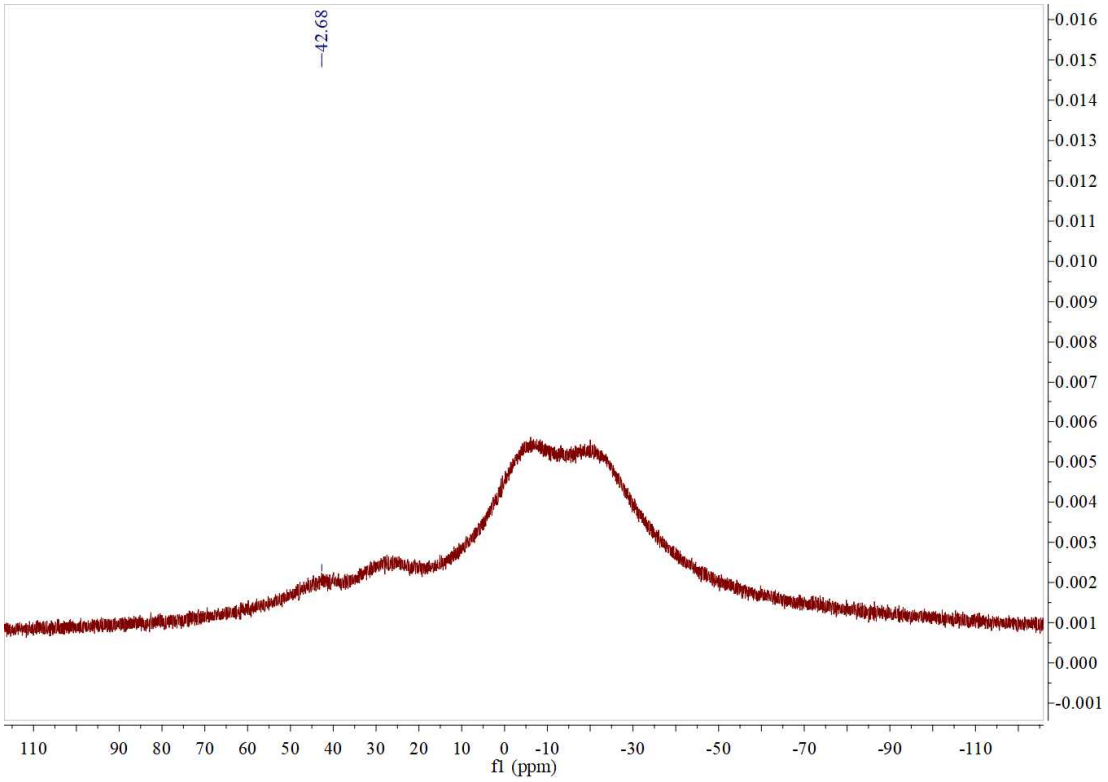


Fig. S42 ^{11}B NMR Spectra of **2** (128 MHz, $CDCl_3$)

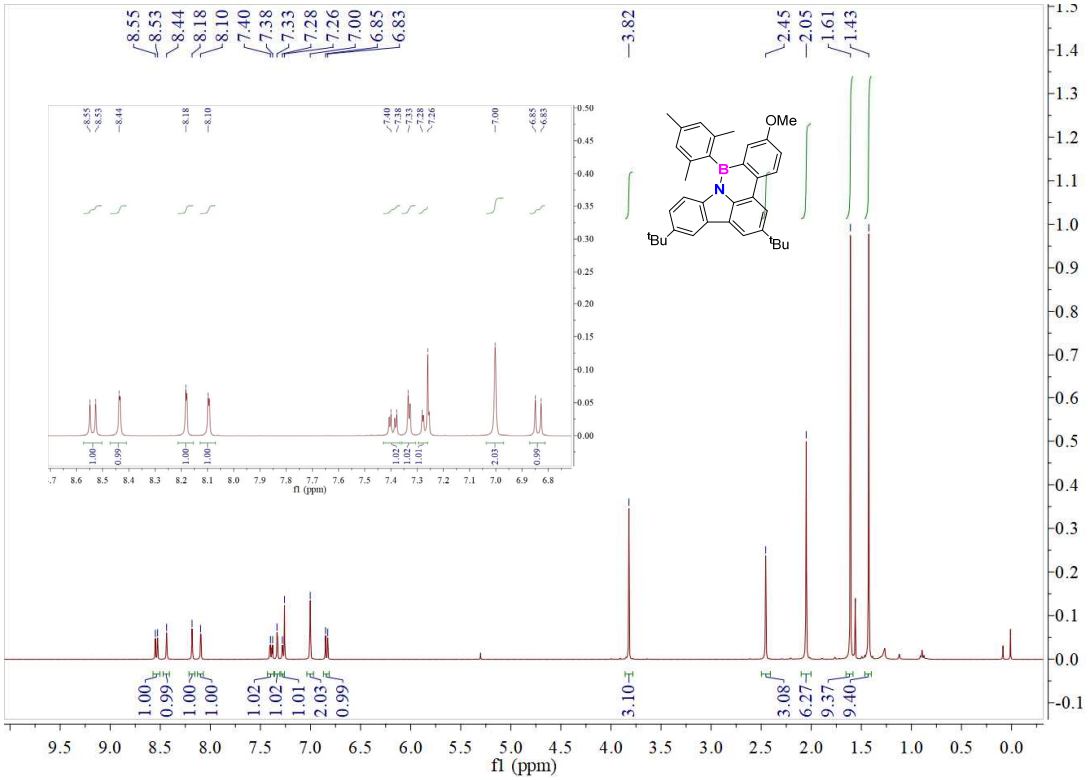


Fig. S43 ^{1}H NMR Spectra of **3** (400 MHz, $CDCl_3$)

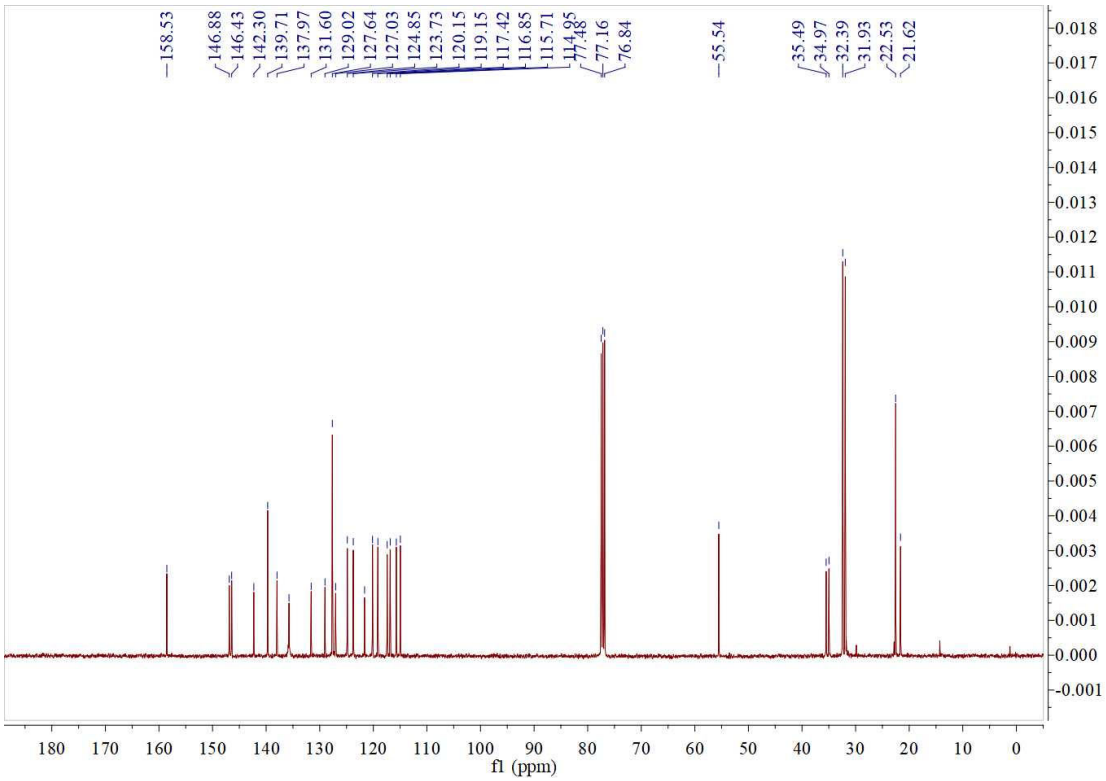


Fig. S44 ^{13}C NMR Spectra of **3** (100 MHz, $CDCl_3$)

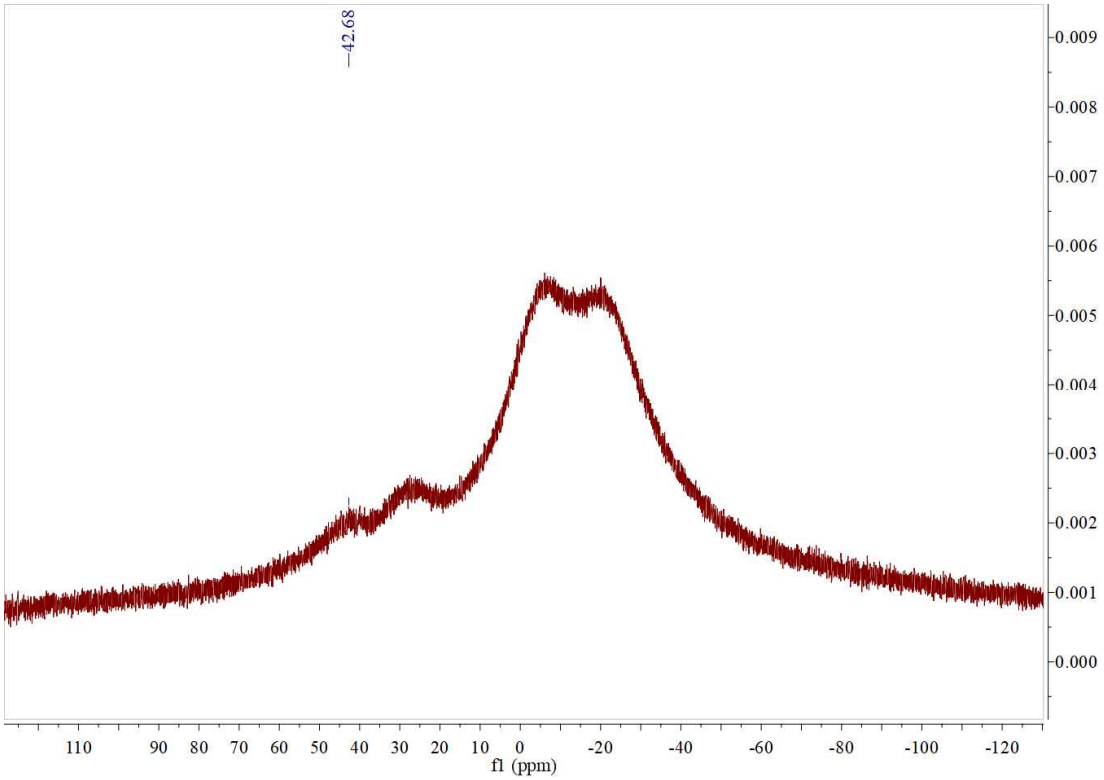


Fig. S45 ^{11}B NMR Spectra of **3** (128 MHz, $CDCl_3$)

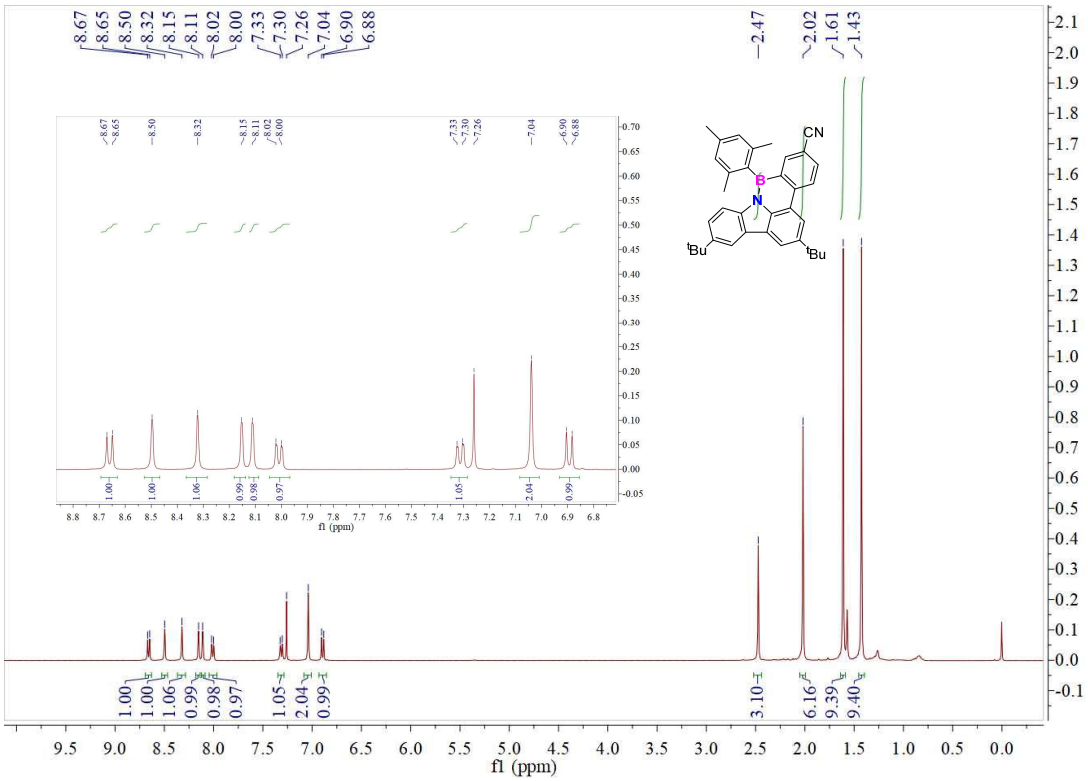


Fig. S46 ^{1}H NMR Spectra of **4** (400 MHz, $CDCl_3$)

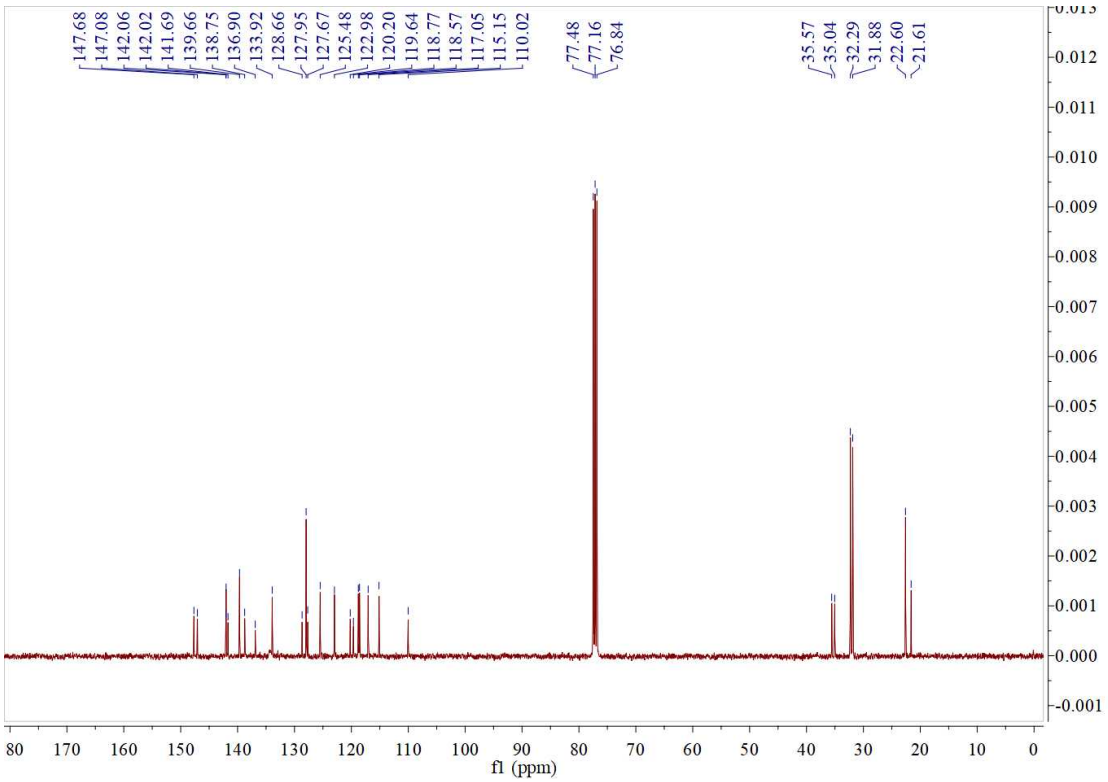


Fig. S47 ^{13}C NMR Spectra of **4** (100 MHz, $CDCl_3$)

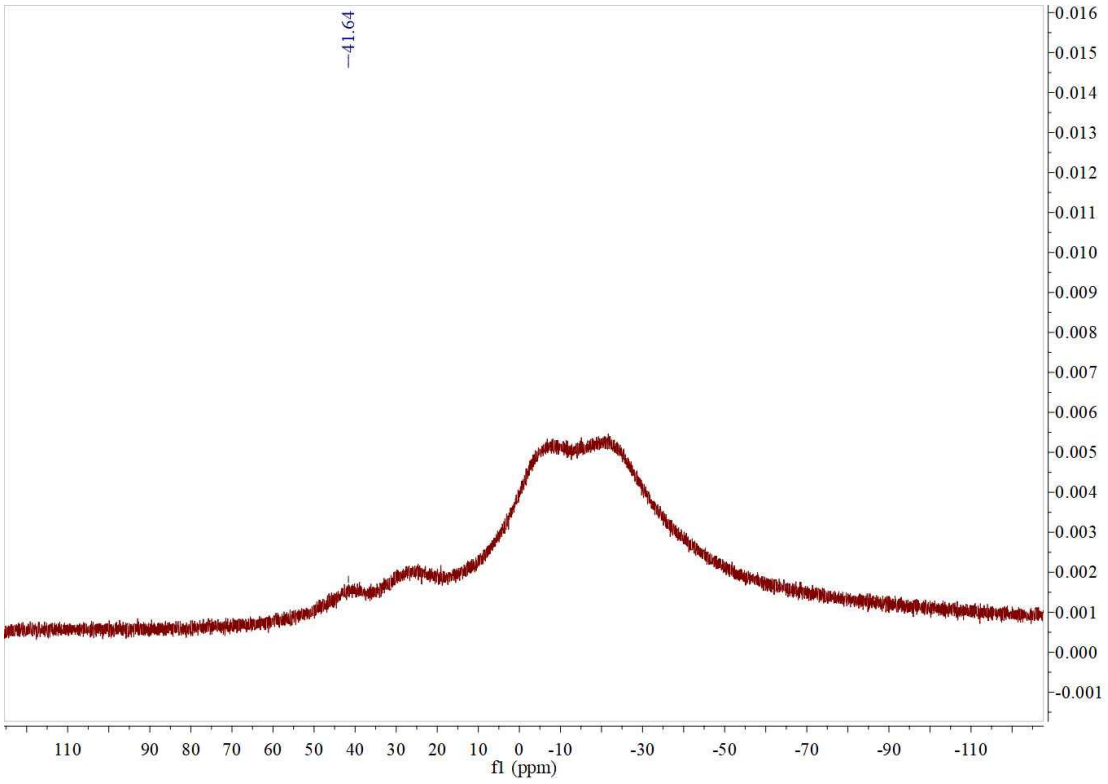


Fig. S48 ^{11}B NMR Spectra of **4** (128 MHz, $CDCl_3$)

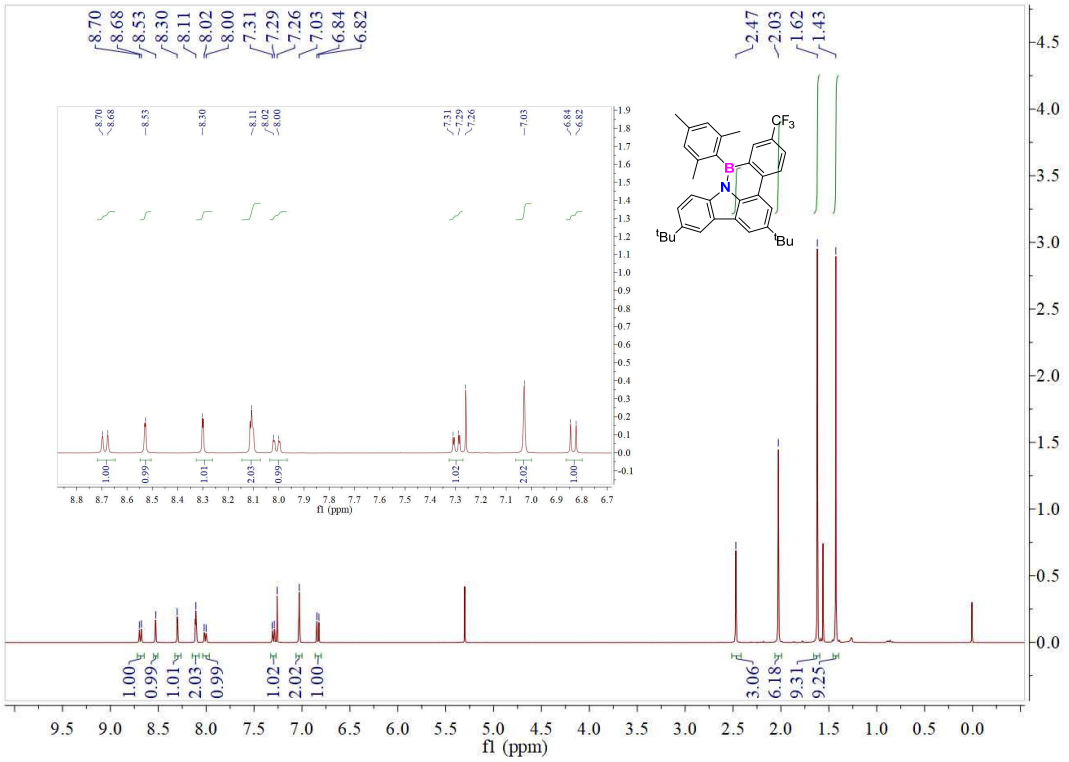


Fig. S49 ^{1}H NMR Spectra of **5** (400 MHz, $CDCl_3$)

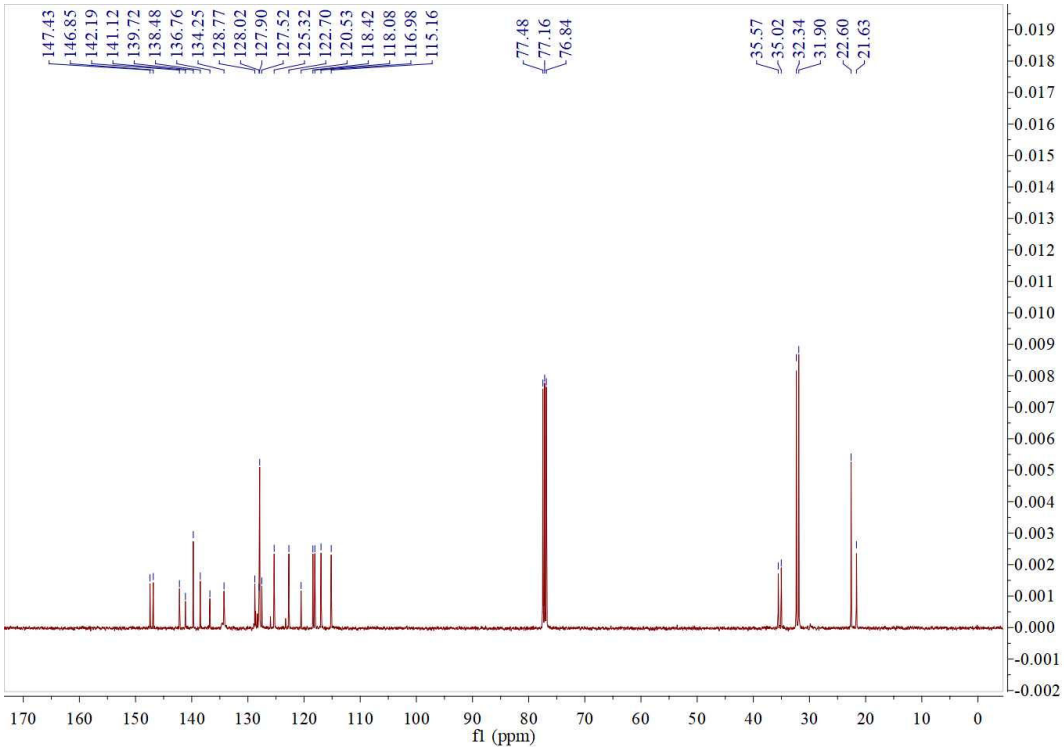


Fig. S50 ^{13}C NMR Spectra of **5** (100 MHz, $CDCl_3$)

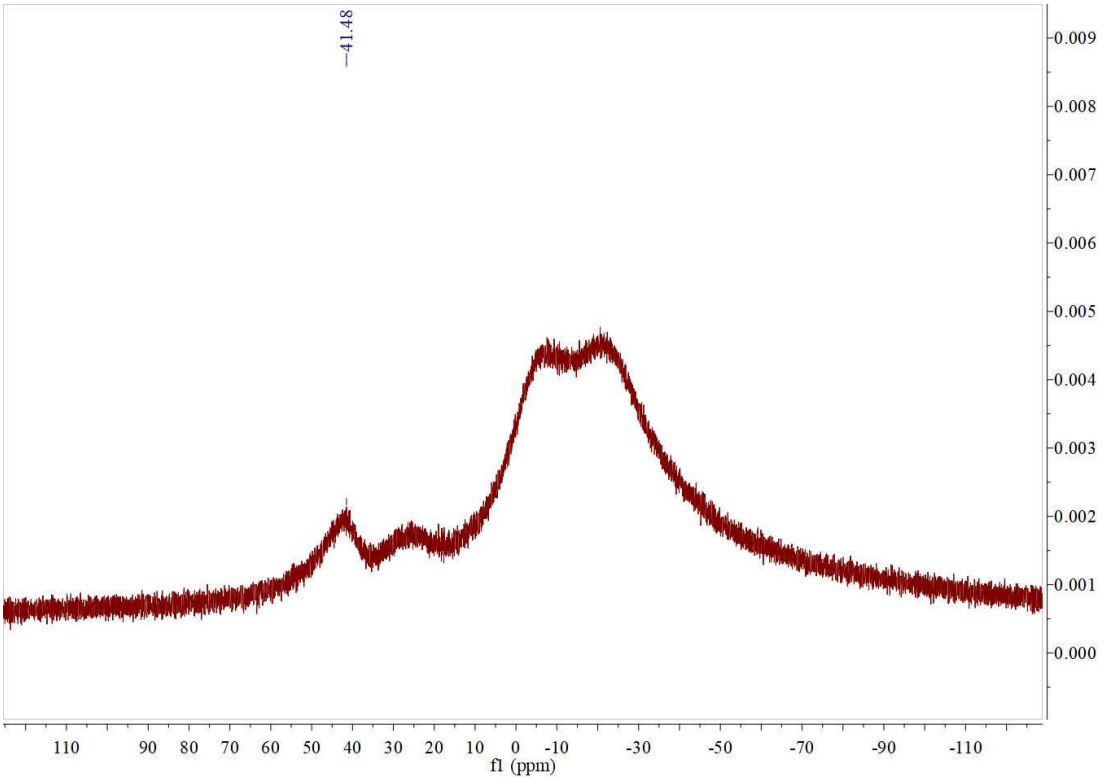


Fig. S51 ^{11}B NMR Spectra of **5** (128 MHz, $CDCl_3$)

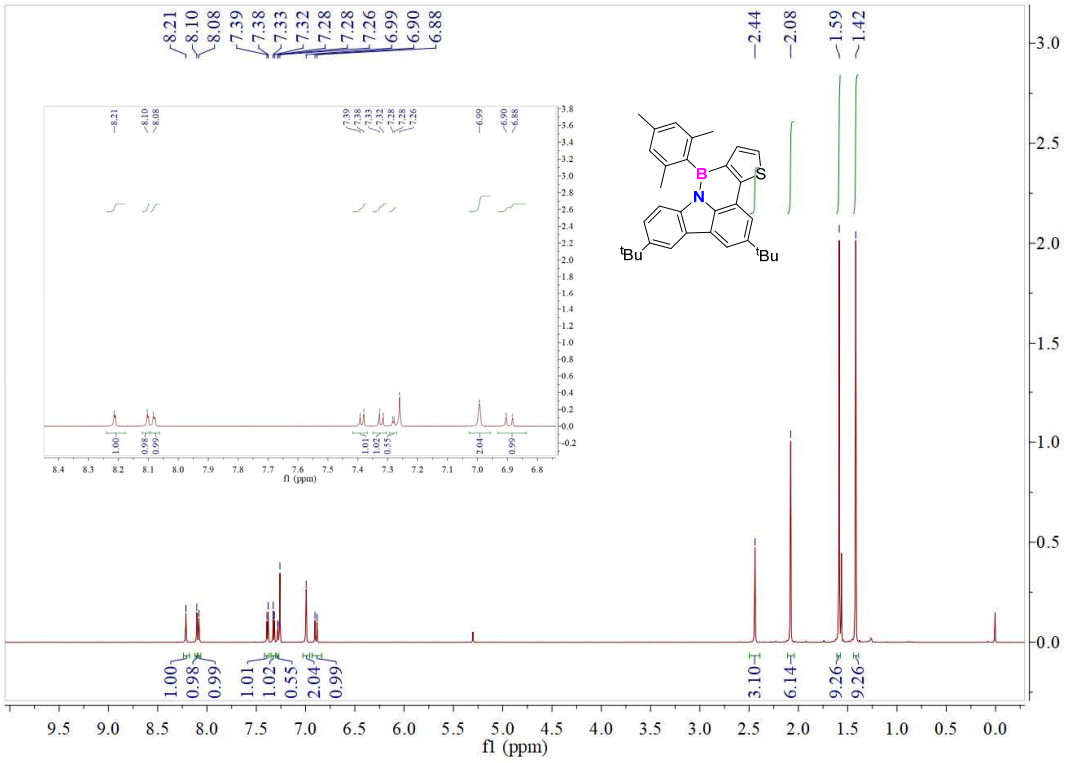


Fig. S52 ^{1}H NMR Spectra of **6** (400 MHz, $CDCl_3$)

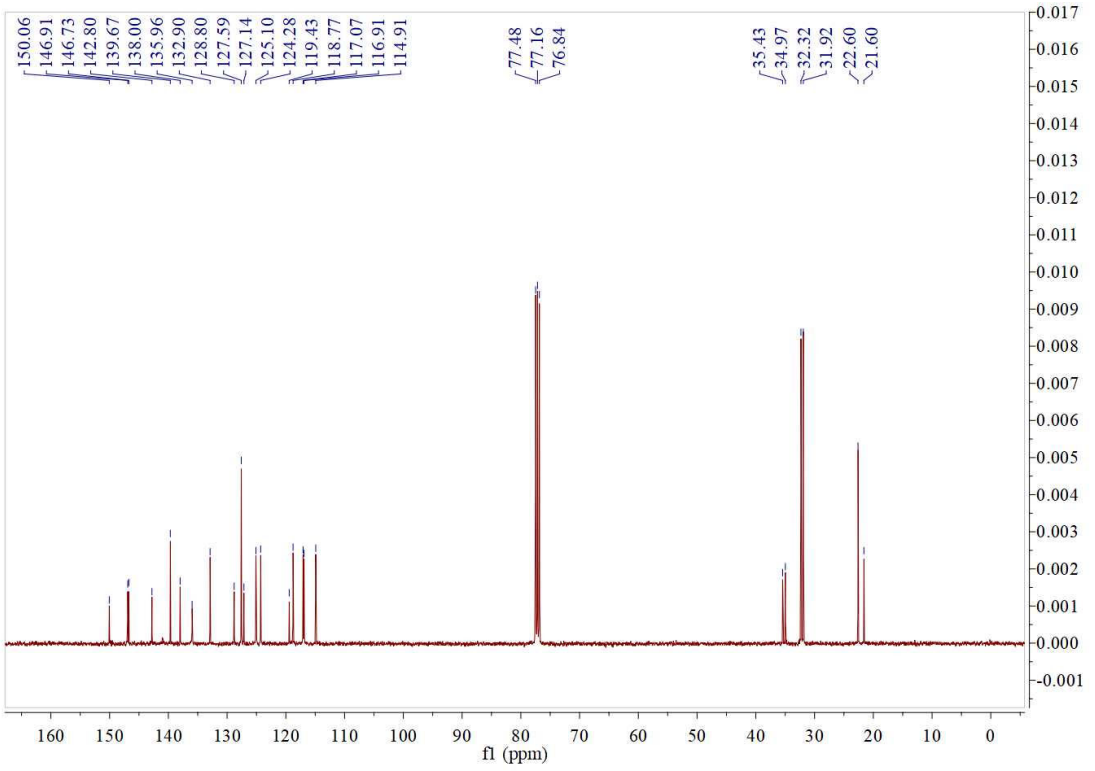


Fig. S53 ^{13}C NMR Spectra of **6** (100 MHz, $CDCl_3$)

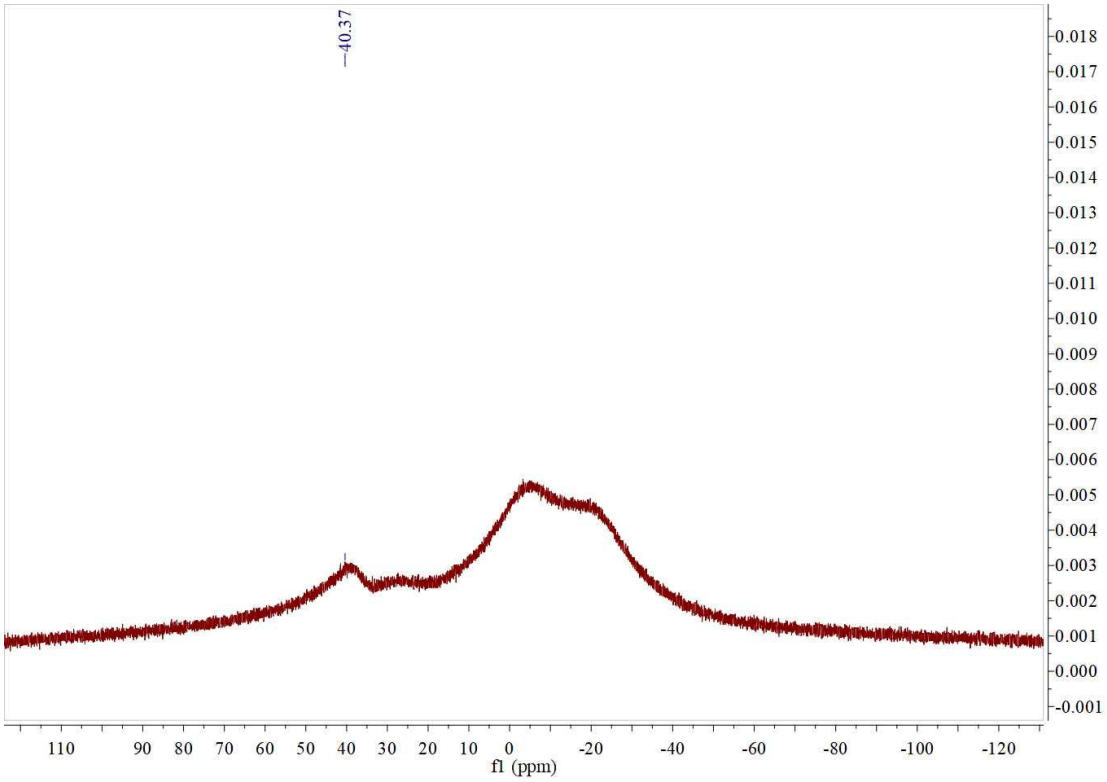


Fig. S54 ^{11}B NMR Spectra of **6** (128 MHz, $CDCl_3$)

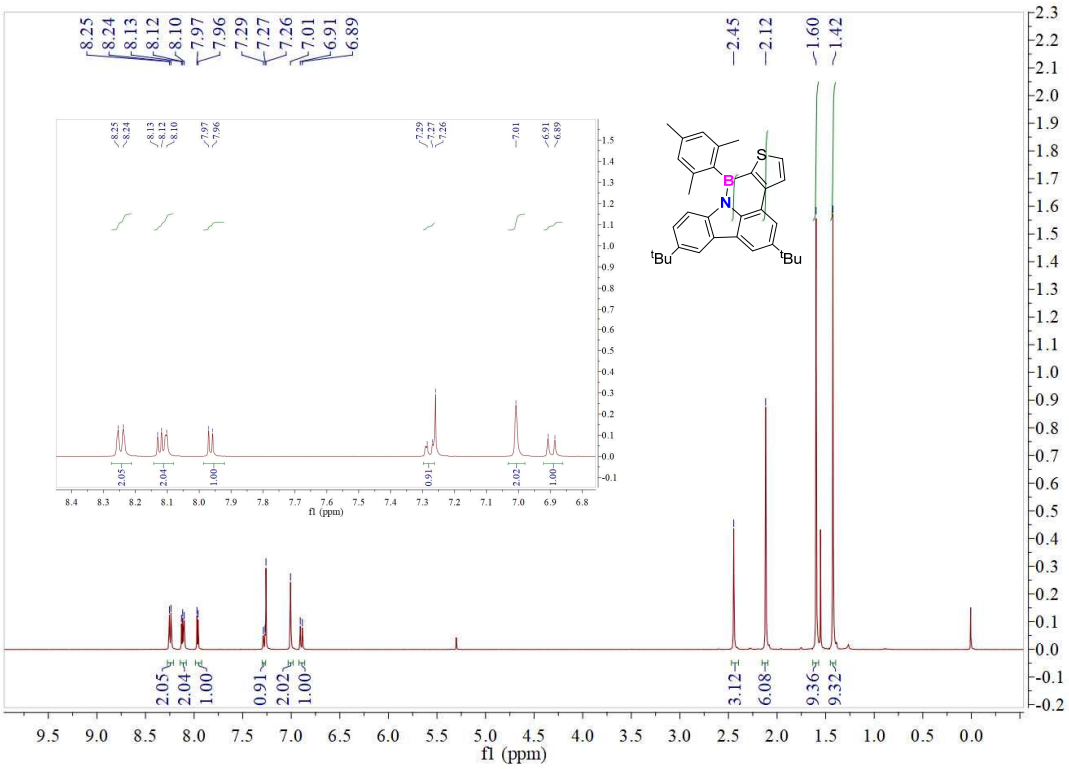


Fig. S55 ^{1}H NMR Spectra of **7** (400 MHz, $CDCl_3$)

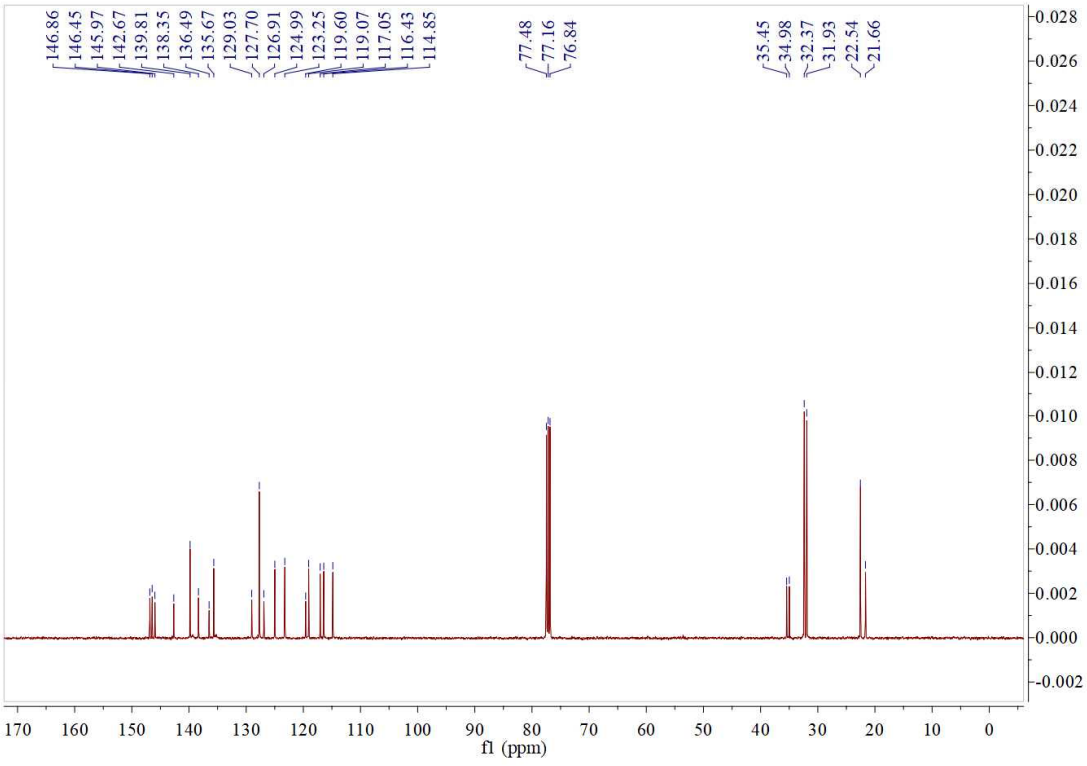


Fig. S56 ^{13}C NMR Spectra of **7** (100 MHz, $CDCl_3$)

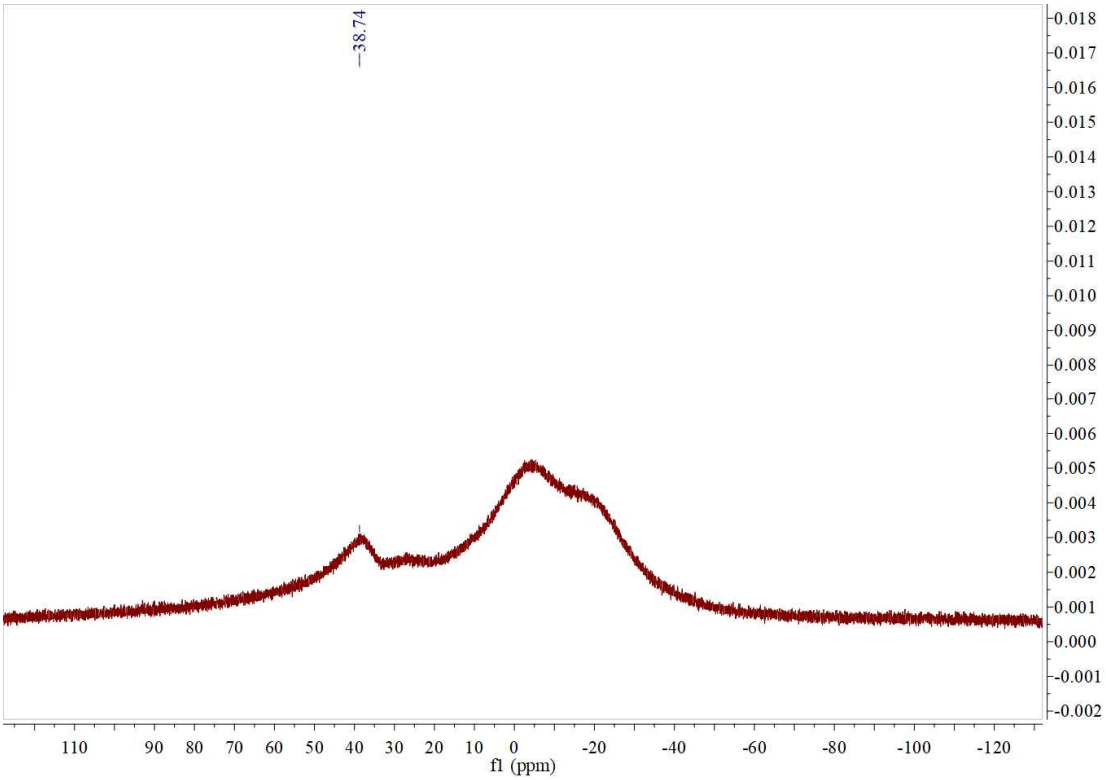


Fig. S57 ^{11}B NMR Spectra of **7** (128 MHz, $CDCl_3$)

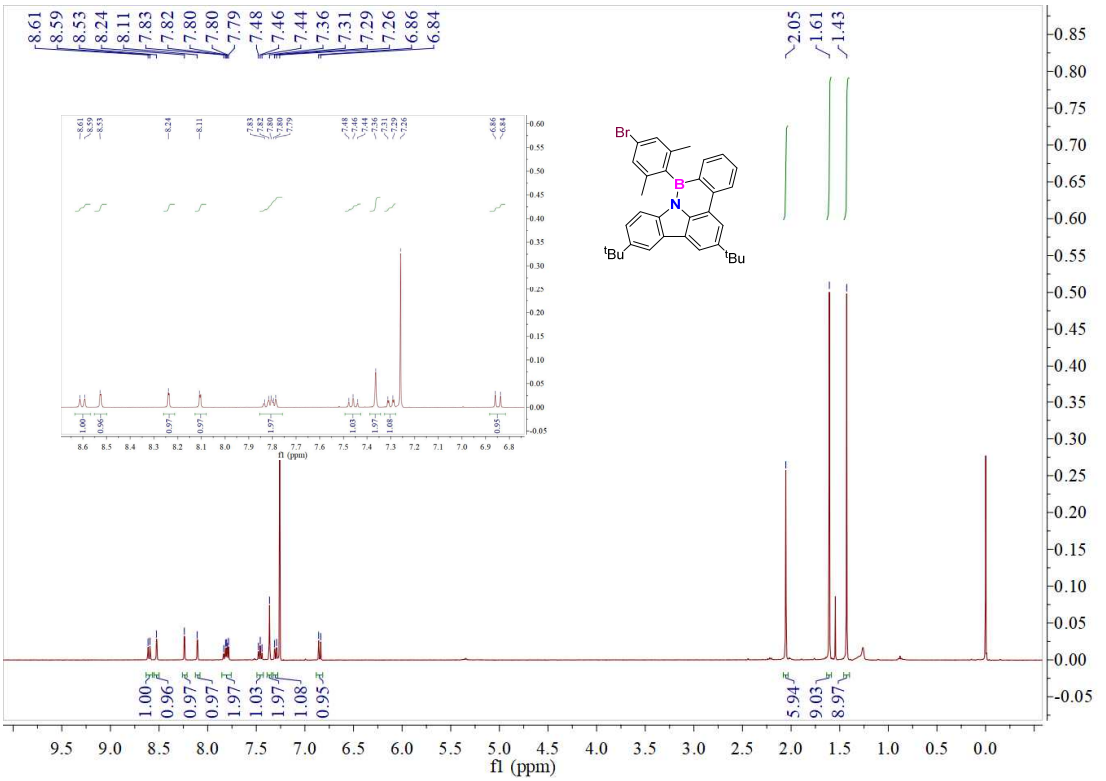


Fig. S58 ^{1}H NMR Spectra of **8** (400 MHz, $CDCl_3$)

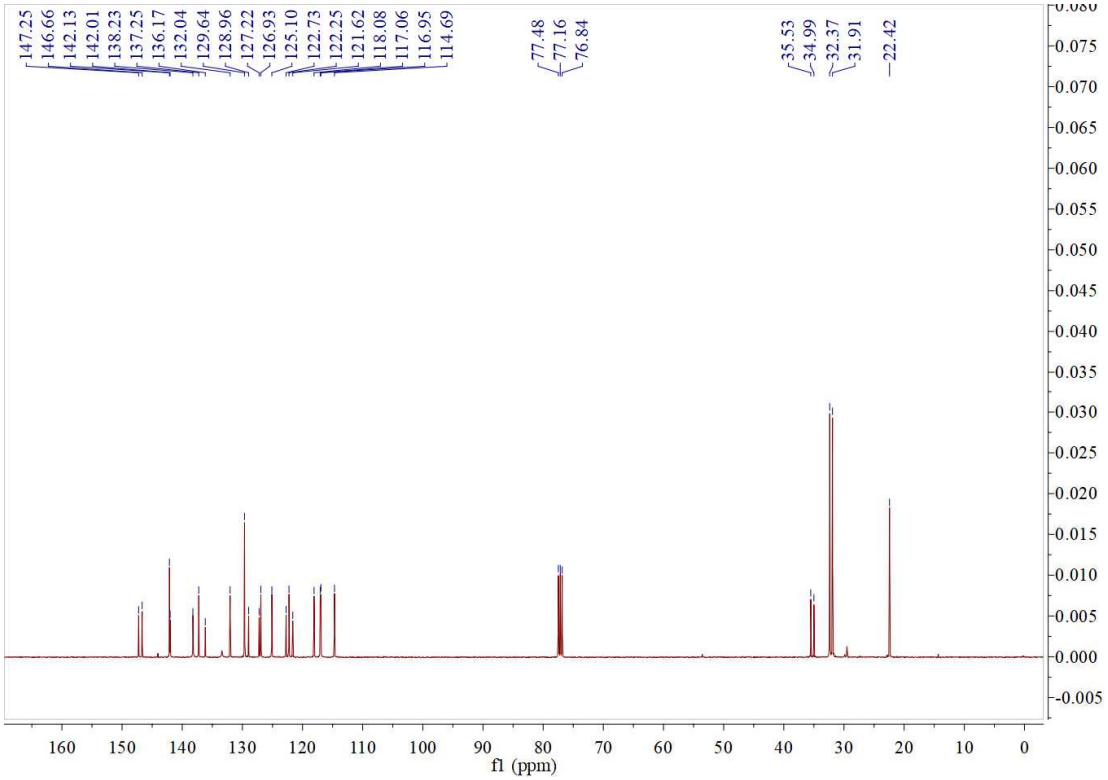


Fig. S59 ^{13}C NMR Spectra of **8** (100 MHz, $CDCl_3$)

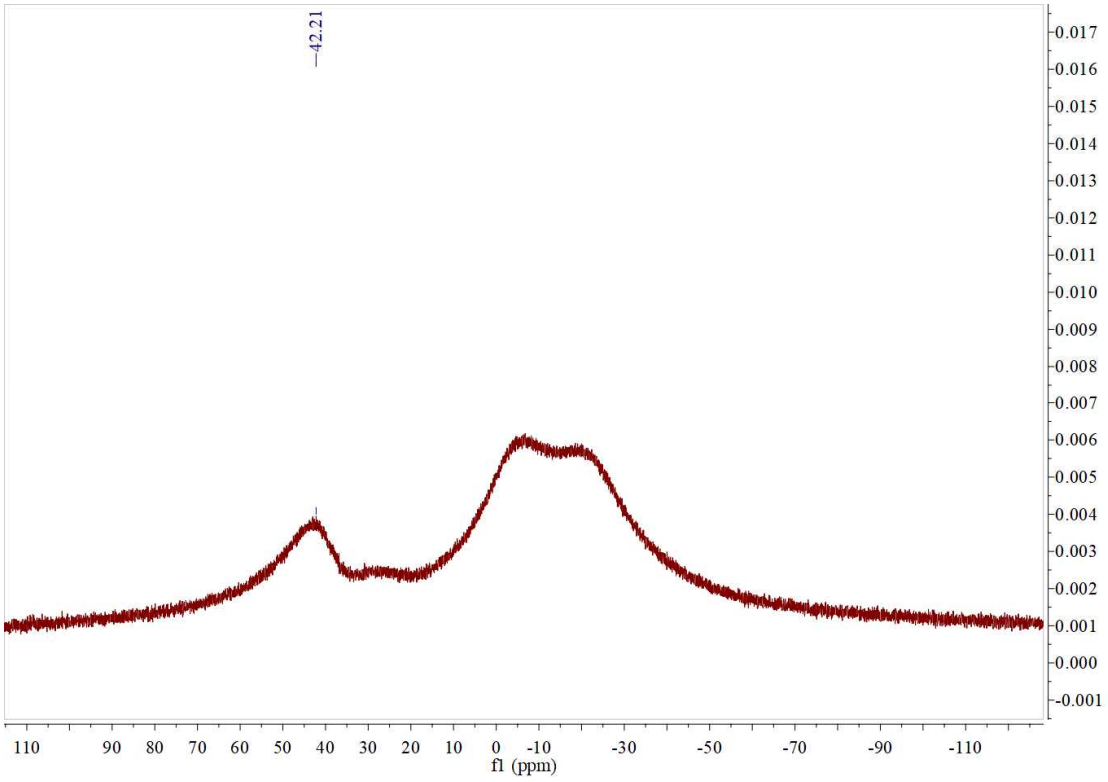


Fig. S60 ^{11}B NMR Spectra of **8** (128 MHz, $CDCl_3$)

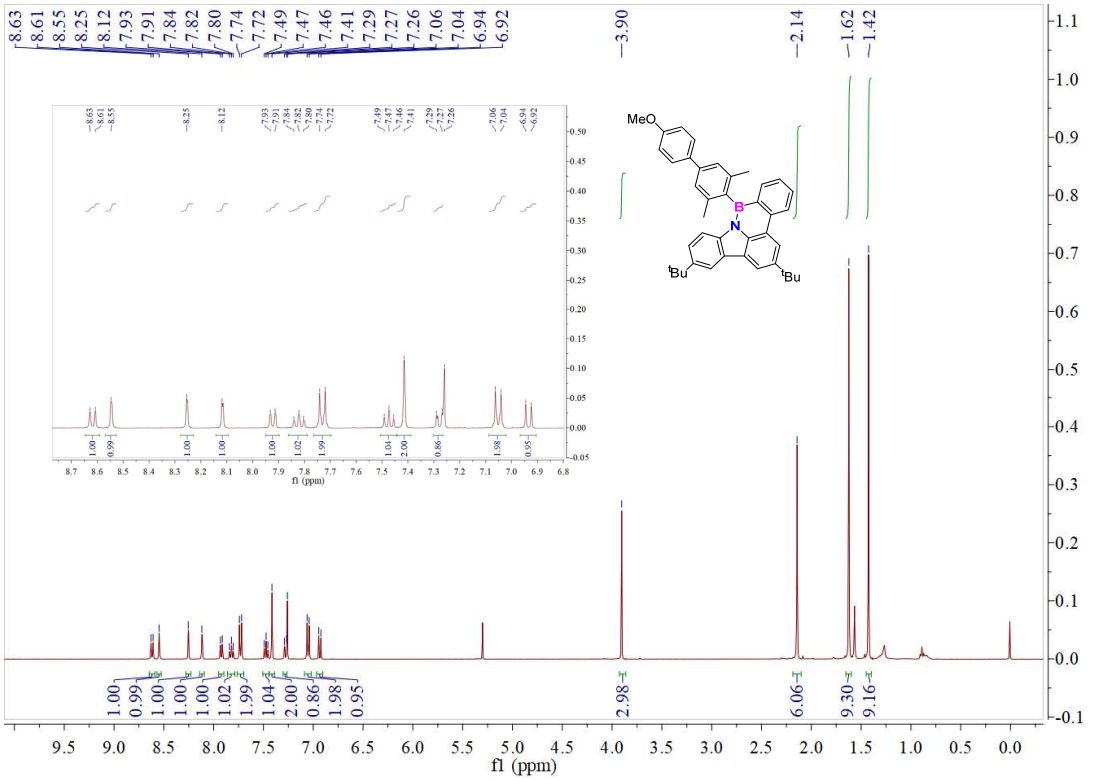


Fig. S61 ^{1}H NMR Spectra of **9** (400 MHz, $CDCl_3$)

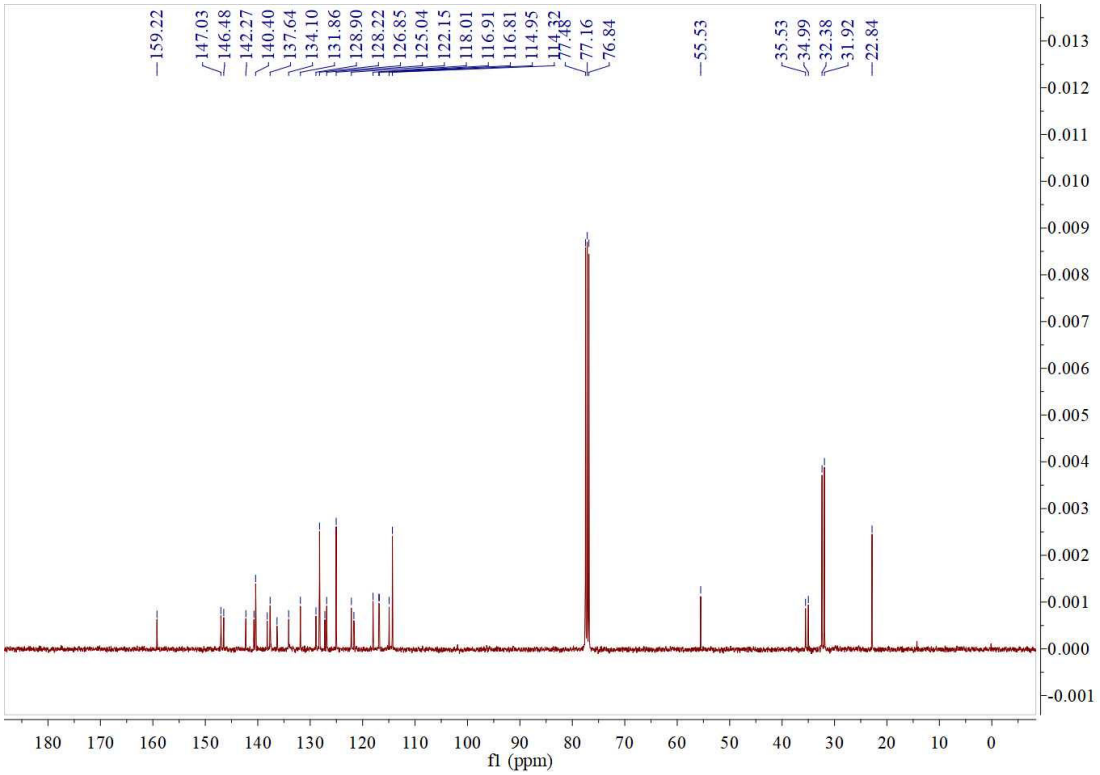


Fig. S62 ^{13}C NMR Spectra of **9** (100 MHz, $CDCl_3$)

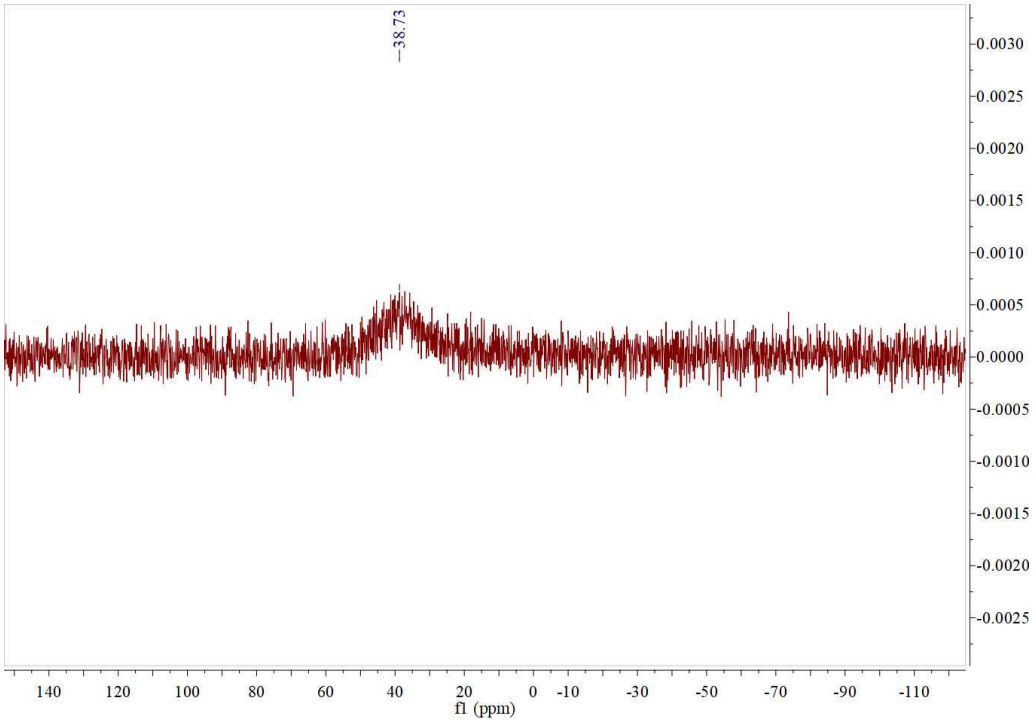


Fig. S63 ^{11}B NMR Spectra of **9** (128 MHz, $CDCl_3$, in quartz NMR tube)

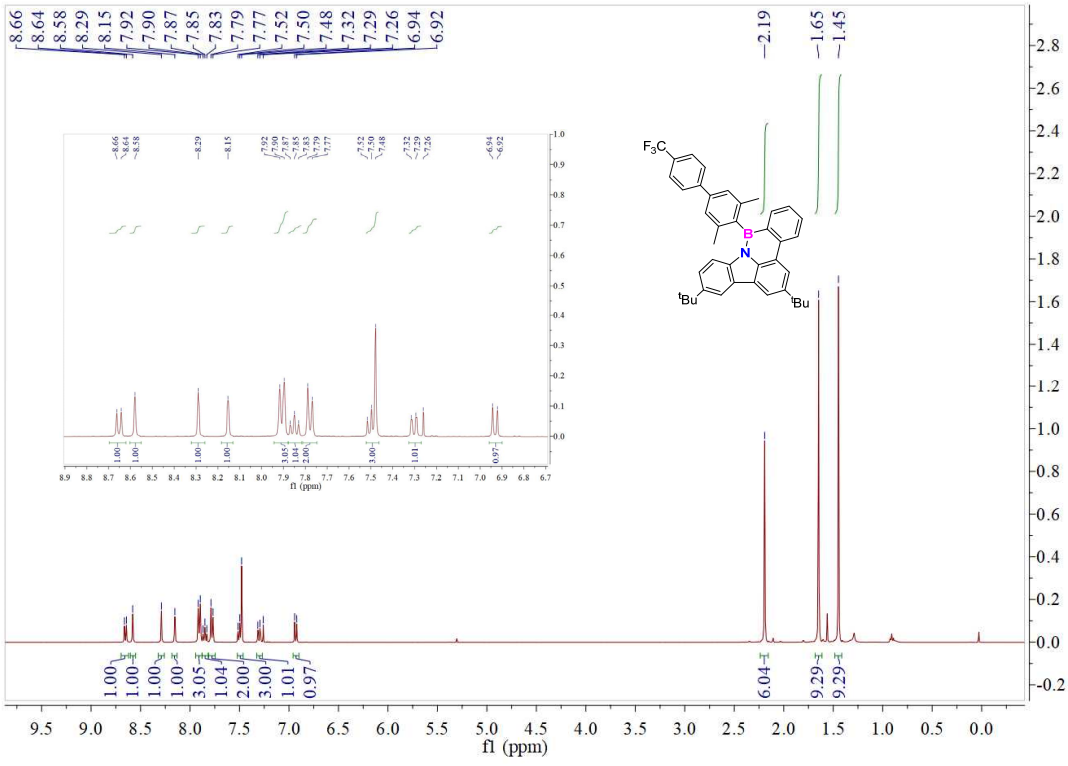


Fig. S64 ^{1}H NMR Spectra of **10** (400 MHz, $CDCl_3$)

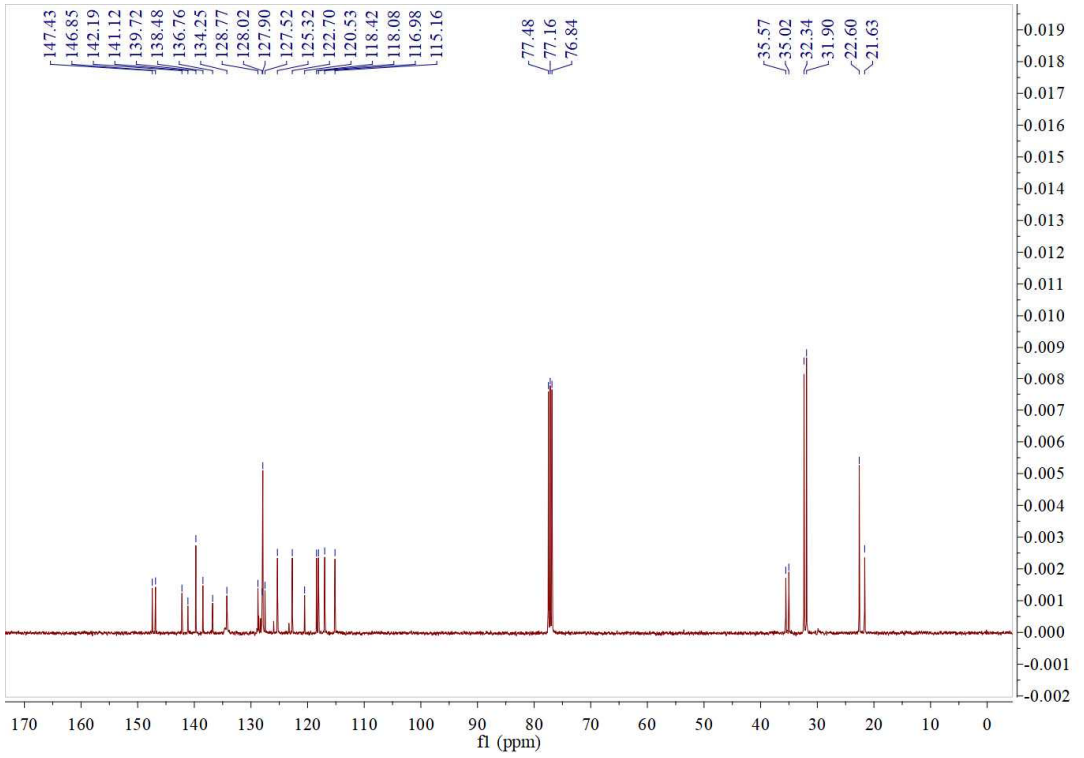


Fig. S65 ^{13}C NMR Spectra of **10** (100 MHz, $CDCl_3$)

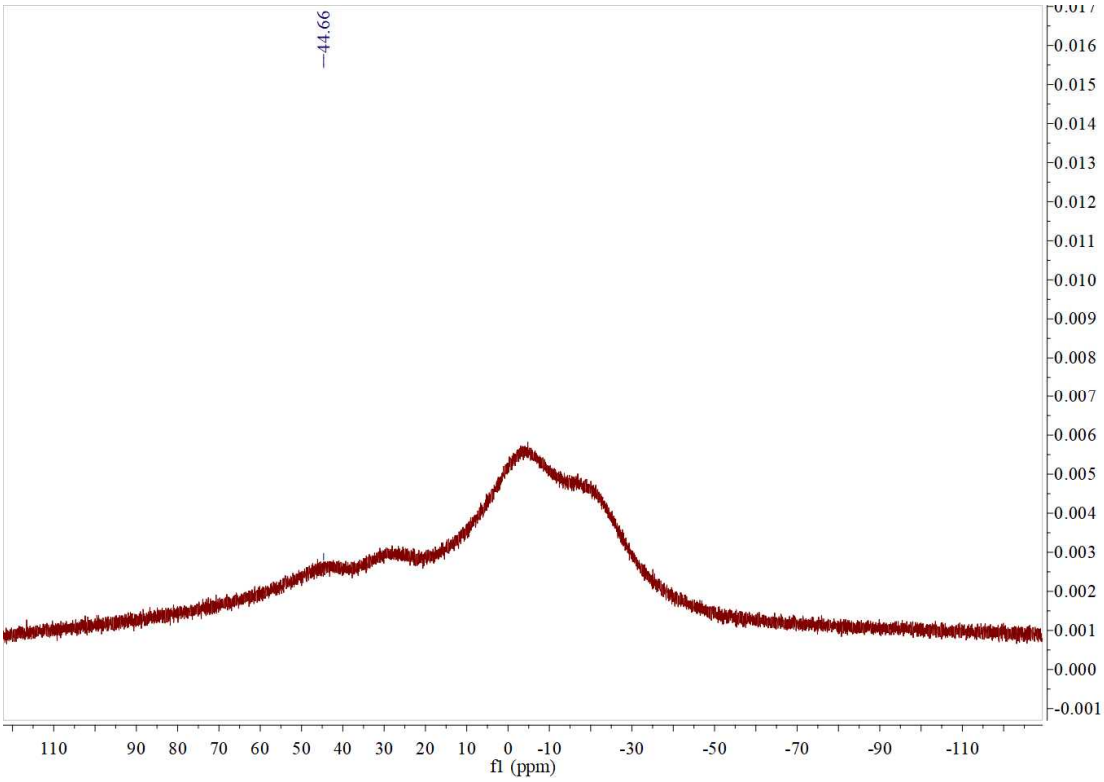


Fig. S66 ^{11}B NMR Spectra of **10** (128 MHz, $CDCl_3$)

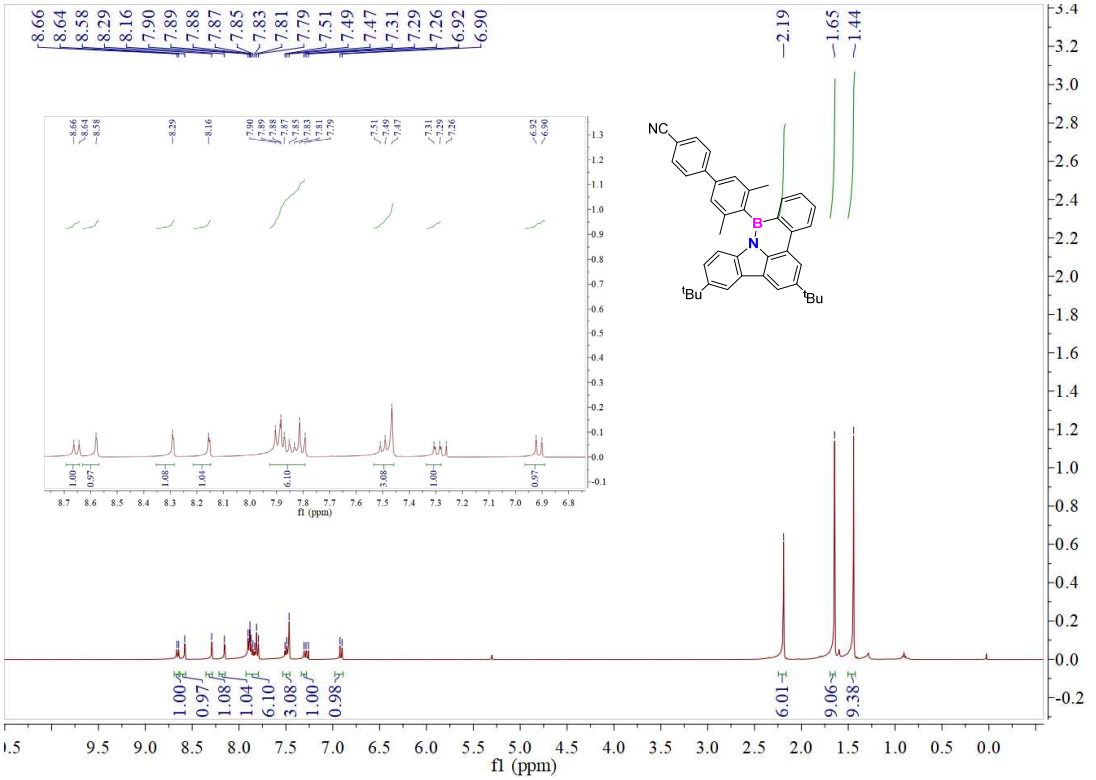


Fig. S67 ^{1}H NMR Spectra of **11** (400 MHz, $CDCl_3$)

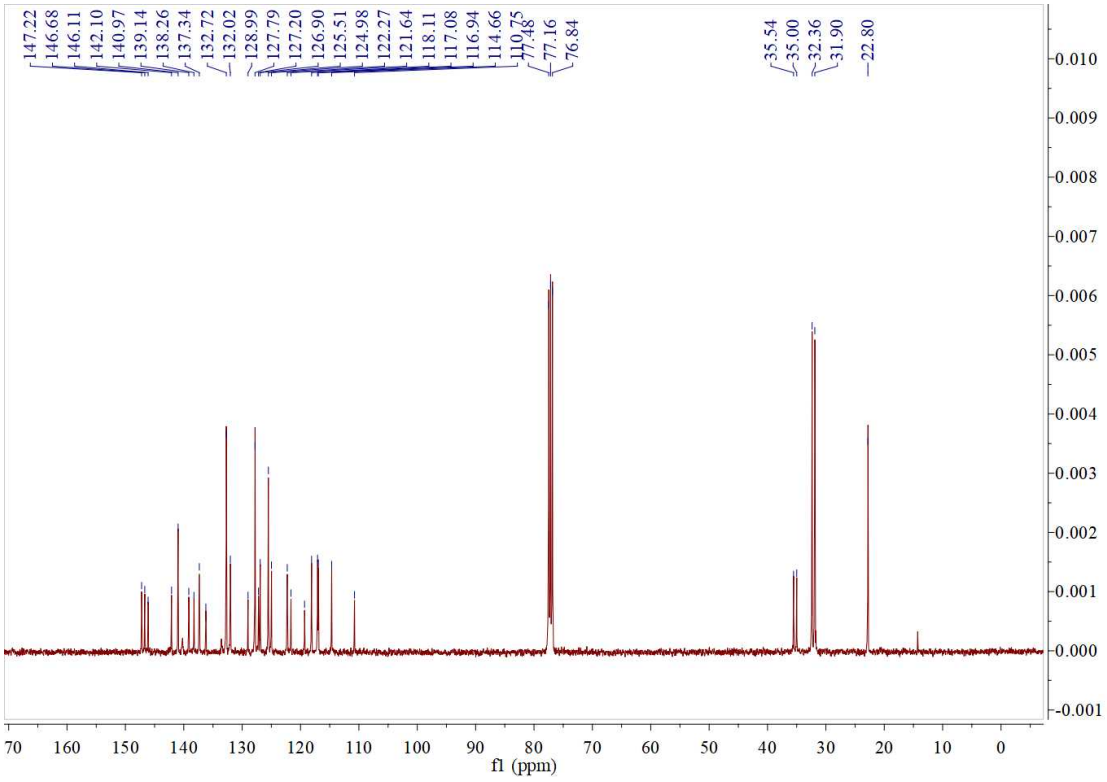


Fig. S68 ^{13}C NMR Spectra of **11** (100 MHz, $CDCl_3$)

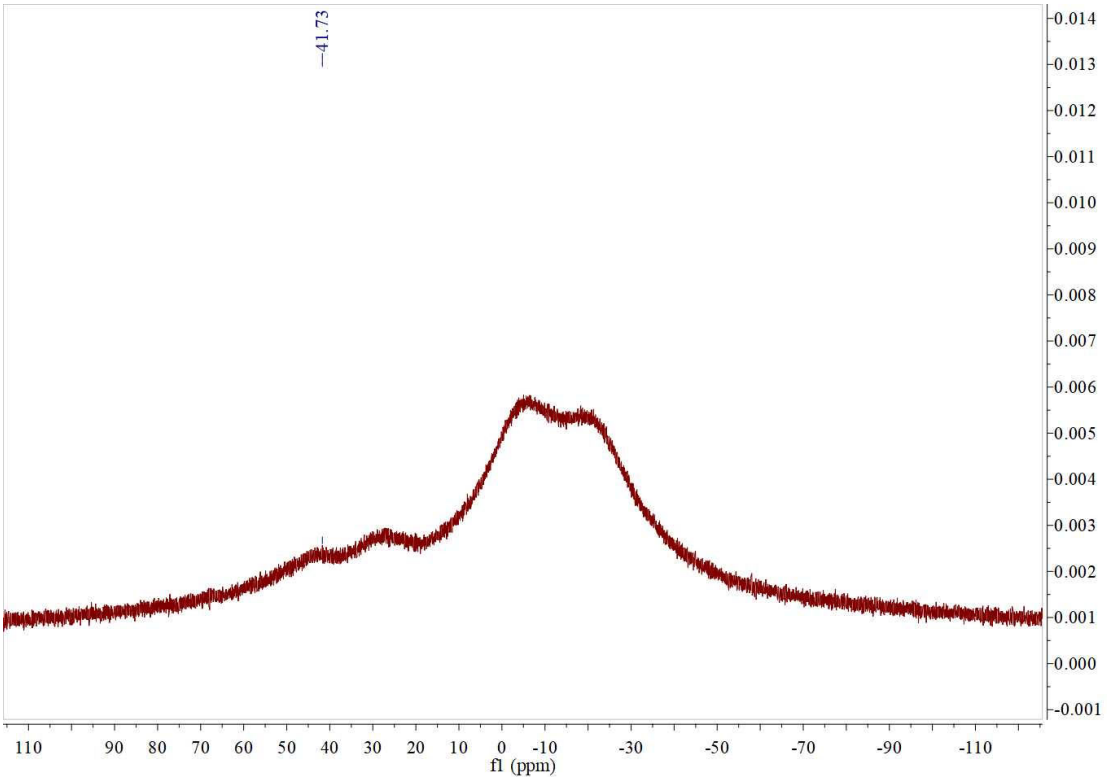


Fig. S69 ^{11}B NMR Spectra of **11** (128 MHz, $CDCl_3$)

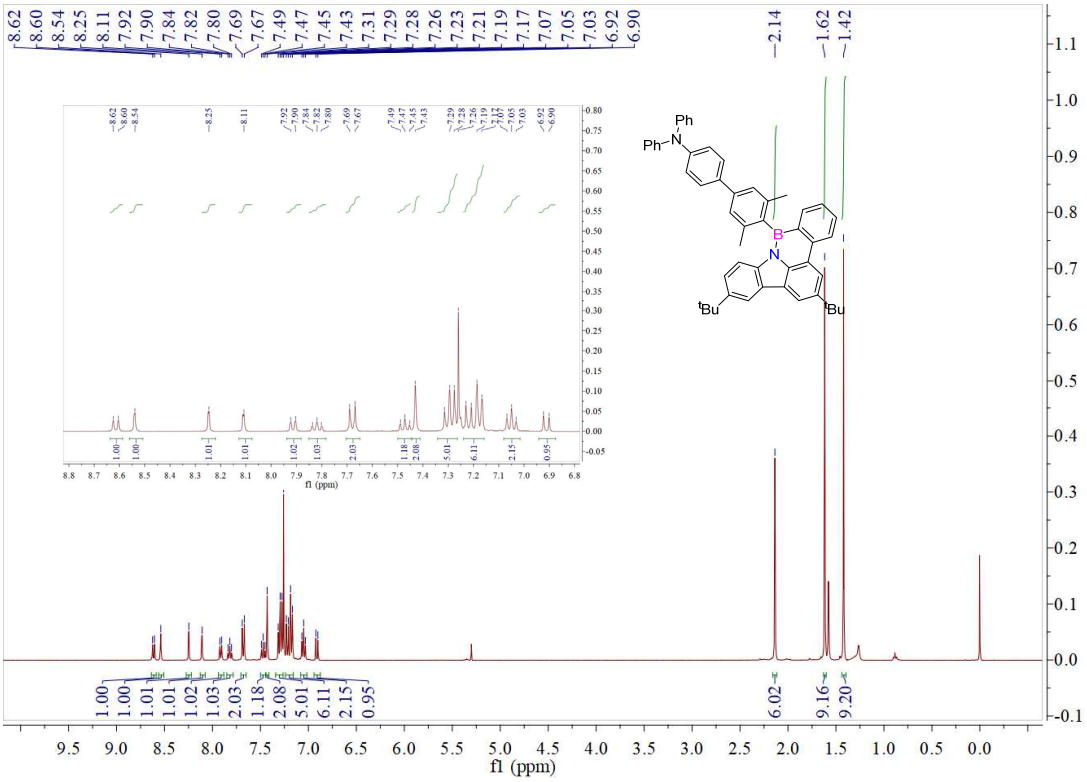


Fig. S70 ^{1}H NMR Spectra of **12** (400 MHz, $CDCl_3$)

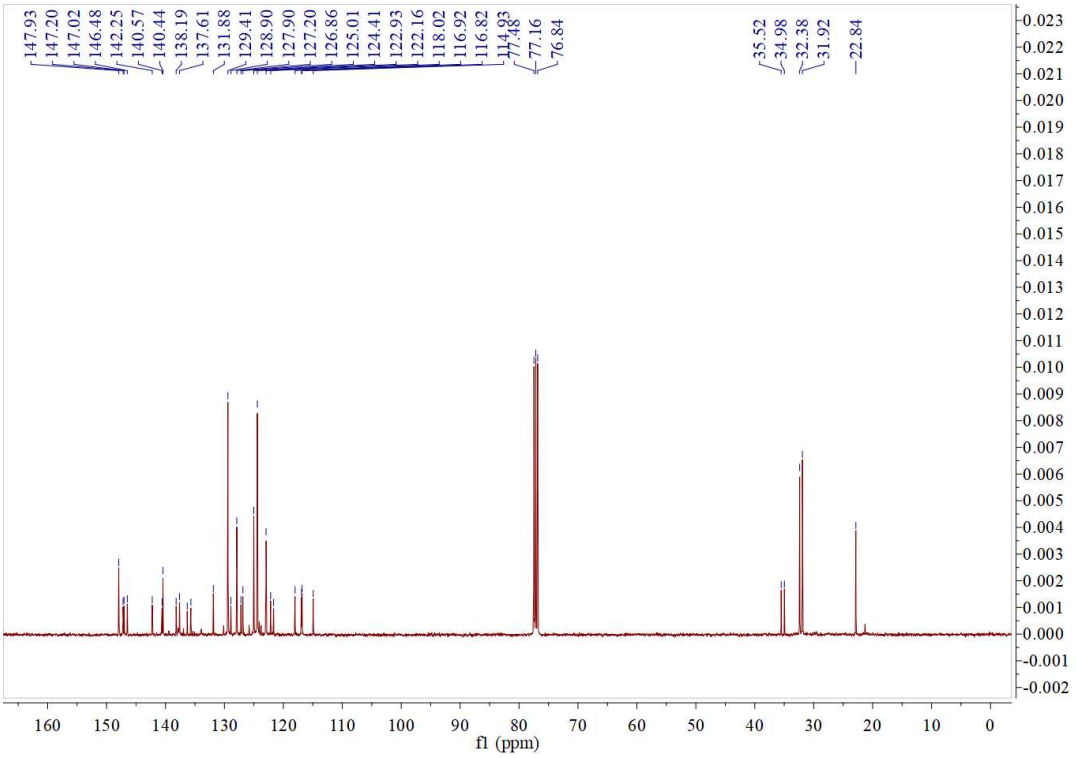


Fig. S71 ^{13}C NMR Spectra of **12** (100 MHz, $CDCl_3$)

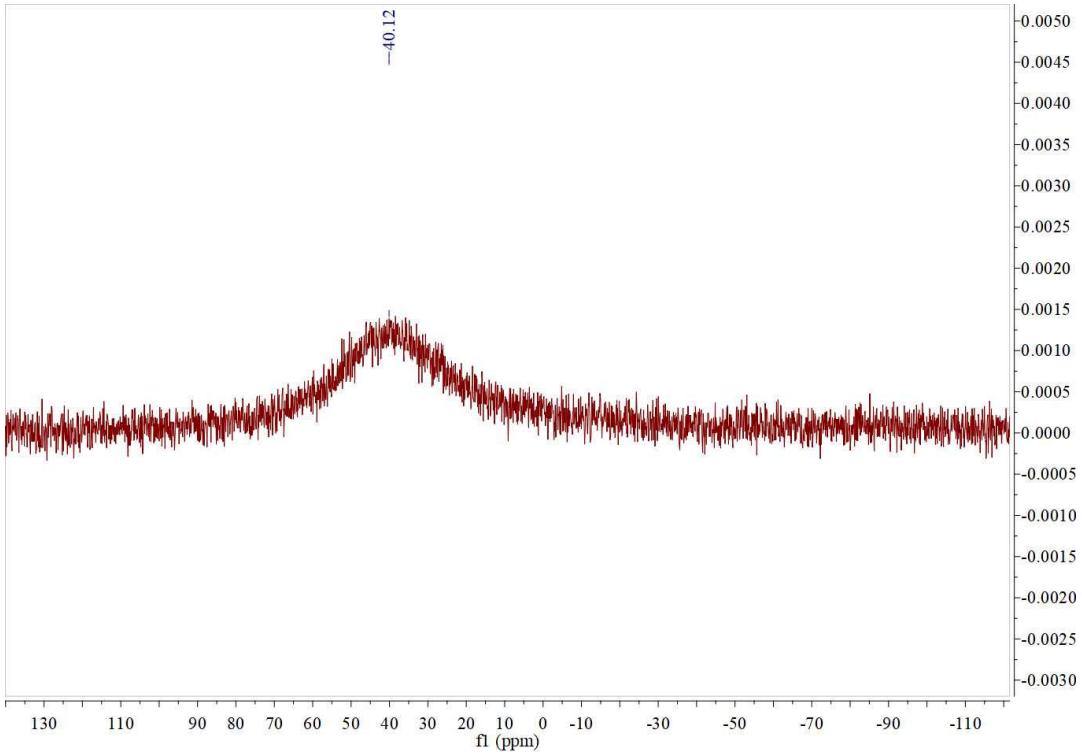


Fig. S72 ^{11}B NMR Spectra of **12** (128 MHz, $CDCl_3$, in quartz NMR tube)

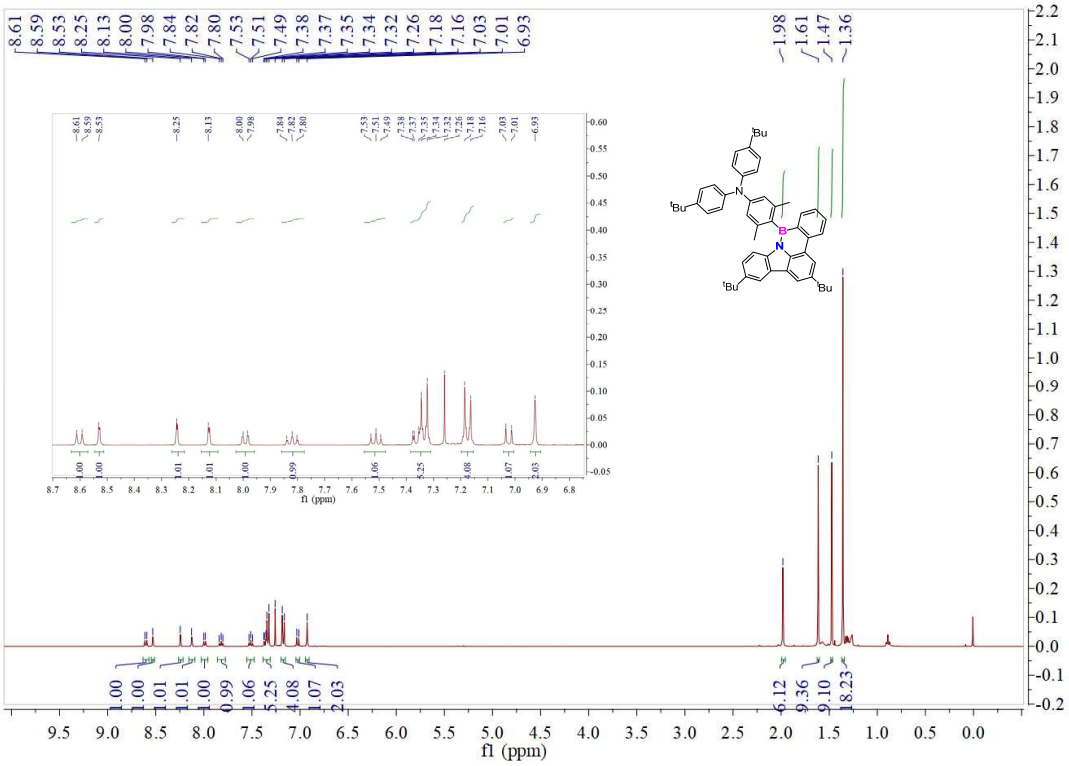


Fig. S73 ^{1}H NMR Spectra of **13** (400 MHz, $CDCl_3$)

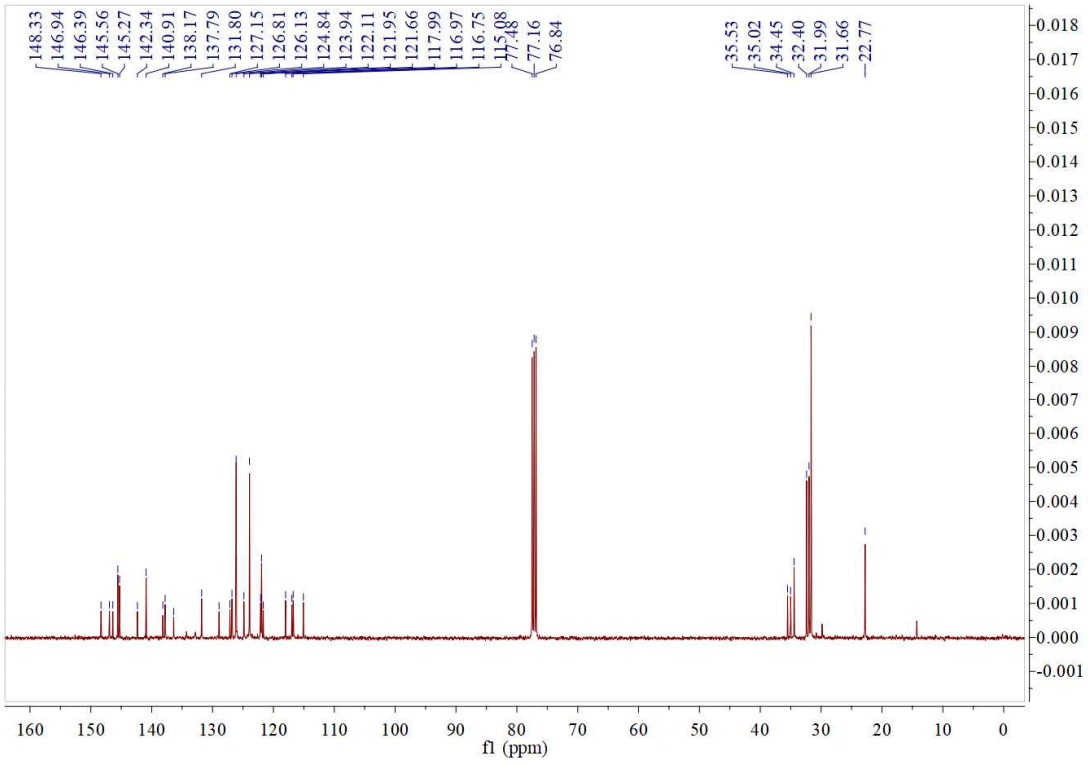


Fig. S74 ^{13}C NMR Spectra of **13** (100 MHz, $CDCl_3$)

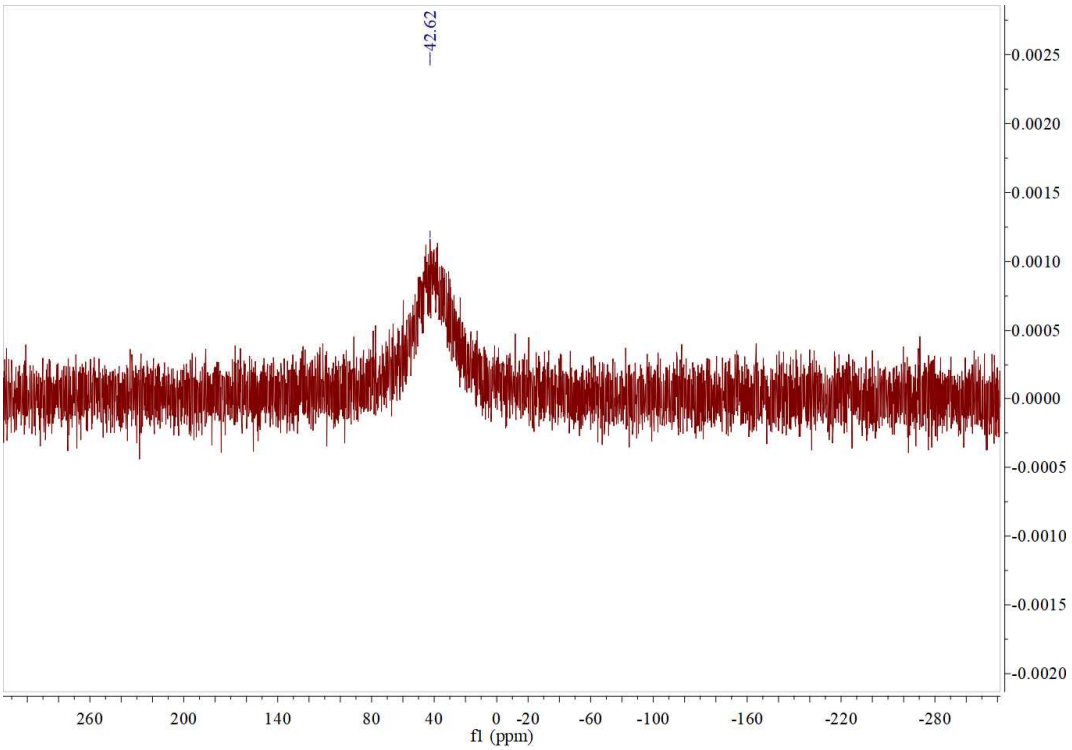


Fig. S75 ^{11}B NMR Spectra of **13** (128 MHz, $CDCl_3$, in quartz NMR tube)