Electronic Supplementary Information

Indole-Fused BN-Heteroarenes as Narrowband Blue Emitters for Organic Light-Emitting Diodes

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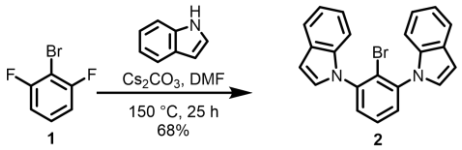
Table of Contents

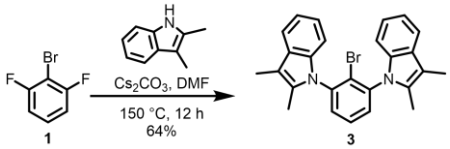
1. General Methods

Unless otherwise noted, all materials were purchased from commercial sources and all these chemicals were used as received without further purification. Thin layer chromatography (TLC) was performed on silica gel with GF254 indicator. All yields given were referred to isolated yields. Nuclear magnetic resonance (NMR) spectra were recorded on AVANCE 400 MHz Bruker spectrometers. Chemical shifts (δ) were reported in ppm. Coupling constants (J values) were reported in Hertz. ^{1}H NMR chemical shifts were referenced to $CHCl_3$ (7.260 ppm), $CHDCl_2$ (5.320 ppm). ^{13}C NMR chemical shifts were referenced to $CDCl_3$ (77.16 ppm), CD_2Cl_2 (54.00 ppm). The following abbreviations were used for multiplicities: s = singlet, d = doublet, t = triplet, m = multiplet. High-resolution mass spectrometry (HRMS) was performed either on Varian 7.0T FTMS by electrospray ionization (ESI) or on a Bruker Solarix scimax MRMS by matrix-assisted laser desorption/ionization (MALDI) with or without tetracyanoquinodimethane (TCNQ) as the matrix. The high-performance liquid chromatography (HPLC) was implemented on a SHIMADZU instrument equipped with a ShimNex HE Sil column (4.6 × 250 mm, 5 μm) by using the eluent CH_2Cl_2/hexane (1 : 4) with a flow rate of 0.8 mL min^{-1}. UV-vis absorption spectra were recorded on an Analytikjena Specord 210 Plus UV-vis spectrophotometer. Fluorescence spectra were recorded on an Edinburgh FS5 Spectrofluorometer and the photoluminescence quantum yields (PLQY) were measured by an integrating sphere on an Edinburgh FSL1000 Spectrofluorometer. The phosphorescence spectra were recorded at 77 K in dilute toluene (1×10^{-5} M) after the solution was bubbled with nitrogen for 10 min on a Hitachi F-7000 Fluorescence Spectrometer. The transient photoluminescence spectra were collected on an Edinburgh FLS1000 Spectrofluorometer equipped with a R928P photomultiplier tube. Transient decay curves for prompt fluorescence were collected with a 442 nm picosecond pulsed LED (EPL450), while the delayed parts were collected with a μF2 micro-flash lamp. Cyclic voltammograms (CV) and differential pulse voltammograms (DPV) were measured under an argon atmosphere in anhydrous THF on a CHI 620E electrochemical workstation. A three-electrode system was adopted with glassy carbon as the working electrode, platinum wire as the counter electrode, and Ag/AgCl as the reference electrode. The redox potentials were calibrated with ferrocene as an external standard. Thermogravimetric analysis (TGA) was performed using a NETZSCH TG 209 analyzer under a nitrogen atmosphere.

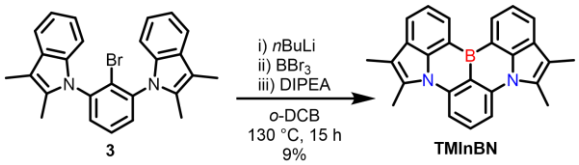
2. Synthetic Procedures



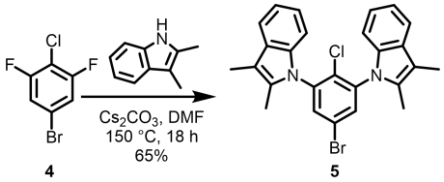
1,1'-(2-bromo-1,3-phenylene)bis(1*H*-indole) **(2)**. To a mixture of indole (918 mg, 7.83 mmol), Cs_2CO_3 (3.30 g, 10.1 mmol), and DMF (10 mL) was added 2-bromo-1,3-difluorobenzene **1** (500 mg, 2.59 mmol) under an argon atmosphere. The mixture was stirred at 150 °C for 25 h. After cooling down to room temperature, the mixture was poured into water and the residue was purified by column chromatography over silica gel (eluent: petroleum ether/CH_2Cl_2 = 5 : 1) and further by recrystallization from CH_2Cl_2/MeOH to afford 689 mg (yield: 68%) of **2** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, ppm) δ 7.74 – 7.69 (m, 2H), 7.63 – 7.54 (m, 3H), 7.32 (s, 2H), 7.28 – 7.17 (m, 6H), 6.74 (d, J = 3.2 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K, ppm) δ 140.65, 136.81, 129.40, 128.89, 128.82, 128.69, 128.60, 122.68, 121.25, 120.68, 110.64, 103.74. HRMS (ESI) *m/z*: Calcd. for $C_{22}H_{16}BrN_2$: 387.0497; Found: 387.0495 $[M + H]^+$.



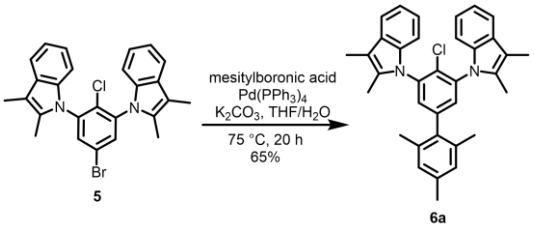
1,1'-(2-bromo-1,3-phenylene)bis(2,3-dimethyl-1*H*-indole) **(3)**. To a mixture of 2,3-dimethylindole (4.50 g, 31.0 mmol), Cs_2CO_3 (13.0 g, 39.9 mmol), and DMF (20 mL) was added 2-bromo-1,3-difluorobenzene **1** (2.00 g, 10.4 mmol) under an argon atmosphere. The mixture was stirred at 150 °C for 12 h. After cooling down to room temperature, the mixture was poured into water and the residue was purified by column chromatography over silica gel (eluent: petroleum ether/CH_2Cl_2 = 5 : 1) to afford 2.95 g (yield: 64%) of **3** as a white solid. ^{1}H NMR (400 MHz, CD_2Cl_2, 298 K, ppm) δ 7.66 (t, J = 8.00 Hz, 1H), 7.56-7.48 (m, 4H), 7.16 – 7.05 (m, 4H), 6.94 – 6.82 (m, 2H), 2.32 (s, 6H), 2.20 (d, J = 9.20 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K, ppm) δ 139.75, 136.95, 132.85, 131.33, 129.05, 128.78, 127.50, 121.51, 119.85, 118.28, 109.43, 108.49, 10.80, 9.04. HRMS (MALDI) *m/z*: Calcd. for $C_{26}H_{23}BrN_2$: 442.1045; Found: 443.1115 $[M]^+$.



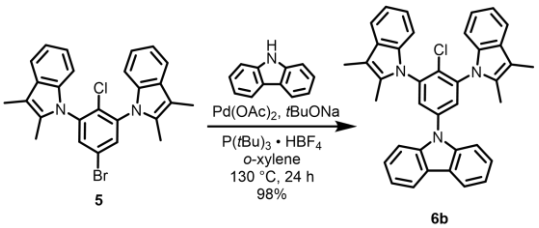
TMInBN. To a solution of **3** (1.28 g, 2.88 mmol) in 1,2-dichlorobenzene (20 mL) was added dropwise *n*BuLi (8.64 mmol, 1.6 M in hexane) at 0 °C under an argon atmosphere. After stirring at 0 °C for 4 h, BBr_3 (8.64 mmol, 1.0 M in heptane) was slowly added to the mixture at 0 °C, and then the mixture was stirred at room temperature for 4 h. Then *N,N*-diisopropylethylamine (DIPEA) (1.05 g, 8.12 mmol) was added at 0 °C, and the mixture was stirred at 130 °C for 15 h. After cooling down to room temperature, the mixture was quenched with MeOH and extracted with CH_2Cl_2 for three times. The combined organic layers were washed with water and brine and dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography over silica gel (eluent: petroleum ether/CH_2Cl_2 = 5 : 1) to afford 95 mg (yield: 9%) of **TMInBN** as a yellow solid. ^{1}H NMR (400 MHz, CD_2Cl_2, 298 K, ppm) δ 8.75 (dd, J = 7.2, 1.2 Hz, 2H), 7.96 (d, J = 8.40 Hz, 2H), 7.85 (dd, J = 7.6, 1.2 Hz, 2H), 7.76 (t, J = 8.4 Hz, 1H), 7.53 (t, J =7.2 Hz, 2H), 2.94 (s, 6H), 2.41 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K, ppm) δ 144.56, 139.07, 133.52, 132.58, 130.27, 128.37, 122.30, 121.74, 114.82, 108.62, 16.37, 9.34. HRMS (MALDI) *m/z*: Calcd. for $C_{26}H_{21}BN_2$: 372.1798; Found: 372.1793 $[M]^+$.



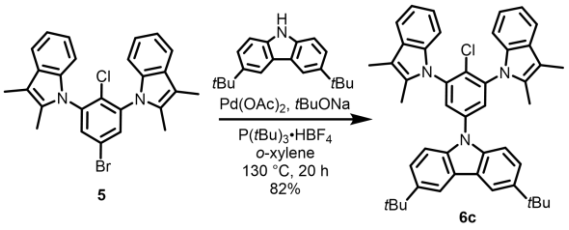
1,1'-(5-bromo-2-chloro-1,3-phenylene)bis(2,3-dimethyl-1*H*-indole) **(5)**. To a mixture of 2,3-dimethylindole (9.58 g, 66.0 mmol), Cs_2CO_3 (57.3 g, 88.0 mmol), and DMF (75 mL) was added 5-bromo-2-chloro-1,3-difluorobenzene **4** (5.00 g, 22.0 mmol) under an argon atmosphere. The mixture was stirred at 150 °C for 18 h. After cooling down to room temperature, the mixture was poured into water and the residue was purified by column chromatography over silica gel (eluent: petroleum ether/CH_2Cl_2 = 5 : 1) to afford 6.81 g (yield: 65%) of **5** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, ppm) δ 7.66 (s, 2H), 7.57 – 7.53 (m, 2H), 7.19 – 7.13 (m, 4H), 6.98 – 6.89 (m, 2H), 2.32 (s, 6H), 2.20 (d, J = 8.4 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K, ppm) δ 138.96, 136.95, 134.13, 132.77, 132.58, 129.28, 121.93, 120.37, 120.21, 118.37, 109.43, 109.27, 10.71, 9.01. HRMS (MALDI) *m/z*: Calcd. for $C_{26}H_{22}BrClN_2$: 476.0655; Found: 479.0705 $[M]^+$.



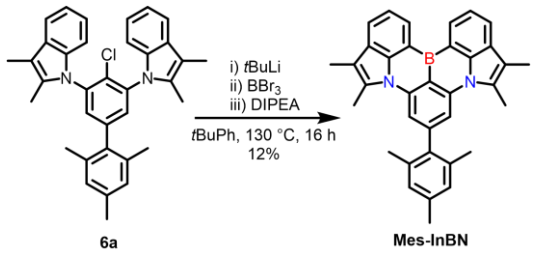
1,1'-(4-chloro-2',4',6'-trimethyl-[1,1'-biphenyl]-3,5-diyl)bis(2,3-dimethyl-1*H*-indole) **(6a)**. To a mixture of **5** (3.00 g, 6.28 mmol), mesitylboronic acid (1.54 g, 9.42 mmol), $Pd(PPh_3)_4$ (363 mg, 0.314 mmol) and K_2CO_3 (1.74 g, 12.6 mmol) was added THF (60 mL) and water (6 mL) under an argon atmosphere. The mixture was stirred at 75 °C for 20 h. After cooling down to room temperature, the mixture was extracted with CH_2Cl_2 for three times. The combined organic layers were washed with water and brine and dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography over silica gel (eluent: petroleum ether/CH_2Cl_2 = 5 : 1) to afford 2.12 g (yield: 65%) of **6a** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, ppm) δ 7.58 – 7.52 (m, 2H), 7.30 (s, 2H), 7.17 – 7.12 (m, 4H), 7.00 – 6.91 (m, 4H), 2.32 (s, 6H), 2.30 (s, 3H), 2.26 (d, J = 9.6 Hz, 6H), 2.15 (t, J = 14.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K, ppm) δ 141.47, 137.76, 137.10, 135.45, 132.92, 132.73, 132.28, 129.29, 128.59, 121.71, 121.59, 119.91, 118.36, 109.47, 109.29, 108.72, 21.17, 20.93, 10.63, 9.04. HRMS (MALDI) *m/z*: Calcd. for $C_{35}H_{33}ClN_2$: 516.2332; Found: 516.2327 $[M]^+$.



9-(4-chloro-3,5-bis(2,3-dimethyl-1*H*-indol-1-yl)phenyl)-9*H*-carbazole **(6b)**. To a mixture of **5** (500 mg, 1.04 mmol), carbazole (260 mg, 1.57 mmol), $Pd(OAc)_2$ (11 mg, 0.05 mmol), *t*BuONa (192 mg, 2.00 mmol) and $P(tBu)_3$•HBF_4 (29 mg, 0.104 mmol) was added *o*-xylene (10 mL) under an argon atmosphere. The mixture was stirred at 130 °C for 24 h. After cooling down to room temperature, the mixture was extracted with CH_2Cl_2 for three times. The combined organic layers were washed with water and brine and dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography over silica gel (eluent: petroleum ether/CH_2Cl_2 = 5 : 1) to afford 581 mg (yield: 98%) of **6b** as a white solid. ^{1}H NMR (400 MHz, CD_2Cl_2, 298 K, ppm) δ 8.15 (dt, J = 8.0, 0.8 Hz, 2H), 7.85 (d, J = 1.6 Hz, 2H), 7.61 – 7.53 (m, 4H), 7.46 (t, J = 8.0 Hz, 2H), 7.33 (td, J = 8.0, 0.8 Hz, 2H), 7.21 – 7.05 (m, 6H). 2.38 – 2.31 (m, 12H). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K, ppm) δ 140.05, 139.14, 137.50, 137.02, 132.77, 132.57, 129.34, 128.82, 126.61, 124.10, 122.02, 121.91, 121.17, 120.80, 120.23, 118.54, 109.47, 109.28, 10.87, 9.05. HRMS (MALDI) *m/z*: Calcd. for $C_{38}H_{30}ClN_3$: 563.2128; Found: 563.2114 $[M]^+$.

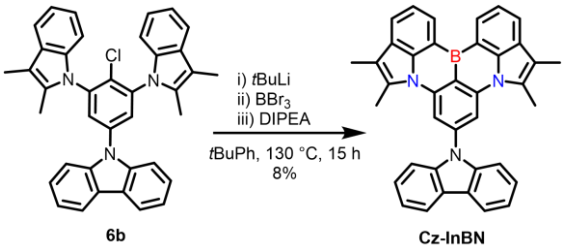


3,6-di-*tert*-butyl-9-(4-chloro-3,5-bis(2,3-dimethyl-1*H*-indol-1-yl)phenyl)-9*H*-carbazole **(6c)**. To a mixture of **5** (1.00 g, 2.09 mmol), 3,6-di-*tert*-butyl-9*H*-carbazole (877 mg, 3.14 mmol), $Pd(OAc)_2$ (23.5 mg, 0.105 mmol), $P(tBu)_3$•HBF_4 (60.7 mg, 0.209 mmol) and *t*BuONa (402 mg, 4.19 mmol) was added *o*-xylene (20 mL) under an argon atmosphere. The mixture was stirred at 130 °C for 20 h, After cooling down to room temperature, the mixture was extracted with CH_2Cl_2 for three times. The combined organic layers were washed with water and brine and dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography over silica gel (eluent: petroleum ether/CH_2Cl_2 = 5 : 1) to afford 1.16 g (yield: 82%) of **6c** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, ppm) δ 8.11 (t, J = 1.2 Hz, 2H), 7.79 (s, 2H), 7.60 – 7.54 (m, 2H), 7.49 (d, J = 1.2 Hz, 4H), 7.23 – 7.15 (m, 4H), 7.12 – 7.03 (m, 2H), 2.34 (d, J = 3.2 Hz, 12H), 1.44 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K, ppm) δ 144.27, 138.98, 138.30, 138.04, 137.06, 132.80, 132.60, 129.37, 128.21, 124.30, 121.87, 120.12, 118.50, 116.71, 109.47, 109.29, 109.12, 109.06, 34.92, 32.05, 10.84, 9.05. HRMS (ESI) *m/z*: Calcd. for $C_{46}H_{47}ClN_3$: 676.3459; Found: 676.3456 $[M + H]^+$.



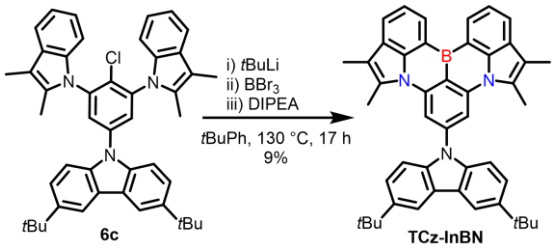
Mes-InBN. To a solution of **6a** (1.20 g, 2.32 mmol) in *t*BuPh (15 mL) was added slowly *t*BuLi (6.96 mmol, 1.3 M in hexane) at 0 °C under an argon atmosphere. After stirring at 60 °C for 3 h, BBr_3 (6.96 mmol, 1.0 M in heptane) was slowly added to the mixture at 0 °C, and then the mixture was stirred at room temperature for 13 h. Then DIPEA (900 mg, 6.96 mmol) was added at 0 °C. The mixture was stirred at 130 °C for 16 h. After cooling down to room temperature, the mixture was quenched with MeOH and extracted with CH_2Cl_2 for three times. The combined organic layers were washed with water and brine and dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography over silica gel (eluent: petroleum ether/CH_2Cl_2 = 5 : 1) to afford 140 mg (yield: 12%) of **Mes-InBN** as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, ppm) δ 8.80 (d, J = 7.6 Hz, 2H), 7.85 (d, J = 7.6 Hz, 2H), 7.72 (s, 2H), 7.55 (t, J = 7.6 Hz, 2H), 7.05 (s, 2H), 2.86 (s, 6H), 2.41 (d, J = 3.2 Hz, 9H), 2.17 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$, 298

K, ppm) δ 145.82, 144.74, 139.70, 139.26, 137.20, 136.03, 133.51, 130.31, 130.28, 128.46, 128.37, 122.35, 121.83, 114.91, 109.94, 108.64, 21.28, 21.00, 16.52, 9.34. HRMS (MALDI) *m/z*: Calcd. for $C_{35}H_{31}BN_2$: 490.2580; Found: 490.2574 $[M]^+$.



6b **Cz-InBN**

Cz-InBN. To a solution of **6b** (650 mg, 1.15 mmol) in *t*BuPh (15 mL) was added slowly *t*BuLi (3.46 mmol, 1.3 M in hexane) at 0 °C under an argon atmosphere. After stirring at 60 °C for 4 h, BBr_3 (3.46 mmol, 1.0 M in heptane) was slowly added to the mixture at 0 °C, and then the mixture was stirred at room temperature for 10 h. Then DIPEA (446 mg, 3.46 mmol) was added at 0 °C. The mixture was stirred at 130 °C for 15 h. After cooling down to room temperature, the mixture was quenched with MeOH and extracted with CH_2Cl_2 for three times. The combined organic layers were washed with water and brine and dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography over silica gel (eluent: petroleum ether/CH_2Cl_2 = 5 : 1) to afford 51 mg (yield: 8%) of **Cz-InBN** as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, ppm) δ 8.84 (d, J = 7.6 Hz, 2H), 8.26 – 8.17 (m, 4H), 7.88 (d, J = 7.6 Hz, 2H), 7.74 (d, J = 8.0 Hz, 2H), 7.59 (t, J = 7.6 Hz, 2H), 7.49 (t, J = 7.6 Hz, 2H), 7.37 (t, J = 7.6 Hz, 2H), 2.86 (s, 6H), 2.41 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K, ppm) δ 145.83, 141.58, 140.79, 139.44, 133.41, 130.59, 128.53, 126.45, 123.97, 122.65, 120.71, 120.59, 115.64, 110.10, 106.77, 16.47, 9.34. HRMS (MALDI) *m/z*: Calcd. for $C_{38}H_{28}BN_3$: 537.2376; Found: 537.2362 $[M]^+$.



6c **TCz-InBN**

TCz-InBN. To a solution of **6c** (1.30 g, 1.92 mmol) in *t*BuPh (20 mL) was added slowly *t*BuLi (5.76 mmol, 1.3 M in hexane) at 0 °C under an argon atmosphere. After stirring at 60 °C for 2 h, BBr_3 (5.76 mmol, 1.0 M in heptane) was slowly added to the mixture at 0 °C, and then the mixture was stirred at room temperature for 5 h. Then DIPEA (743 mg, 5.76 mmol) was added at 0 °C. The mixture was stirred at 130 °C for 17 h. After cooling down to room temperature, the mixture was quenched with MeOH and extracted with CH_2Cl_2 for three times. The combined organic layers were washed with water and brine and dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by column chromatography over silica gel (eluent: petroleum ether/CH_2Cl_2 = 5 : 1) to afford 111 mg (yield: 9%) of **TCz-InBN** as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, ppm) δ 8.83 (d, J = 7.6 Hz 2H), 8.23 – 8.15 (m, 4H), 7.86 (d, J = 7.6 Hz 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.58 (t, J = 7.6 Hz, 2H), 7.52 (dd, J = 8.4, 2.0 Hz, 2H), 2.87 (s, 6H), 2.41 (s, 6H), 1.50 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K, ppm) δ 145.71, 143.56, 142.03, 139.36, 139.06, 133.42, 130.46, 128.44, 124.07, 123.93, 122.49, 122.08, 116.63, 115.42, 109.53, 106.42, 34.96, 32.18, 16.56, 9.34. HRMS (MALDI) *m/z*: Calcd. for $C_{46}H_{44}BN_3$: 649.3628; Found: 649.3628 $[M]^+$.

3. Thermal Properties

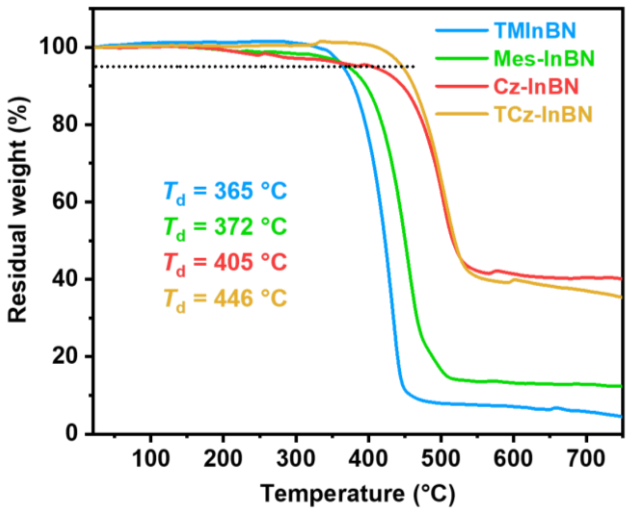


Figure S1. TGA curves of TMInBN, Mes-InBN, Cz-InBN, and TCz-InBN at a heating rate of 10 °C min^{-1} under a nitrogen atmosphere. Decomposition temperature (T_d): 5% weight loss.

4. Photophysical and Electrochemical Properties

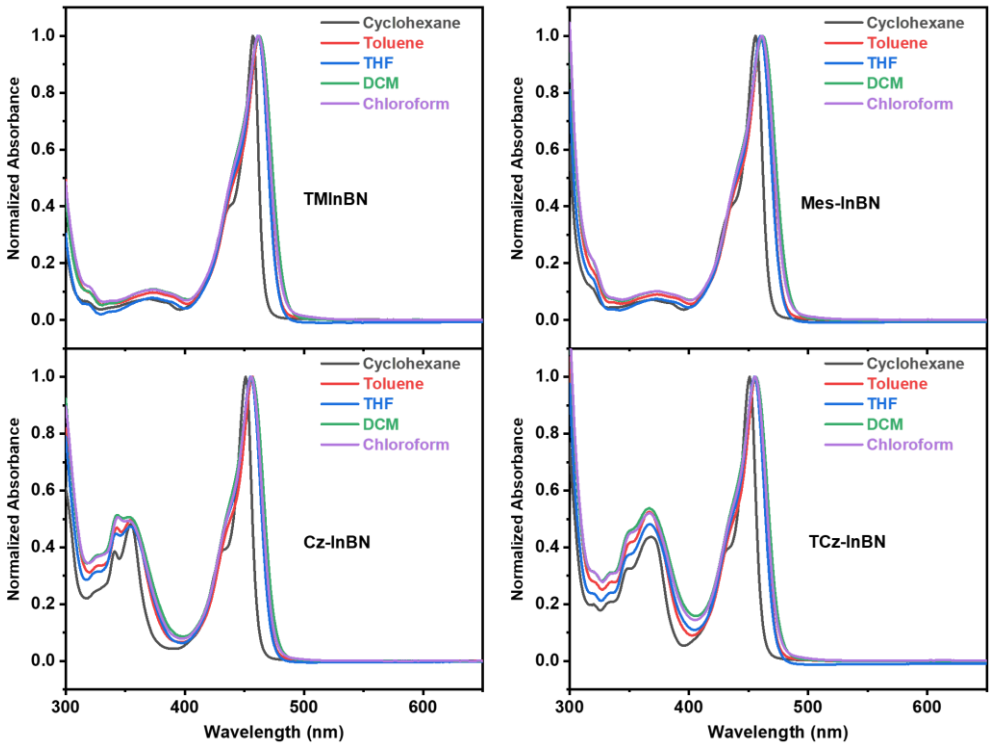


Figure S2. UV-vis absorption spectra of TMInBN, Mes-InBN, Cz-InBN, and TCz-InBN in different solvents (1×10^{-5} M).

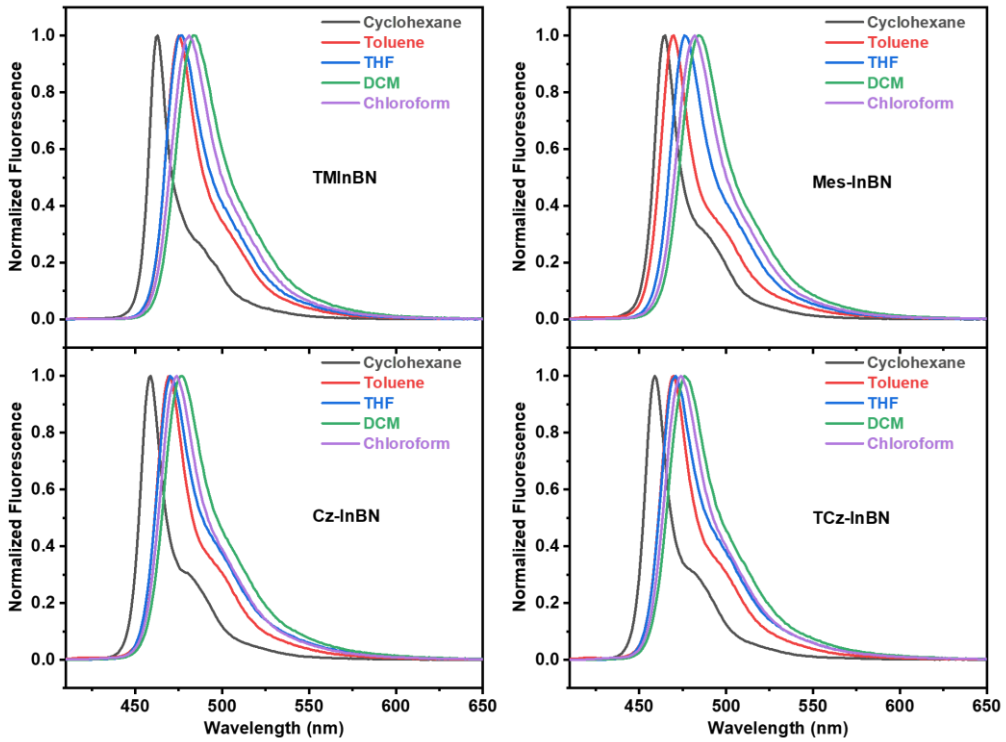


Figure S3. Normalized emission spectra of TMInBN, Mes-InBN, Cz-InBN, and TCz-InBN in different solvents (1×10^{-5} M).

Table S1. Summary of emission maxima and FWHMs (in parentheses) of TMInBN, Mes-InBN, Cz-InBN, and TCz-InBN in different solvents.

Compound	Cyclohexane (nm)	Toluene (nm)	THF (nm)	DCM (nm)	Chloroform (nm)
TMInBN	462 (14)	475 (23)	477 (27)	484 (33)	481 (31)
Mes-InBN	465 (17)	470 (22)	476 (27)	484 (32)	482 (30)
Cz-InBN	459 (16)	470 (22)	470 (27)	477 (32)	474 (28)
TCz-InBN	459 (16)	470 (22)	471 (28)	476 (31)	474 (29)

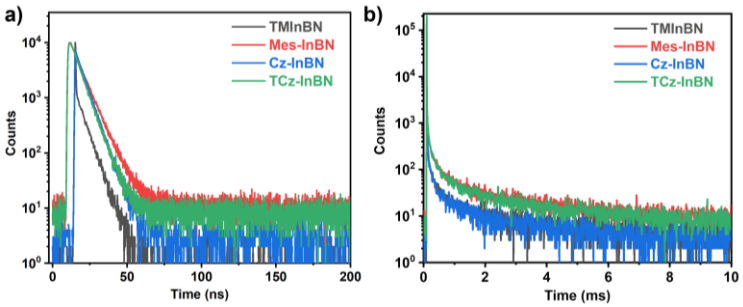


Figure S4. a) Prompt and b) delayed photoluminescence decay curves of TMInBN, Mes-InBN, Cz-InBN, and TCz-InBN in degassed toluene (1×10^{-5} M, 298 K).

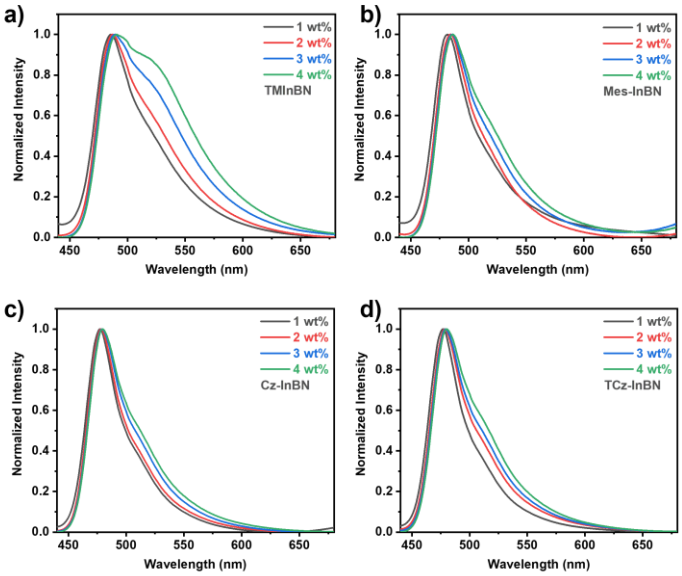


Figure S5. Normalized emission spectra of a) TMInBN, b) Mes-InBN, c) Cz-InBN, and d) TCz-InBN doped in mCPBC films with different dopant concentrations. mCPBC: 9-(3-(9*H*-carbazol-9-yl)phenyl)-9*H*-3,9'-bicarbazole.

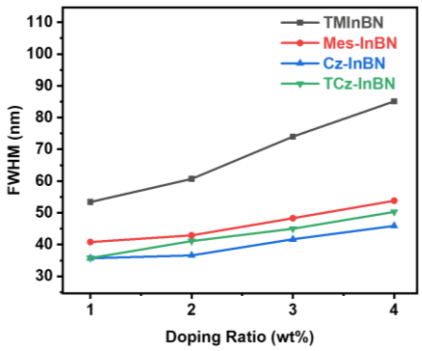


Figure S6. The full width at half maximum (FWHM) of TMInBN, Mes-InBN, Cz-InBN, and TCz-InBN at different dopant concentrations (in mCPBC).

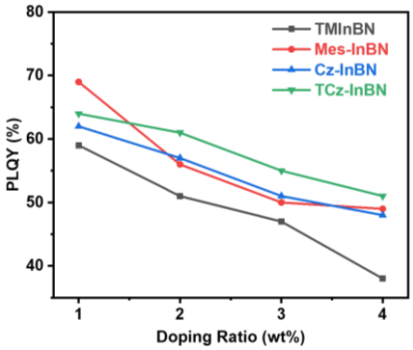


Figure S7. The PLQYs of TMInBN, Mes-InBN, Cz-InBN, and TCz-InBN at different dopant concentrations (in mCPBC).

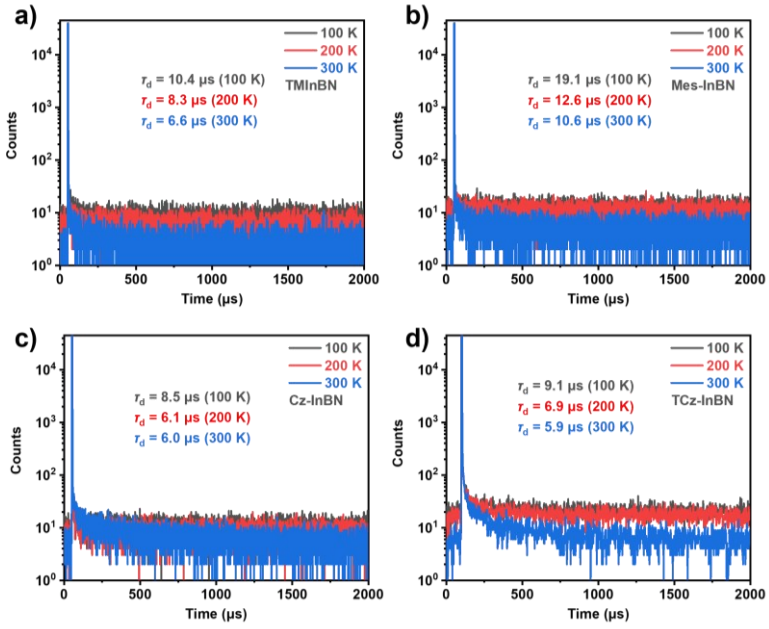


Figure S8. Variable-temperature transient photoluminescence decay curves of a) TMInBN, b) Mes-InBN, c) Cz-InBN, and d) TCz-InBN in mCPBC doped film (1 wt%).

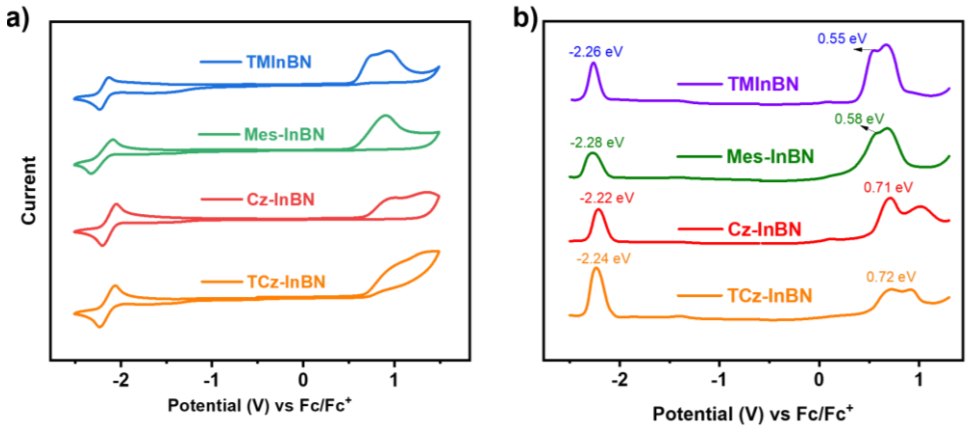


Figure S9. a) Cyclic voltammograms (scan rate: 100 mV s^{-1}) and b) differential pulse voltammograms of TMInBN, Mes-InBN, Cz-InBN, and TCz-InBN in THF (1 mM) at room temperature with 0.1 M *n*-Bu_4NPF_6 as supporting electrolyte and ferrocene as an external standard.

Table S2. Summary of the photophysical and electrochemical properties of TMInBN, Mes-InBN, Cz-InBN, and TCz-InBN.

Compound	λ_{onset} (nm)	E_g^{opt} (eV)	λ_{PL} (nm)	$HOMO^{CV}$ (eV)	$LUMO^{CV}$ (eV)	E_g^{CV} (eV)	$HOMO^{DPV}$ (eV)	$LUMO^{DPV}$ (eV)	E_g^{DPV} (eV)
TMInBN	477	2.60	475	-5.37	-2.69	2.68	-5.35	-2.54	2.81
Mes-InBN	477	2.60	475	-5.37	-2.67	2.70	-5.38	-2.52	2.86
Cz-InBN	471	2.63	470	-5.49	-2.75	2.74	-5.51	-2.58	2.93
TCz-InBN	471	2.63	470	-5.48	-2.73	2.75	-5.52	-2.56	2.96

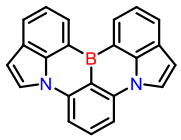
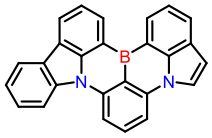
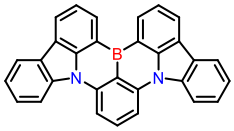
λ_{onset} is the lowest-energy absorption onset; E_g^{opt} is the optical energy gap derived from the lowest-energy absorption onset in the absorption spectrum; λ_{em} is emission maximum; the $HOMO^{CV}$ and $LUMO^{CV}$ energy levels are calculated according to the equations $HOMO = -(4.80 + E_{ox}^{CV})$ and $LUMO = -(4.80 + E_{red}^{CV})$, where E_{ox}^{CV} and E_{red}^{CV} are the onset potentials of the first oxidative and reductive waves, respectively; the $HOMO^{DPV}$ and $LUMO^{DPV}$ energy levels are calculated according to the equations $HOMO = -(4.80 + E_{ox}^{DPV})$ and $LUMO = -(4.80 + E_{red}^{DPV})$, where E_{ox}^{DPV} and E_{red}^{DPV} are the peak potentials of the first oxidative and reductive waves, respectively.

5. Theoretical Calculations

Theoretical calculations were performed using the Gaussian 09 software package.[1] All calculations were carried out using the density functional theory (DFT) method. The geometries were optimized at the B3LYP/6-31G(d,p) level, and the energies were calculated at the same level of theory. Time-dependent DFT (TD-DFT) calculations were performed at the B3LYP/6-311G(d,p) or B3LYP/6-311G(d) level. The electron excitation analysis of major molecular orbital (MO) transitions in all excited states was carried out by Multiwfn.[2] The spin-orbit coupling (SOC) matrix elements between triplets and singlets ($<S_1|\hat{H}_{SOC}|T_n>$) were calculated by the ORCA 4.1.0 software package by the B3LYP method with the TZVP basis set.[3] The $<S_1|\hat{H}_{SOC}|T_n>$ is defined by the square root of the sum of squares of the real and imaginary parts (*Re* and *Im*) of the matrix elements (eq. S1). The root-mean-square deviation (RMSD) values were calculated by VMD 1.9.4.[4] The Spin-Component Scaling second-order approximate Coupled-Cluster (SCS-CC2) calculations were performed using the MRCC Program with the cc-pVDZ basis set.[5,6]

$$\langle S_1|\hat{H}_{SOC}|T_n\rangle = \sum_{m=0,\pm1}\left[\left(\mathrm{Re}\langle S_1|\hat{H}_{SOC}|T_n\rangle\right)^2+\left(\mathrm{Im}\langle S_1|\hat{H}_{SOC}|T_n\rangle\right)^2\right]^{1/2} \qquad \text{eq. S1}$$

Table S3. TD-DFT calculation results at the B3LYP/6-311G(d) level for InBN, InCzBN and CzBN at the optimized S_0 and S_1 geometries.

Compound	Transition	Wavelength (nm)	Energy (eV)	Oscillator strength
 InBN	$S_0 \rightarrow S_1$	418.56	2.9622	0.2657
	$S_1 \rightarrow S_0$	440.45	2.8149	0.2235
 InCzBN	$S_0 \rightarrow S_1$	423.99	2.9242	0.3016
	$S_1 \rightarrow S_0$	446.69	2.7756	0.2528
 CzBN	$S_0 \rightarrow S_1$	427.92	2.8973	0.3337
	$S_1 \rightarrow S_0$	450.34	2.7531	0.2746

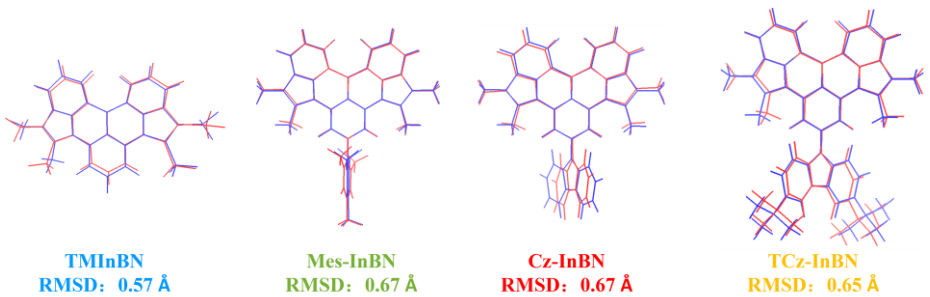


Figure S10. Overlap diagrams of optimized S_0 (blue) and S_1 (red) geometries of TMInBN, Mes-InBN, Cz-InBN, and TCz-InBN, respectively.

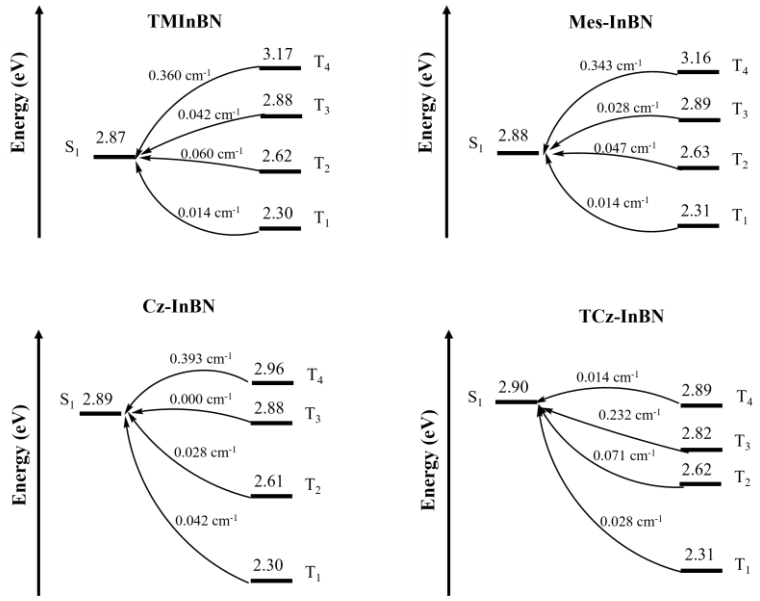


Figure S11. SOC matrix elements between the T_m and S_1 states of TMInBN, Mes-InBN, Cz-InBN, and TCz-InBN, respectively.

Table S4. Calculated energy levels of TMInBN, Mes-InBN, Cz-InBN, and TCz-InBN by using the SCS-CC2 method.

Compound	S_1 (eV)	T_1 (eV)	ΔE_{ST} (eV)
TMInBN	3.1828	2.8842	0.2986
Mes-InBN	3.1612	2.8755	0.2857
Cz-InBN	3.1838	2.8855	0.2983
TCz-InBN	3.1865	2.8916	0.2949

Table S5. Summary of the TD-DFT calculation results of TMInBN at the optimized S_0 geometry.

Excited States	Energy (eV)	Wavelength (nm)	Oscillator Strength	Major Contributions
S_1	2.8886	429.22	0.2621	HOMO→LUMO (98%)
S_2	3.2694	379.23	0.0236	HOMO-1→LUMO (97%)
S_3	3.4639	357.93	0.0590	HOMO-2→LUMO (98%)
S_4	3.8441	322.53	0.0045	HOMO-3→LUMO (85%) HOMO→LUMO+1 (10%)
S_5	4.0950	302.77	0.0269	HOMO→LUMO+1 (91%) HOMO-4→LUMO (29%) HOMO-3→LUMO (11%)
S_6	4.2063	294.76	0.0012	HOMO→LUMO+2 (95%)
S_7	4.3404	285.65	0.0553	HOMO-5→LUMO (74%) HOMO-1→LUMO+1 (19%)
S_8	4.3841	282.80	0.0934	HOMO-4→LUMO (40%) HOMO→LUMO+3 (33%) HOMO→LUMO+1 (16%)
S_9	4.4758	277.01	0.1046	HOMO→LUMO+3 (61%) HOMO-4→LUMO (17%) HOMO→LUMO+1 (9%)

S_{10}	4.5214	274.22	0.0819	HOMO-1→LUMO+1 (71%) HOMO-5→LUMO (13%) HOMO-1→LUMO+3 (6%)

Table S6. Summary of the TD-DFT calculation results of Mes-InBN at the optimized S_0 geometry.

Excited States	Energy (eV)	Wavelength (nm)	Oscillator Strength	Major Contributions
S_1	2.8892	429.13	0.2527	HOMO→LUMO (98%)
S_2	3.2701	379.14	0.0227	HOMO-1→LUMO (97%)
S_3	3.4642	357.90	0.0537	HOMO-2→LUMO (98%)
S_4	3.8403	322.85	0.0037	HOMO-3→LUMO (81%) HOMO→LUMO+1 (12%)
S_5	4.0443	306.57	0.0035	HOMO-4→LUMO (60%) HOMO→LUMO+1 (21%) HOMO-6→LUMO (11%) HOMO-3→LUMO (7%)
S_6	4.0869	303.37	0.0308	HOMO-4→LUMO (38%) HOMO→LUMO+1 (32%) HOMO-6→LUMO (21%) HOMO-3→LUMO (7%)
S_7	4.1886	296.00	0.0005	HOMO→LUMO+2 (92%)
S_8	4.2154	294.12	0.0017	HOMO-5→LUMO (97%)
S_9	4.3350	286.01	0.3211	HOMO-6→LUMO (51%) HOMO→LUMO+1 (26%) HOMO→LUMO+3 (10%)
S_{10}	4.3403	285.66	0.0432	HOMO-7→LUMO (70%) HOMO-1→LUMO+1 (23%)

Table S7. Summary of the TD-DFT calculation results of Cz-InBN at the optimized S_0 geometry.

Excited States	Energy (eV)	Wavelength (nm)	Oscillator Strength	Major Contributions
S_1	2.9016	427.30	0.2474	HOMO→LUMO (98%)
S_2	3.1384	395.06	0.0467	HOMO-1→LUMO (89%) HOMO-2→LUMO (10%)
S_3	3.2680	379.39	0.0963	HOMO-2→LUMO (88%) HOMO-1→LUMO (10%)
S_4	3.4305	361.42	0.0592	HOMO-3→LUMO (96%)
S_5	3.5822	343.11	0.0001	HOMO-4→LUMO (98%)
S_6	3.8377	323.07	0.0009	HOMO-5→LUMO (86%) HOMO→LUMO+2 (8%)
S_7	3.9254	315.85	0.0002	HOMO→LUMO+1 (99%)
S_8	3.9572	313.31	0.0667	HOMO-1→LUMO+1 (92%)
S_9	4.0809	303.82	0.1004	HOMO→LUMO+2 (71%) HOMO-6→LUMO (17%) HOMO-5→LUMO (10%)
S_{10}	4.1055	302.00	0.0012	HOMO→LUMO+3 (79%) HOMO-1→LUMO+2 (17%)

Table S8. Summary of the TD-DFT calculation results of TCz-InBN at the optimized S_0 geometry.

Excited States	Energy (eV)	Wavelength (nm)	Oscillator Strength	Major Contributions
S_1	2.9070	426.50	0.2422	HOMO→LUMO (98%)
S_2	3.0054	412.54	0.1228	HOMO-1→LUMO (97%)
S_3	3.2632	379.95	0.0648	HOMO-2→LUMO (96%)
S_4	3.4407	360.35	0.0563	HOMO-4→LUMO (97%)
S_5	3.5489	349.36	0.0001	HOMO-3→LUMO (99%)
S_6	3.8086	325.54	0.0529	HOMO-1→LUMO+1 (94%)
S_7	3.8418	322.72	0.0003	HOMO-5→LUMO (85%) HOMO→LUMO+2 (9%)
S_8	3.9257	315.83	0.0001	HOMO→LUMO+1 (99%)
S_9	4.0535	305.87	0.0058	HOMO-1→LUMO+2 (61%) HOMO→LUMO+3 (33%)
S_{10}	4.0911	303.06	0.1234	HOMO→LUMO+2 (70%) HOMO-7→LUMO (18%) HOMO-5→LUMO (10%)

Cartesian coordinates obtained in gas-phase DFT calculations

TMInBN (S_0)

E(B3LYP/6-31G(d,p)) = -1137.893280 Hartree

Tag	Symbol	X	Y	Z
1	C	6.13717900	-0.10151700	0.10034000
2	C	4.20894100	-2.59479200	0.51918100
3	C	-4.20991600	-2.59499200	-0.51579500
4	C	-6.13730100	-0.10103800	-0.09730100
5	C	4.09183600	2.40518200	-0.35460800
6	C	3.01853800	3.29162300	-0.49577200
7	C	1.69588400	2.84515000	-0.41025300
8	C	-1.69552500	2.84531900	0.40887400
9	C	-3.01809800	3.29192300	0.49489000
10	C	-4.09149300	2.40546900	0.35465300
11	C	3.79517700	-1.19409500	0.18913600
12	C	4.63943900	-0.12098400	0.04441100
13	C	3.82263700	1.04979300	-0.15447600
14	C	-3.82245100	1.04999800	0.15486100
15	C	-4.63950700	-0.12078800	-0.04271800
16	C	-3.79546800	-1.19403800	-0.18770600
17	N	2.44234100	-0.74807200	0.06781300
18	C	2.47713500	0.62903600	-0.10622500
19	C	1.37397500	1.48891200	-0.19038500
20	B	0.00006700	0.82132400	-0.00044400
21	C	-1.37380200	1.48899500	0.18928500
22	C	-2.47702100	0.62912000	0.10581600
23	N	-2.44244600	-0.74807300	-0.06786800
24	C	0.00011500	-3.53976600	-0.00238800
25	C	1.21413800	-2.86709500	-0.01708100
26	C	1.22751400	-1.46624300	0.02307300
27	C	-0.00001300	-0.72583400	-0.00036700
28	C	-1.22753400	-1.46626300	-0.02439900
29	C	-1.21395500	-2.86719000	0.01349900
30	H	6.49617900	0.56305200	0.89568600

31	H	6.56617600	-1.09013300	0.27764000
32	H	6.55990200	0.27125800	-0.84072300
33	H	4.10761800	-3.28839400	-0.32403000
34	H	5.26222200	-2.59305700	0.80451100
35	H	3.64374200	-3.00323000	1.36226700
36	H	-5.26416300	-2.59367900	-0.79748900
37	H	-3.64759800	-3.00364700	-1.36071900
38	H	-4.10543700	-3.28817100	0.32736600
39	H	-6.55885600	0.27592600	0.84260500
40	H	-6.49691700	0.56028100	-0.89508800
41	H	-6.56688600	-1.09022200	-0.26990600
42	H	5.11481900	2.76774200	-0.40655900
43	H	3.21649800	4.34560600	-0.66809200
44	H	0.89575400	3.56682800	-0.53382500
45	H	-0.89527400	3.56694900	0.53193100
46	H	-3.21590600	4.34597700	0.66695000
47	H	-5.11444300	2.76805300	0.40707500
48	H	0.00012100	-4.62607000	-0.00340800
49	H	2.12203500	-3.44181800	-0.06603900
50	H	-2.12172900	-3.44217600	0.06118800

TMInBN (S_1)

E(B3LYP/6-311G(d)) = -1137.983438 Hartree

Tag	Symbol	X	Y	Z
1	C	6.05146395	-0.25499790	0.53102880
2	C	4.02773023	-2.63984436	0.62127871
3	C	-4.13759426	-2.64358848	0.36867038
4	C	-6.09625314	-0.12637573	0.39909604
5	C	4.18330101	2.40963105	-0.08333714
6	C	3.14005435	3.29847601	-0.26306844
7	C	1.79928622	2.86792448	-0.31787713
8	C	-1.70789602	2.89365851	-0.06571244
9	C	-3.03160745	3.33241962	0.03479128
10	C	-4.09641223	2.43777941	0.12366536
11	C	3.66588304	-1.23804067	0.27274497
12	C	4.59227094	-0.14168583	0.26099330
13	C	3.85163260	1.03566342	0.00304963
14	C	-3.81033873	1.06135455	0.10431429
15	C	-4.60989361	-0.12663364	0.21493245
16	C	-3.76453949	-1.21098420	0.15282820
17	N	2.42675297	-0.77219143	-0.00688838
18	C	2.50354397	0.65108582	-0.11238652
19	C	1.41519200	1.51044018	-0.21286204
20	B	0.00366138	0.84234769	-0.13227925
21	C	-1.36361473	1.51554822	-0.09181835
22	C	-2.47220263	0.65173110	-0.01751574
23	N	-2.43465289	-0.74294373	-0.02430258
24	C	-0.02188016	-3.48633320	-0.71944283
25	C	1.19572243	-2.82207150	-0.54213310
26	C	1.18971134	-1.47173240	-0.21878204
27	C	-0.00613515	-0.69703043	-0.14149199
28	C	-1.22983299	-1.44007862	-0.21349868
29	C	-1.21680841	-2.80696074	-0.53801278
30	H	6.25024013	-0.43076981	1.59625580
31	H	6.50799083	-1.08589230	-0.01553019
32	H	6.57465695	0.65958802	0.25133349
33	H	4.23276885	-3.25252003	-0.26377321
34	H	4.93444202	-2.64277913	1.22801153
35	H	3.23248426	-3.13255982	1.18223470

36	H	-5.13506784	-2.69154543	0.80631735
37	H	-4.16981092	-3.23813827	-0.55198168
38	H	-3.45871348	-3.14654922	1.06275064
39	H	-6.38690925	0.41721609	1.30537364
40	H	-6.59719085	0.37050760	-0.43945677
41	H	-6.51485145	-1.13165823	0.47090663
42	H	5.20968933	2.75070160	-0.00566223
43	H	3.34997030	4.36035616	-0.34460701
44	H	1.03369595	3.62297756	-0.44244661
45	H	-0.92623706	3.64275097	-0.09869248
46	H	-3.23263494	4.40006416	0.05279619
47	H	-5.11679546	2.79773783	0.21036511
48	H	-0.03131003	-4.53170743	-1.00575243
49	H	2.11487667	-3.35997969	-0.71503980
50	H	-2.13899995	-3.33972091	-0.70039482

Mes-InBN (S_0)

E(B3LYP/6-31G(d,p)) = -1486.912580 Hartree

Tag	Symbol	X	Y	Z
1	C	0.98227900	4.21014900	0.51319100
2	C	-1.51477900	6.13484300	0.10663200
3	C	-4.00970200	-4.10064600	0.33751100
4	C	-4.89983600	-3.03031500	0.47697700
5	C	-4.45667000	-1.70632600	0.39541800
6	C	-4.46127600	1.69409000	-0.39676600
7	C	-4.90812100	3.01683700	-0.47844700
8	C	-4.02108900	4.08966400	-0.33841100
9	C	-0.40898100	-3.79449600	-0.19169400
10	C	-2.65446400	-3.82703400	0.14229100
11	C	-2.66517900	3.81987000	-0.14250700
12	C	-1.49403900	4.63703400	0.05199400
13	C	-0.41981900	3.79358000	0.19282400
14	C	-1.48089800	-4.64093900	-0.05136400
15	C	-2.23718500	-2.48048600	0.09609300
16	C	-3.10071300	-1.38001900	0.18058700
17	B	-2.43632200	-0.00326900	-0.00014800
18	C	-3.10451300	1.37159300	-0.18125500
19	C	-2.24414400	2.47448700	-0.09624200
20	N	-0.86603000	2.44000700	0.07428300
21	C	1.94760100	0.00296100	0.00029400
22	C	1.25508700	-1.20755700	0.00801000
23	C	-0.14525100	-1.22465700	-0.02781800
24	C	-0.89030200	-0.00109700	0.00022200
25	C	-0.14873400	1.22457600	0.02844600
26	C	1.25163100	1.21150200	-0.00734800
27	C	0.99450900	-4.20724800	-0.51088800
28	C	3.44735500	0.00479100	0.00014600
29	C	-1.49742600	-6.13881100	-0.10585100
30	N	-0.85907100	-2.44213000	-0.07368500
31	C	4.15321300	-0.02427200	1.22034100
32	C	5.55190800	-0.01868100	1.19710000
33	C	6.27121600	0.01267800	-0.00022000
34	C	5.55129700	0.04515600	-1.19751000
35	C	4.15290300	0.04049900	-1.22041500
36	C	3.42378300	-0.05571200	2.54483500
37	C	3.42273800	0.07652600	-2.54438900
38	C	7.78164800	-0.01461300	-0.00205000
39	H	0.98196500	5.26670100	0.78594000

40	H	1.39409500	3.65539100	1.36157200
41	H	1.67336500	4.09790400	-0.33039700
42	H	-1.89635500	6.55596500	-0.83160600
43	H	-2.17294600	6.49381100	0.90731900
44	H	-0.52533000	6.56542300	0.27492800
45	H	-4.36912400	-5.12484300	0.38717700
46	H	-5.95384200	-3.23152100	0.64535800
47	H	-5.18102200	-0.90856900	0.51849600
48	H	-5.18332600	0.89431400	-0.52027400
49	H	-5.96260400	3.21508500	-0.64735500
50	H	-4.38337500	5.11284700	-0.38818100
51	H	1.83175900	-2.11494200	0.04609300
52	H	1.82566100	2.12056700	-0.04550800
53	H	0.99740600	-5.26402200	-0.78276400
54	H	1.40523900	-3.65199400	-1.35947500
55	H	1.68472300	-4.09229400	0.33305000
56	H	-2.15376900	-6.49971300	-0.90716900
57	H	-0.50661400	-6.56666600	-0.27309900
58	H	-1.87877500	-6.56087200	0.83204900
59	H	6.09202200	-0.03729300	2.14129700
60	H	6.09099000	0.07579300	-2.14168100
61	H	2.79274500	-0.94614600	2.63756300
62	H	4.12967500	-0.05349800	3.37943700
63	H	2.75932900	0.80737700	2.65964700
64	H	4.12817500	0.07735100	-3.37937700
65	H	2.75874600	-0.78658200	-2.66155200
66	H	2.79109600	0.96687700	-2.63392200
67	H	8.19129600	0.42598500	0.91177900
68	H	8.16056500	-1.04250300	-0.06533900
69	H	8.19126400	0.53370200	-0.85587700

Mes-InBN (S_1)

E(B3LYP/6-311G(d)) = -1487.055729 Hartree

Tag	Symbol	X	Y	Z
1	C	-0.82569030	-4.03983843	1.19439267
2	C	1.54694857	-6.02608207	0.74167805
3	C	3.96046552	4.15762545	-0.25064154
4	C	4.84753860	3.10589978	-0.47210787
5	C	4.42356907	1.77367727	-0.47318612
6	C	4.42299696	-1.74090733	-0.64227438
7	C	4.87862962	-3.07403824	-0.64096278
8	C	4.04654090	-4.12711289	-0.30922785
9	C	0.37641136	3.76950514	0.40292852
10	C	2.60664346	3.84906294	-0.03072953
11	C	2.69949562	-3.81367223	-0.00663935
12	C	1.59078344	-4.56848109	0.44399542
13	C	0.49549296	-3.65913156	0.62257098
14	C	1.43966643	4.63231470	0.26498989
15	C	2.20784172	2.50245678	-0.05702170
16	C	3.06811894	1.40690822	-0.25784987
17	B	2.42389419	0.02840856	-0.16096834
18	C	3.09333432	-1.37471931	-0.32615356
19	C	2.27928689	-2.47316160	-0.07328580
20	N	0.89010738	-2.41588508	0.26018634
21	C	-1.96400801	-0.01949375	-0.01520698
22	C	-1.26477219	1.18326834	0.04038489
23	C	0.13687479	1.22305125	0.12578483
24	C	0.90576154	0.01509506	0.08620522
25	C	0.14736448	-1.19063428	0.15376299

26	C	-1.23717494	-1.21921836	0.06188594
27	C	-1.00541755	4.12692834	0.85062054
28	C	-3.45209313	-0.04252675	-0.16583214
29	C	1.44369753	6.12215103	0.41852437
30	N	0.83259473	2.44289985	0.17416868
31	C	-4.28448830	0.18690520	0.94776641
32	C	-5.67106912	0.15182733	0.78276713
33	C	-6.26140936	-0.09953903	-0.45542508
34	C	-5.42117215	-0.32478754	-1.54571774
35	C	-4.03005328	-0.30048434	-1.42538693
36	C	-3.70484662	0.46263552	2.31643434
37	C	-3.17121697	-0.53630300	-2.64693233
38	C	-7.76244825	-0.09739050	-0.61707252
39	H	-0.71708174	-4.94618333	1.79174453
40	H	-1.23125292	-3.25174583	1.83026602
41	H	-1.57283826	-4.25268797	0.42187858
42	H	2.41537977	-6.53781002	0.32650540
43	H	1.54381450	-6.21521113	1.82298656
44	H	0.64877465	-6.50206701	0.33645261
45	H	4.30996869	5.18526915	-0.24400513
46	H	5.89856888	3.32441480	-0.63992047
47	H	5.17072850	1.00367671	-0.62170737
48	H	5.13590073	-0.96641107	-0.89448290
49	H	5.91701287	-3.27024453	-0.88905307
50	H	4.41188993	-5.14753423	-0.27612135
51	H	-1.83145494	2.09602572	-0.04251455
52	H	-1.78148532	-2.14878540	0.00087912
53	H	-0.99736980	5.13546425	1.26474582
54	H	-1.74961177	4.12345594	0.04595826
55	H	-1.36834912	3.46078563	1.63843403
56	H	1.78691261	6.61172830	-0.49987336
57	H	0.45673291	6.52779682	0.64701686
58	H	2.12379341	6.44020629	1.21705759
59	H	-6.30682346	0.32318057	1.64817405
60	H	-5.85965482	-0.52038235	-2.52135932
61	H	-3.22246567	1.44381220	2.36324709
62	H	-4.48325133	0.44267217	3.08204752
63	H	-2.94062856	-0.26941944	2.59008182
64	H	-3.78188193	-0.58068724	-3.55102336
65	H	-2.42983210	0.25606120	-2.77764490
66	H	-2.61131566	-1.47422276	-2.58024899
67	H	-8.26690065	-0.40790002	0.30132320
68	H	-8.13277671	0.90324862	-0.86663253
69	H	-8.08250349	-0.76839251	-1.41808378

Cz-InBN (S_0)

E(B3LYP/6-31G(d,p)) = -1654.177624 Hartree

Tag	Symbol	X	Y	Z
1	C	-1.93075600	-6.11563700	0.53254100
2	C	0.56756100	-4.23662700	-0.04747600
3	C	0.56337400	4.23784800	0.04676000
4	C	-1.93714400	6.11454100	-0.53134100
5	C	-4.44416200	-4.04409800	0.74450700
6	C	-5.33497700	-2.96535000	0.76968200
7	C	-4.89162500	-1.65667700	0.55550400
8	C	-4.89337400	1.65253400	-0.55545700
9	C	-5.33812000	2.96082100	-0.76907200
10	C	-4.44841600	4.04048200	-0.74361700
11	C	-0.84032500	-3.79424500	0.20548800
12	C	-1.91343700	-4.62061000	0.42700500

13	C	-3.08838200	-3.79109600	0.52822300
14	C	-3.09232800	3.78879600	-0.52773900
15	C	-1.91825700	4.61949800	-0.42633300
16	C	-0.84421600	3.79414500	-0.20546400
17	N	-1.29224200	-2.43616700	0.17677200
18	C	-2.67163100	-2.45671600	0.34437000
19	C	-3.53460000	-1.35336900	0.31313700
20	B	-2.86989900	-0.00107900	-0.00019900
21	C	-3.53599400	1.35053600	-0.31345300
22	C	-2.67413100	2.45476200	-0.34459200
23	N	-1.29469800	2.43559000	-0.17731400
24	C	1.49685600	0.00108400	-0.00060500
25	C	0.81955700	-1.20718100	0.13422200
26	C	-0.58020100	-1.22293100	0.09327100
27	C	-1.32324600	-0.00029700	-0.00024300
28	C	-0.58144100	1.22305800	-0.09390500
29	C	0.81833800	1.20866800	-0.13525400
30	N	2.91851500	0.00183400	-0.00080400
31	C	3.73762100	-0.71563100	-0.88032400
32	C	5.09495100	-0.45554400	-0.56149000
33	C	5.09460500	0.45838200	0.56191000
34	C	3.73707700	0.71883000	0.87961600
35	C	3.38208900	-1.53903400	-1.95238100
36	C	4.40997300	-2.12219300	-2.69013800
37	C	5.76012000	-1.88944500	-2.37719000
38	C	6.10785400	-1.05505000	-1.31913300
39	C	6.10703400	1.05762500	1.32039100
40	C	5.75864200	1.89206300	2.37819900
41	C	4.40829900	2.12513200	2.69005000
42	C	3.38087400	1.54229200	1.95139900
43	H	-2.59640200	-6.55756500	-0.21876100
44	H	-0.94227300	-6.56045100	0.40010800
45	H	-2.30172300	-6.43500500	1.51413900
46	H	1.24470600	-4.03058800	0.78983300
47	H	0.57420100	-5.31679100	-0.20119600
48	H	0.99439100	-3.77968700	-0.94518700
49	H	0.56907900	5.31800900	0.20054000
50	H	0.99122800	3.78126000	0.94416100
51	H	1.24017000	4.03254900	-0.79101400
52	H	-2.60389200	6.55538500	0.21961400
53	H	-0.94928400	6.56041900	-0.39783800
54	H	-2.30765700	6.43395400	-1.51310100
55	H	-4.80361900	-5.05785700	0.89792900
56	H	-6.38956200	-3.14870000	0.95365800
57	H	-5.61647100	-0.85103600	0.59493400
58	H	-5.61739300	0.84615400	-0.59502000
59	H	-6.39292900	3.14315500	-0.95277400
60	H	-4.80895600	5.05393600	-0.89651100
61	H	1.40210000	-2.09660900	0.29220300
62	H	1.39996600	2.09866200	-0.29340800
63	H	2.34223300	-1.70889500	-2.20868600
64	H	4.15917100	-2.76635500	-3.52779600
65	H	6.53687800	-2.36080500	-2.97131100
66	H	7.15196900	-0.86645500	-1.08619100
67	H	7.15129400	0.86878600	1.08829500
68	H	6.53503200	2.36320600	2.97297300
69	H	4.15697000	2.76931100	3.52753500
70	H	2.34085300	1.71238800	2.20687400

Cz-InBN (S_1)

E(B3LYP/6-311G(d)) = -1654.358802 Hartree

Tag	Symbol	X	Y	Z
1	C	1.73598537	6.12491667	-0.17662544
2	C	-0.55502477	4.09945334	-0.82244132
3	C	-0.41487110	-4.09248481	-1.21449239
4	C	2.12551635	-6.00731686	-0.98708102
5	C	4.31075724	4.23235993	0.69657898
6	C	5.17950070	3.18672715	0.93242825
7	C	4.77341573	1.84071396	0.80220156
8	C	4.92128052	-1.63014212	0.27893055
9	C	5.40323786	-2.93698110	0.15284212
10	C	4.55981638	-4.00081503	-0.15930989
11	C	0.78168211	3.71438519	-0.29460288
12	C	1.84346790	4.64873196	-0.02414811
13	C	2.97607253	3.89885104	0.35551959
14	C	3.19255890	-3.73399604	-0.34363438
15	C	2.05787628	-4.53846882	-0.70169589
16	C	0.95766531	-3.71469164	-0.75533847
17	N	1.22441063	2.46012497	-0.05186216
18	C	2.60690872	2.54007959	0.29160090
19	C	3.46313692	1.45609797	0.44410903
20	B	2.84593808	0.04659004	0.14379890
21	C	3.55057626	-1.30640526	0.10625674
22	C	2.73605621	-2.41387378	-0.19265855
23	N	1.35850537	-2.39387820	-0.41153798
24	C	-1.51542278	-0.06592777	-0.02490617
25	C	-0.85389971	1.17099070	0.02150780
26	C	0.52613067	1.20002854	-0.06657546
27	C	1.33274410	0.02125162	-0.10300948
28	C	0.61216648	-1.21453967	-0.25376819
29	C	-0.78695383	-1.23894845	-0.18304147
30	N	-2.93330240	-0.10931659	0.09804200
31	C	-3.84588307	0.35949960	-0.84606251
32	C	-5.16104094	0.19895710	-0.34083796
33	C	-5.03240567	-0.40059671	0.97036514
34	C	-3.64535747	-0.57205941	1.20653249
35	C	-3.60821991	0.89354271	-2.11366637
36	C	-4.70898963	1.28188032	-2.87033417
37	C	-6.01735001	1.14041490	-2.38213689
38	C	-6.24860169	0.59755661	-1.12365684
39	C	-5.94822486	-0.79424390	1.95103932
40	C	-5.47672957	-1.34224532	3.13755827
41	C	-4.09860823	-1.49780672	3.35596986
42	C	-3.16531232	-1.11579383	2.39859845
43	H	1.68998363	6.41751533	-1.23336248
44	H	0.83340292	6.52162376	0.29866473
45	H	2.59681356	6.62890873	0.26261289
46	H	-1.29981774	4.21113716	-0.02652642
47	H	-0.48433556	5.06263118	-1.32938850
48	H	-0.94196906	3.36248228	-1.52665977
49	H	-0.37364910	-5.06816825	-1.69876254
50	H	-1.14678517	-4.17598246	-0.40294496
51	H	-0.81437106	-3.38818243	-1.94944200
52	H	2.50149085	-6.56010553	-0.11887908
53	H	1.15466577	-6.43497246	-1.24215590
54	H	2.80834265	-6.22227337	-1.81694055
55	H	4.63621202	5.26448361	0.76305473
56	H	6.20878920	3.39580979	1.20567555
57	H	5.51527108	1.07413671	0.98522841
58	H	5.63611421	-0.84506373	0.49269040

59	H	6.46407425	-3.12369947	0.29418220
60	H	4.95299180	-5.00739528	-0.26147309
61	H	-1.44576043	2.05787230	0.18098522
62	H	-1.33436068	-2.16564066	-0.21144055
63	H	-2.59980620	0.98520075	-2.50175076
64	H	-4.55148640	1.69544487	-3.86155967
65	H	-6.85468495	1.45200677	-2.99778569
66	H	-7.26339093	0.48110970	-0.75562808
67	H	-7.01488749	-0.67236682	1.78912485
68	H	-6.17809305	-1.65300020	3.90486703
69	H	-3.75176652	-1.92477683	4.29159048
70	H	-2.10191527	-1.23480666	2.57244471

TCz-InBN (S_0)

E(B3LYP/6-31G(d,p)) = -1968.706997 Hartree

Tag	Symbol	X	Y	Z
1	C	3.29803600	5.70598800	-2.26499700
2	C	0.79541100	3.77383800	-1.93797100
3	C	0.79377800	-3.77870900	1.92878900
4	C	3.29751600	-5.70860000	2.25989400
5	C	5.80838500	3.94421100	-1.15486100
6	C	6.69853700	2.99084900	-0.64899500
7	C	6.25362600	1.72607700	-0.25182200
8	C	6.25423700	-1.72449700	0.25721600
9	C	6.69924300	-2.98923900	0.65434800
10	C	5.80868800	-3.94362500	1.15754300
11	C	2.20311200	3.48565600	-1.51645500
12	C	3.27770300	4.32150400	-1.69089800
13	C	4.45224500	3.62199900	-1.23384000
14	C	4.45217500	-3.62239100	1.23399300
15	C	3.27720600	-4.32334100	1.68765700
16	C	2.20232400	-3.48817800	1.51179500
17	N	2.65399600	2.25589100	-0.93820000
18	C	4.03399900	2.34720300	-0.80021700
19	C	4.89635600	1.34751400	-0.33105000
20	B	4.23025000	0.00007100	0.00083900
21	C	4.89655000	-1.34692600	0.33398400
22	C	4.03389200	-2.34747300	0.80079000
23	N	2.65353500	-2.25720400	0.93618100
24	C	-0.13862900	-0.00006100	-0.00052700
25	C	0.54195700	1.12866500	-0.44933500
26	C	1.94133200	1.13442600	-0.46516900
27	C	2.68489600	-0.00042900	-0.00053200
28	C	1.94111200	-1.13538800	0.46354600
29	C	0.54171200	-1.12904100	0.44801000
30	N	-1.55790200	0.00019400	-0.00018100
31	C	-2.38059800	-0.97533900	-0.57989800
32	C	-3.73655100	-0.62238900	-0.37093900
33	C	-3.73616800	0.62337700	0.37181600
34	C	-2.38000000	0.97595900	0.58000500
35	C	-2.04730800	-2.11742700	-1.30666500
36	C	-3.08510200	-2.91041200	-1.79734400
37	C	-4.44584400	-2.60082200	-1.59436600
38	C	-4.75142300	-1.43765400	-0.87558300
39	C	-4.75053200	1.43891800	0.87703600
40	C	-4.44422500	2.60200100	1.59564300
41	C	-3.08328200	2.91123100	1.79782700
42	C	-2.04598200	2.11796900	1.30655500

43	C	-5.58461500	3.48610800	2.13886800
44	C	-5.06112300	4.71797200	2.90157200
45	C	-6.45610800	3.98663100	0.96258300
46	C	-6.46266600	2.66060900	3.10905000
47	C	-5.58678700	-3.48462700	-2.13692200
48	C	-5.06406900	-4.71665700	-2.89989100
49	C	-6.45774700	-3.98487900	-0.96012600
50	C	-6.46516000	-2.65890900	-3.10662400
51	H	2.30607700	6.05904900	-2.55453400
52	H	3.69956300	6.42422400	-1.53977200
53	H	3.93997900	5.75742900	-3.15285900
54	H	0.78629900	4.69257500	-2.52620200
55	H	0.38166300	2.98186700	-2.57005100
56	H	0.11061000	3.92779000	-1.09596900
57	H	0.78370400	-4.69996000	2.51304400
58	H	0.37812000	-2.98969500	2.56334400
59	H	0.11108500	-3.92936800	1.08450600
60	H	3.70111800	-6.42551200	1.53451000
61	H	3.93773200	-5.76067000	3.14896500
62	H	2.30531200	-6.06291000	2.54703700
63	H	6.16812400	4.91910000	-1.47213400
64	H	7.75345900	3.23606200	-0.56736400
65	H	6.97792500	1.02387700	0.14591700
66	H	6.97881400	-1.02152500	-0.13864200
67	H	7.75449700	-3.23366200	0.57467500
68	H	6.16840100	-4.91856500	1.47468800
69	H	-0.04073100	1.96519300	-0.78696900
70	H	-0.04127300	-1.96512000	0.78616400
71	H	-1.01396500	-2.38345100	-1.49953600
72	H	-2.81490900	-3.79607000	-2.35989500
73	H	-5.78677700	-1.15526700	-0.70781000
74	H	-5.78605900	1.15681300	0.70985500
75	H	-2.81252700	3.79682600	2.36020800
76	H	-1.01246000	2.38374800	1.49879800
77	H	-5.90549500	5.31324900	3.26386700
78	H	-4.46095300	4.43441100	3.77230800
79	H	-4.45223200	5.36543600	2.26207700
80	H	-7.27689800	4.61207100	1.33202900
81	H	-6.89681100	3.15735200	0.40141300
82	H	-5.86238800	4.58356500	0.26257500
83	H	-5.87316500	2.29865400	3.95767600
84	H	-7.28241800	3.27377600	3.50068300
85	H	-6.90534200	1.78994200	2.61634200
86	H	-5.90881200	-5.31172300	-3.26166900
87	H	-4.46433600	-4.43328800	-3.77099000
88	H	-4.45497500	-5.36425900	-2.26072900
89	H	-7.27892700	-4.61009400	-1.32908700
90	H	-6.89789200	-3.15546300	-0.39872200
91	H	-5.86379400	-4.58196500	-0.26044700
92	H	-5.87604100	-2.29713900	-3.95559500
93	H	-7.28530800	-3.27185600	-3.49777400
94	H	-6.90730800	-1.78810600	-2.61368400

TCz-InBN (S_1)

E(B3LYP/6-311G(d)) = -1968.928111 Hartree

Tag	Symbol	X	Y	Z
1	C	3.26929035	-5.17305422	3.17619562
2	C	0.93288824	-3.12931748	2.79821992

3	C	0.84219590	4.17458024	-0.91061776
4	C	3.32870192	5.78445900	-2.09339724
5	C	5.77437378	-3.92218054	1.40524740
6	C	6.61000154	-3.11539027	0.65976832
7	C	6.16892051	-1.88799168	0.11991499
8	C	6.23287300	1.40456429	-1.10998288
9	C	6.68040477	2.61540251	-1.64809166
10	C	5.81113318	3.67907264	-1.87975460
11	C	2.24828605	-3.03960219	2.10826489
12	C	3.33127387	-3.96719524	2.30672115
13	C	4.43627328	-3.48640162	1.57258015
14	C	4.45276817	3.50958249	-1.56161950
15	C	3.29938293	4.36346775	-1.62070788
16	C	2.22216019	3.64962132	-1.14931308
17	N	2.65105340	-2.06510319	1.26235954
18	C	4.03023805	-2.28121761	0.96592613
19	C	4.85366917	-1.39855469	0.27742526
20	B	4.20344433	-0.03273667	-0.13394898
21	C	4.87247768	1.17967042	-0.77436709
22	C	4.03101164	2.27582146	-1.03848465
23	N	2.65611971	2.33841878	-0.80991541
24	C	-0.15832208	0.06614650	0.05174353
25	C	0.53665371	-1.01630651	0.61503927
26	C	1.91823307	-0.97727041	0.66637332
27	C	2.69298354	0.08295033	0.10379371
28	C	1.94085796	1.22014768	-0.35183565
29	C	0.54138767	1.17414100	-0.41136309
30	N	-1.57703519	0.02341231	-0.03313814
31	C	-2.46584753	0.83830055	0.67197585
32	C	-3.79409225	0.46920303	0.34939353
33	C	-3.70328306	-0.62871000	-0.59341536
34	C	-2.32406950	-0.87071499	-0.80292758
35	C	-2.21158681	1.85879839	1.58278863
36	C	-3.29963128	2.51438097	2.15487875
37	C	-4.63496880	2.18438049	1.85107496
38	C	-4.86043259	1.14664630	0.94019209
39	C	-4.64852718	-1.39932556	-1.26984695
40	C	-4.25165732	-2.40787272	-2.15472915
41	C	-2.87056605	-2.61278627	-2.34217228
42	C	-1.90004411	-1.86110193	-1.68352627
43	C	-5.31917826	-3.24320612	-2.88814896
44	C	-4.70136424	-4.29479311	-3.82692290
45	C	-6.19715126	-3.98545733	-1.85520529
46	C	-6.21235495	-2.31290329	-3.73994390
47	C	-5.83332878	2.91906677	2.48307543
48	C	-5.39687921	4.02991307	3.45484020
49	C	-6.68792617	3.56935742	1.37148971
50	C	-6.70315399	1.91333766	3.27085728
51	H	2.37021541	-5.76833460	2.98851535
52	H	4.13637948	-5.81481276	3.02033746
53	H	3.25077923	-4.90121448	4.23931601
54	H	1.03856471	-3.71556490	3.71189608
55	H	0.54594056	-2.14369184	3.05958639
56	H	0.17374831	-3.62695084	2.18455955
57	H	0.86051190	5.26343250	-0.95958807
58	H	0.10596897	3.83976651	-1.65025782
59	H	0.46040974	3.90587395	0.07815313
60	H	4.01589840	6.39133174	-1.49289681
61	H	3.67732306	5.84752666	-3.13034566
62	H	2.34935304	6.26410319	-2.05584751
63	H	6.12794467	-4.84609099	1.84913779
64	H	7.64039675	-3.41518599	0.49770779

65	H	6.88592514	-1.29915835	-0.43762646
66	H	6.96682275	0.62963952	-0.92563515
67	H	7.73481843	2.73012668	-1.88331430
68	H	6.17795869	4.61430377	-2.29087616
69	H	-0.03511256	-1.86406047	0.95591034
70	H	-0.02563124	1.97038076	-0.86321148
71	H	-1.19771643	2.13811070	1.84675630
72	H	-3.09007952	3.30841485	2.86044915
73	H	-5.87461461	0.85617169	0.68474487
74	H	-5.70319002	-1.20322193	-1.10422490
75	H	-2.52962461	-3.37805274	-3.02800640
76	H	-0.84607510	-2.03823902	-1.86671434
77	H	-5.49532258	-4.85948740	-4.32336450
78	H	-4.08933656	-3.83750322	-4.60909853
79	H	-4.08011593	-5.01384617	-3.28573783
80	H	-6.96333600	-4.58392185	-2.35866068
81	H	-6.70887773	-3.29351969	-1.18216204
82	H	-5.59370388	-4.65866264	-1.23987721
83	H	-5.61956874	-1.77487393	-4.48464830
84	H	-6.97683912	-2.89065827	-4.26942874
85	H	-6.72721579	-1.56846987	-3.12826005
86	H	-6.27869928	4.52222302	3.87402211
87	H	-4.81442978	3.63702628	4.29277372
88	H	-4.80035956	4.79933069	2.95709583
89	H	-7.54525878	4.09652430	1.80241419
90	H	-7.07603424	2.82859869	0.66848409
91	H	-6.10078285	4.29192083	0.79812439
92	H	-6.12696315	1.43914919	4.07021025
93	H	-7.56063905	2.41883565	3.72671803
94	H	-7.09206757	1.11936767	2.62903468

InBN (S_0)

E(B3LYP/6-31G(d,p)) = -980.620635 Hartree

Tag	Symbol	X	Y	Z
1	C	-1.21132200	1.72602400	0.00042300
2	C	-1.21269700	3.12600600	0.00035500
3	C	0.00000000	3.80625400	-0.00011800
4	C	1.21269700	3.12600600	-0.00051600
5	C	1.21132100	1.72602400	-0.00043900
6	C	0.00000000	0.97338000	0.00001200
7	N	-2.42047800	1.01876000	0.00085300
8	B	0.00000000	-0.58324000	-0.00000300
9	N	2.42047900	1.01876000	-0.00078600
10	C	-2.49082800	-0.36274600	0.00009100
11	C	-3.85634000	-0.73957600	0.00011600
12	C	-4.62006400	0.48340400	0.00106900
13	C	-3.73033400	1.51634800	0.00146300
14	C	3.73033400	1.51634800	-0.00128200
15	C	4.62006400	0.48340500	-0.00088200
16	C	3.85634000	-0.73957500	-0.00004100
17	C	2.49082800	-0.36274500	-0.00007500
18	C	-1.39994700	-1.24659600	-0.00064200
19	C	-1.76829200	-2.60844900	-0.00183000
20	C	-3.10594200	-3.02377400	-0.00192100
21	C	-4.15895900	-2.10347000	-0.00086600
22	C	4.15896000	-2.10347000	0.00088300
23	C	3.10594200	-3.02377400	0.00184000
24	C	1.76829200	-2.60844900	0.00171800
25	C	1.39994700	-1.24659600	0.00058500
26	H	-2.13959600	3.68569300	0.00058800
27	H	0.00000000	4.89219500	-0.00018400

28	H	2.13959600	3.68569300	-0.00083700
29	H	-5.69646100	0.58046600	0.00143500
30	H	-3.91986300	2.57737600	0.00217800
31	H	3.91986200	2.57737700	-0.00189000
32	H	5.69646100	0.58046700	-0.00115000
33	H	-0.99957800	-3.37248600	-0.00293000
34	H	-3.33038600	-4.08642000	-0.00285100
35	H	-5.19003700	-2.44588500	-0.00091400
36	H	5.19003800	-2.44588400	0.00096500
37	H	3.33038700	-4.08642000	0.00272300
38	H	0.99957800	-3.37248700	0.00275700

InBN (S_1)

E(B3LYP/6-311G(d)) = -980.686448 Hartree

Tag	Symbol	X	Y	Z
1	C	-1.19903200	-1.71412600	-0.00012700
2	C	-1.20069900	-3.13087100	-0.00009600
3	C	0.00000000	-3.82780100	0.00001600
4	C	1.20069900	-3.13087100	0.00011800
5	C	1.19903200	-1.71412600	0.00012900
6	C	0.00000000	-0.95794400	0.00000000
7	N	-2.40675300	-1.02893600	-0.00026300
8	B	0.00000000	0.60021300	0.00000100
9	N	2.40675300	-1.02893600	0.00025200
10	C	-2.48614400	0.37596300	0.00000700
11	C	-3.84269700	0.73684200	-0.00000100
12	C	-4.59525400	-0.49145300	-0.00033300
13	C	-3.70704700	-1.53306700	-0.00046400
14	C	3.70704700	-1.53306700	0.00043700
15	C	4.59525400	-0.49145300	0.00030200
16	C	3.84269700	0.73684200	-0.00000800
17	C	2.48614400	0.37596300	-0.00000900
18	C	-1.39219300	1.25289400	0.00022500
19	C	-1.77908700	2.62381600	0.00062900
20	C	-3.11774700	3.02227900	0.00066600
21	C	-4.17031600	2.10271000	0.00031900
22	C	4.17031600	2.10271000	-0.00031900
23	C	3.11774700	3.02227900	-0.00065200
24	C	1.77908700	2.62381600	-0.00061100
25	C	1.39219300	1.25289400	-0.00021700
26	H	-2.13215700	-3.68114400	-0.00014200
27	H	0.00000000	-4.91136500	0.00002600
28	H	2.13215700	-3.68114400	0.00017900
29	H	-5.67113400	-0.59419700	-0.00047100
30	H	-3.90086800	-2.59168000	-0.00074100
31	H	3.90086800	-2.59168000	0.00069500
32	H	5.67113400	-0.59419700	0.00042400
33	H	-1.01647500	3.39257500	0.00104900
34	H	-3.34737200	4.08391800	0.00097100
35	H	-5.20274000	2.43555200	0.00031300
36	H	5.20274000	2.43555200	-0.00031800
37	H	3.34737200	4.08391800	-0.00095100
38	H	1.01647500	3.39257500	-0.00102100

InCzBN (S_0)

E(B3LYP/6-31G(d,p)) = -1134.272393 Hartree

Tag	Symbol	X	Y	Z
1	C	-0.70109300	-1.33666300	-0.13192800
2	C	-0.94582000	-2.70110600	-0.34095200
3	C	0.12394500	-3.58705300	-0.41899800

4	C	1.43921200	-3.15496700	-0.30179400
5	C	1.69004100	-1.78693800	-0.14907000
6	C	0.63425300	-0.83052400	-0.08179100
7	N	-1.75770300	-0.41867100	-0.00968300
8	B	0.92893500	0.69030500	-0.04090800
9	N	3.00783500	-1.31461700	-0.07115000
10	C	-1.55344400	0.95596300	-0.13935800
11	C	-2.79654200	1.62437200	-0.17437900
12	C	-3.81714100	0.61193500	0.00735100
13	C	-3.15110800	-0.63650300	0.13913000
14	C	4.20506700	-2.04263000	-0.07257000
15	C	5.26445100	-1.19706800	0.07755100
16	C	4.73409700	0.13972400	0.18405100
17	C	3.32677900	0.02238400	0.08184500
18	C	-0.30766200	1.59899800	-0.20422000
19	C	-0.37607900	2.99782700	-0.38634900
20	C	-1.59030800	3.68406500	-0.46009500
21	C	-2.81023700	3.00692100	-0.34116800
22	C	5.27064800	1.41804800	0.36146100
23	C	4.39814200	2.50881700	0.43774500
24	C	3.01073900	2.34914200	0.32422000
25	C	2.41435600	1.08694500	0.12495200
26	C	-5.20711000	0.68688300	0.11698000
27	C	-5.93136600	-0.47200000	0.38304600
28	C	-5.26489200	-1.68991100	0.56604000
29	C	-3.87694100	-1.78947100	0.45520700
30	H	-1.94718700	-3.06980300	-0.49695000
31	H	-0.07624500	-4.64180400	-0.58297700
32	H	2.24788600	-3.87308500	-0.35452300
33	H	4.20086800	-3.11542500	-0.17696700
34	H	6.30380800	-1.49165100	0.10953600
35	H	0.54390200	3.56314600	-0.48705500
36	H	-1.58945500	4.76039800	-0.60330300
37	H	-3.74847500	3.55288700	-0.38284700
38	H	6.34363100	1.56499600	0.44806100
39	H	4.80611600	3.50366400	0.59081200
40	H	2.38331600	3.22925300	0.41445500
41	H	-5.71203500	1.64258700	0.01085600
42	H	-7.01240800	-0.42904600	0.47114200
43	H	-5.83388800	-2.58163000	0.81119900
44	H	-3.39735400	-2.73613700	0.65747800

InCzBN (S_1)

E(B3LYP/6-311G(d)) = -1134.365391 Hartree

Tag	Symbol	X	Y	Z
1	C	-0.69388800	-1.31005400	-0.15793500
2	C	-0.95162800	-2.67674300	-0.42317500
3	C	0.09811300	-3.58752400	-0.49084900
4	C	1.40233200	-3.15110700	-0.32714000
5	C	1.66533100	-1.76901300	-0.14626500
6	C	0.63066900	-0.80452900	-0.09338300
7	N	-1.74664000	-0.40891200	-0.02479100
8	B	0.93027300	0.72154000	-0.03577000
9	N	2.97783900	-1.33191500	-0.03183500
10	C	-1.55223600	0.98764900	-0.14699000
11	C	-2.79607100	1.62977200	-0.18369100
12	C	-3.80318400	0.60613300	-0.00317000
13	C	-3.12949200	-0.64021700	0.13807800
14	C	4.15878500	-2.07882700	0.00009900
15	C	5.22379900	-1.23382400	0.14157900
16	C	4.71733600	0.11427100	0.20661900

17	C	3.31988300	0.02287500	0.09699400
18	C	-0.29988300	1.62502700	-0.18623400
19	C	-0.38892700	3.03481700	-0.34419100
20	C	-1.61447200	3.70146400	-0.41688000
21	C	-2.83341600	3.02506000	-0.32772700
22	C	5.29117400	1.38768900	0.34582900
23	C	4.43222600	2.49049100	0.37238500
24	C	3.04627800	2.35928700	0.25581400
25	C	2.41445000	1.09407700	0.10325900
26	C	-5.19016100	0.65722300	0.11275300
27	C	-5.89586200	-0.50986400	0.40119800
28	C	-5.22033700	-1.71734100	0.60645900
29	C	-3.83302400	-1.79442400	0.49056500
30	H	-1.95535100	-3.01201700	-0.63314900
31	H	-0.10559000	-4.63318800	-0.68947200
32	H	2.21331800	-3.86546200	-0.37694900
33	H	4.14663000	-3.15272200	-0.07115900
34	H	6.25814100	-1.54236900	0.19542500
35	H	0.52069600	3.61737200	-0.42304700
36	H	-1.61831500	4.78104400	-0.53571000
37	H	-3.77346500	3.56441800	-0.36449200
38	H	6.36491600	1.51581600	0.43294600
39	H	4.85602600	3.48379800	0.48828800
40	H	2.43874700	3.25475300	0.30678200
41	H	-5.71441600	1.60024300	-0.00170700
42	H	-6.97605000	-0.47627000	0.49685000
43	H	-5.77646600	-2.60737400	0.87992000
44	H	-3.33534000	-2.72416900	0.72667800

CzBN (S_0)

E(B3LYP/6-31G(d,p)) = -1287.923748 Hartree

Tag	Symbol	X	Y	Z
1	C	1.22292800	1.24543600	0.00801300
2	C	1.21294100	2.64502100	0.07040100
3	C	0.00012000	3.31971600	-0.00015400
4	C	-1.21274700	2.64508400	-0.07064700
5	C	-1.22288000	1.24549300	-0.00816100
6	C	0.00000900	0.50428900	-0.00008000
7	N	-2.43251100	0.52818100	0.02033000
8	C	-2.47490600	-0.84897600	-0.20369500
9	C	-1.36455900	-1.70325500	-0.26406800
10	C	1.36453400	-1.70330200	0.26399400
11	C	2.47490300	-0.84905200	0.20367600
12	N	2.43252300	0.52809200	-0.02038100
13	C	1.66928500	-3.05363500	0.54154600
14	C	2.98184900	-3.50201100	0.70757200
15	C	4.06534300	-2.62278600	0.58724900
16	C	3.81365400	-1.27779000	0.32654600
17	C	-3.81365800	-1.27772500	-0.32651600
18	C	-4.06537400	-2.62271600	-0.58722100
19	C	-2.98190000	-3.50195400	-0.70759100
20	C	-1.66933100	-3.05358500	-0.54161100
21	C	-3.77113100	0.98402300	0.14433600
22	C	3.77112800	0.98396600	-0.14426600
23	C	-4.29627500	2.22330000	0.52535600
24	C	-5.68352800	2.36808500	0.58361100
25	C	-6.54687900	1.30684300	0.28589100
26	C	-6.02786700	0.05806900	-0.04454400
27	C	-4.64320100	-0.11108700	-0.10340500
28	C	4.64320000	-0.11113800	0.10347500
29	C	6.02786000	0.05807400	0.04465500

30	C	6.54682500	1.30689100	-0.28571300
31	C	5.68344800	2.36813200	-0.58338800
32	C	4.29620000	2.22329700	-0.52517800
33	B	-0.00000100	-1.03843700	-0.00008800
34	H	2.12364500	3.20705300	0.19917100
35	H	0.00015800	4.40588000	-0.00020700
36	H	-2.12336700	3.20719500	-0.19950700
37	H	0.85845000	-3.76708400	0.64571100
38	H	3.16710600	-4.54983500	0.92383500
39	H	5.08286600	-2.98664400	0.69844700
40	H	-5.08290600	-2.98656400	-0.69837600
41	H	-3.16717500	-4.54977500	-0.92385500
42	H	-0.85850600	-3.76703800	-0.64582500
43	H	-3.66873900	3.05205400	0.81811900
44	H	-6.09518100	3.32843600	0.87905900
45	H	-7.62124800	1.45350400	0.33550900
46	H	-6.68843200	-0.78165700	-0.23970800
47	H	6.68845400	-0.78163100	0.23981100
48	H	7.62119000	1.45359700	-0.33528500
49	H	6.09507500	3.32851900	-0.87875500
50	H	3.66859000	3.05204500	-0.81785300

CzBN (S_1)

E(B3LYP/6-311G(d)) = -1288.043364 Hartree

Tag	Symbol	X	Y	Z
1	C	-1.20691000	-1.21629900	-0.01167600
2	C	-1.19723400	-2.63117100	-0.10576600
3	C	0.00004700	-3.32417900	-0.00012500
4	C	1.19730900	-2.63114500	0.10557600
5	C	1.20693300	-1.21627000	0.01159700
6	C	0.00000300	-0.47201600	-0.00002500
7	N	2.41448200	-0.52225700	-0.01196100
8	C	2.47530900	0.87161100	0.21639000
9	C	1.36367800	1.73052500	0.25041200
10	C	-1.36368800	1.73052200	-0.25042000
11	C	-2.47531600	0.87158200	-0.21639600
12	N	-2.41447300	-0.52229900	0.01193600
13	C	-1.69856400	3.08662100	-0.50747700
14	C	-3.01933700	3.50693700	-0.67976600
15	C	-4.09548200	2.62001600	-0.59408700
16	C	-3.81193200	1.26857900	-0.34859800
17	C	3.81193500	1.26862200	0.34858700
18	C	4.09546000	2.62005100	0.59406400
19	C	3.01928900	3.50697100	0.67974100
20	C	1.69853700	3.08664700	0.50746500
21	C	3.74284600	-0.99447400	-0.14177300
22	C	-3.74284200	-0.99450100	0.14181800
23	C	4.24849600	-2.22707200	-0.56133800
24	C	5.63159000	-2.39575400	-0.61855700
25	C	6.50205600	-1.35197000	-0.28982800
26	C	6.00151200	-0.10165900	0.06586100
27	C	4.62303900	0.09166500	0.12546700
28	C	-4.62303900	0.09163100	-0.12545600
29	C	-6.00151200	-0.10167200	-0.06581900
30	C	-6.50206600	-1.35195800	0.28993900
31	C	-5.63160600	-2.39572600	0.61872600
32	C	-4.24851200	-2.22706300	0.56147900
33	B	-0.00000700	1.08118000	0.00000600
34	H	-7.57423400	-1.50942400	0.34193400
35	H	7.57422400	-1.50944900	-0.34179800
36	H	3.21571400	4.55708700	0.87523900

37	H	-3.21573800	4.55705500	-0.87527600
38	H	-2.11028100	-3.17633900	-0.28268200
39	H	0.00006500	-4.40805200	-0.00018100
40	H	2.11038600	-3.17629600	0.28241400
41	H	-0.90520300	3.82008700	-0.58996500
42	H	-5.11537200	2.97107300	-0.70673800
43	H	5.11533500	2.97115400	0.70670300
44	H	0.90514400	3.82007800	0.58994900
45	H	3.61049800	-3.03279000	-0.89389700
46	H	6.03144700	-3.35031900	-0.94307200
47	H	6.67785300	0.72043600	0.27579400
48	H	-6.67784600	0.72042300	-0.27577400
49	H	-6.03147300	-3.35026400	0.94330800
50	H	-3.61053200	-3.03276500	0.89409900

6. Device Fabrication and Measurement

All compounds were purified by temperature-gradient sublimation under a high vacuum before use. Organic light-emitting diodes (OLEDs) were fabricated on ITO-coated glass substrates with multiple organic layers sandwiched between the transparent bottom ITO anode and the top metal cathode. The ITO glass substrates were first cleaned carefully. Then different layers of organic materials were deposited by thermal evaporation in a vacuum chamber with a base pressure of 10^{-6} torr. The deposition system permits the fabrication of the complete device in a single vacuum pump-down without breaking vacuum. The deposition rate of organic layers was kept at 0.1−0.2 nm s^{-1}. The doping layer was obtained by co-evaporation from separate sources with different evaporation rates. The current density, voltage, luminance, current efficiency (CE), power efficiency (PE), external quantum efficiency (EQE), electroluminescence (EL) spectra and other device characteristics were measured at the same time with a Keithley 2400 source meter and a Hamamatsu C9920-12 instrument, which is equipped with Hamamatsu PMA-12 Photonic multichannel analyzer C10027-02.

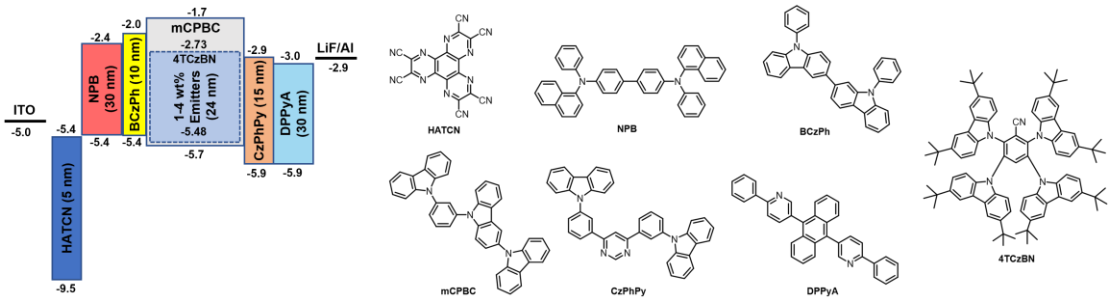


Figure S12. The energy diagrams of the device and the molecular structures of the materials used in the device fabrication.

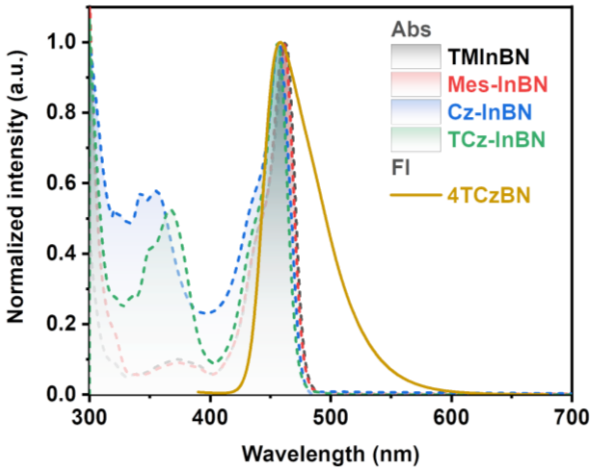


Figure S13. UV-vis absorption spectra of the MR emitters and the fluorescence spectrum of the sensitizer 4TCzBN in toluene solution.

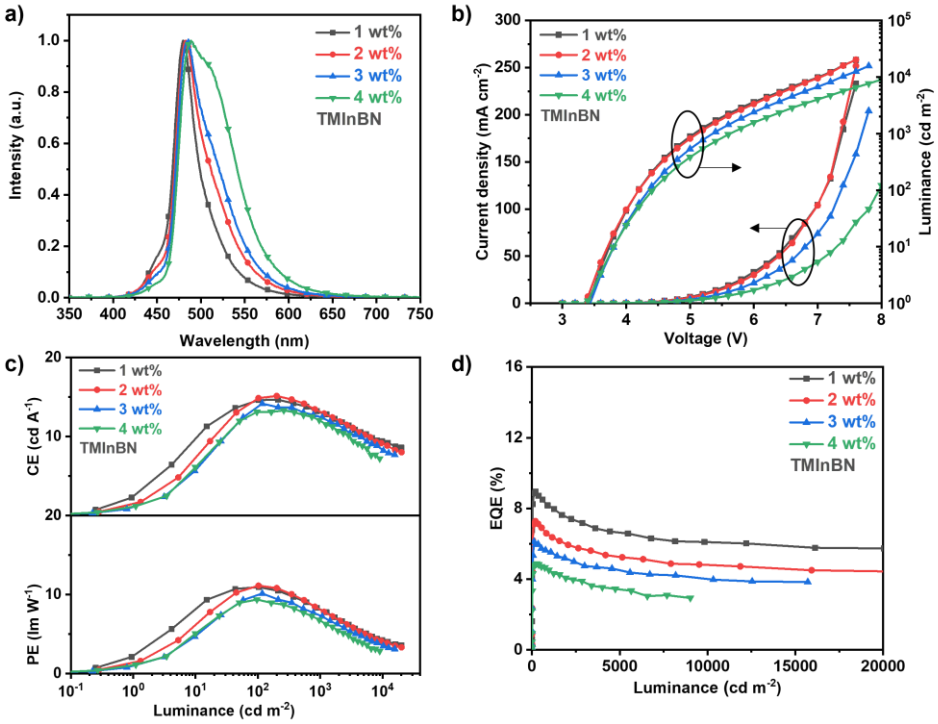


Figure S14. (a) EL spectra, (b) current density and luminance versus voltage, (c) current efficiency (CE) and power efficiency (PE) versus luminance, and (d) external quantum efficiency versus luminance curves of OLED devices based on TMInBN.

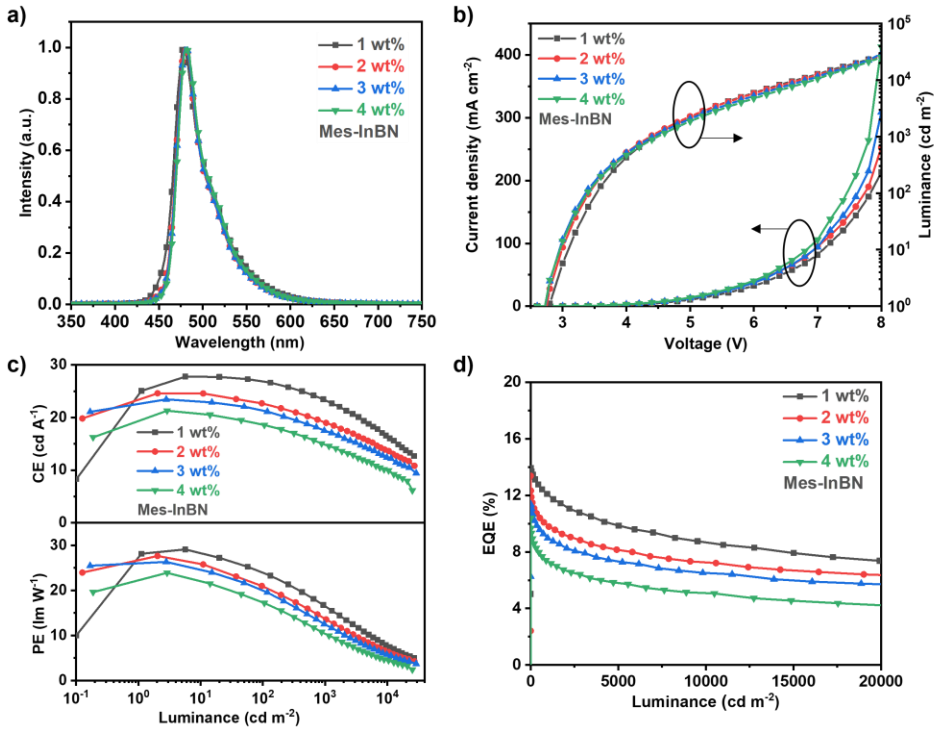


Figure S15. (a) EL spectra, (b) current density and luminance versus voltage, (c) current efficiency (CE) and power efficiency (PE) versus luminance, and (d) external quantum efficiency versus luminance curves of OLED devices based on Mes-InBN.

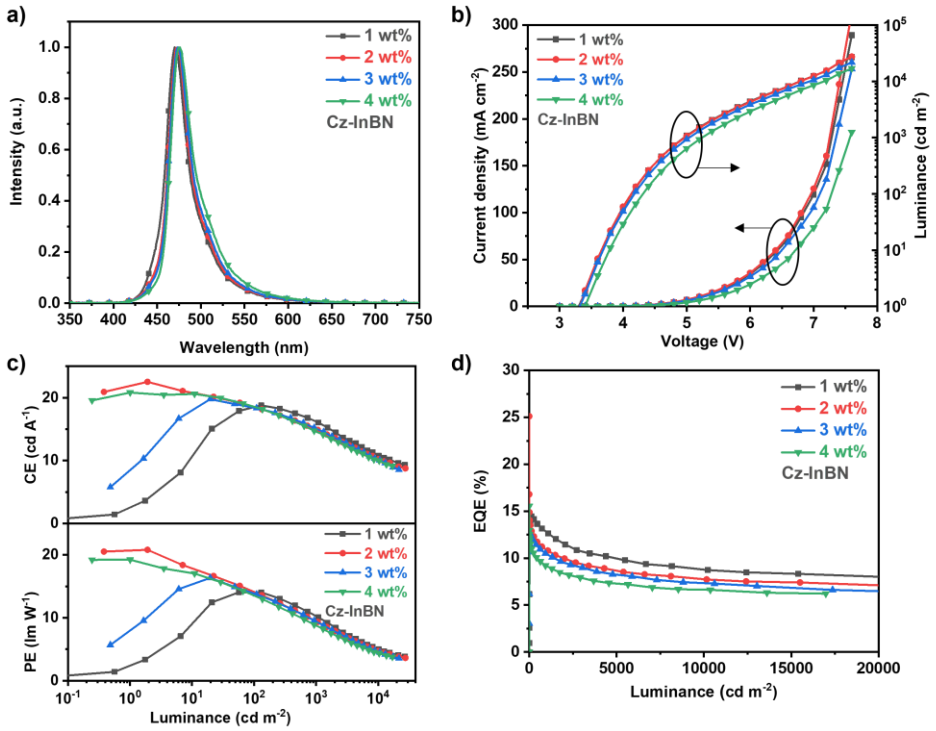


Figure S16. (a) EL spectra, (b) current density and luminance versus voltage, (c) current efficiency (CE) and power efficiency (PE) versus luminance, and (d) external quantum efficiency versus luminance curves of OLED devices based on Cz-InBN.

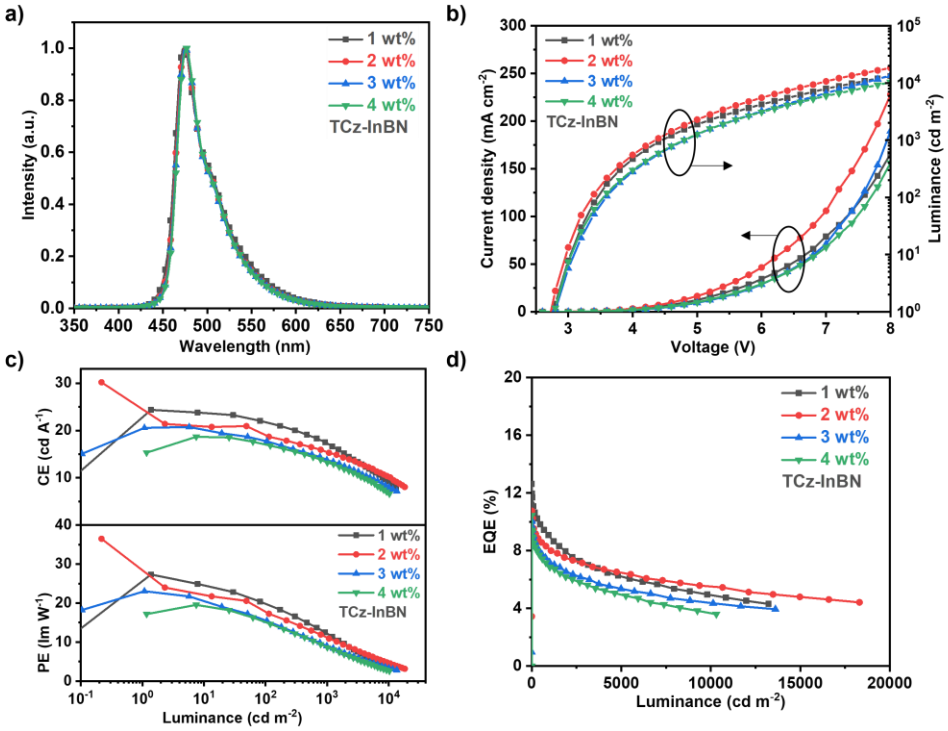


Figure S17. (a) EL spectra, (b) current density and luminance versus voltage, (c) current efficiency (CE) and power efficiency (PE) versus luminance, and (d) external quantum efficiency versus luminance curves of OLED devices based on TCz-InBN.

7. References

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[6] MRCC, a quantum chemical program suite written by M. Kállay, P. R. Nagy, D. Mester, L. Gyevi-Nagy, J. Csóka, P. B. Szabó, Z. Rolik, G. Samu, J. Csontos, B. Hégely, Á. Ganyecz, I. Ladjánszki, L. Szegedy, B. Ladóczki, K. Petrov, M. Farkas, P. D. Mezei, and R. A. Horváth. See www.mrcc.hu.

8. NMR and HRMS Spectra

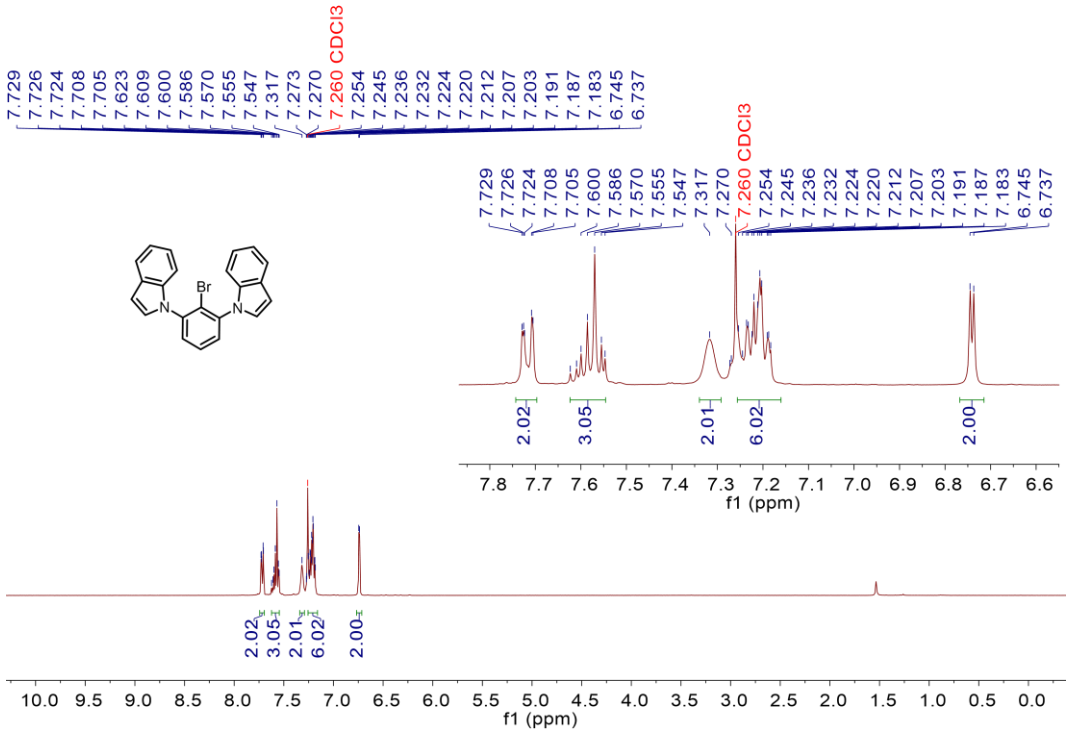

Figure S18. ^{1}H NMR spectrum of **2** (400 MHz, $CDCl_3$, 298 K).

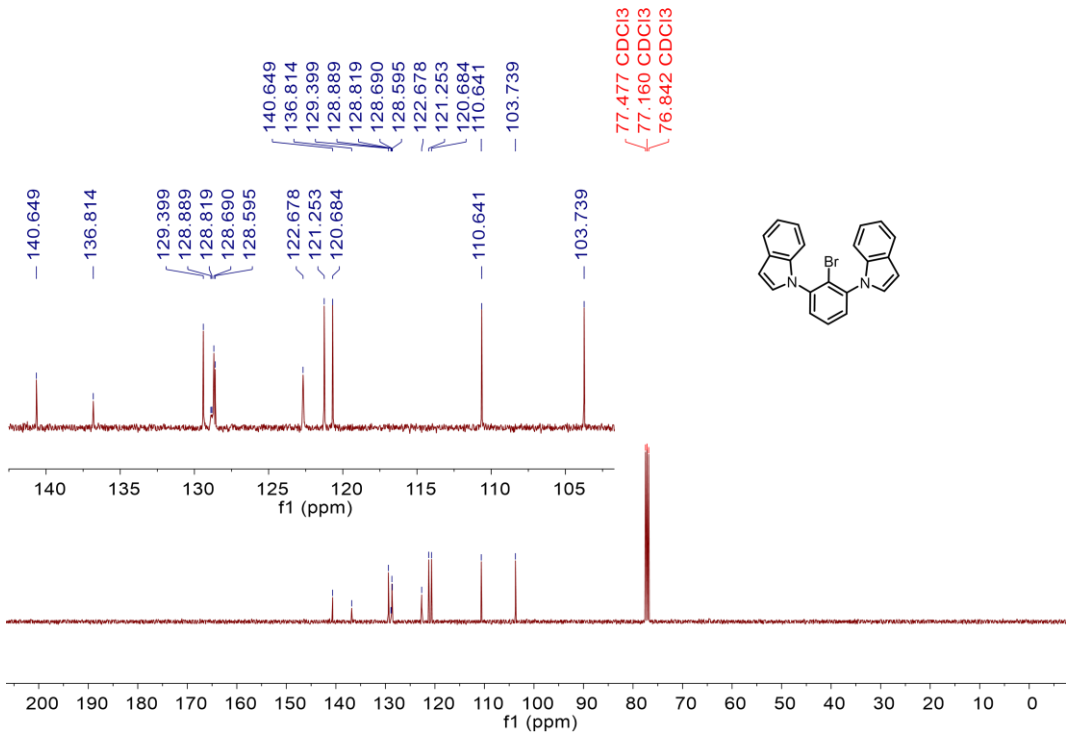

Figure S19. ^{13}C NMR spectrum of **2** (101 MHz, $CDCl_3$, 298 K).

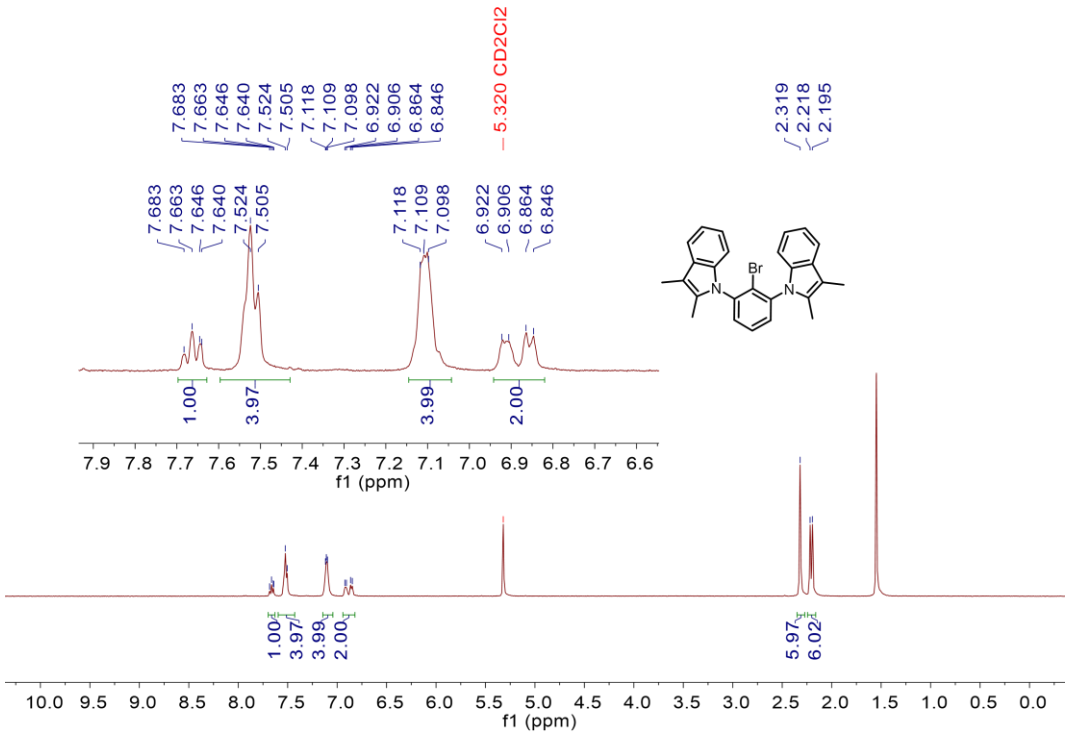

Figure S20. ^{1}H NMR spectrum of **3** (400 MHz, CD_2Cl_2, 298 K).

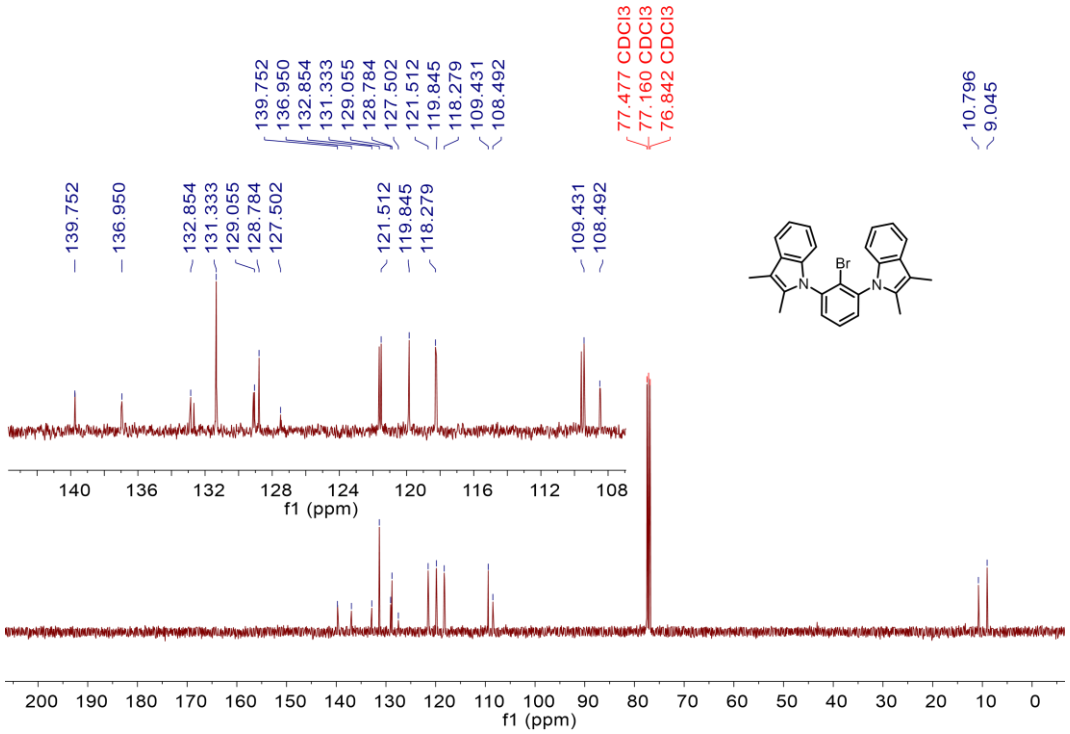

Figure S21. ^{13}C NMR spectrum of **3** (101 MHz, $CDCl_3$, 298 K).

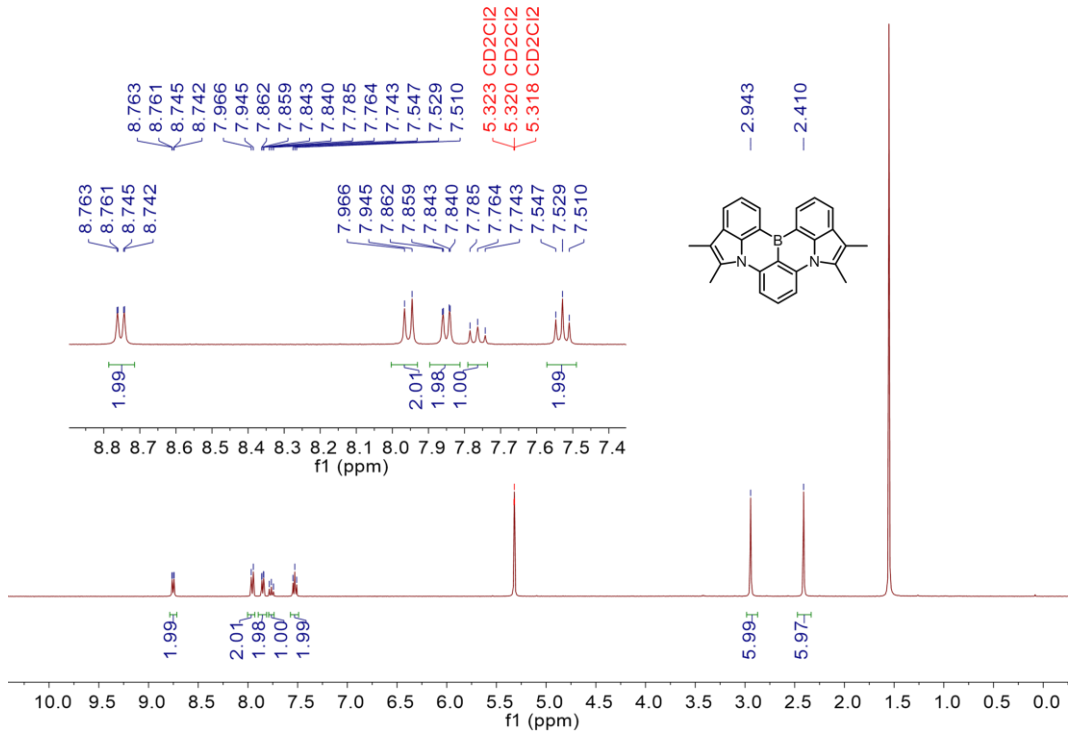

Figure S22. ^{1}H NMR spectrum of **TMInBN** (400 MHz, CD_2Cl_2, 298 K).

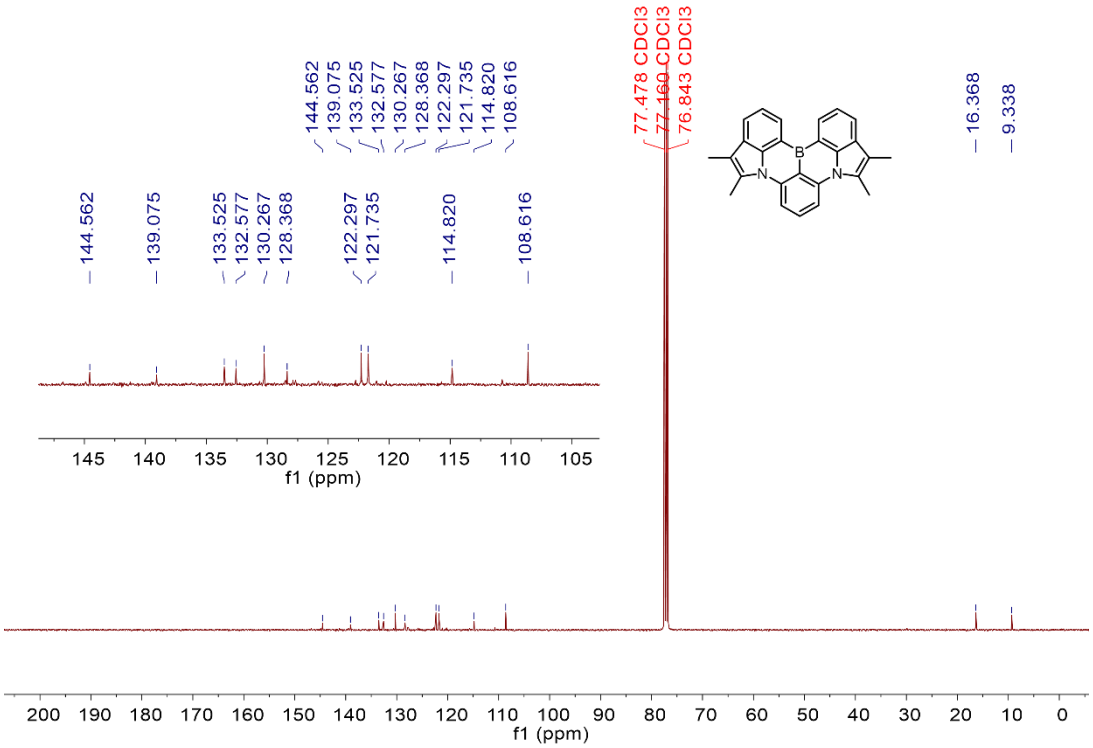

Figure S23. ^{13}C NMR spectrum of **TMInBN** (101 MHz, $CDCl_3$, 298 K).

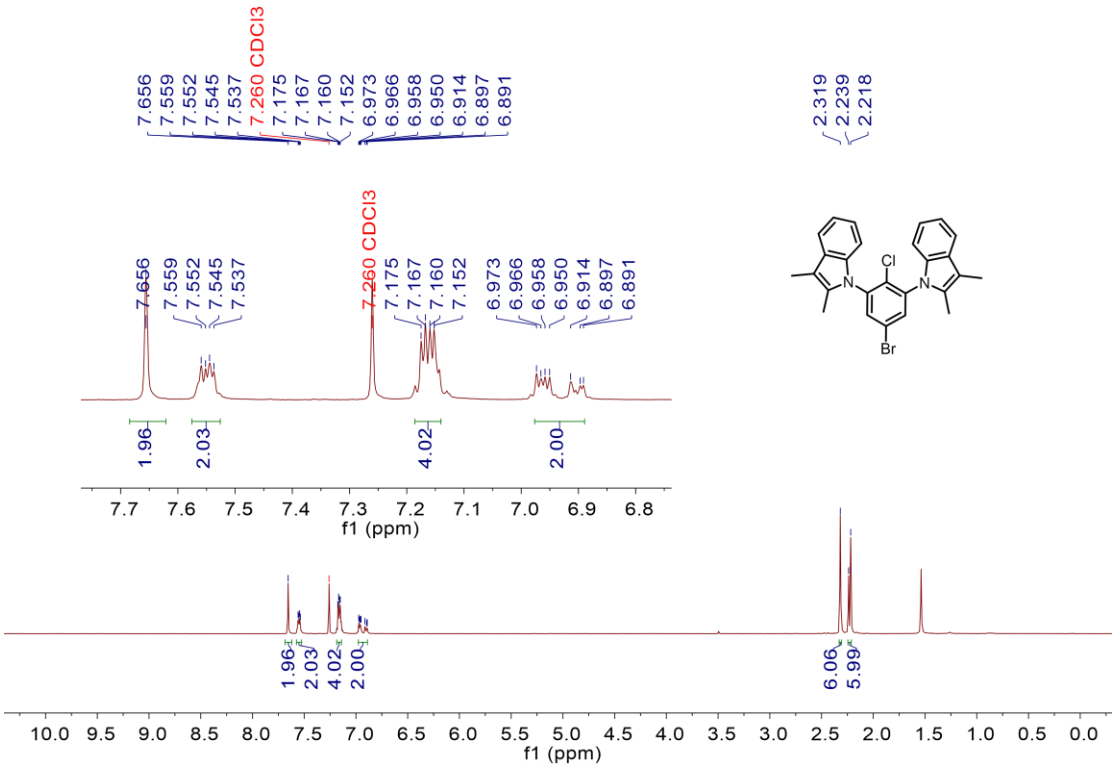

Figure S24. ^{1}H NMR spectrum of **5** (400 MHz, $CDCl_3$, 298 K).

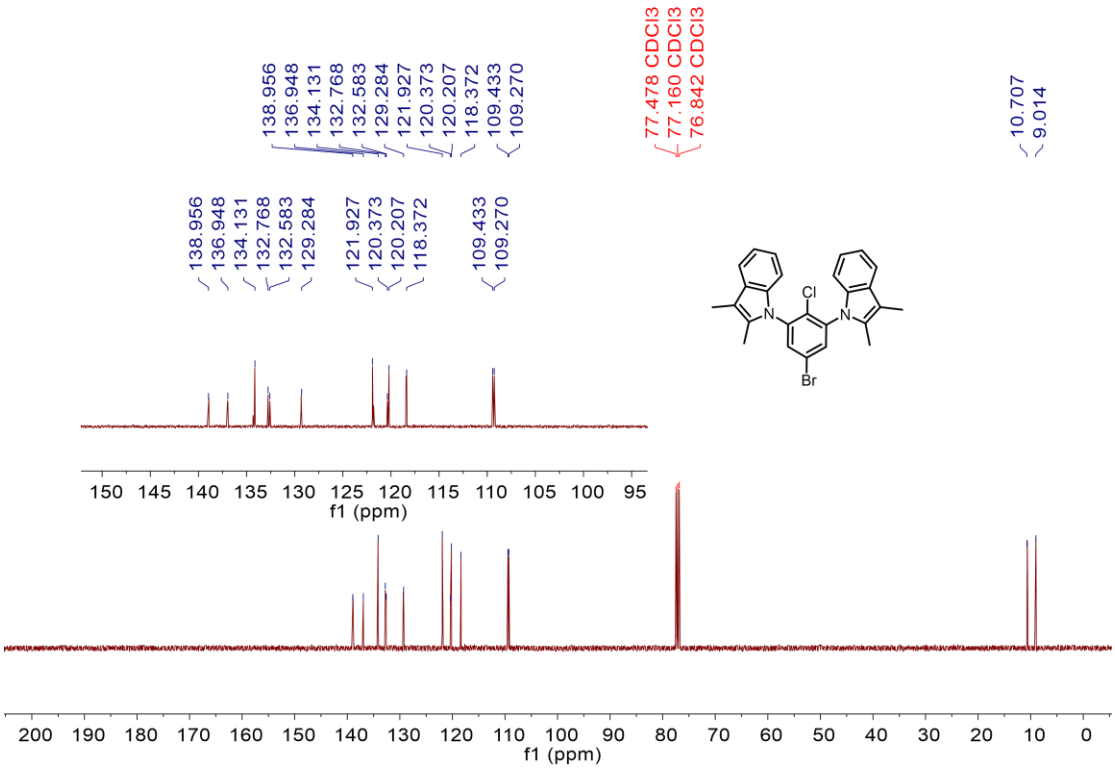

Figure S25. ^{13}C NMR spectrum of **5** (101 MHz, $CDCl_3$, 298 K).

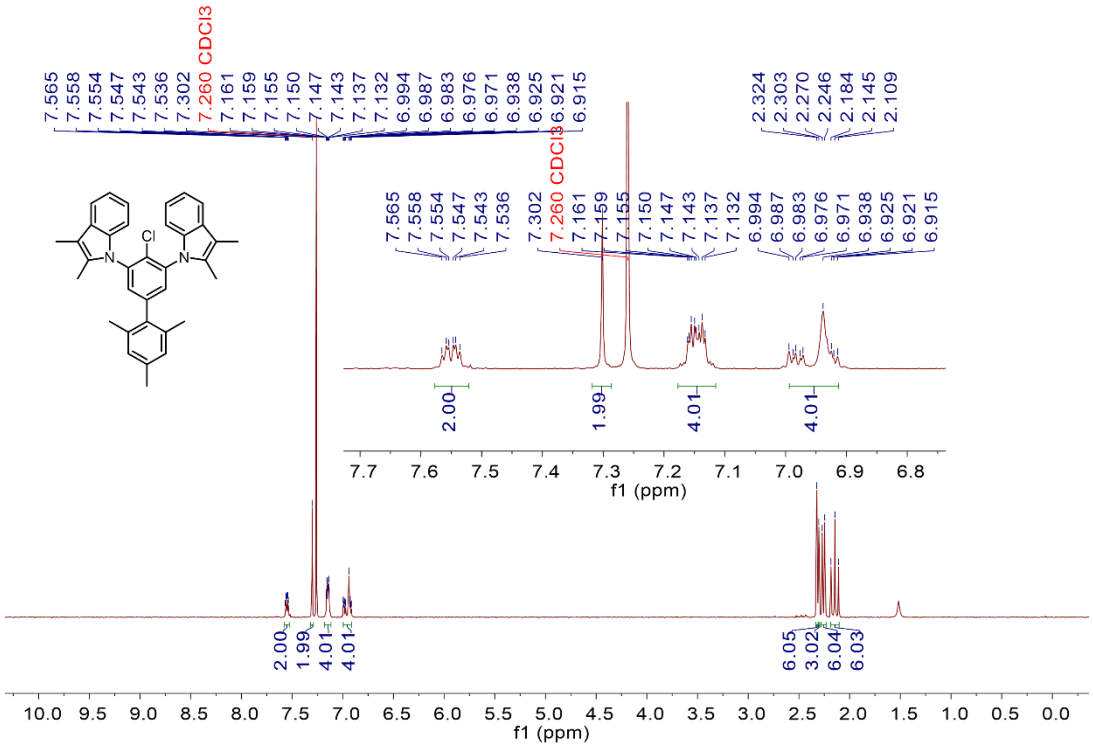

Figure S26. ^{1}H NMR spectrum of **6a** (400 MHz, $CDCl_3$, 298 K).

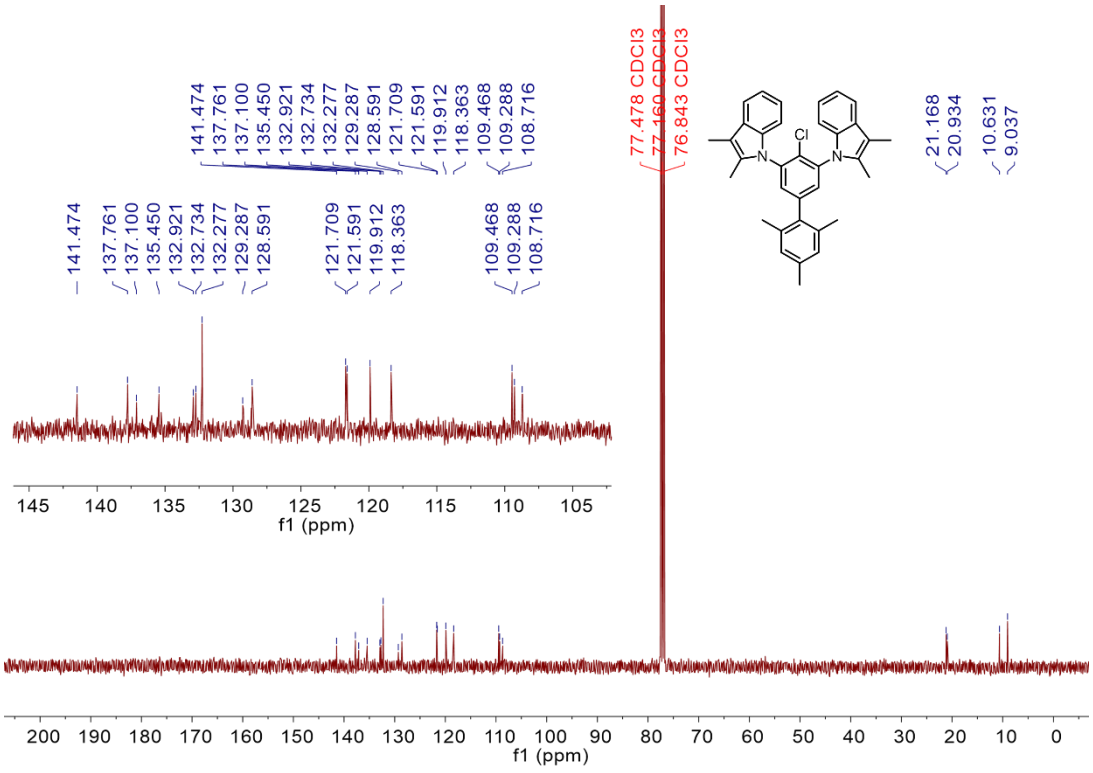

Figure S27. ^{13}C NMR spectrum of **6a** (101 MHz, $CDCl_3$, 298 K).

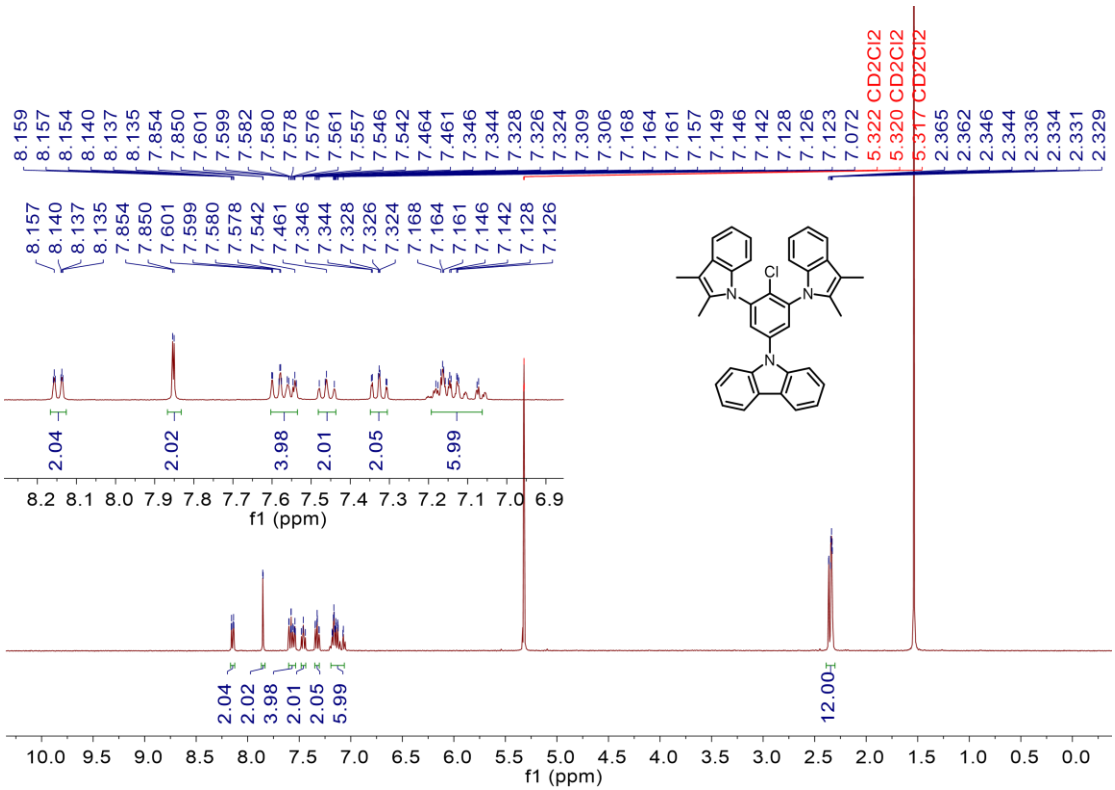

Figure S28. ^{1}H NMR spectrum of **6b** (400 MHz, CD_2Cl_2, 298 K).

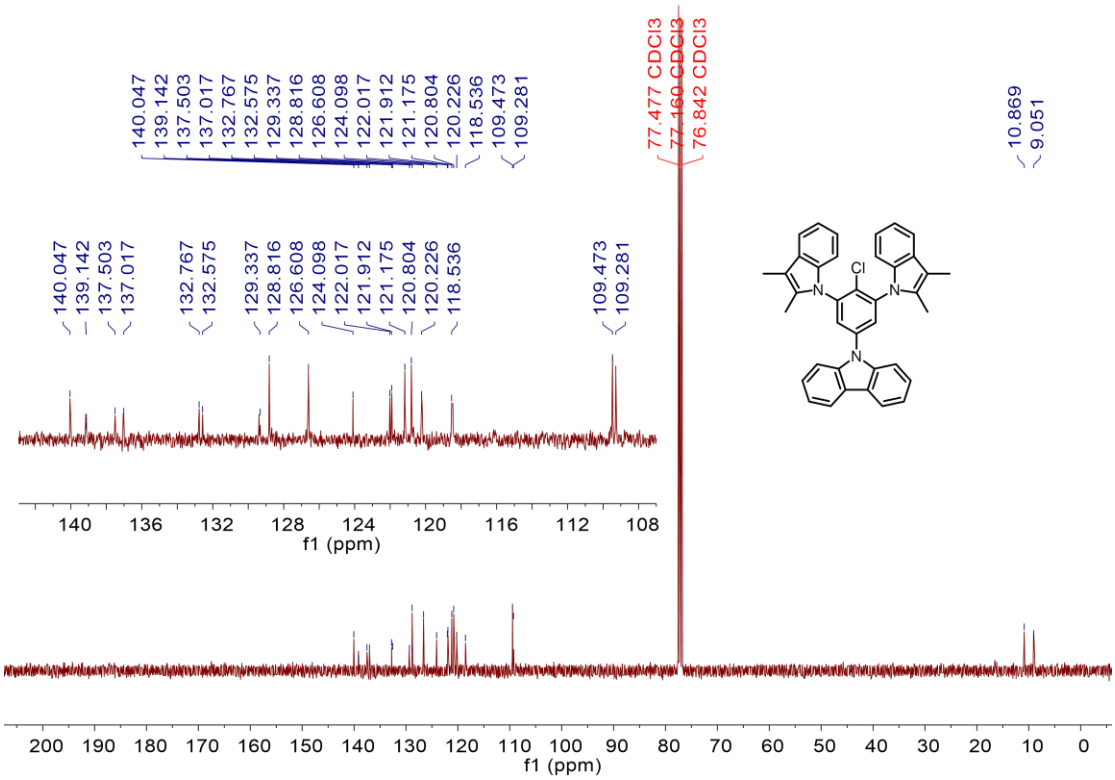

Figure S29. ^{13}C NMR spectrum of **6b** (101 MHz, $CDCl_3$, 298 K).

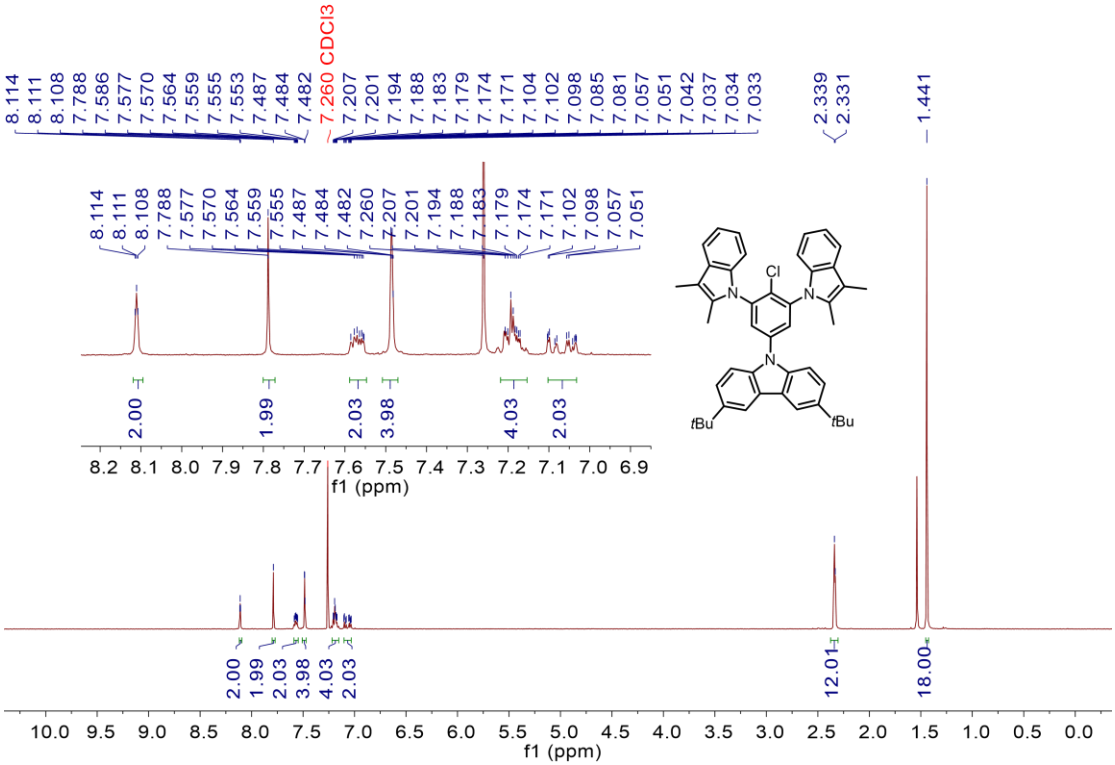

Figure S30. ^{1}H NMR spectrum of **6c** (400 MHz, $CDCl_3$, 298 K).

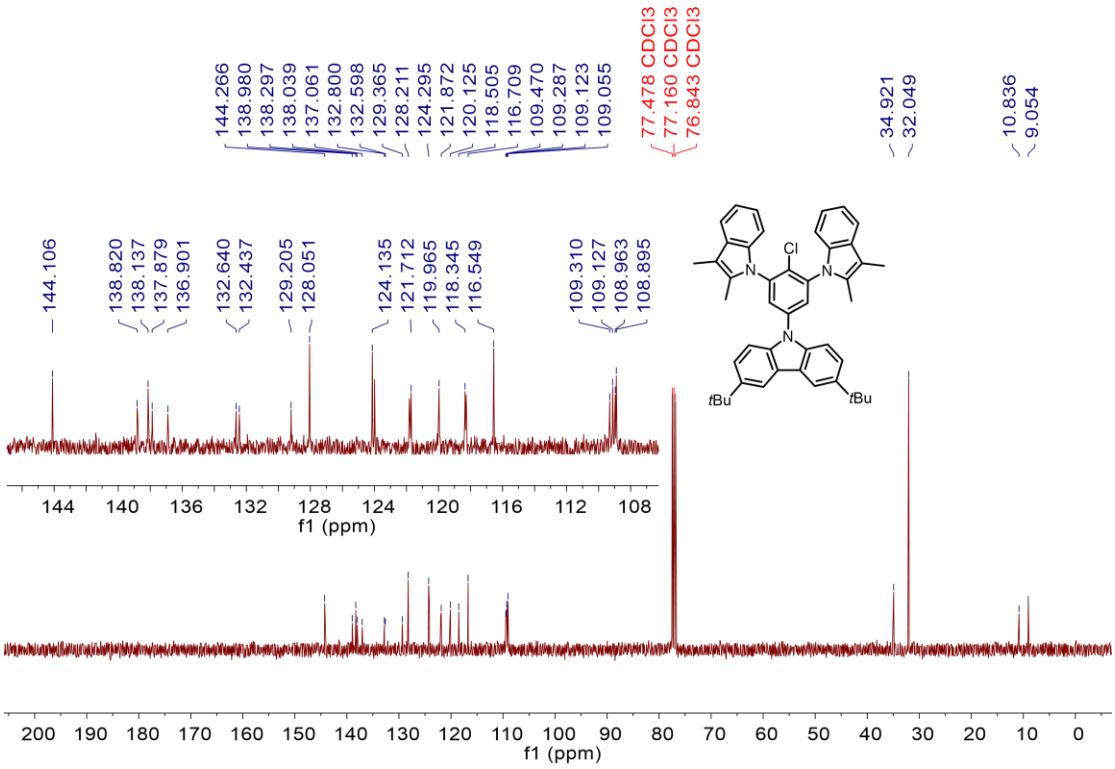

Figure S31. ^{13}C NMR spectrum of **6c** (101 MHz, $CDCl_3$, 298 K).

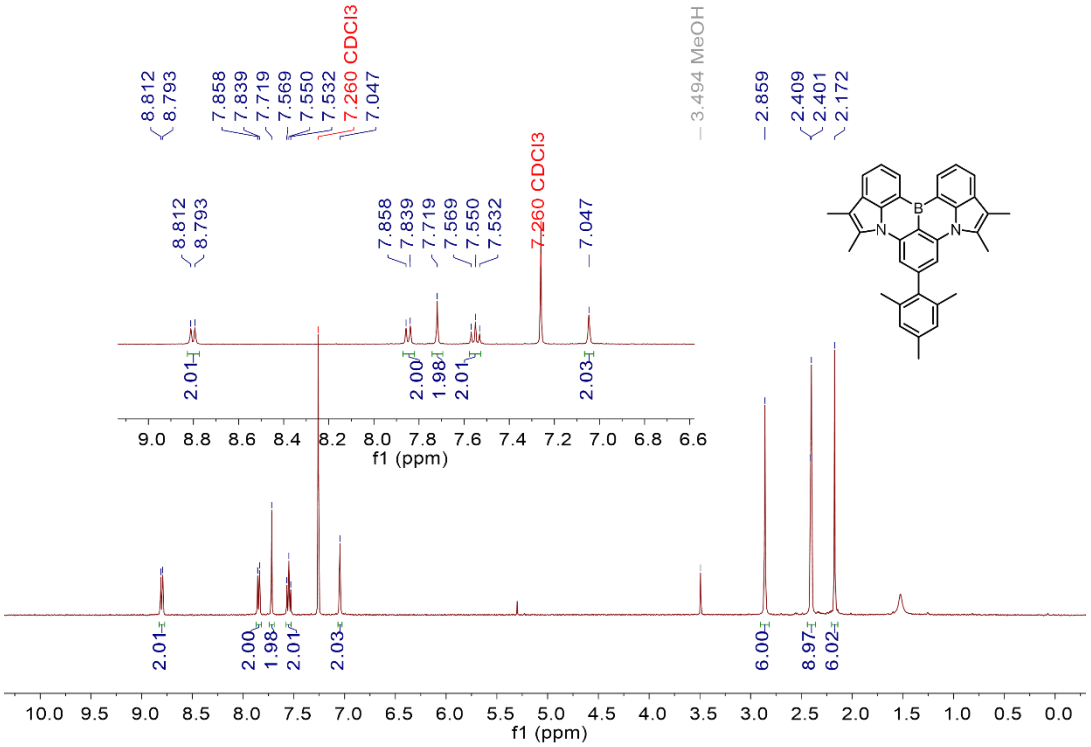

Figure S32. ^{1}H NMR spectrum of **Mes-InBN** (400 MHz, $CDCl_3$, 298 K).

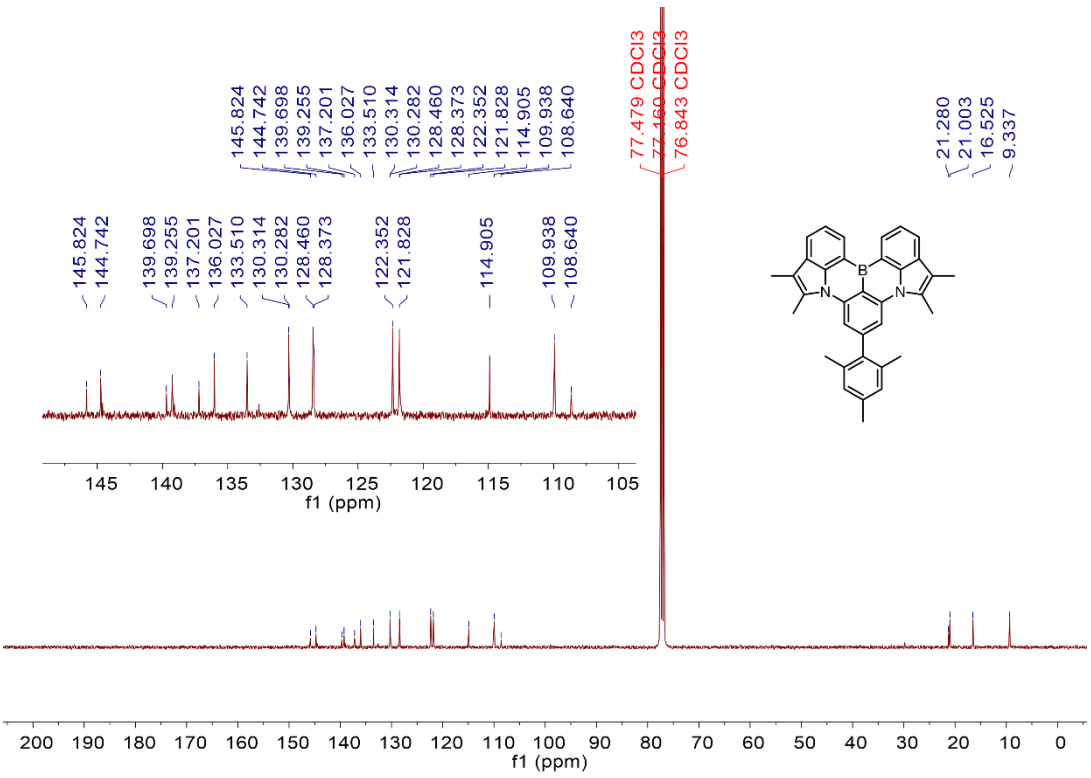

Figure S33. ^{13}C NMR spectrum of **Mes-InBN** (101 MHz, $CDCl_3$, 298 K).

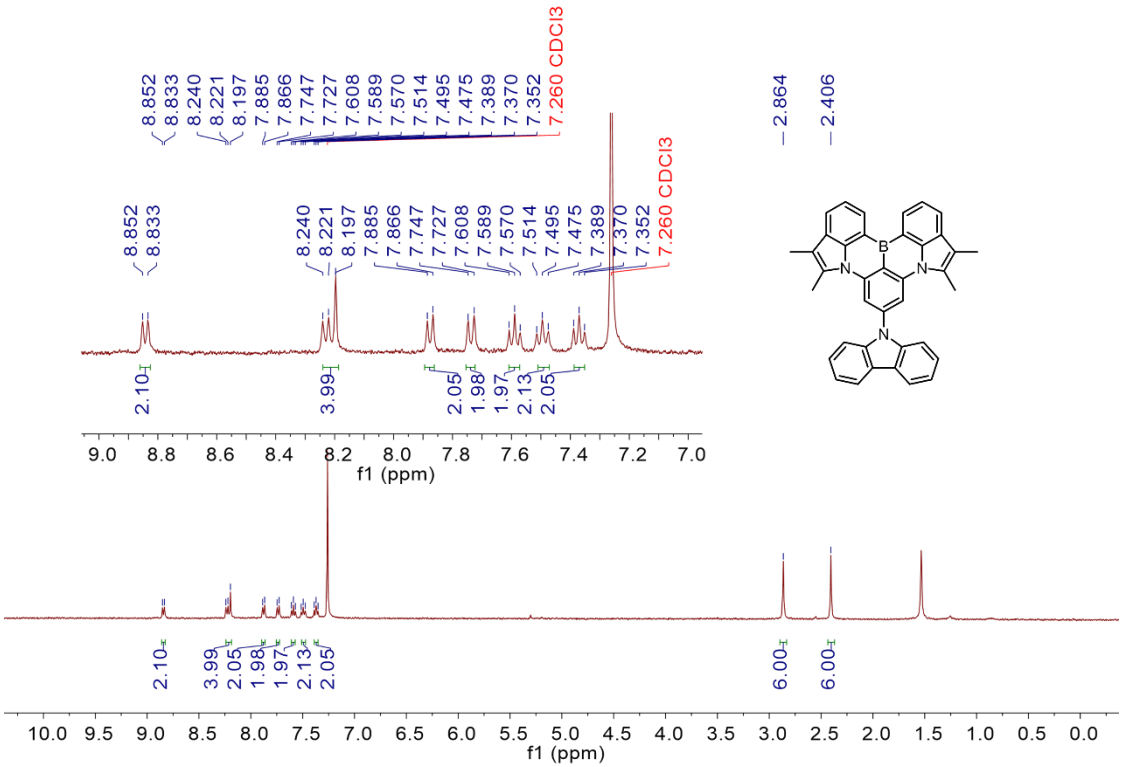

Figure S34. ^{1}H NMR spectrum of **Cz-InBN** (400 MHz, $CDCl_3$, 298 K).

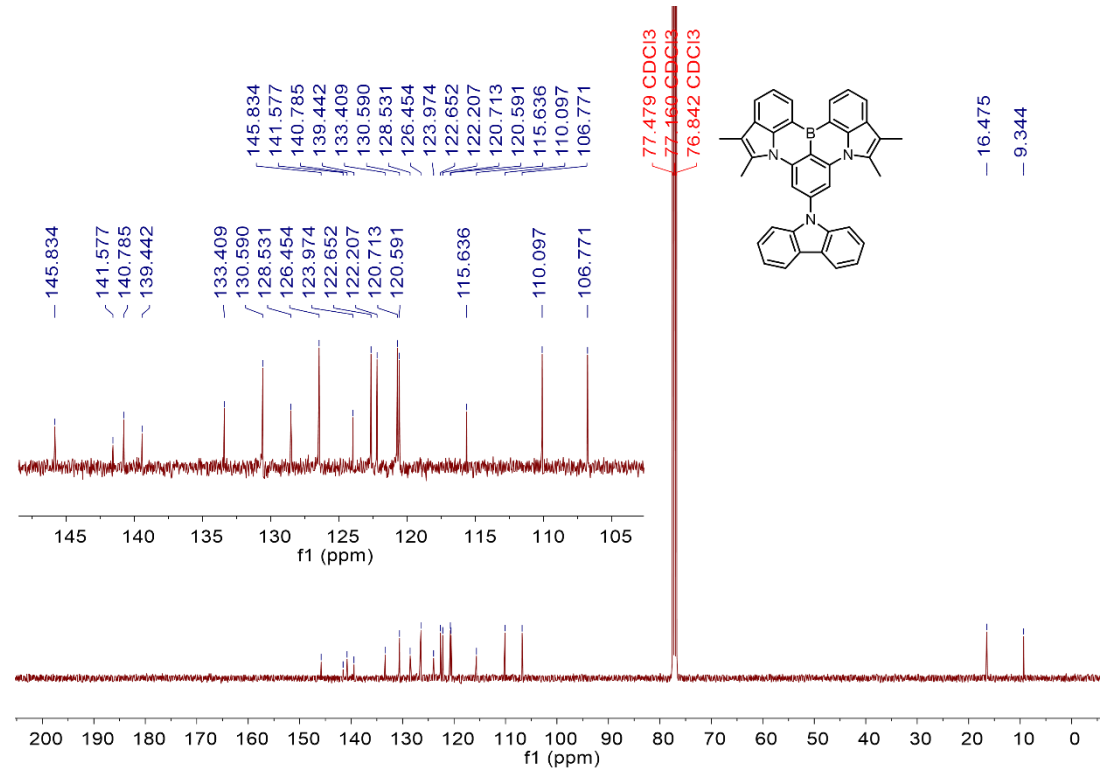

Figure S35. ^{13}C NMR spectrum of **Cz-InBN** (101 MHz, $CDCl_3$, 298 K).

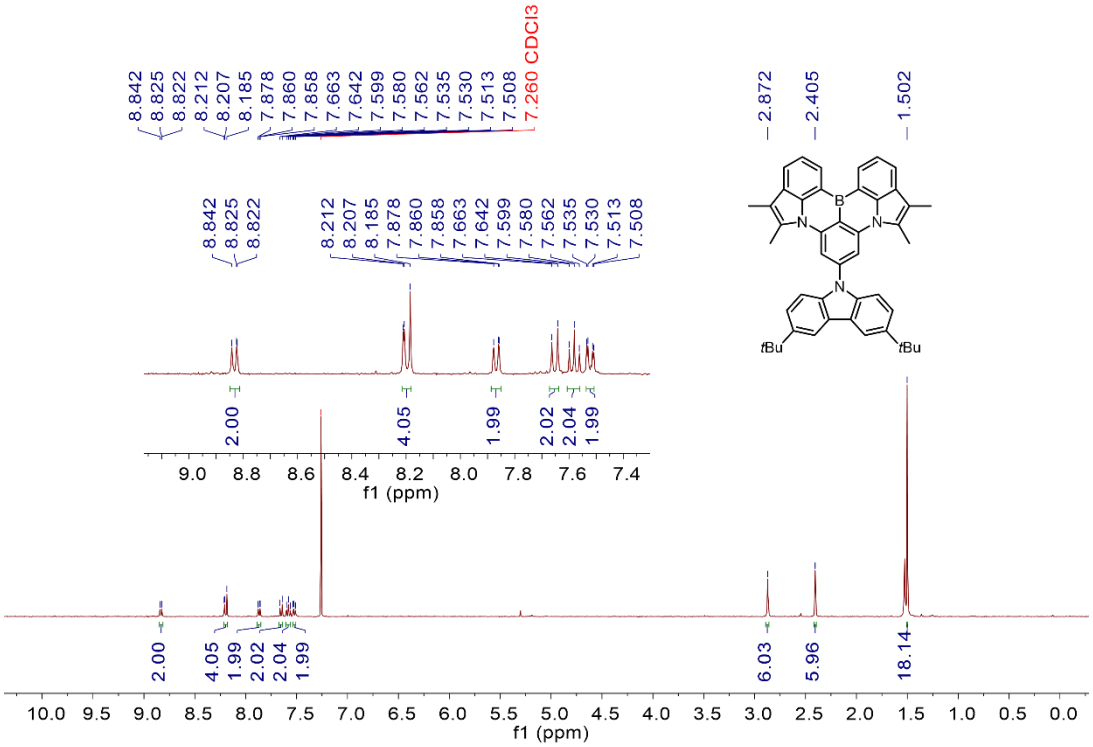

Figure S36. ^{1}H NMR spectrum of **TCz-InBN** (400 MHz, $CDCl_3$, 298 K).

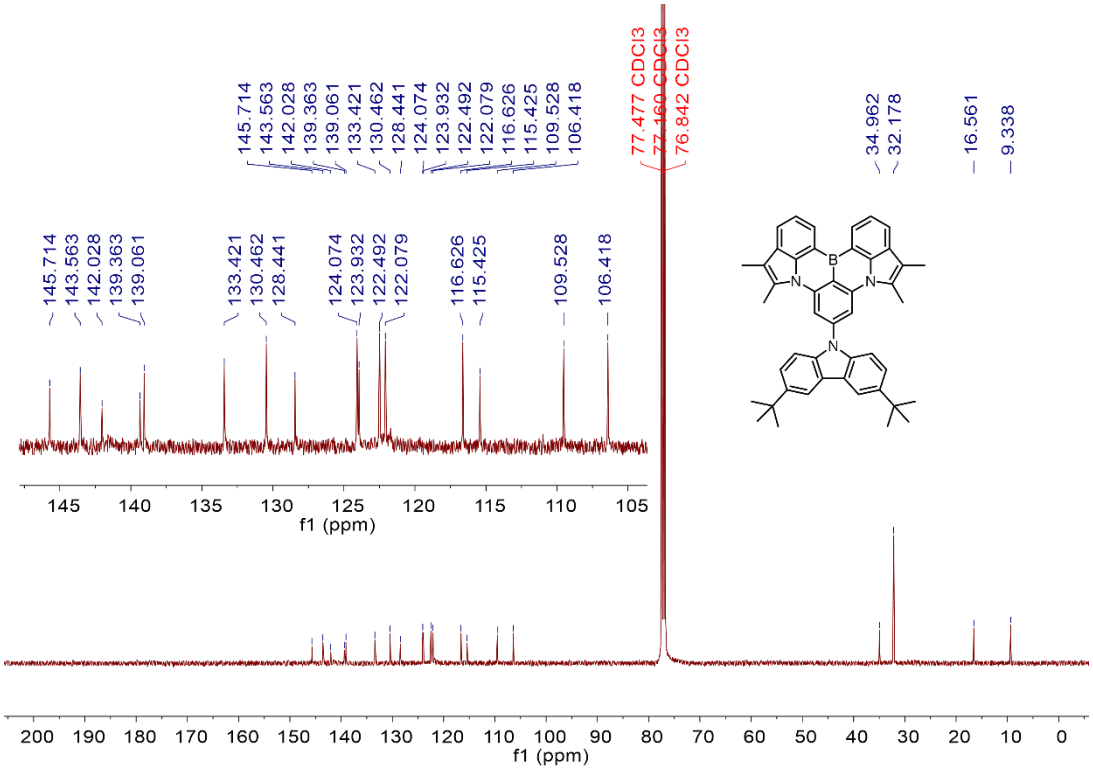

Figure S37. ^{13}C NMR spectrum of **TCz-InBN** (101 MHz, $CDCl_3$, 298 K).

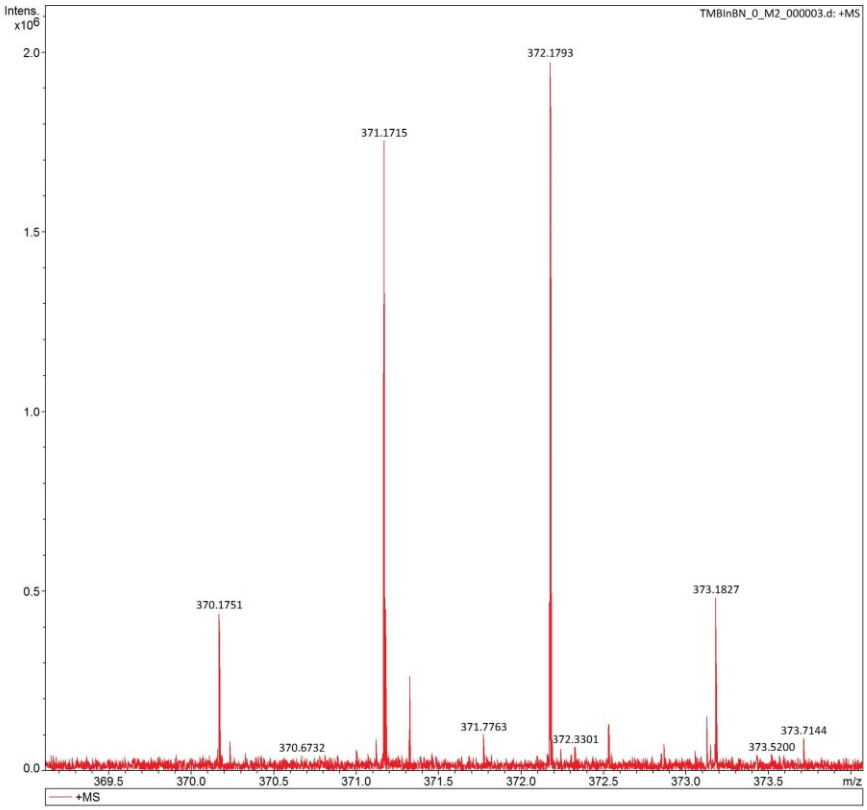

Figure S38. High-resolution MALDI-MS spectrum of **TMInBN**.

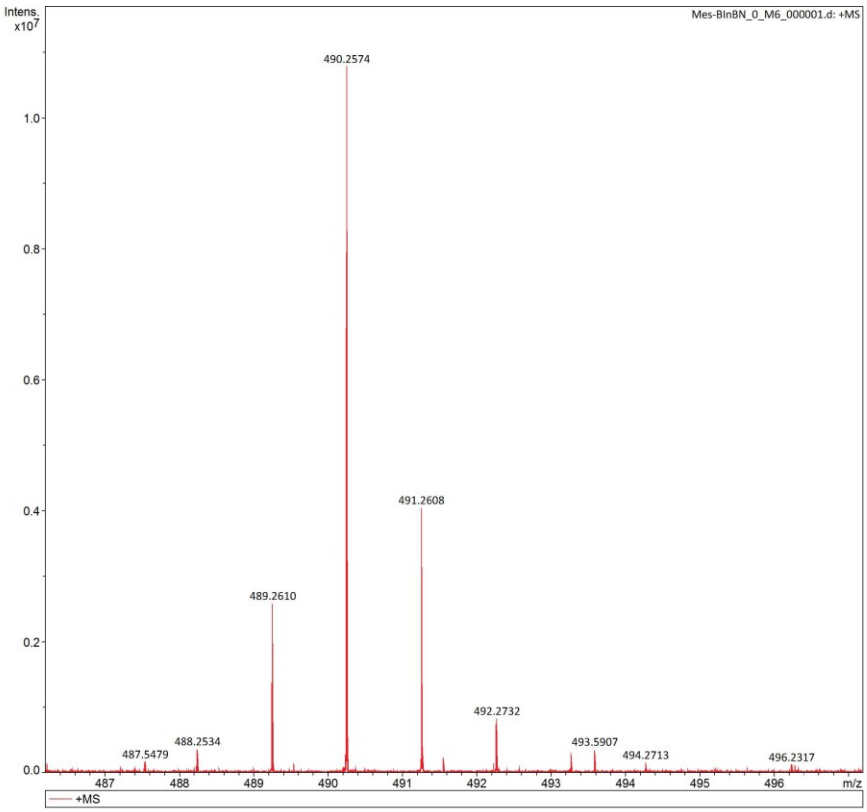

Figure S39. High-resolution MALDI-MS spectrum of **Mes-InBN**.

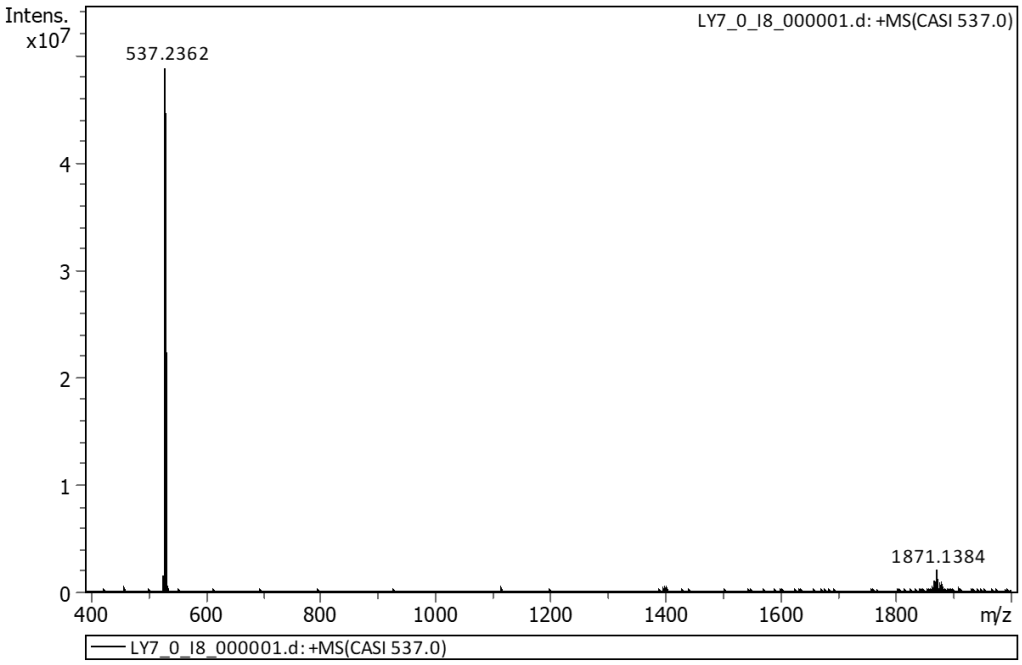

Figure S40. High-resolution MALDI-MS spectrum of **Cz-InBN**.

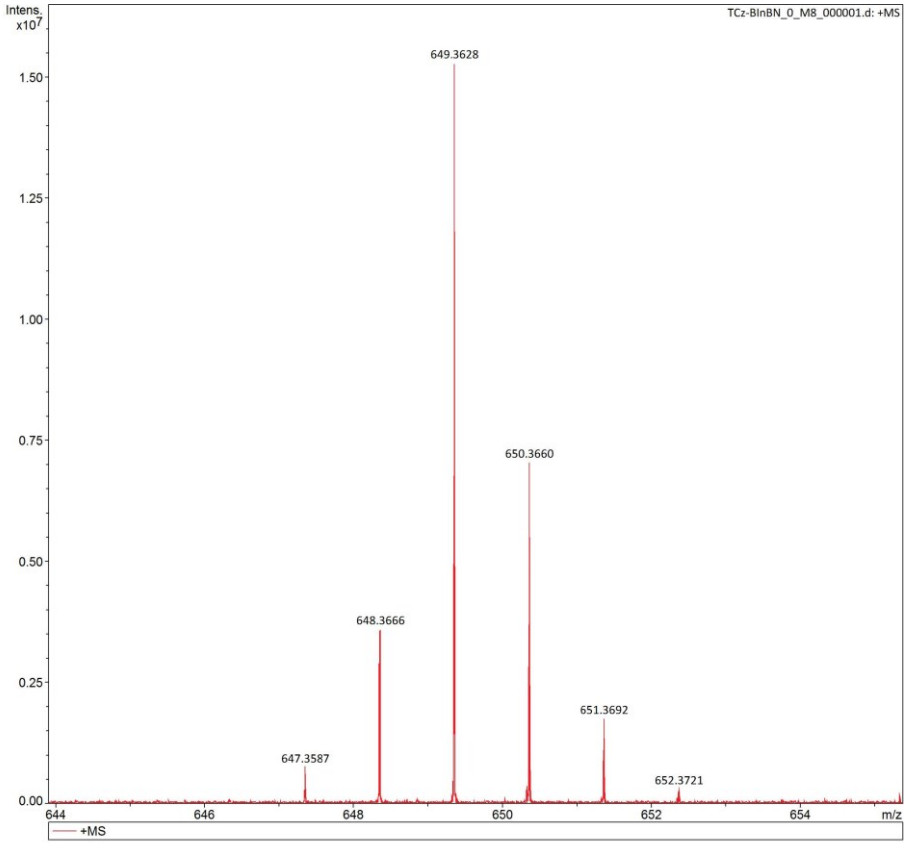

Figure S41. High-resolution MALDI-MS spectrum of **TCz-InBN**.

9. HPLC Analysis Report

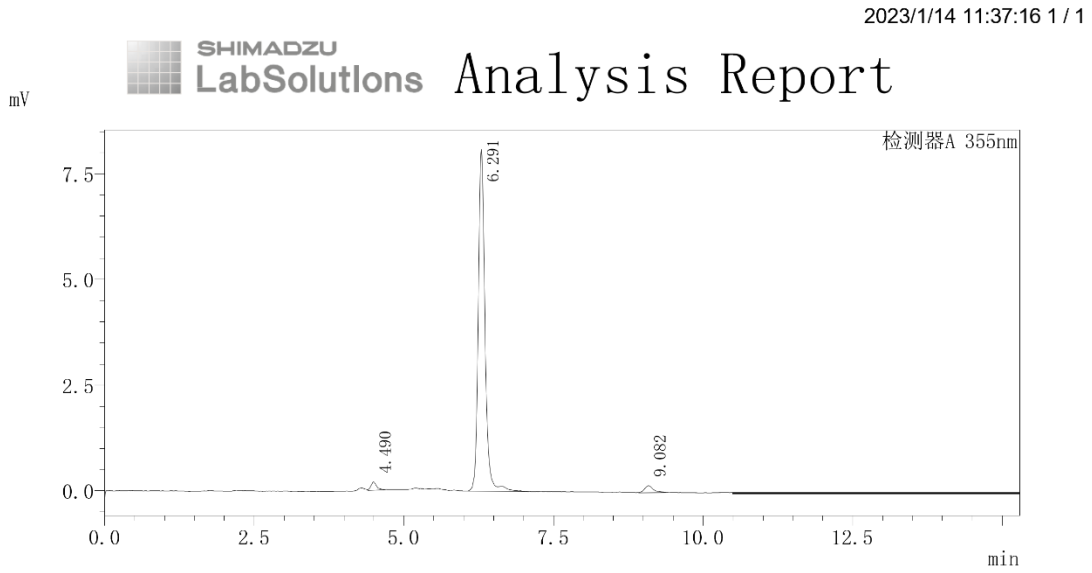

Figure S42. The HPLC trace of **TMInBN**.

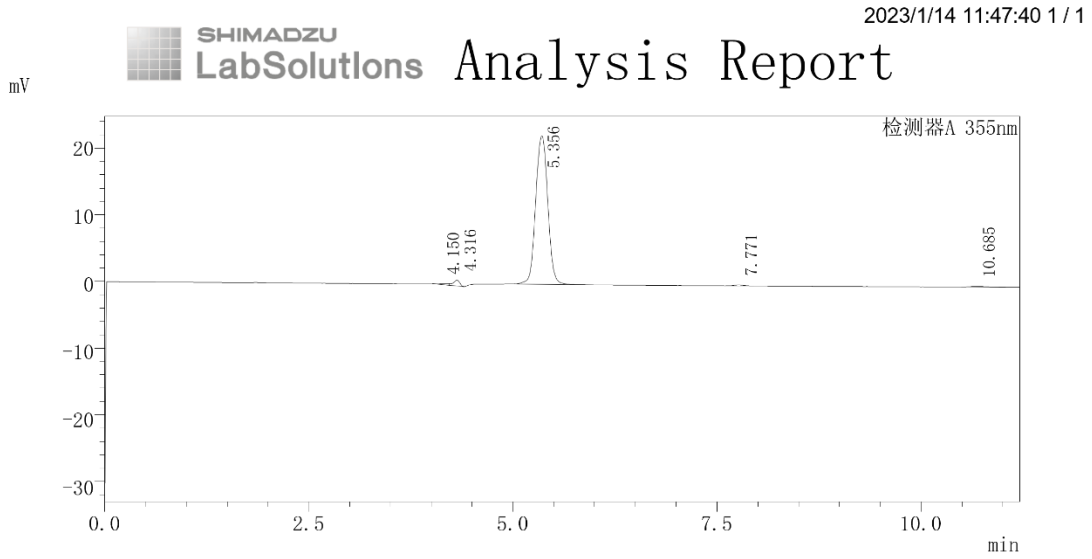

Figure S43. The HPLC trace of **Mes-InBN**.

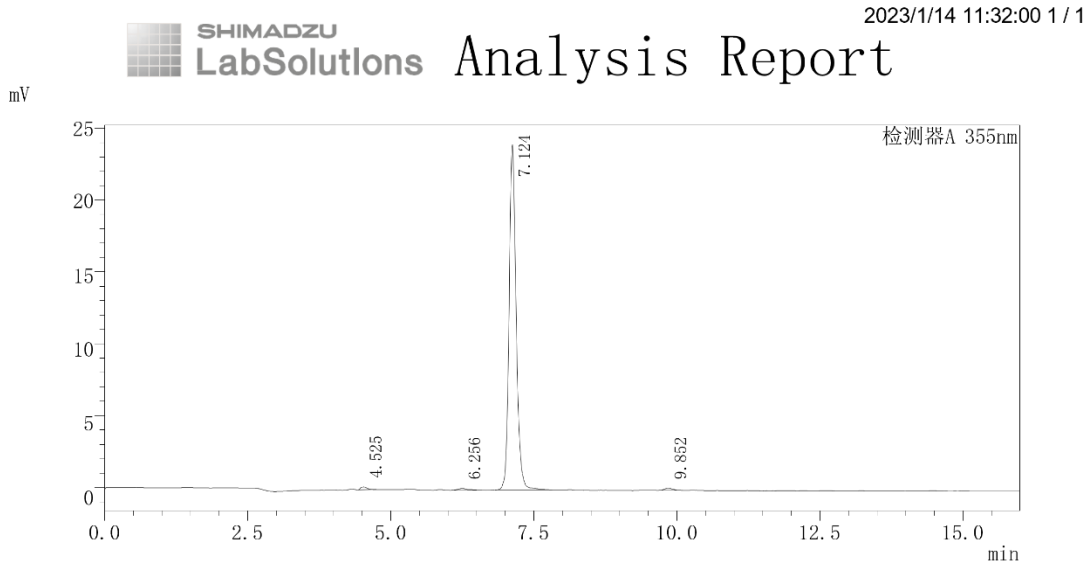

Figure S44. The HPLC trace of **Cz-InBN**.

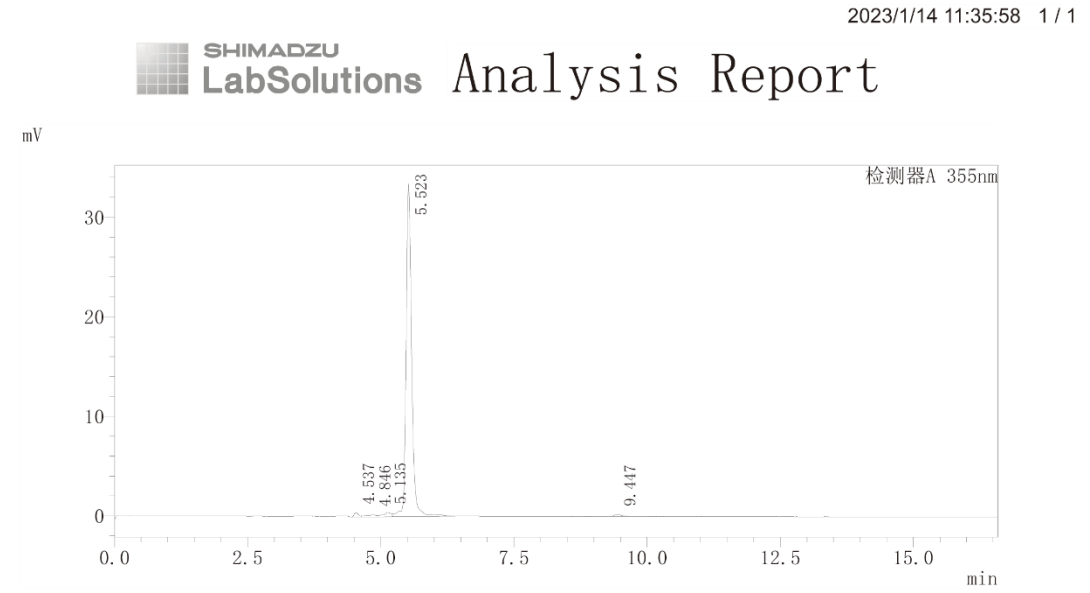

Figure S45. The HPLC trace of **TCz-InBN**.