Supporting Information

Multi-Resonance Emitters with Room-Temperature Phosphorescence in Amorphous State and Excited by Visible Light

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Table of contents

Experimental Details

General information

The chemicals and reagents were obtained from Sigma-Aldrich and Energy Chemical and used directly unless otherwise noted. Tetrahydrofuran and toluene were distilled from sodium/benzophenone, while *N, N*-dimethylformamide and *N*-methylpyrrolidone were dried by CaH_2 before use. ^{1}H and ^{13}C NMR spectrum were recorded by Bruker Avance NMR spectrometers in $CDCl_3$ or $C_2D_2Cl_4$ with tetramethylsilane as internal standard. Matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectra was measured on AXIMA CFR MS apparatus (COMPACT). Thermal gravimetric analysis was performed on Perkin-Elmer-TGA 7 at heating rate of 10 ^{o}C/min with continuous nitrogen flow. Cyclic voltammetry was carried out in electrochemical workstation (Shanghai CH instruments, CHI610E) with three-electrode cell using *n*-Bu_4NClO_4 (0.1 M) as supporting electrolyte and ferrocene as reference at a scan rate of 50 $mV{\cdot}s^{-1}$.

Single-crystal analysis

Single crystals for the emitters were grown by slow sublimation of the samples under vacuum. The crystallographic data were collected by Bruker D8 VENTURE diffractometer equipped with graphite monochromated Cu K_α radiation (λ =1.54184 Å) at 293 K, using the phi and omega scans technique. The structure was solved by direct methods, and all the non-hydrogen atoms were refined anisotropically on F2 by full-matrix least-squares using SHELXL package.

Photophysical measurements

UV-visible absorption spectra were measured by PerkinElmer Lambda 35 UV-vis spectrometer, and steady-state photoluminescence (PL) spectra were measured by HORIBA FluoroMax spectrofluorometer. Transient PL spectra and time-resolved spectroscopy were detected on Edinburgh fluorescence spectrometer (FLSP-980). PLQY values were measured by integrating sphere coupled with a photonic multichannel analyzer on Hamamatsu Photonics C9920-2.

Computational method

The calculations were performed with Gaussian 09 package using density functional theory (DFT) for HOMO/LUMO distributions, and time-dependent density functional theory (TD-DFT) for optimization of excited-state configuration and electron transition analysis at the M062X/def2SVP level of theory. The SOC matrix elements are calculated by ORCA software package (version 4.1) at the same theory level. Natural transition orbitals (NTO) were performed by Multiwfn (version 3.5)[1] and drawn by VMD software (version 1.9.3). The excited-state energy levels were calculated by SCS-CC2 calculations using the MRCC Program[2] with cc-pVDZ basis set to consider electron correlation in the form of double excitations[3].

Calculation for kinetic parameters

The calculation formulas for rate constant of radiative decay from S_1 (k_r^F), radiative decay and non-radiative decay from T_1 (k_r^P and k_{nr}^P), intersystem crossing (k_{ISC}) from S_1 to T_1 and reverse intersystem crossing (k_{RISC}) from T_1 to S_1 are expressed as follows. For α-ThBSS, α-DThBSS and α-DThBSS-Cz with fluorescence and RTP emissions[4]:

$$k_r^F = \Phi_F / \tau_F$$

$$k_r^P = \Phi_{Ph} / \tau_{Ph}$$

$$k_{nr}^P = (1-\Phi_{Ph})/\tau_{Ph}$$

$$k_{ISC} = \Phi_{Ph} / \tau_F$$

where τ_F and τ_{Ph} are lifetimes of fluorescence and phosphorescence emissions, and Φ_F and Φ_{Ph} are quantum efficiencies for fluorescence and phosphorescence components. For β-ThBSS, β-DThBSS and β-DThBSS-Cz with TADF and RTP emissions[5]:

$$k_r^P = \Phi_{Ph} / \tau_{Ph}$$

$$k_{nr}^P = (1-\Phi_{Ph})/\tau_{Ph}$$

$$k_r^F = \Phi_{PF} / \tau_p$$

$$k_{ISC} = (1-\Phi_{PF})/\tau_p$$

$$k_{RISC} = (\Phi_{PL}-\Phi_{PF})R_{DE}^{DF}/[\Phi_{PF}\ (1-\Phi_{PF})\tau_d]$$

where τ_p and τ_d are lifetimes of prompt and delayed emissions for TADF emission component, while τ_{Ph} is lifetime of phosphorescence component. Φ_{PL} is total photoluminescenct quantum efficiency, while Φ_{PF} and Φ_{Ph} are quantum efficiency for prompt fluorescence and phosphorescence components respectively. R_{DE}^{DF} is the ratio of the delayed fluorescence component of the delayed. Note that due to the fast intersystem crossing process for B, S-doped PAHs, the non-radiative decay from S_1 (k_{nr}^F) could be ignored, thus we assume that $\Phi_{PF} + \Phi_{ISC} = 1$.

Preparation of RTP films and patterning

The emitters (α-ThBSS, α-DThBSS and α-DThBSS-Cz) are mixed (1 wt% for each emitter) with poly (methyl methacrylate) which are dissolved in chlorobenzene to form the inks with 10 mg/mL concentration. Then films with butterfly and digital patterns are fabricated by coating the prepared inks on wood-free paper via cotton swab, which are dried at room temperature under vacuum for 6 h. For multi-color anti-counterfeiting applications, the α-DThBSS-Cz and α-ThBSS ink was successively coated through a flower-shaped mask and a leaf-shaped mask on the same paper, and are dried at room temperature under vacuum for 6 h after each coating step.

Synthetic Procedures

Benzo[b]thiophene-3-thiol (2)

3-Bromobenzo[*b*]thiophene (**1**, 42.6 g, 200.0 mmol) was dissolved in tetrahydrofuran (THF) (300 mL) under argon atmosphere and cooled to -78 ºC. Afterwards a solution of *n*-butyllithium in hexane (80.0 mL, 2.5 M, 200.0 mmol) was added dropwise and the mixture was stirred at -78 ºC for 1 hour. After adding grounded sulfur (7.04 g, 220.0 mmol) in 3 portions, the mixture was kept at -78 ºC for 3 hours and then quenched with 1 M aq. HCl (100 mL). After warming to room temperature, the organic layer was separated and the aqueous layer was extracted with ethyl acetate three times (100 mL×3). The combined organic phases were made alkaline with 1.5 M aq. NaOH (150 mL). The aqueous phase was separated and acidized by 1 M aq. HCl (250 mL) and then extracted three times with ethyl acetate (100 mL×3). The organic phases were combined and dried over anhydrous $MgSO_4$. After the solvent was removed under vacuum, the product **2** was obtained as yellow liquid (25.2 g) and used directly for next step. Yield: 76%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 8.8 Hz, 2H), 7.49-7.39 (m, 3H), 3.30 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.55, 139.40, 126.89, 124.82, 124.58, 122.82, 122.49, 118.93.

3-((2,5-Dibromo-3-fluorophenyl)thio)benzo[b]thiophene (3)

A mixture of **2** (5.00 g, 30.1 mmol), 2,5-dibromo-1,3-difluorobenzene (9.00 g, 33.1 mmol) and K_2CO_3 (8.32 g, 60.2 mmol) in dry *N*-methylpyrrolidone (NMP, 150 mL) was stirred at 60 ºC for 24 hours under argon atmosphere and then cooled to room temperature. The mixture was slowly poured into deionized water (600 mL) and the aqueous layer was extracted with dichloromethane three times (100 mL×3). The combined organic fractions were dried over anhydrous $MgSO_4$ and the solvent was removed under vacuum. The crude product was purified by silica gel chromatography using hexane as eluent to afford **3** as a white solid (11.0 g). Yield: 88%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dd, *J* = 6.8, 1.6 Hz, 1H), 7. 91 (s, 1H), 7.77 (dd, *J* = 6.8, 1.6 Hz, 1H), 7.46-7.43 (m, 2H), 7.04 (dd, *J* =7.2, 1.6 Hz, 1H), 6.42 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.09, 140.14, 138.36, 135.69, 125.54, 125.36, 124.66, 123.21, 122.74, 121.45, 121.36, 121.00, 116.45, 116.19.

3-((2,5-Dibromo-3-(phenylthio)phenyl)thio)benzo[b]thiophene (4)

A mixture of **3** (4.18 g, 10.0 mmol) and sodium thiophenolate (1.20 g, 9.0 mmol) in dry

NMP (100 mL) was stirred at 60 °C for 24 hours under argon atmosphere and then cooled to room temperature. The mixture was slowly poured into NH_4Cl solution (400 mL), which was extracted with dichloromethane three times (50 mL×3). The combined organic fractions were dried over anhydrous $MgSO_4$ and the solvent was removed under vacuum. The crude product was purified by silica gel chromatography using hexane/dichloromethane (8/1, v/v) as eluent to afford **4** as a white solid (4.10 g). Yield: 90%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 7.0, 2.5 Hz, 1H), 7.89 (s, 1H), 7.79 (dd, *J* =7.0, 2.5 Hz, 1H), 7.54-7.51 (m, 2H), 7.45-7.42 (m, 5H), 6.54 (d, *J* = 2.0 Hz, 1H), 6.36 (d, *J* = 2.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.13, 142.06, 140.09, 138.46, 135.37, 134.81, 131.15, 130.03, 129.59, 126.84, 125.75, 125.43, 125.25, 123.12, 122.86, 121.92, 121.77, 117.14.

7-Bromo-5,9,14-trithia-14b-borafluoreno[3,2,1-de]anthracene (α-ThBSS-Br)

A solution of *n*-butyllithium in hexane (1.68 mL, 2.5 M, 4.2 mmol) was added slowly to a solution of **4** (2.03 g, 4.0 mmol) in anhydrous *m*-xylene (50 mL) at -30 °C under argon atmosphere. The reaction mixture was stirred for 30 minutes before heating at 40 °C for 1 hour. BBr_3 (0.46 mL, 4.8 mmol) was slowly added to the mixture at -30 °C, which was then heated to 50 °C and stirred for 3 hours. After addition of $(i\text{-Pr})_2$NEt (1.4 mL, 8.0 mmol) at 0 °C, the reaction mixture was stirred at 120 °C for 24 hours, which was then cooled to room temperature and slowly quenched by 2 mL deionized water. Subsequently, the reaction mixture was filtered and the residue was washed with methanol (40 mL) to afford the desired compound ***α*-ThBSS-Br** as a yellow solid (786.6 mg). Yield: 45%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.06 (d, *J* = 8.0 Hz, 1H), 8.08 (d, *J* = 8.0 Hz, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.83 (d, *J* =1.5 Hz, 1H), 7.73 (d, *J* =1.5 Hz,1H), 7.64-7.57 (m, 3H), 7.54-7.49 (m, 2H). ^{13}C NMR (126 MHz, $C_2D_2Cl_4$) δ 146.05, 144.42, 144.20, 142.81, 139.94, 138.11, 136.96, 131.65, 127.95, 125.44, 124.86, 124.59, 124.41, 124.29, 122.89, 122.54.

5,9,14-Trithia-14b-borafluoreno[3,2,1-de]anthracene (α-ThBSS)

A mixture of ***α*-ThBSS-Br** (437.0 mg, 1.0 mmol), Pd(dppf)Cl_2 (22.0 mg, 0.03 mmol), *N,N,N′,N′*-tetramethylethylenediamine (TMEDA, 27.8 mg, 5.0 mmol), $NaBH_4$ (230.4 mg, 5.0 mmol) and THF (50 mL) was stirred at room temperature under argon atmosphere for 12 hours. After the mixture was poured into deionized water (200 mL), the precipitate was filtered, dried under vacuum, and then subjected to silica gel chromatography using hexane/dichloromethane (6/1, v/v) as eluent to afford ***α*-ThBSS** as a yellow solid (304.0 mg). Yield: 85%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.07 (dd, *J* =

7.5, 1.0 Hz, 1H), 8.10 (d, *J* = 7.5 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.71 (dd, *J* =7.5, 1.0 Hz, 1H), 7.63 (t, *J* =7.5 Hz,2H), 7.60-7.48 (m, 5H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.90, 143.81, 143.31, 142.44, 140.39, 137.90, 136.93, 131.28, 129.38, 127.61, 125.36, 124.92, 124.53, 122.74, 122.46, 122.14, 121.68. High-Resolution Mass Spectra (HRMS): calcd for $C_{20}H_{11}BS_3$: 358.0116, found: 358.0098 $[M]^+$. Anal. calcd (%): C, 67.04; H, 3.09; S, 26.84. found: C, 67.27; H, 2.98; S, 26.94. Melting point: 234 ℃.

Benzo[b]thiophene-2-thiol (6)

A mixture of 2-bromobenzo[b]thiophene (**5**, 42.6 g, 200.0 mmol) and sodium thiomethoxide (57.6 g, 800.0 mmol) in dry *N, N*-dimethylformamide (DMF, 500 mL) was stirred at reflux for 12 hours under argon atmosphere. After cooling to room temperature, the mixture was slowly poured into 3 M aq. HCl (400 mL) and the aqueous layer was extracted with ethyl acetate three times (100 mL×3). The combined organic phases were washed with brine three times (100 mL×3) and were made alkaline with 1.5 M aq. NaOH (150 mL). The aqueous phase was separated and acidized by 1 M aq. HCl (250 mL) and then extracted three times with ethyl acetate (100 mL×3). The organic phases were combined and dried over anhydrous $MgSO_4$. After the solvent was removed under vacuum, the product **6** was obtained as a yellow solid (26.5 g) and used directly for the next step. Yield: 80%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 7.5 Hz, 1H), 7.31 (dd, *J* = 8.0, 7.5 Hz, 2H), 7.28 (s, 1H), 3.68 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.64, 139.93, 128.67, 127.65, 124.53, 124.41, 122.82, 121.60.

2-((2,5-Dibromo-3-fluorophenyl)thio)benzo[b]thiophene (7)

A mixture of **6** (5.00 g, 30.1 mmol), 2,5-dibromo-1,3-difluorobenzene (9.00 g, 33.1 mmol) and K_2CO_3 (8.32 g, 60.2 mmol) in dry NMP (150 mL) was stirred at 60 ºC for 24 hours under argon atmosphere and then cooled to room temperature. The mixture was slowly poured into deionized water (600 mL) and the aqueous layer was extracted with dichloromethane three times (100 mL×3). The combined organic fractions were dried over anhydrous $MgSO_4$ and the solvent was removed under vacuum. The crude product was purified by silica gel chromatography using hexane as eluent to afford **7** as a white solid (9.80 g). Yield: 78%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86-7.84 (m, 2H), 7.65 (s, 1H), 7.45-7.43 (m, 2H), 7.10 (dd, *J* =7.6, 2.0 Hz, 1H), 6.84 (s,1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.27, 157.76, 143.79, 143.49, 139.47, 134.95, 129.46, 125.99, 125.15, 124.92, 124.34, 122.45, 116.98, 116.77.

2-((2,5-Dibromo-3-(phenylthio)phenyl)thio)benzo[b]thiophene (8)

A mixture of **7** (4.18 g, 10.0 mmol) and sodium thiophenolate (1.20 g, 9.0 mmol) in dry NMP (100 mL) was stirred at 60 ºC for 24 hours under argon atmosphere and then cooled to room temperature. The mixture was slowly poured into NH_4Cl solution (1 M, 400 mL), which was extracted with dichloromethane three times (50 mL×3). The combined organic fractions were dried over anhydrous $MgSO_4$ and the solvent was removed under vacuum. The crude product was purified by silica gel chromatography using hexane/dichloromethane (10/1, v/v) as eluent to afford **8** as a white solid (3.30 g). Yield: 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.82 (m, 2H), 7.63 (s, 1H), 7.53-7.51 (m, 2H), 7.46-7.44 (m, 3H), 7.43-7.41 (m, 2H), 6.79 (d, *J* = 2.0 Hz, 1H), 6.62 (d, *J* = 2.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.74, 143.20, 142.54, 139.50, 134.76, 134.64, 131.18, 130.40, 130.06, 129.60, 127.51, 126.29, 125.84, 124.83, 124.26, 122.42, 122.17, 117.43.

7-Bromo-5,9,10-trithia-14c-borafluoreno[2,3,4-de]anthracene (β-ThBSS-Br)

A solution of *n*-butyllithium in hexane (1.68 mL, 2.5 M, 4.2 mmol) was added slowly to a solution of **8** (2.03 g, 4.0 mmol) in anhydrous *m*-xylene (50 mL) at -30 ºC under argon atmosphere. The reaction mixture was stirred for 30 minutes before heating at 40 ºC for 1 hour. BBr_3 (0.46 mL, 4.8 mmol) was slowly added to the mixture at -30 ºC, which was then heated to 50 ºC and stirred for 3 hours. After addition of $(i\text{-Pr})_2$NEt (1.4 mL, 8.0 mmol) at 0 ºC, the reaction mixture was stirred at 120 ºC for 24 hours, which was then cooled to room temperature and slowly quenched by 2 mL deionized water. Subsequently, organic solvent in the reaction mixture was removed under vacuum, and the crude product was purified by silica gel chromatography using hexane/dichloromethane (8/1, v/v) as eluent to afford ***β*-ThBSS-Br** as a light-yellow solid (875.0 mg). Yield: 50%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (dd, *J* = 8.0, 1.0 Hz, 1H), 8.09 (d, *J* = 7.5 Hz, 1H), 7.87 (d, *J* = 7.5 Hz, 1H), 7.77 (d, *J* =1.5 Hz, 1H), 7.73 (d, *J* =1.5 Hz,1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.33-7.29 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.61, 144.62, 142.57, 141.96, 141.81, 139.09, 137.78, 131.51, 125.87, 125.34, 124.81, 124.74, 124.29, 123.82, 123.68, 121.55.

5,9,10-Trithia-14c-borafluoreno[2,3,4-de]anthracene (β-ThBSS)

A mixture of ***β*-ThBSS-Br** (437.0 mg, 1.0 mmol), $Pd(dppf)Cl_2$ (22.0 mg, 0.03 mmol), TMEDA (27.8 mg, 5.0 mmol), $NaBH_4$ (230.4 mg, 5.0 mmol) and THF (50 mL) was

stirred at room temperature under argon atmosphere for 12 hours. After the mixture was poured into deionized water (200 mL), the precipitate was filtered, dried under vacuum, and then subjected to silica gel chromatography using hexane/dichloromethane (6/1, v/v) as eluent to afford ***β*-ThBSS** as a light-yellow solid (286.5 mg). Yield: 80%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (dd, *J* = 7.5, 1.5 Hz, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* =8.0 Hz, 1H), 7.65 (dd, *J* =7.5, 1.0 Hz,1H), 7.60 (d, *J* = 7.5, 1.0 Hz, 1H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.30 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.30, 143.94, 143.67, 143.03, 142.05, 139.98, 138.75, 132.23, 130.15, 126.84, 126.28, 125.52, 125.38, 125.15, 123.36, 122.46, 122.42. HRMS: calcd for $C_{20}H_{11}BS_3$: 358.0116, found: 358.0111 $[M]^+$. Anal. calcd (%): C, 67.04; H, 3.09; S, 26.84. found: C, 67.31; H, 2.93; S, 27.14. Melting point: 217 °C.

3,3'-((2,5-Dibromo-1,3-phenylene)bis(sulfanediyl))bis(benzo[b]thiophene) (9)

A mixture of **2** (13.3 g, 80.0 mmol), 2,5-dibromo-1,3-difluorobenzene (10.9 g, 40.0 mmol) and K_2CO_3 (22.1 g, 160.0 mmol) in dry NMP (200 mL) was stirred at 60 °C for 48 hours under argon atmosphere and then cooled to room temperature. The mixture was slowly poured into NH_4Cl solution (1 M, 600 mL) and the precipitate was filtered and dried in vacuum at 80 °C. Afterwards, the crude product was purified by silica gel chromatography using cyclohexane/dichloromethane (6/1, v/v) as eluent to afford **9** as a white solid (13.1 g). Yield: 58%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94-7.92 (m, 2H), 7.92 (s, 2H), 7.80-7.78 (m, 2H), 7.44-7.42 (m, 4H), 6.32 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.05, 140.10, 138.51, 135.43, 125.62, 125.45, 125.28, 123.15, 122.86, 122.00, 121.67, 115.93.

7-Bromo-5,9,14,15-tetrathia-14b-boradiindeno[2,1-a:1',2'-j]phenalene (α-DThBSS-Br)

A solution of *n*-butyllithium in hexane (5.04 mL, 2.5 M, 12.6 mmol) was added slowly to a solution of **9** (6.77 g, 12.0 mmol) in anhydrous *m*-xylene (200 mL) at -30 °C under argon atmosphere. The reaction mixture was stirred for 30 minutes before heating at 40 °C for 1 hour. BBr_3 (1.39 mL, 14.4 mmol) was slowly added to the mixture at -30 °C, which was then heated to 50 °C and stirred for 3 hours. After addition of $(i\text{-}Pr)_2NEt$ (4.18 mL, 24.0 mmol) at 0 °C, the reaction mixture was stirred at 120 °C for 24 hours, which was then cooled to room temperature and slowly quenched by 6 mL deionized water. Subsequently, the reaction mixture was filtered, and the residue was washed with acetone (30 mL) to afford the desired compound ***α*-DThBSS-Br** as a yellow solid (1.18

g). Yield: 20%. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$) δ 8.15-8.07 (m, 4H), 7.92 (s, 2H), 7.66-7.54 (m, 4H). ^{13}C NMR could not be measured due to its poor solubility.

5,9,14,15-Tetrathia-14b-boradiindeno[2,1-a:1',2'-j]phenalene (α-DThBSS)

A mixture of ***α*-DThBSS-Br** (492.0 mg, 1.0 mmol), Pd(dppf)Cl_2 (22.0 mg, 0.03 mmol), TMEDA (27.8 mg, 5.0 mmol), $NaBH_4$ (230.4 mg, 5.0 mmol) and THF (80 mL) was stirred at room temperature under argon atmosphere for 12 hours. After the mixture was poured into deionized water (200 mL), the precipitate was filtered, dried under vacuum, and then subjected to silica gel chromatography using cyclohexane/dichloromethane (4/1, v/v) as eluent to afford ***α*-DThBSS** as a yellow solid (200.0 mg). Yield: 48%. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$) δ 8.10 (t, *J* = 8.5 Hz, 4H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.62-7.59 (m, 3H), 7.56 (t, *J* = 8.0 Hz, 2H). ^{13}C NMR (126 MHz, $C_2D_2Cl_4$) δ 144.43, 142.90, 137.16, 129.16, 127.69, 124.72, 123.19, 122.94, 122.47. HRMS: calcd for $C_{22}H_{11}BS_4$: 413.9837, found: 413.9823 $[M]^+$. Anal. calcd (%): C, 63.77; H, 2.68; S, 30.95. found: C, 63.75; H, 2.51; S, 30.97. Melting point was not observed before decomposition temperature.

9-(5,9,14,15-Tetrathia-14b-boradiindeno[2,1-a:1',2'-j]phenalen-7-yl)-3,6-di-tert-butyl-9H-carbazole (α-DThBSS-Cz)

A mixture of ***α*-DThBSS-Br** (591.6 mg, 1.2 mmol), 3,6-bis(*t*-butyl)carbazole (402.3 mg, 1.44 mmol), $Pd_2(dba)_3$ (22.0 mg, 0.024 mmol), *t*-$Bu_3P{\cdot}BF_4$ (27.8 mg, 0.096 mmol), sodium *t*-butoxide (230.4 g, 2.4 mmol) and toluene (50 mL) was heated to 100 ºC and stirred for 12 hours under argon. After cooling to room temperature, the mixture was washed with brine (100 mL). The organic phase was dried over anhydrous $MgSO_4$, and the solvent was removed under vacuum. The crude product was purified by silica gel chromatography using cyclohexane/dichloromethane (4/1, v/v) as eluent to afford ***α*-DThBSS-Cz** as a yellow solid (580.6 mg). Yield: 70%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 (d, *J* = 1.5 Hz, 2H), 8.06 (d, *J* = 8.0 Hz, 2H), 8.02 (d, *J* = 7.5 Hz, 2H), 7.96 (s, 2H), 7.59-7.50 (m, 8H), 1.50 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.31, 144.97, 144.87, 140.04, 140.01, 139.60, 137.76, 128.61, 125.64, 125.01, 124.09, 123.28, 120.75, 117.49, 110.34. HRMS: calcd for $C_{42}H_{34}BNS_4$: 691.1667, found: 691.1638 $[M]^+$. Anal. calcd (%): C, 72.92; H, 4.95; N, 2.02; S, 18.54. found: C, 73.22; H, 4.88; N, 2.07; S, 18.68. Melting point was not observed before decomposition temperature.

2,2'-((2,5-Dibromo-1,3-phenylene)bis(sulfanediyl))bis(benzo[b]thiophene) (10)

A mixture of **6** (13.3 g, 80.0 mmol), 2,5-dibromo-1,3-difluorobenzene (10.9 g, 40.0

mmol) and K_2CO_3 (22.1 g, 160.0 mmol) in dry NMP (200 mL) was stirred at 60 °C for 48 hours under argon atmosphere and then cooled to room temperature. The mixture was slowly poured into NH_4Cl solution (1 M, 600 mL) and the precipitate was filtered and dried under vacuum at 80 °C. Afterwards, the crude product was purified by silica gel chromatography using cyclohexane/dichloromethane (6/1, v/v) as eluent to afford **10** as a white solid (14.6 g). Yield: 65%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85-7.83 (m, 4H), 7.63 (s, 2H), 7.43-7.41 (m, 4H), 6.82 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.75, 142.54, 139.49, 134.71, 130.19, 126.70, 125.87, 124.85, 124.28, 122.46, 122.43.

8-Bromo-5,6,10,11-tetrathia-15c-boradiindeno[1,2-a:2',1'-j]phenalene (β-DThBSS-Br)

A solution of *n*-butyllithium in hexane (5.04 mL, 2.5 M, 12.6 mmol) was added slowly to a solution of **9** (6.77 g, 12.0 mmol) in anhydrous *m*-xylene (200 mL) at -30 °C under argon atmosphere. The reaction mixture was stirred for 30 minutes before heating at 40 °C for 1 hour. BBr_3 (1.39 mL, 14.4 mmol) was slowly added to the mixture at -30 °C, which was then heated to 50 °C and stirred for 3 hours. After addition of $(i\text{-Pr})_2NEt$ (4.18 mL, 24.0 mmol) at 0 °C, the reaction mixture was stirred at 120 °C for 24 hours, which was then cooled to room temperature and slowly quenched by 6 mL deionized water. Subsequently, the reaction mixture was filtered, and the residue was washed with methanol (30 mL) to afford the desired compound ***β*-DThBSS-Br** as a light-yellow solid (3.55 g). Yield: 60%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, J = 8.0 Hz, 2H), 7.81 (s, 2H), 7.33 (dd, J = 8.0, 8.0 Hz, 4H), 7.07 (t, J = 8.0 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.49, 142.35, 141.17, 138.75, 126.82, 124.82, 124.67, 124.10, 121.19.

5,6,10,11-Tetrathia-15c-boradiindeno[1,2-a:2',1'-j]phenalene (β-DThBSS)

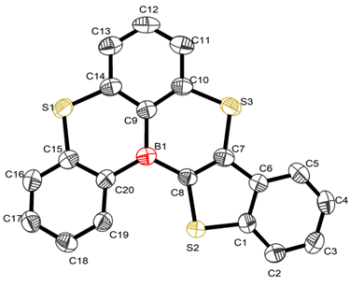
A mixture of ***β*-DThBSS-Br** (493.0 mg, 1.0 mmol), $Pd(dppf)Cl_2$ (22.0 mg, 0.03 mmol), TMEDA (27.8 mg, 5.0 mmol), $NaBH_4$ (230.4 mg, 5.0 mmol) and THF (50 mL) was stirred at room temperature under argon atmosphere for 12 hours. After the mixture was poured into deionized water (200 mL), the precipitate was filtered, dried under vacuum, and then subjected to silica gel chromatography using hexane/dichloromethane (4/1, v/v) as eluent to afford ***β*-DThBSS** as a light-yellow solid (273.0 mg). Yield: 66%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, J = 8.0 Hz, 2H), 7.68 (d, J =7.5 Hz, 2H), 7.51 (t, J = 7.5 Hz, 1H), 7.34 (d, J = 8.0 Hz, 2H), 7.30 (t, J = 7.0 Hz, 2H), 7.07 (t, J = 7.0 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.18, 141.36, 140.79, 138.63, 128.35, 126.74, 124.44, 123.96, 122.42, 121.09. HRMS: calcd for $C_{22}H_{11}BS_4$: 413.9837, found:

413.9792 $[M]^+$. Anal. calcd (%): C, 63.77; H, 2.68; S, 30.95. found: C, 63.85; H, 2.50; S, 31.26. Melting point: 268 ℃.

9-(5,6,10,11-Tetrathia-15c-boradiindeno[1,2-a:2',1'-j]phenalen-8-yl)-3,6-di-tert-butyl-9H-carbazole (β-DThBSS-Cz)

A mixture of ***β*-DThBSS-Br** (591.6 mg, 1.2 mmol), 3,6-bis(*t*-butyl)carbazole (402.3 mg, 1.44 mmol), $Pd_2(dba)_3$ (22.0 mg, 0.024 mmol), *t*-$Bu_3P{\cdot}BF_4$ (27.8 mg, 0.096 mmol), sodium *t*-butoxide (230.4 g, 2.4 mmol) and toluene (50 mL) was heated to 100 ºC and stirred for 12 hours under argon. After cooling to room temperature, the mixture was washed with brine (100 mL). The organic phase was dried over anhydrous $MgSO_4$, and the solvent was removed under vacuum. The crude product was purified by silica gel chromatography using hexane/dichloromethane (4/1, v/v) as eluent to afford ***β*-DThBSS-Cz** as a light-yellow solid (655.0 mg). Yield: 79%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 1.5 Hz, 2H), 7.92 (s, 2H), 7.89 (d, *J* = 8.0 Hz, 2H), 7.50 (dd, *J* = 8.5, 1.5 Hz, 2H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.10 (t, *J* = 7.5 Hz, 2H), 1.49 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.72, 143.88, 142.54, 141.31, 138.76, 138.68, 138.35, 126.84, 124.62, 124.09, 124.02, 123.96, 121.19, 119.75, 116.52, 109.21. HRMS: calcd for $C_{42}H_{34}BNS_4$: 691.1667, found: 691.1694 $[M]^+$. Anal. calcd (%): C, 72.92; H, 4.95; N, 2.02; S, 18.54. found: C, 73.22; H, 4.88; N, 2.05; S, 18.49. Melting point: 347 ℃.

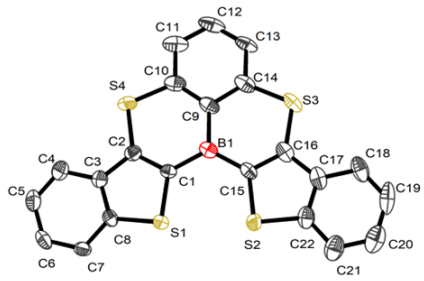
Single-Crystal Structures



Angles [°]		Bond lengths [Å]	
C(8)-B(1)-C(9)	116.6(3)	B(1)-C(8)	1.546(4)
C(8)-B(1)-C(20)	123.4(3)	B(1)-C(9)	1.550(4)
C(9)-B(1)-C(20)	120.0(3)	B(1)-C(20)	1.556(4)
C(14)-S(1)-C(15)	107.10(15)	S(1)-C(14)	1.742(3)
C(1)-S(2)-C(8)	93.11(15)	S(1)-C(15)	1.745(3)
C(7)-S(3)-C(10)	105.10(15)	S(2)-C(1)	1.725(3)
		S(2)-C(8)	1.755(3)
		S(3)-C(7)	1.710(3)
		S(3)-C(10)	1.755(3)
		C(9)-C(10)	1.420(4)
		C(9)-C(14)	1.421(4)
		C(1)-C(2)	1.394(4)
		C(1)-C(6)	1.400(4)
		C(6)-C(7)	1.443(4)
		C(7)-C(8)	1.386(4)
		C(15)-C(20)	1.407(4)

Empirical formula	$C_{20}H_{11}BS_3$
Formula weight	358.28
Temperature	301(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 3.9616(2) Å a = 90°. b = 19.6770(11) Å b = 90°. c = 19.9810(9) Å g = 90°.
Volume	1557.57(14) Å^3
Z	4
Calculated density	1.528 Mg/m^3
Absorption coefficient	0.472 mm^{-1}
F(000)	736
Crystal size	0.21 x 0.19 x 0.16 mm^3
Theta range for data collection	2.29 to 33.75°.
Limiting indices	-6<=h<=5, -25<=k<=30, -30<=l<=31
Reflections collected / unique	21434 / 6188 [R(int) = 0.0557]
Completeness to theta = 33.75°	99.6%
Absorption correction	None
Max. and min. transmission	0.9282 and 0.9073
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6188 / 0 / 217
Goodness-of-fit on F^2	1.007
Final R indices [I>2sigma(I)]	R1 = 0.0585, wR2 = 0.1252
R indices (all data)	R1 = 0.1268, wR2 = 0.1575
Absolute structure parameter	0.08(4)
Largest diff. peak and hole	0.806 and -0.320 e. Å^{-3}

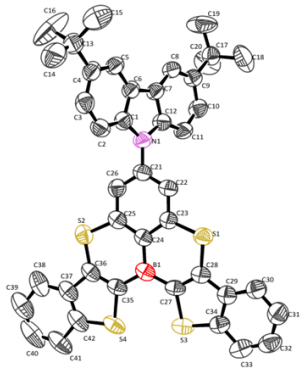
Figure S1. X-ray crystal structure and refinement information for ***α*-ThBSS** (Thermal ellipsoids are set at 50% probability level).



Angles [°]		Bond lengths [Å]	
C(8)-S(1)-C(1)	92.9(3)	S(1)-C(8)	1.734(7)
C(15)-S(2)-C(22)	91.8(3)	S(1)-C(1)	1.746(6)
C(16)-S(3)-C(14)	104.8(4)	S(2)-C(15)	1.745(7)
C(2)-S(4)-C(10)	105.4(3)	S(2)-C(22)	1.747(7)
C(1)-B(1)-C(9)	118.4(6)	S(3)-C(16)	1.716(8)
C(1)-B(1)-C(15)	123.6(6)	S(3)-C(14)	1.760(9)
C(9)-B(1)-C(15)	118.0(6)	S(4)-C(2)	1.731(7)
		S(4)-C(10)	1.769(8)
		B(1)-C(1)	1.533(10)
		B(1)-C(9)	1.536(10)
		B(1)-C(15)	1.554(11)
		C(1)-C(2)	1.377(10)
		C(2)-C(3)	1.436(10)
		C(3)-C(8)	1.388(10)
		C(9)-C(10)	1.415(11)
		C(9)-C(14)	1.422(10)
		C(15)-C(16)	1.379(9)
		C(16)-C(17)	1.434(11)
		C(17)-C(22)	1.384(11)

Empirical formula	$C_{22}H_{11}BS_4$
Formula weight	414.36
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P2(1)/n
Unit cell dimensions	a = 15.8412(18) Å a = 90°. b = 3.9132(4) Å b = 102.031(3)°. c = 28.452(3) Å g = 90°.
Volume	1725.0(3) Å^3
Z	4
Calculated density	1.596 Mg/m^3
Absorption coefficient	0.555 mm^{-1}
F(000)	848
Crystal size	0.21 x 0.19 x 0.12 mm^3
Theta range for data collection	1.36 to 24.67°.
Limiting indices	-18<=h<=18, -4<=k<=4, -33<=l<=33
Reflections collected / unique	18495 / 2891 [R(int) = 0.0456]
Completeness to theta = 24.67°	98.1%
Absorption correction	None
Max. and min. transmission	0.9364 and 0.8923
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2891 / 0 / 244
Goodness-of-fit on F^2	1.105
Final R indices [I>2sigma(I)]	R1 = 0.0969, wR2 = 0.2766
R indices (all data)	R1 = 0.1050, wR2 = 0.2846
Largest diff. peak and hole	2.529 and -0.751 e. Å^{-3}

Figure S2. X-ray crystal structure and refinement information for ***α*-DThBSS** (Thermal ellipsoids are set at 50% probability level).



Empirical formula	$C_{42}H_{34}BNS_4$
Formula weight	691.75
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 50.501(11) Å a = 90°.
	b = 14.437(3) Å b = 110.306(6)°.
	c = 20.652(5) Å g = 90°.
Volume	14121(5) Å^3
Z	16
Calculated density	1.301 Mg/m^3
Absorption coefficient	0.301 mm^{-1}
F(000)	5792
Crystal size	0.220 x 0.150 x 0.100 mm^3
Theta range for data collection	1.896 to 25.027°.
Index ranges	-60<=h<=60, -17<=k<=17, -24<=l<=24
Reflections collected	116587
Independent reflections	12471 [R(int) = 0.1073]
Completeness to theta = 25.027°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.971 and 0.910
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12471 / 20 / 896
Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 = 0.0770, wR2 = 0.1842
R indices (all data)	R1 = 0.1531, wR2 = 0.2362
Extinction coefficient	0.00031(5)
Largest diff. peak and hole	0.828 and -0.835 e.Å^{-3}

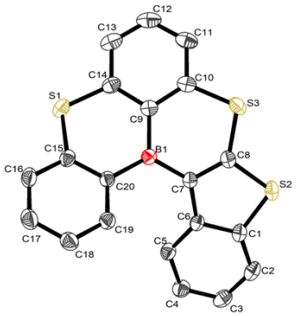
Angles [°]

C(28)-S(1)-C(23)	104.7(3)
C(36)-S(2)-C(25)	104.6(3)
C(34)-S(3)-C(27)	92.5(3)
C(42)-S(4)-C(35)	92.9(3)
C(1)-N(1)-C(12)	108.7(4)
C(1)-N(1)-C(21)	125.3(5)
C(12)-N(1)-C(21)	126.0(5)
C(27)-B(1)-C(35)	125.2(5)
C(27)-B(1)-C(24)	117.3(5)
C(35)-B(1)-C(24)	117.4(5)

Bond lengths [Å]

S(1A)-C(28A)	1.724(5)
S(1A)-C(23A)	1.746(5)
S(2A)-C(36A)	1.709(6)
S(2A)-C(25A)	1.747(5)
S(3A)-C(34A)	1.720(6)
S(3A)-C(27A)	1.752(5)
S(4A)-C(42A)	1.731(6)
S(4A)-C(35A)	1.744(5)
N(1A)-C(1A)	1.382(6)
N(1A)-C(12A)	1.386(6)
N(1A)-C(21A)	1.428(6)
B(1A)-C(27A)	1.525(8)
B(1A)-C(35A)	1.532(8)
B(1A)-C(24A)	1.534(8)
C(23A)-C(24A)	1.430(6)
C(24A)-C(25A)	1.424(7)
C(27A)-C(28A)	1.371(7)
C(28A)-C(29A)	1.439(7)
C(29A)-C(34A)	1.406(7)
C(35A)-C(36A)	1.380(7)
C(36A)-C(37A)	1.446(7)
C(37A)-C(42A)	1.392(8)

Figure S3. X-ray crystal structure and refinement information for ***α*-DThBSS-Cz** (Thermal ellipsoids are set at 50% probability level).



Empirical formula	$C_{20}H_{11}BS_3$
Formula weight	358.28
Temperature	281(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 18.0631(8) Å a = 90°.
	b = 7.5560(3) Å b = 90°.
	c = 22.9236(11) Å g = 90°.
Volume	3128.7(2) Å^3
Z	8
Calculated density	1.521 Mg/m^3
Absorption coefficient	0.470 mm^{-1}
F(000)	1472
Crystal size	0.21 x 0.19 x 0.12 mm^3
Theta range for data collection	3.05 to 30.38°.
Limiting indices	-25<=h<=25, -10<=k<=10, -32<=l<=32
Reflections collected / unique	129837 / 4696 [R(int) = 0.0489]
Completeness to theta = 30.38°	99.4%
Absorption correction	None
Max. and min. transmission	0.9457 and 0.9077
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4696 / 0 / 217
Goodness-of-fit on F^2	1.007
Final R indices [I>2sigma(I)]	R1 = 0.0305, wR2 = 0.0832
R indices (all data)	R1 = 0.0371, wR2 = 0.0893
Largest diff. peak and hole	0.436 and -0.277 e. Å^{-3}

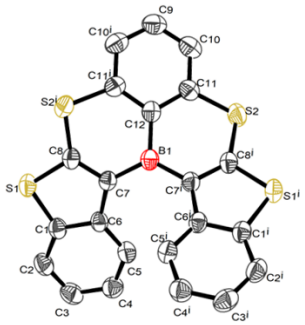
Angles [°]

C(15)-S(1)-C(14)	105.17(6)
C(8)-S(2)-C(1)	90.70(5)
C(8)-S(3)-C(10)	102.99(6)
C(7)-B(1)-C(9)	117.61(10)
C(7)-B(1)-C(20)	123.80(10)
C(9)-B(1)-C(20)	118.49(10)

Bond lengths [Å]

S(1)-C(15)	1.7491(12)
S(1)-C(14)	1.7521(13)
S(2)-C(8)	1.7400(12)
S(2)-C(1)	1.7403(13)
S(3)-C(8)	1.7290(12)
S(3)-C(10)	1.7568(13)
B(1)-C(7)	1.5377(16)
B(1)-C(9)	1.5446(17)
B(1)-C(20)	1.5582(17)
C(1)-C(6)	1.4108(15)
C(6)-C(7)	1.4571(15)
C(7)-C(8)	1.3842(15)
C(9)-C(10)	1.4142(16)
C(9)-C(14)	1.4176(16)
C(15)-C(16)	1.4028(17)

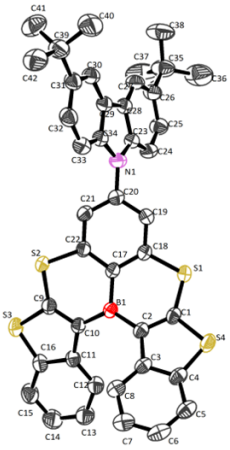
Figure S4. X-ray crystal structure and refinement information for ***β*-ThBSS** (Thermal ellipsoids are set at 50% probability level).



Angles [°]			
C(8)-S(1)-C(1)	90.74(11)	B(1)-C(12)	1.542(5)
C(8)#1-S(2)-C(11)	102.15(11)	B(1)-C(7)	1.545(3)
C(12)-B(1)-C(7)	116.75(15)	B(1)-C(7)#1	1.545(3)
C(12)-B(1)-C(7)#1	116.75(15)	C(1)-C(6)	1.408(3)
C(7)-B(1)-C(7)#1	126.5(3)	C(6)-C(7)	1.460(3)
		C(7)-C(8)	1.373(3)
Bond lengths [Å]		C(8)-S(2)#1	1.724(3)
S(1)-C(8)	1.739(2)	C(11)-C(12)	1.418(3)
S(1)-C(1)	1.743(2)	C(12)-C(11)#1	1.418(3)
S(2)-C(8)#1	1.724(3)		
S(2)-C(11)	1.753(3)		

Empirical formula	$C_{11}H_{5.5}B_{0.5}S2_2$
Formula weight	207.18
Temperature	(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pnna
Unit cell dimensions	a = 13.5070(10) Å a = 90°.
	b = 7.4267(5) Å b = 90°.
	c = 19.9470(15) Å g = 90°.
Volume	2000.9(3) Å^3
Z	8
Calculated density	1.375 Mg/m^3
Absorption coefficient	0.479 mm^{-1}
F(000)	848
Crystal size	0.21 x 0.19 x 0.12 mm^3
Theta range for data collection	1.82 to 26.39°.
Limiting indices	-15<=h<=16, -6<=k<=9, -24<=l<=24
Reflections collected / unique	10311 / 2056 [R(int) = 0.0501]
Completeness to theta = 26.39°	99.7%
Max. and min. transmission	0.9448 and 0.9062
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2056 / 0 / 124
Goodness-of-fit on F^2	0.995
Final R indices [I>2sigma(I)]	R1 = 0.0449, wR2 = 0.1105
R indices (all data)	R1 = 0.0666, wR2 = 0.1220
Largest diff. peak and hole	0.296 and -0.200 e. Å^{-3}

Figure S5. X-ray crystal structure and refinement information for ***β*-DThBSS** with symmetrical structure (Thermal ellipsoids are set at 50% probability level).



Angles [°]		C(9)-S(2)-C(22)	103.31(14)
C(10)-B(1)-C(17)	117.3(3)	C(16)-S(3)-C(9)	90.54(14)
C(10)-B(1)-C(2)	126.6(3)	C(1)-S(4)-C(4)	90.44(14)
C(17)-B(1)-C(2)	116.1(3)		
C(23)-N(1)-C(34)	108.1(2)	Bond lengths [Å]	
C(23)-N(1)-C(20)	124.3(3)	B(1)-C(10)	1.542(4)
C(34)-N(1)-C(20)	126.6(3)	B(1)-C(17)	1.545(4)
C(1)-S(1)-C(18)	102.04(14)	B(1)-C(2)	1.546(4)
		N(1)-C(23)	1.393(4)
		N(1)-C(34)	1.400(4)
		N(1)-C(20)	1.425(4)
		S(1)-C(1)	1.734(3)
		S(1)-C(18)	1.759(3)
		S(2)-C(9)	1.721(3)
		S(2)-C(22)	1.753(3)
		S(3)-C(16)	1.736(3)
		S(3)-C(9)	1.737(3)
		S(4)-C(1)	1.736(3)
		S(4)-C(4)	1.740(3)
		C(1)-C(2)	1.376(4)
		C(2)-C(3)	1.462(4)
		C(3)-C(4)	1.411(4)
		C(9)-C(10)	1.388(4)
		C(10)-C(11)	1.453(4)
		C(11)-C(16)	1.406(4)
		C(17)-C(22)	1.415(4)
		C(17)-C(18)	1.421(4)

Empirical formula	$C_{84}H_{68}B_2N_2S_8$
Formula weight	1383.50
Temperature	300(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 12.5062(10) Å a = 96.768(3)°.
	b = 13.0995(13) Å b = 96.462(3)°.
	c = 22.288(2) Å g = 90.512(3)°.
Volume	3602.0(6) Å^3
Z	2
Calculated density	1.276 Mg/m^3
Absorption coefficient	0.295 mm^{-1}
F(000)	1448
Crystal size	0.21 x 0.19 x 0.12 mm^3
Theta range for data collection	1.91 to 25.00°.
Limiting indices	-14<=h<=14, -15<=k<=15, -26<=l<=26
Reflections collected / unique	112019 / 12697 [R(int) = 0.0774]
Completeness to theta = 25.00°	99.9%
Absorption correction	None
Max. and min. transmission	0.9654 and 0.9406
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12697 / 2199 / 892
Goodness-of-fit on F^2	1.080
Final R indices [I>2sigma(I)]	R1 = 0.0508, wR2 = 0.1425
R indices (all data)	R1 = 0.0719, wR2 = 0.1539
Largest diff. peak and hole	0.777 and -0.498 e. Å^{-3}

Figure S6. X-ray crystal structure and refinement information for ***β*-DThBSS-Cz** (Thermal ellipsoids are set at 50% probability level).

Theoretical Calculations

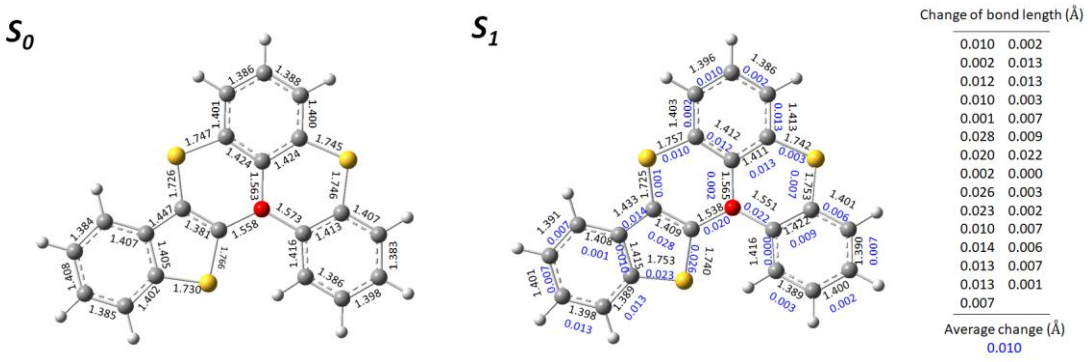


Figure S7. Bond lengths of optimized structures for S_0 and S_1 states of ***α*-ThBSS**, with the change of bond length between S_0 and S_1 states shown in blue color.

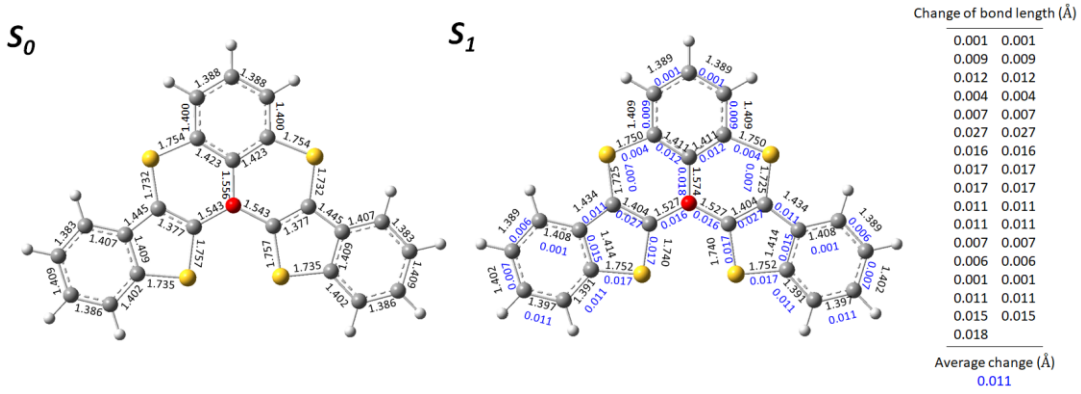


Figure S8. Bond lengths of optimized structures for S_0 and S_1 states of ***α*-DThBSS**, with the change of bond length between S_0 and S_1 states shown in blue color.

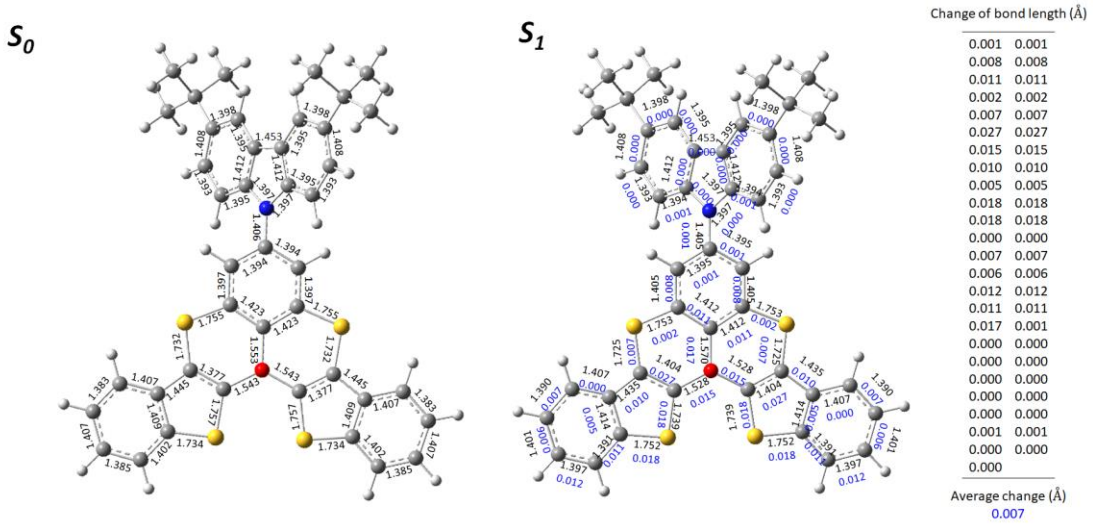


Figure S9. Bond lengths of optimized structures for S_0 and S_1 states of ***α*-DThBSS-Cz**, with the change of bond length between S_0 and S_1 states shown in blue color.

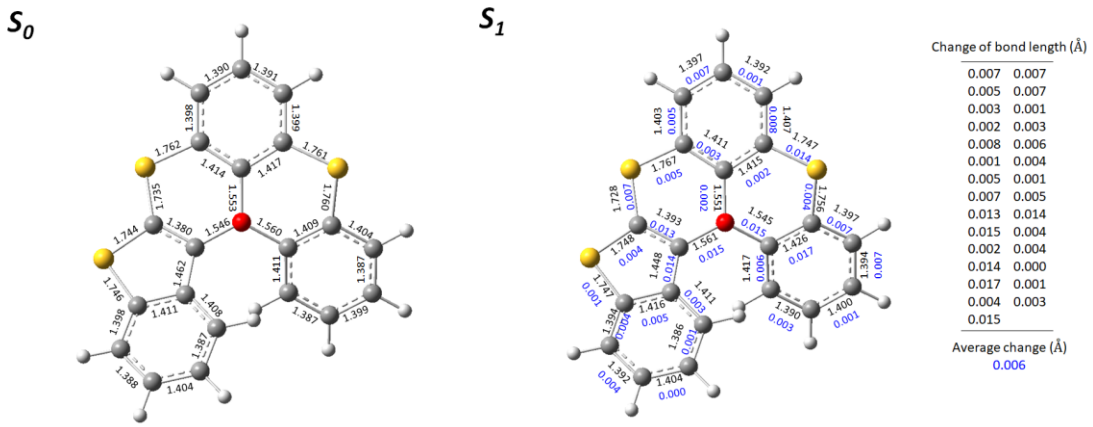


Figure S10. Bond lengths of optimized structures for S_0 and S_1 states of ***β*-ThBSS**, with the change of bond length between S_0 and S_1 states shown in blue color.

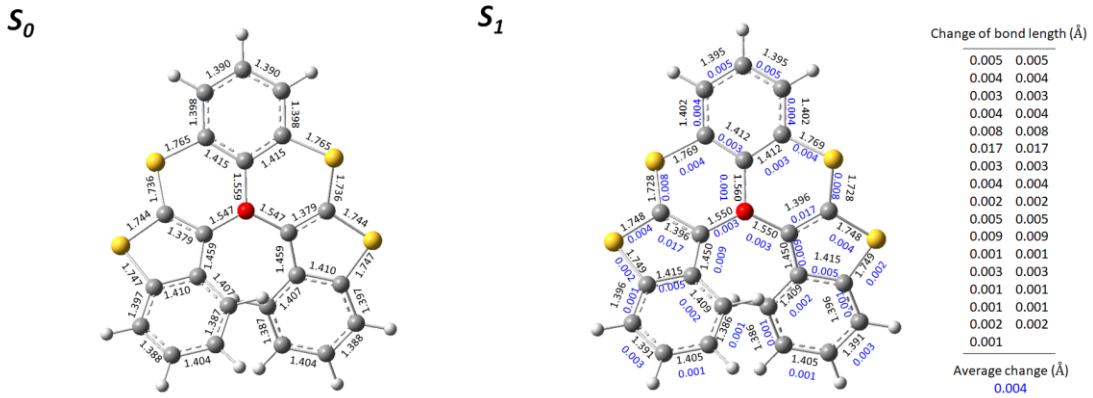


Figure S11. Bond lengths of optimized structures for S_0 and S_1 states of ***β*-DThBSS**, with the change of bond length between S_0 and S_1 states shown in blue color.

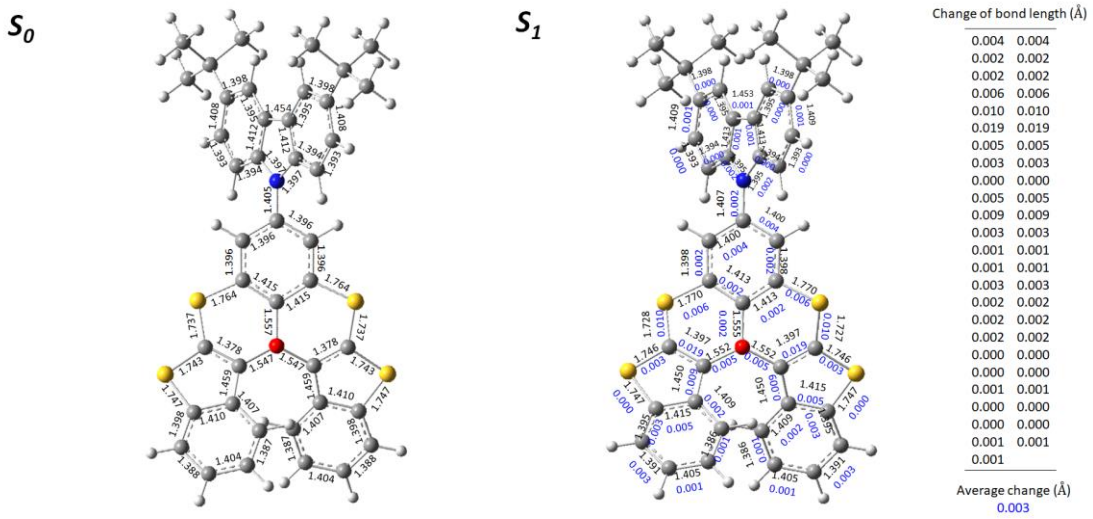


Figure S12. Bond lengths of optimized structures for S_0 and S_1 states of ***β*-DThBSS-Cz**, with the change of bond length between S_0 and S_1 states shown in blue color.

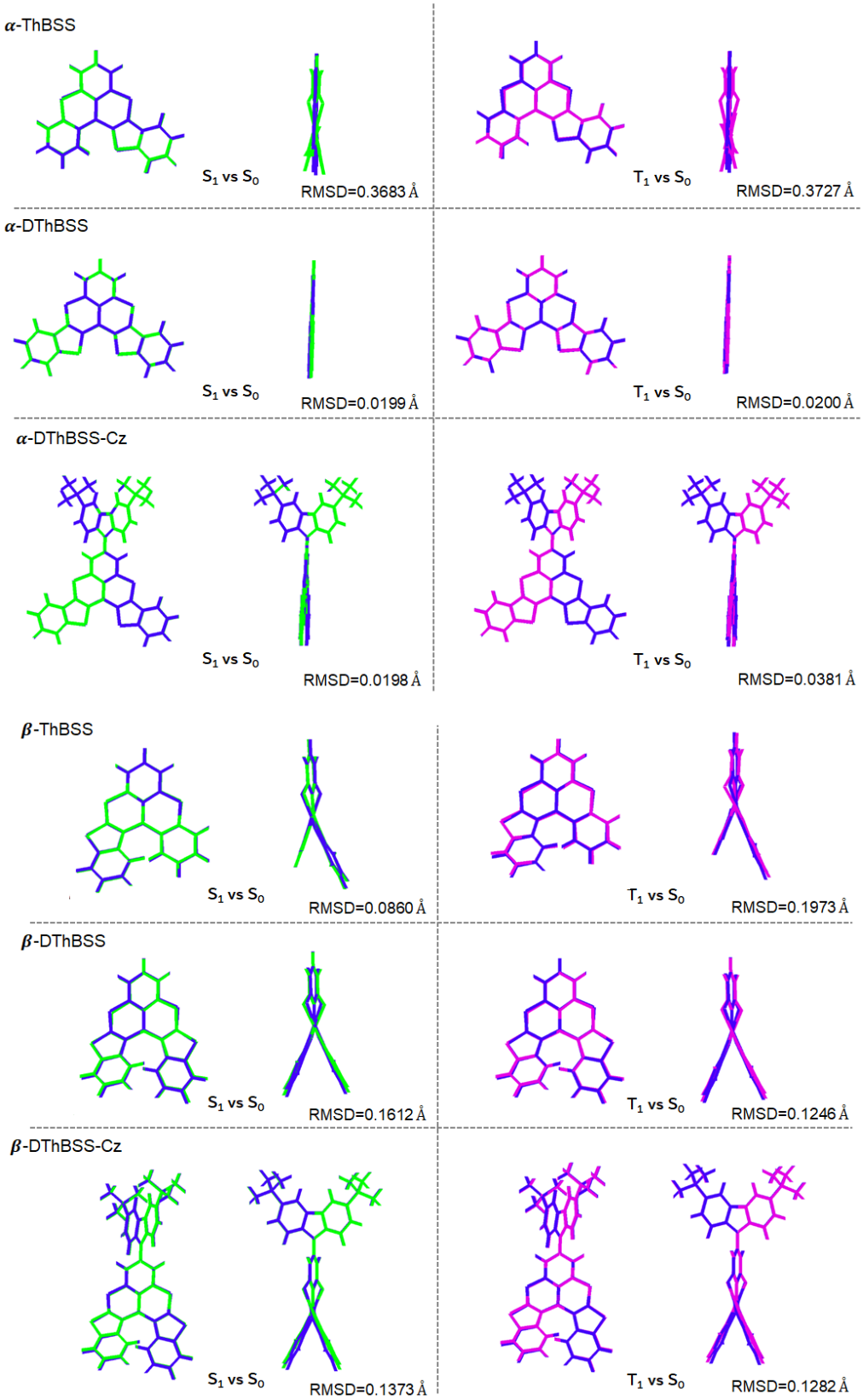
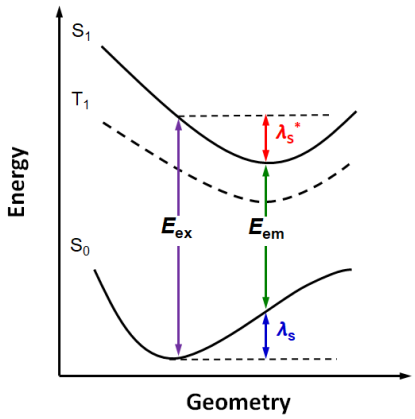


Figure S13. Excited-state molecular configuration and root mean square displacement (RMSD) between S_0 and S_1/T_1 state for the emitters.



	$\lambda_S + \lambda_S^*$ (S_1, eV)	$\lambda_S + \lambda_S^*$ (T_1, eV)
α-ThBSS	0.174	0.544
α-DThBSS	0.197	0.299
α-DThBSS-Cz	0.193	0.308
β-ThBSS	0.208	0.514
β-DThBSS	0.234	0.275
β-DThBSS-Cz	0.218	0.283

Figure S14. Reorganization energy (λ_S and λ_S^*) for the emitters.

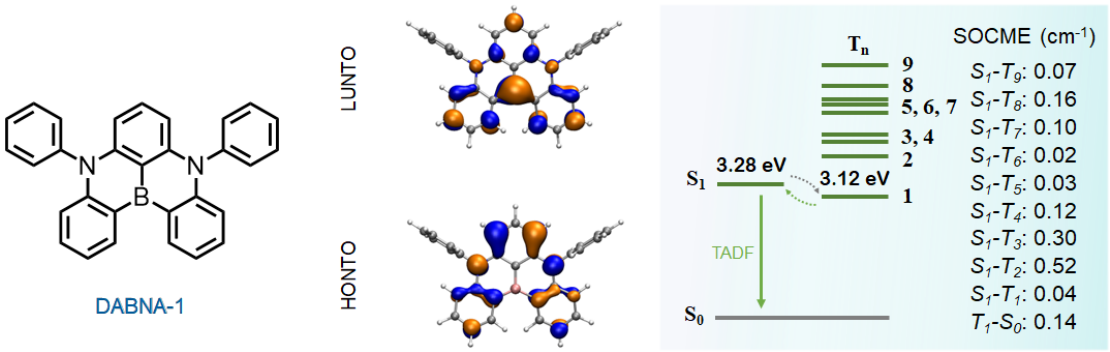


Figure S15. Nature transition orbitals (NTO) of S_1 state, and SOC matrix element for a typical B, N-based MR-TADF emitter (DABNA-1) by TD-DFT calculation (M062X/def2SVP level).

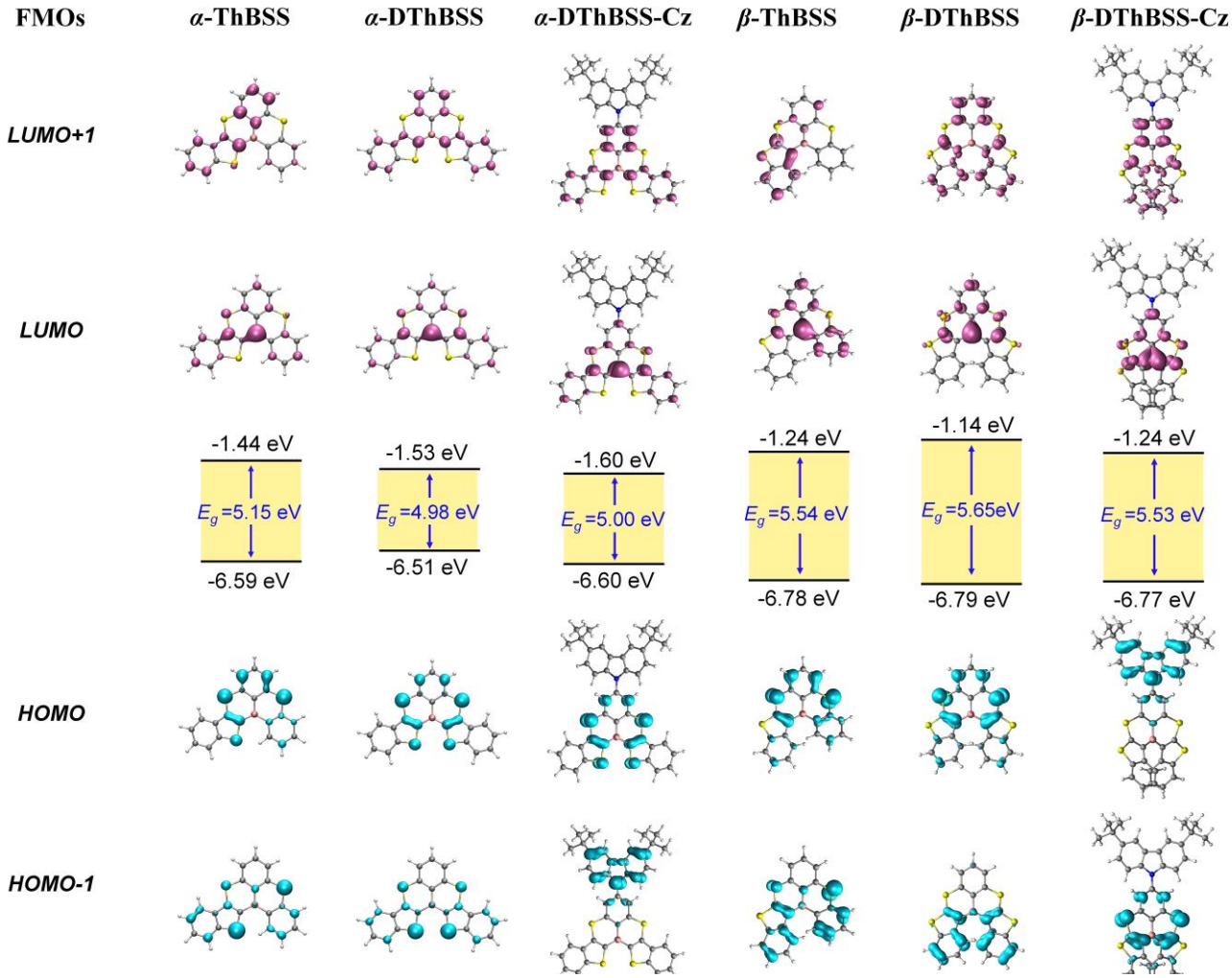


Figure S16. Frontier molecular orbitals (HOMOs and LUMOs) for the emitters at M062X/def2SVP level (note that for *β*-DThBSS-Cz, HOMO-1 orbital contributes most to S_0-S_1 transition).

Table S1. Summary of TD-DFT calculation (M062X/def2SVP level) results for the emitters.

Compound	State	Excitation Energy [eV]	Oscillator Strength [*f*]	Main Configuration
α-ThBSS	S_1	3.2935	0.2089	H→L (0.9652)
	T_1	2.5736		H→L (0.8554), H-1→L (0.0449)
α-DThBSS	S_1	3.1824	0.2650	H→L (0.9685)
	T_1	2.4150		H→L (0.9011), H-1→L+1 (0.0283)
α-DThBSS-Cz	S_1	3.2139	0.2537	H→L (0.9646)
	T_1	2.4456		H→L (0.8953), H-3→L+1 (0.0242)
β-ThBSS	S_1	3.5136	0.1599	H→L (0.9568)
	T_1	2.9169		H→L (0.8744), H→L+1 (0.0233)
β-DThBSS	S_1	3.6024	0.1633	H→L (0.9489)
	T_1	2.9060		H→L (0.8643), H-1→L+1 (0.0298), H→L+2 (0.0233)
β-DThBSS-Cz	S_1	3.6151	0.1475	H-1→L (0.9345)
	T_1	2.9300		H-1→L (0.8373), H-1→L+2 (0.0436), H-3→L+1 (0.0279)

Electrochemical Measurements

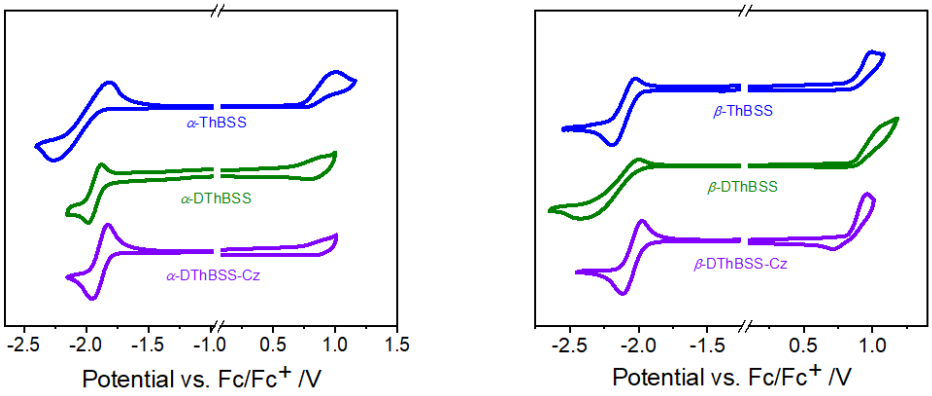


Figure S17. Cyclic voltammetry (CV) characteristics for the emitters. The oxidation and reduction curves were recorded in dichloromethane (DCM) and tetrahydrofuran (THF) respectively, using ferrocene as the reference and *n*-Bu_4NClO_4 as the supporting electrolyte.

Table S2. Summary of electrochemical parameters for the emitters.

Emitters	E_{onset}^{ox} [V]	E_{onset}^{red} [V]	HOMO [eV]	LUMO [eV]
α-ThBSS	0.76	-1.86	-5.56	-2.94
α-DThBSS	0.68	-1.79	-5.48	-3.01
α-DThBSS-Cz	0.73	-1.76	-5.53	-3.04
β-ThBSS	0.82	-1.97	-5.62	-2.83
β-DThBSS	0.84	-2.00	-5.64	-2.80
β-DThBSS-Cz	0.81	-1.98	-5.61	-2.82

The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energy levels of the emitters were calculated according to equations of $E_{HOMO}/E_{LUMO} = -(4.80 + E_{onset}^{ox}/E_{onset}^{red})$, in which E_{onset}^{ox} and E_{onset}^{red} are the onset of oxidation and reduction potentials respectively.

Thermal Properties

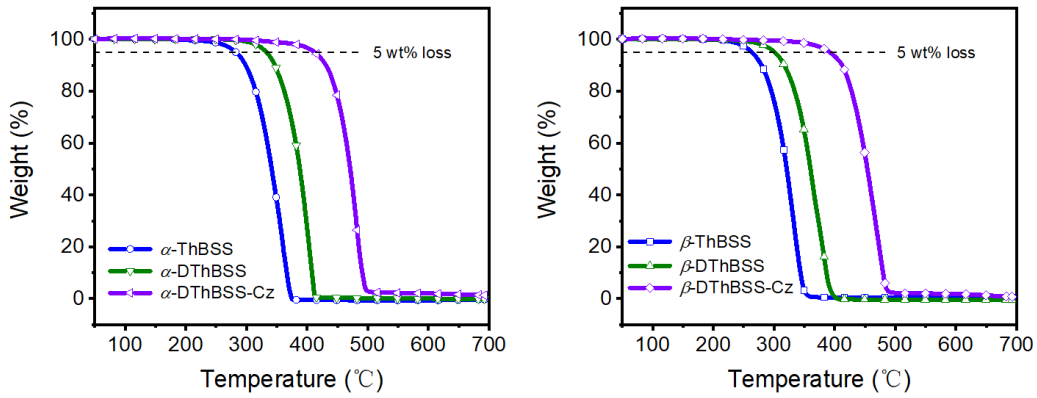


Figure S18. Thermogravimetric analysis (TGA) curves for the emitters.

Photophysical Properties

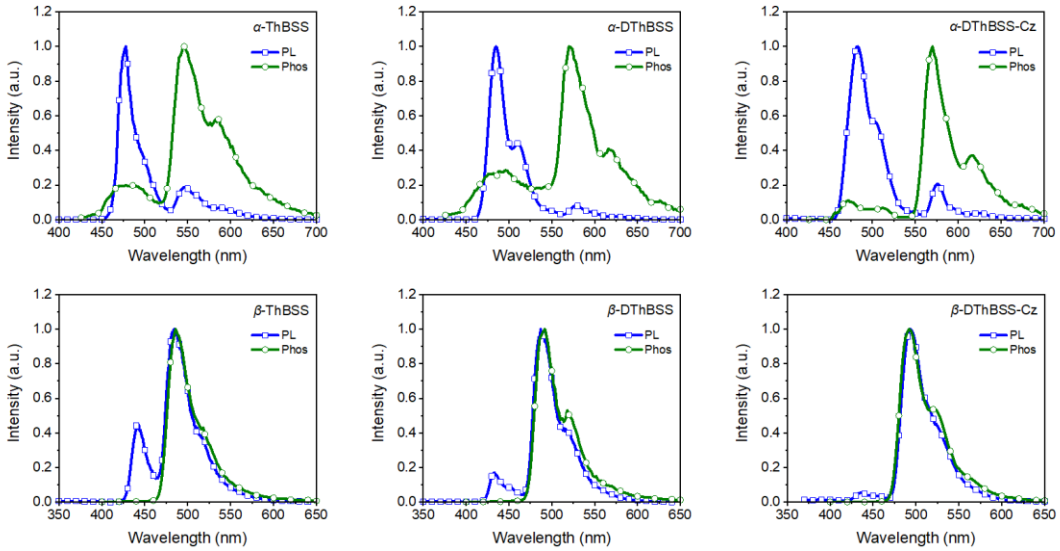


Figure S19. Fluorescence and phosphorescence (delay time: 10 ms) spectra in toluene at 77 K.

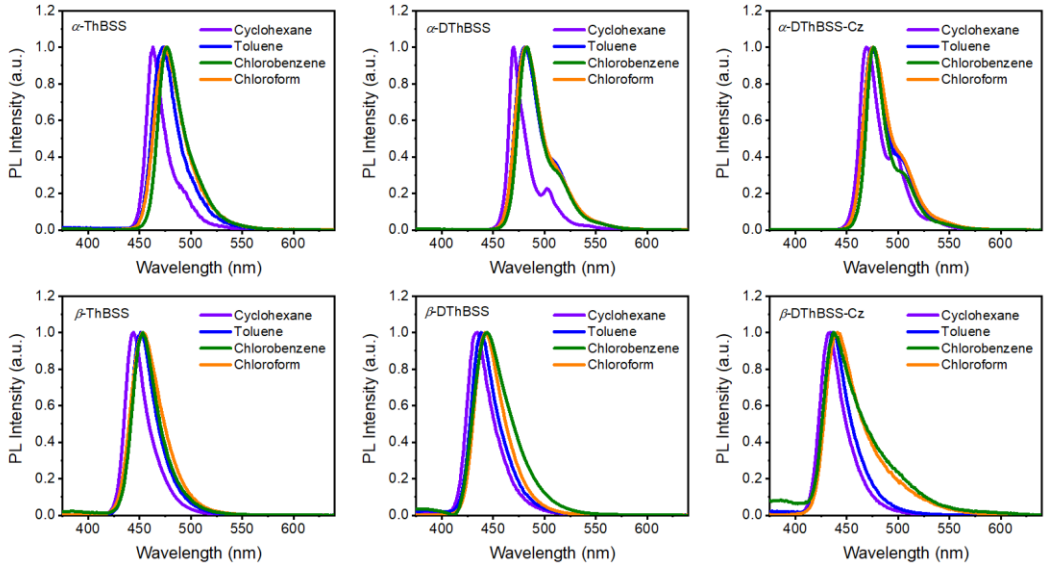


Figure S20. PL spectra in solvents with different polarity (10^{-5} mol L^{-1}).

Table S3. Summary of photophysical properties for the emitters in toluene (10^{-5} mol L^{-1}).

Emitters	λ_{abs} [a] [nm]	λ_{em} [b] [nm]	λ_{ph} [c] [nm]	Stokes shift [d] [nm]	FWHM [e] [nm]
α-ThBSS	318, 360, 451	473	546	22	28
α-DThBSS	310, 335, 360, 465	481	570	16	27
α-DThBSS-Cz	310, 340, 360, 385, 459	475	569	16	26
β-ThBSS	312, 427	451	486	24	27
β-DThBSS	312, 415	438	492	23	27
β-DThBSS-Cz	314, 332, 380, 413	437	491	24	26

[a] Absorption peaks; [b] Emission peak; [c] Phosphorescence peak (77 K, delay time: 10 ms); [d] Stokes shift ($\lambda_{em}-\lambda_{abs}$); [e] Full width at half-maximum for PL spectra.

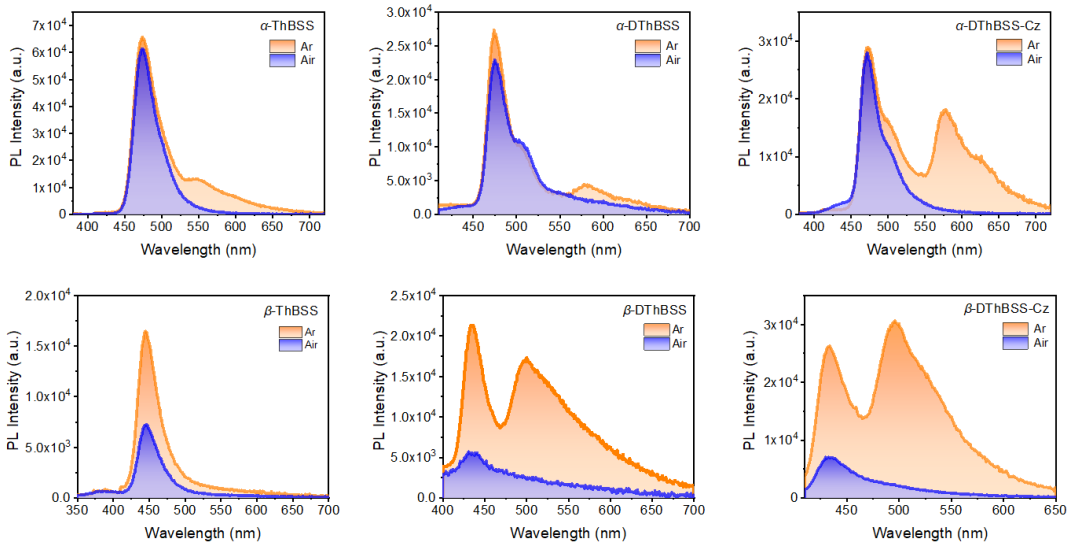


Figure S21. Steady-state PL spectra for the emitters in PMMA matrix (1 wt%) under argon and air atmosphere.

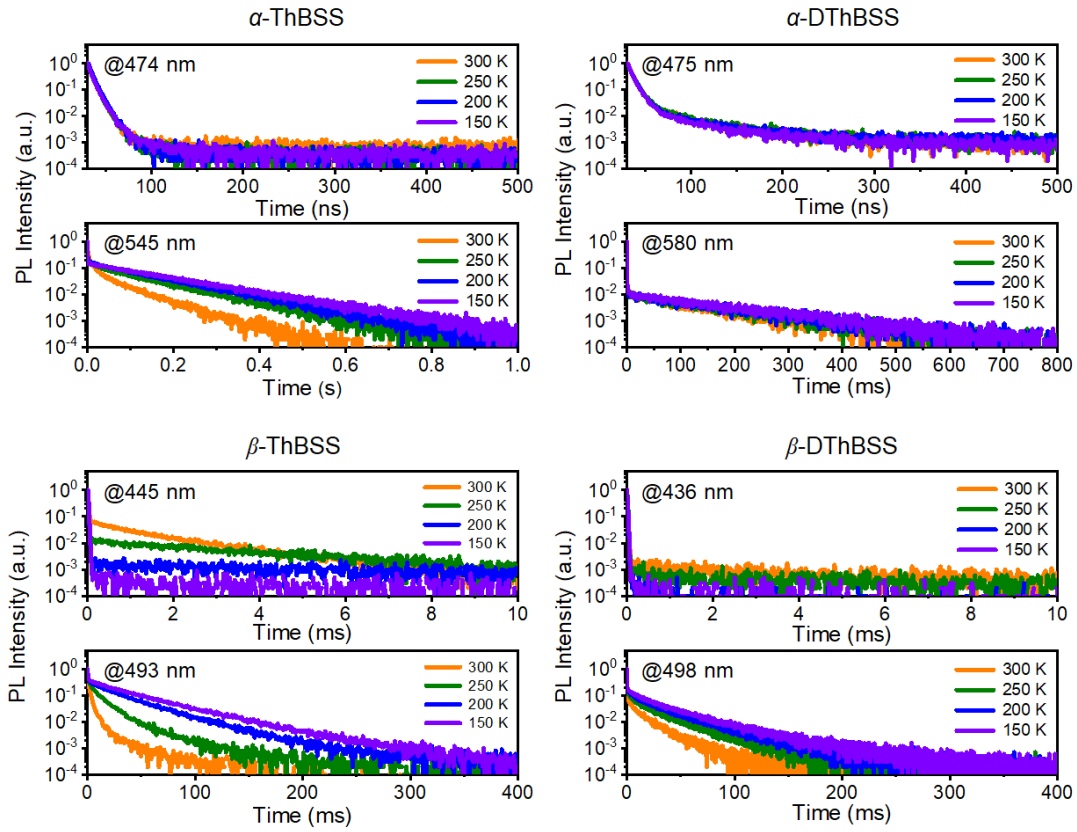


Figure S22. Temperature-dependent transient PL decay characteristics for the emitters in PMMA matrix (1 wt%).

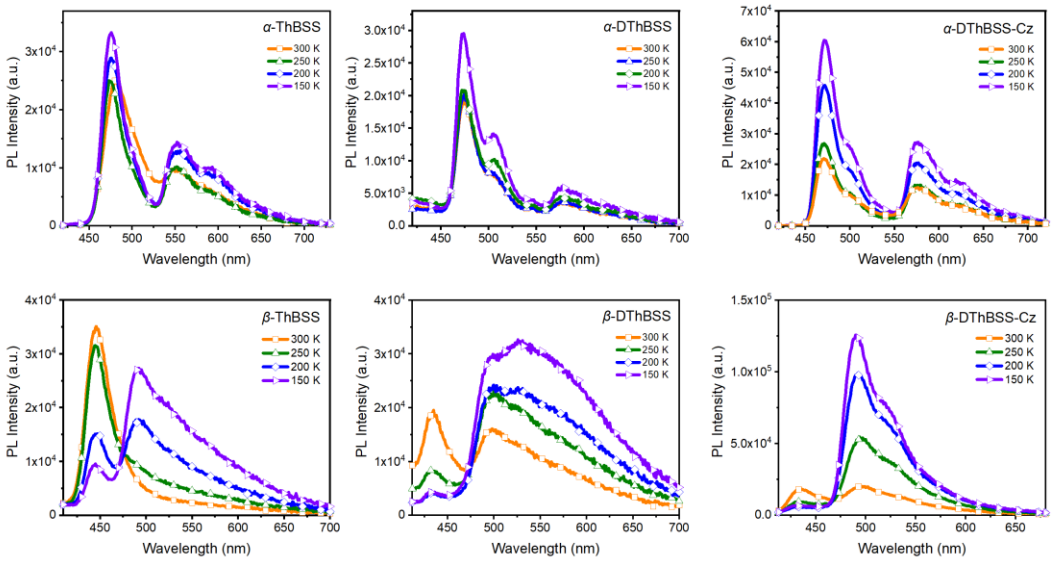


Figure 23. Temperature-dependent PL spectra for the emitters in doped PMMA films (1 wt%).

Table S4. Summary of kinetic parameters for the emitters in doped PMMA films (1 wt%).

Compounds	k_r^F [10^8 s^{-1}]	k_{ISC} [10^8 s^{-1}]	k_{RISC} [10^3 s^{-1}]	k_r^P [10^1 s^{-1}]	k_{nr}^P [10^1 s^{-1}]
α-ThBSS	1.19	0.50	--	0.54	1.56
α-DThBSS	0.92	0.25	--	0.12	0.76
α-DThBSS-Cz	1.15	0.92	--	0.26	0.57
β-ThBSS	0.61	7.33	5.17	1.56	13.18
β-DThBSS	0.22	2.43	0.44	2.51	10.84
β-DThBSS-Cz	0.22	6.36	0.48	1.76	6.22

k_r^F: radiative decay rate constant from S_1; k_r^P and k_{nr}^P: radiative and non-radiative decay rate constant from T_1; k_{ISC}: intersystem crossing rate constant from S_1 to T_1; k_{RISC}: reverse intersystem crossing rate constant from T_1 to S_1.

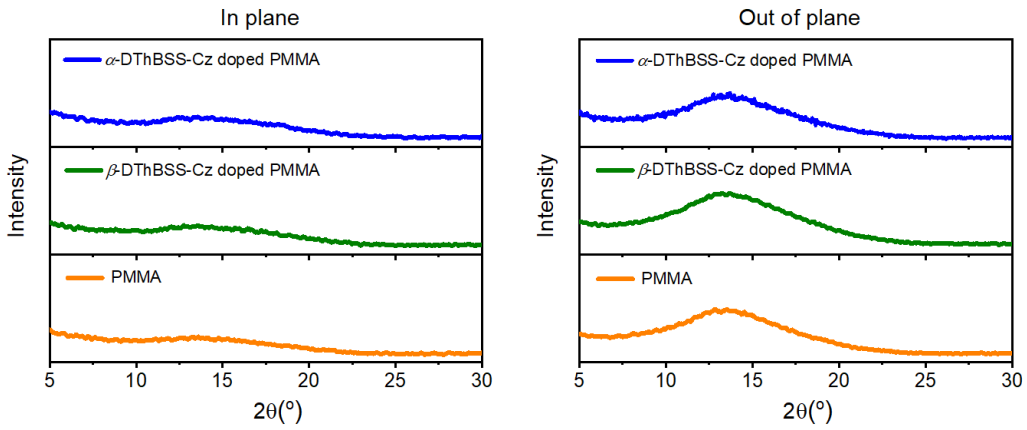


Figure S24. X-Ray diffraction (XRD) pattern for *α*-DThBSS-Cz and *β*-DThBSS-Cz doped PMMA films (1 wt% doping concentration) as well as pure PMMA film.

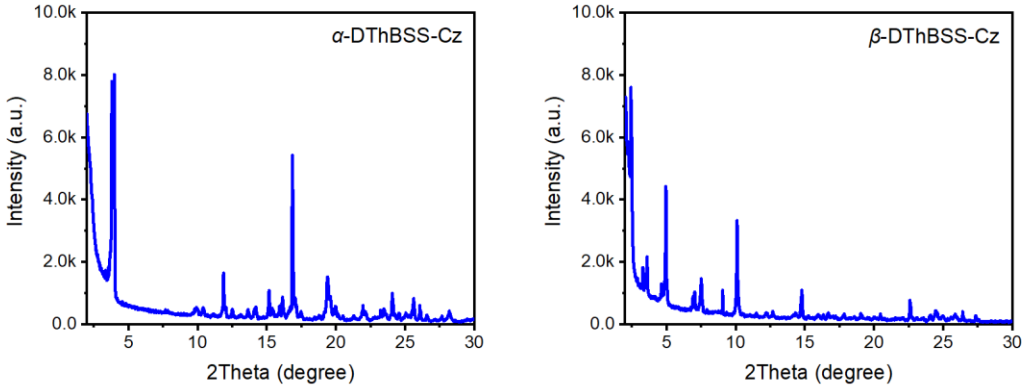


Figure 25. XRD pattern for *α*-DThBSS-Cz and *β*-DThBSS-Cz powders.

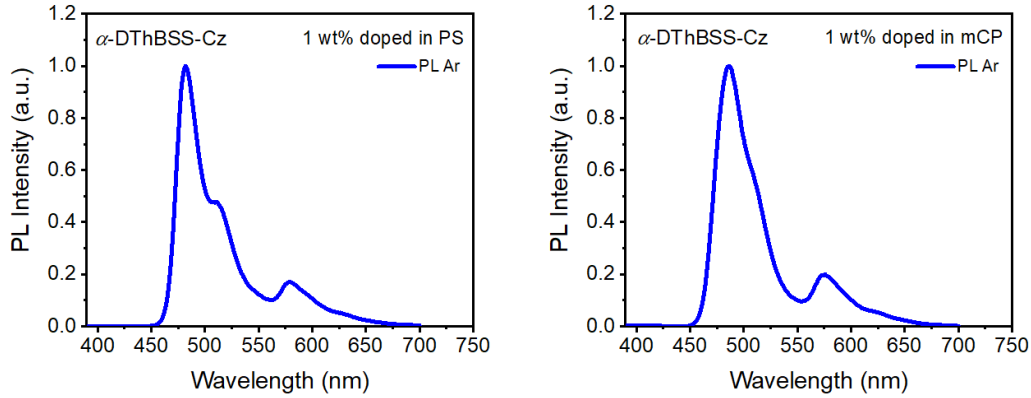


Figure S26. Steady-state PL spectra for *α*-DThBSS-Cz doped in polystyrene (PS) and 1,3-bis(carbazol-9-yl)benzene (mCP) at room temperature.

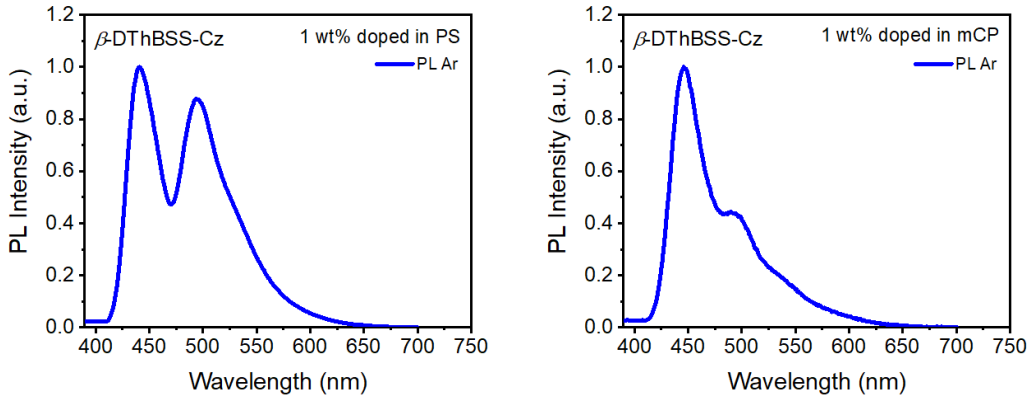


Figure S27. Steady-state PL spectra for *β*-DThBSS-Cz doped in PS and mCP at room temperature.

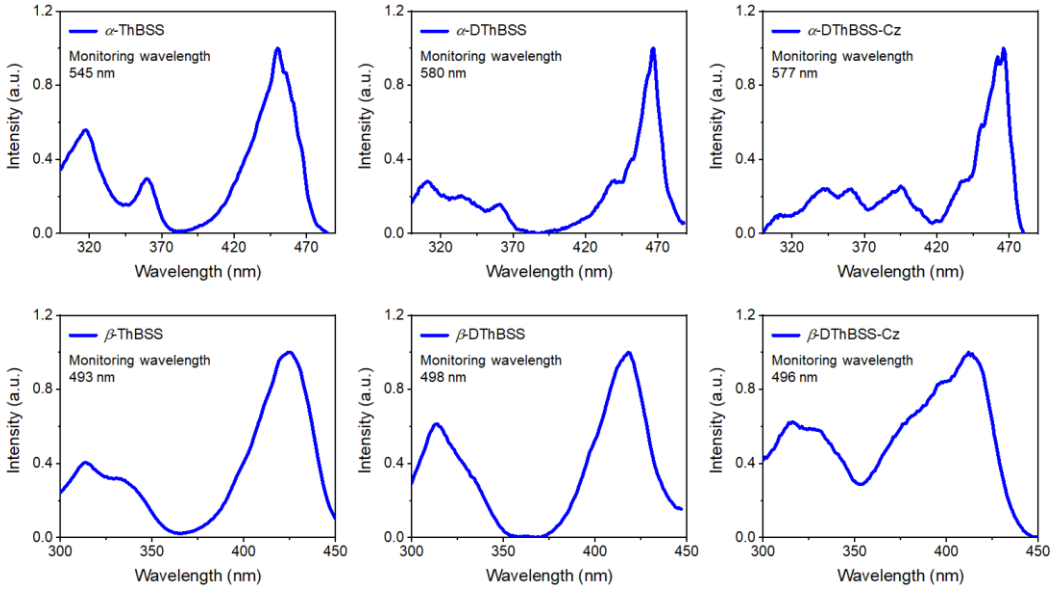


Figure S28. Excitation spectra for the emitters in doped films (1 wt% in PMMA). Note that the multi-resonance molecules exhibit restricted excited-state structure relaxation owing to their non-bonding molecular orbitals as well as the rigid and planar molecular skeleton, which indicates that the nuclear displacement from excited state to ground state can be greatly reduced, leading to small Stokes shift of 16-24 nm for resultant emitters. Such small Stokes-shift values mean that the absorption bands are very close to emission bands, making the emitters with blue emissions can be excited by visible light at 400-450 nm.

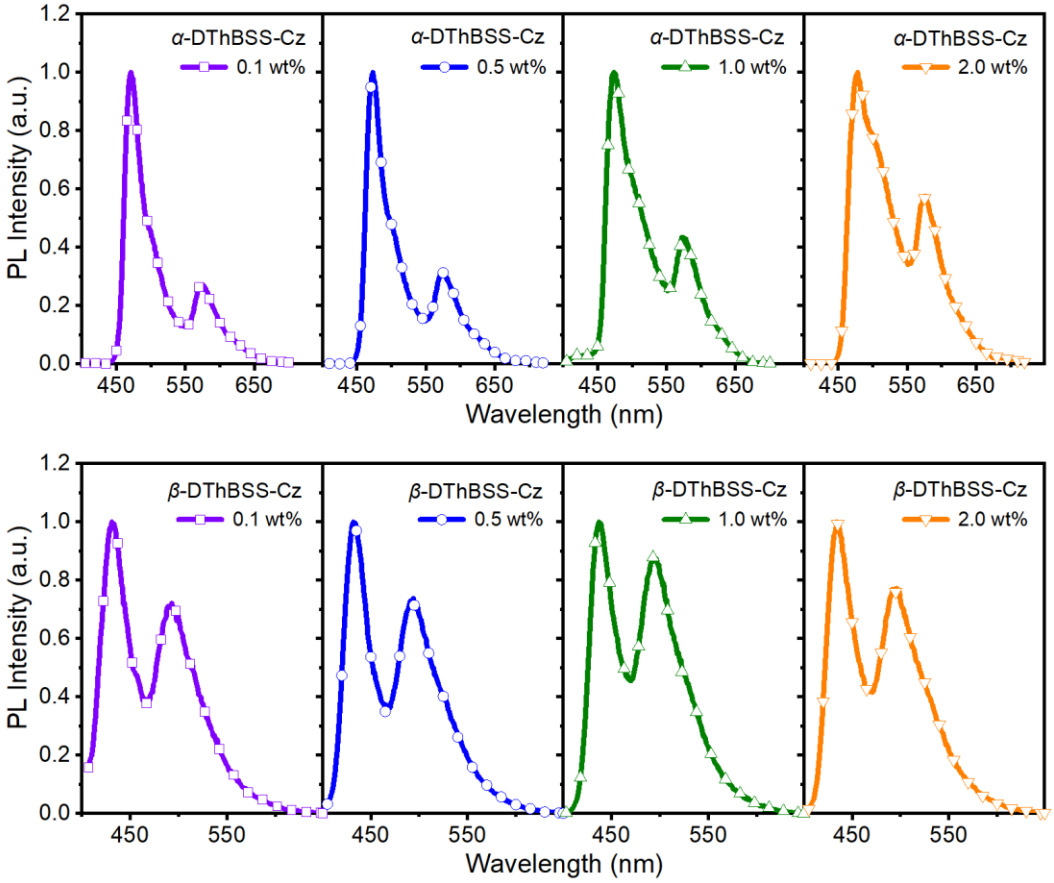


Figure 29. Steady-state PL spectra of *α*-DThBSS-Cz and *β*-DThBSS-Cz doped in PMMA films with different concentrations.

References

1 T. Lu and F. Chen, *J Comput Chem*, 2012, **33**, 580.

2 M. Kallay, P. R. Nagy, D. Mester, Z. Rolik, G. Samu, J. Csontos, J. Csoka, P. B. Szabo, L. Gyevi-Nagy, B. Hegely, I. Ladjanszki, L. Szegedy, B. Ladoczki, K. Petrov, M. Farkas, P. D. Mezei and A. Ganyecz, *J Chem Phys*, 2020, **152**, 074107.

3 A. Pershin, D. Hall, V. Lemaur, J. C. Sancho-Garcia, L. Muccioli, E. Zysman-Colman, D. Beljonne and Y. Olivier, *Nat Commun*, 2019, **10**, 597.

4 S. Tian, H. Ma, X. Wang, A. Lv, H. Shi, Y. Geng, J. Li, F. Liang, Z. M. Su, Z. An and W. Huang, *Angew. Chem. Int. Ed*, 2019, **58**, 6645.

5 Y. Tsuchiya, S. Diesing, F. Bencheikh, Y. Wada, P. L. Dos Santos, H. Kaji, E. Zysman-Colman, I. D. W. Samuel and C. Adachi, *J Phys Chem A*, 2021, **125**, 8074.

NMR Spectra

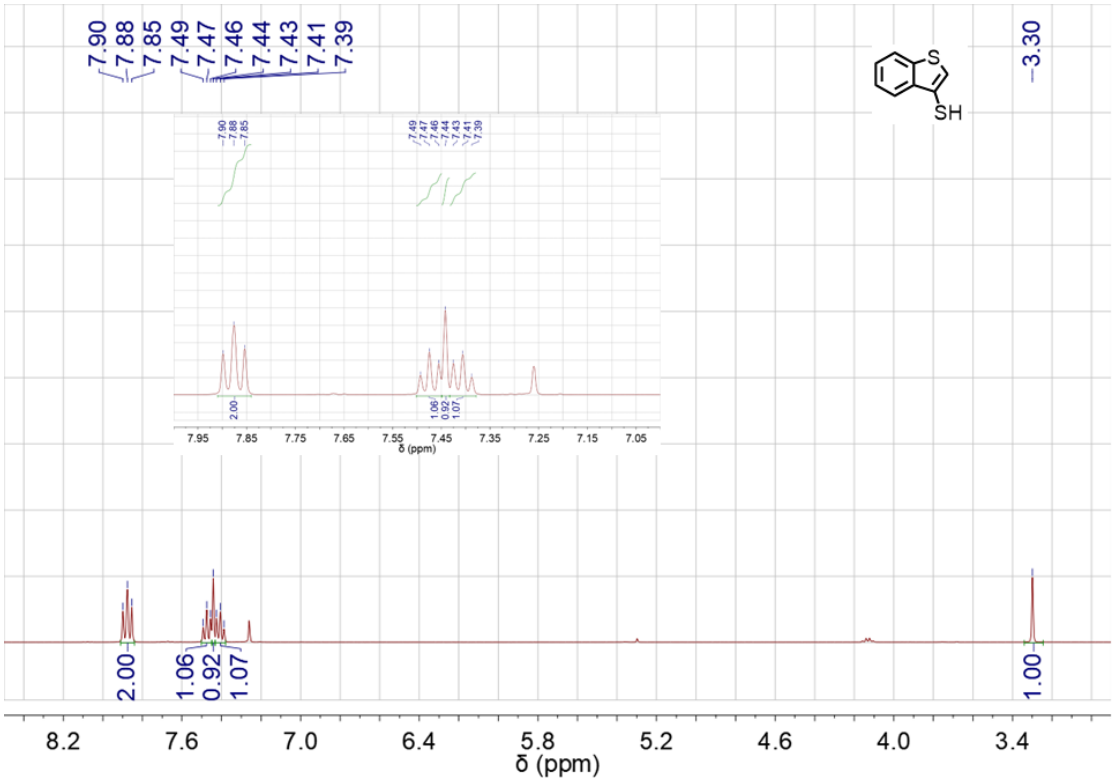


Figure S30. ^{1}H NMR spectrum of **2**.

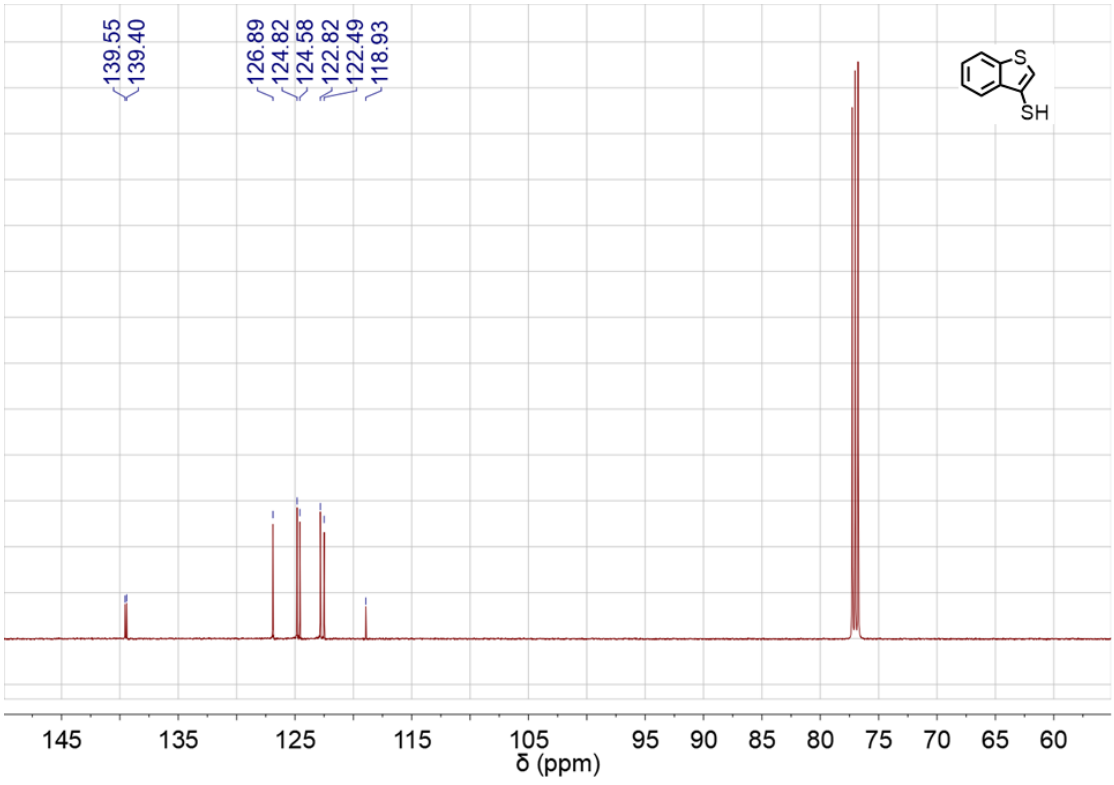


Figure S31. ^{13}C NMR spectrum of **2**.

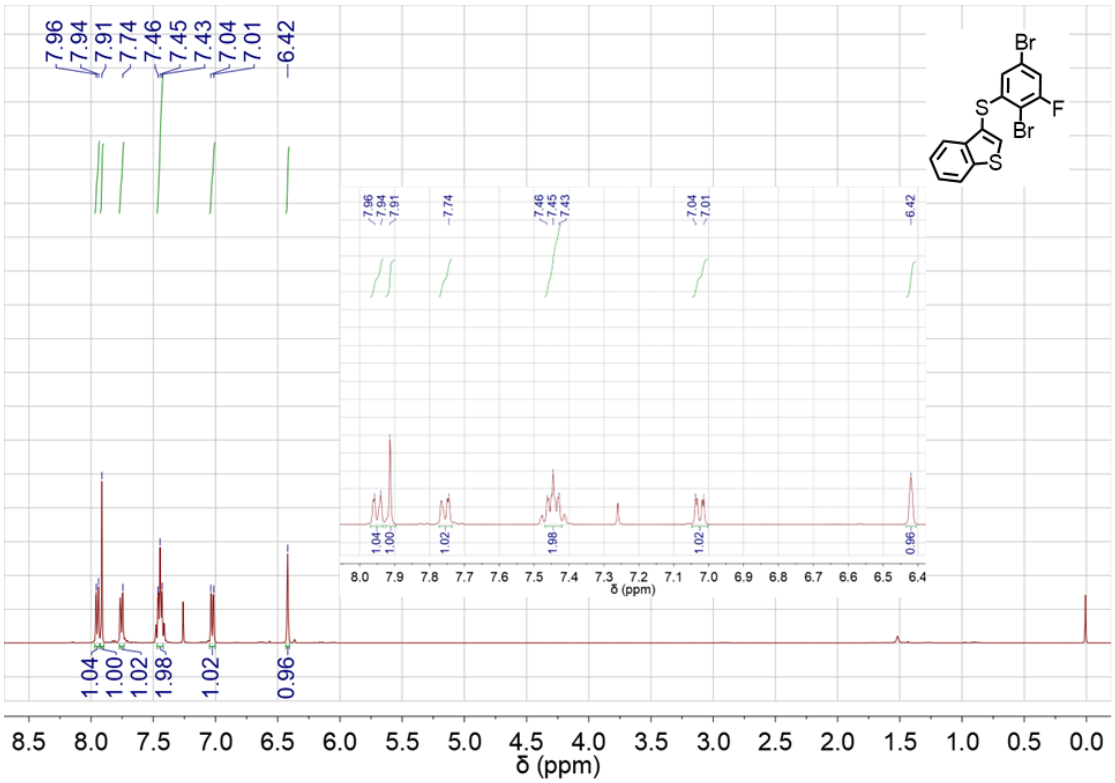


Figure S32. ^{1}H NMR spectrum of **3**.

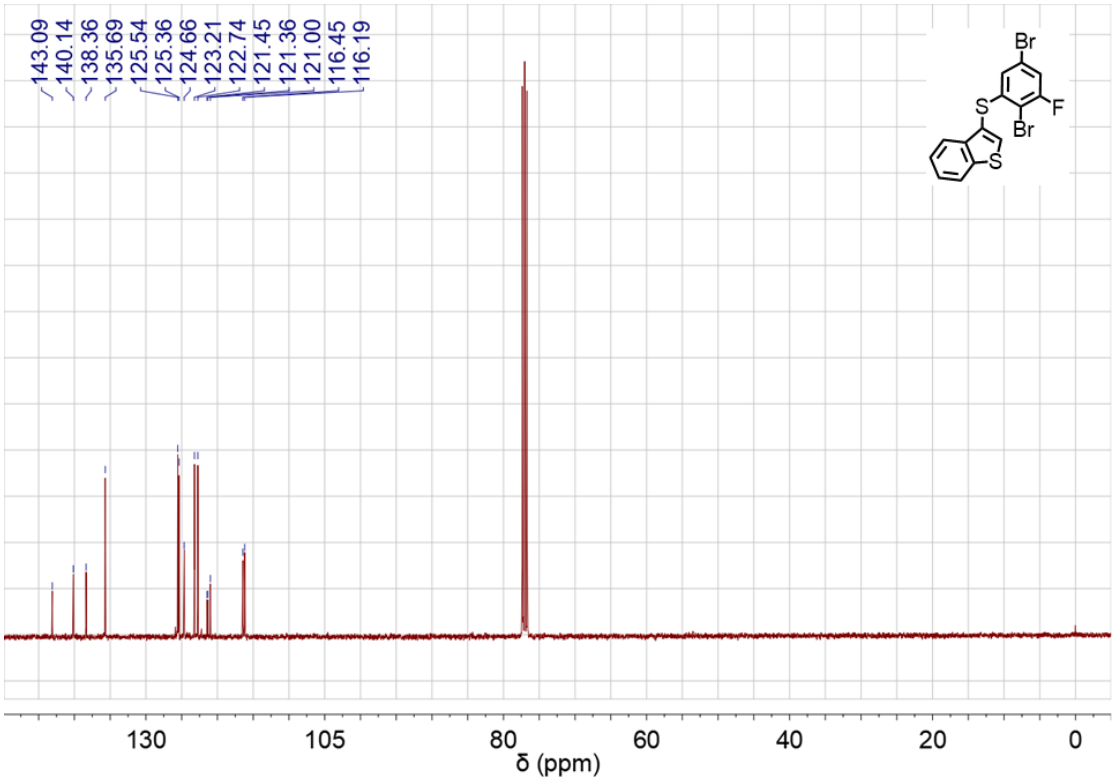


Figure S33. ^{13}C NMR spectrum of **3**.

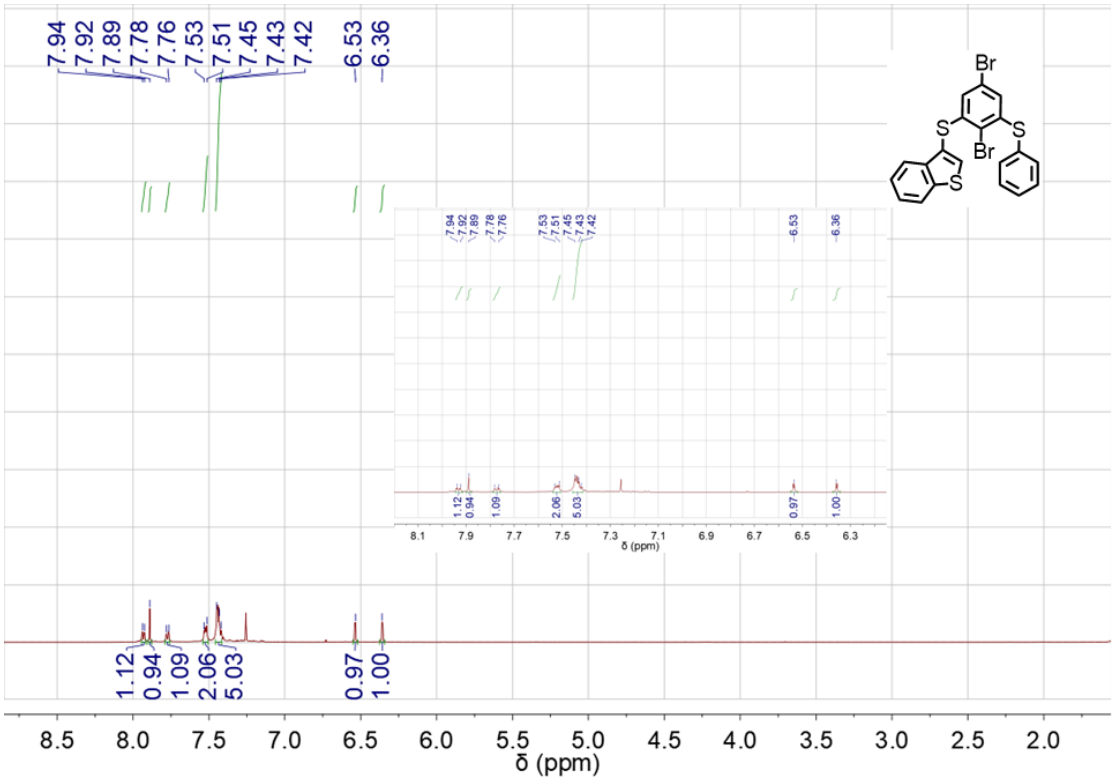


Figure S34. ^{1}H NMR spectrum of **4**.

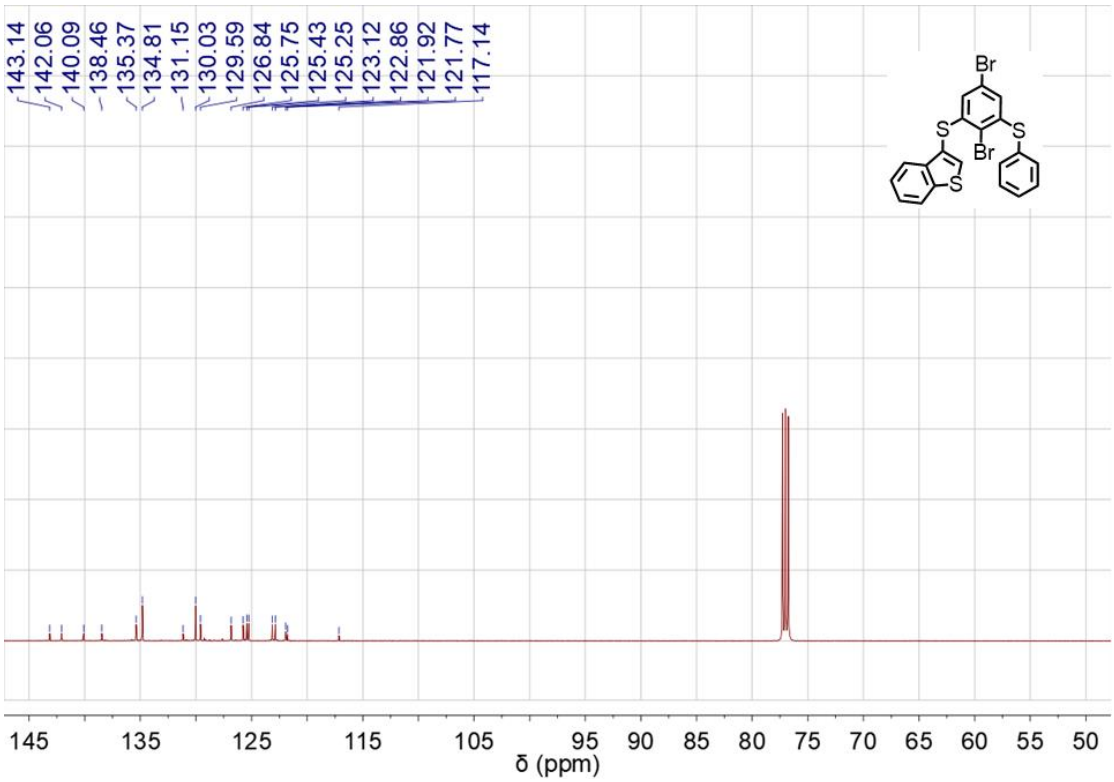


Figure S35. ^{13}C NMR spectrum of **4**.

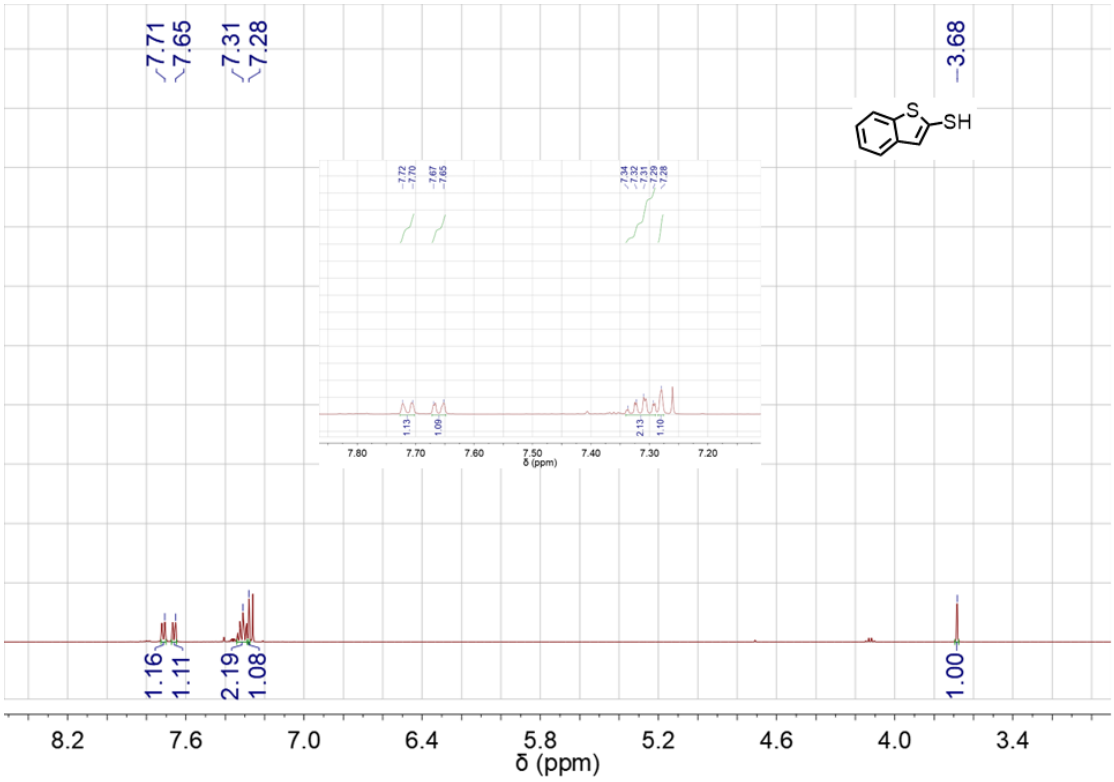


Figure S36. ^{1}H NMR spectrum of **6**.

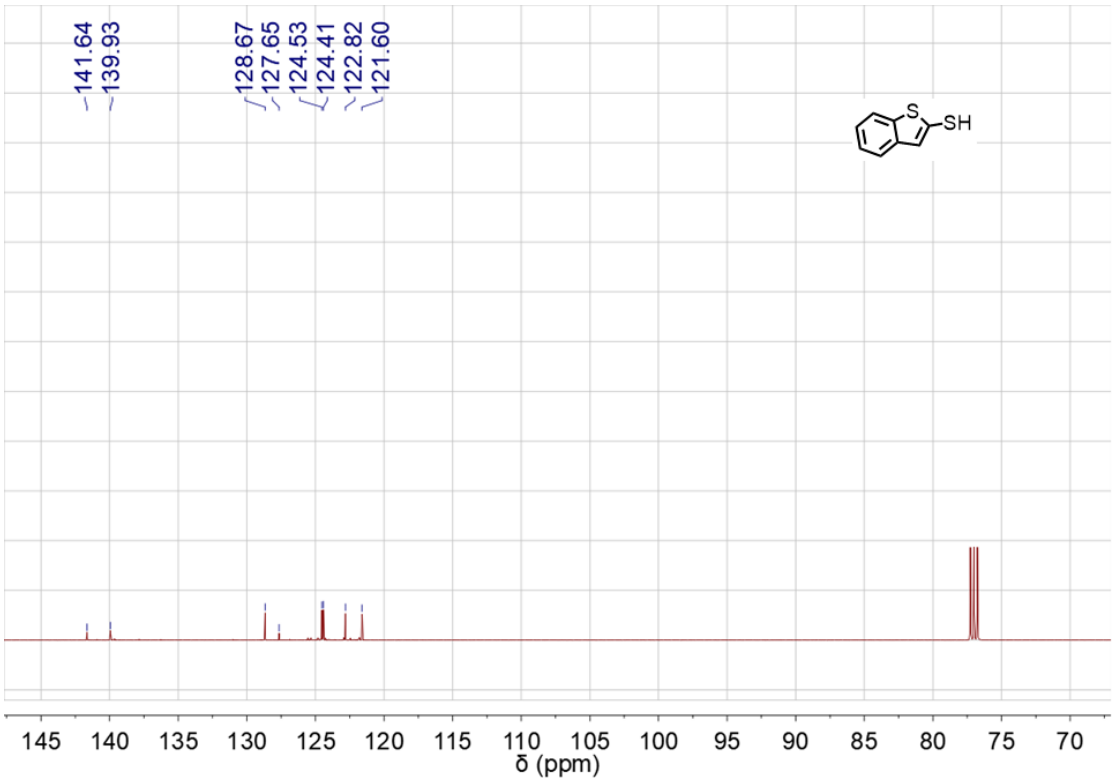


Figure S37. ^{13}C NMR spectrum of **6**.

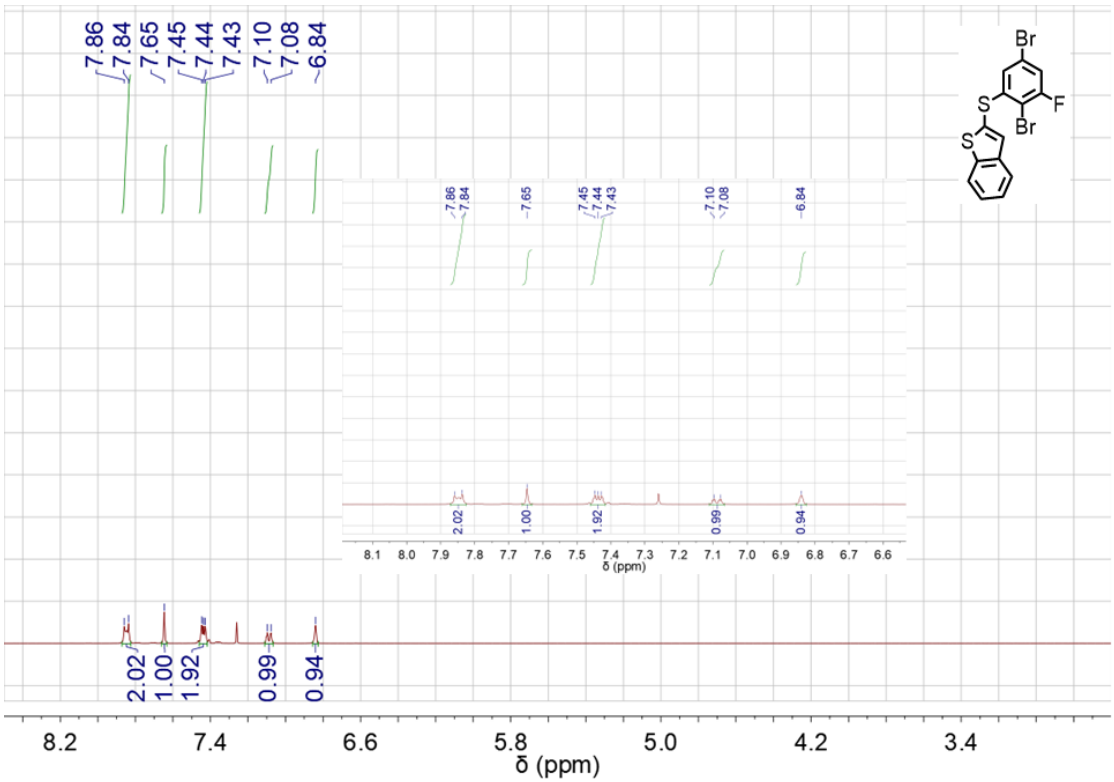


Figure S38. ^{1}H NMR spectrum of **7**.

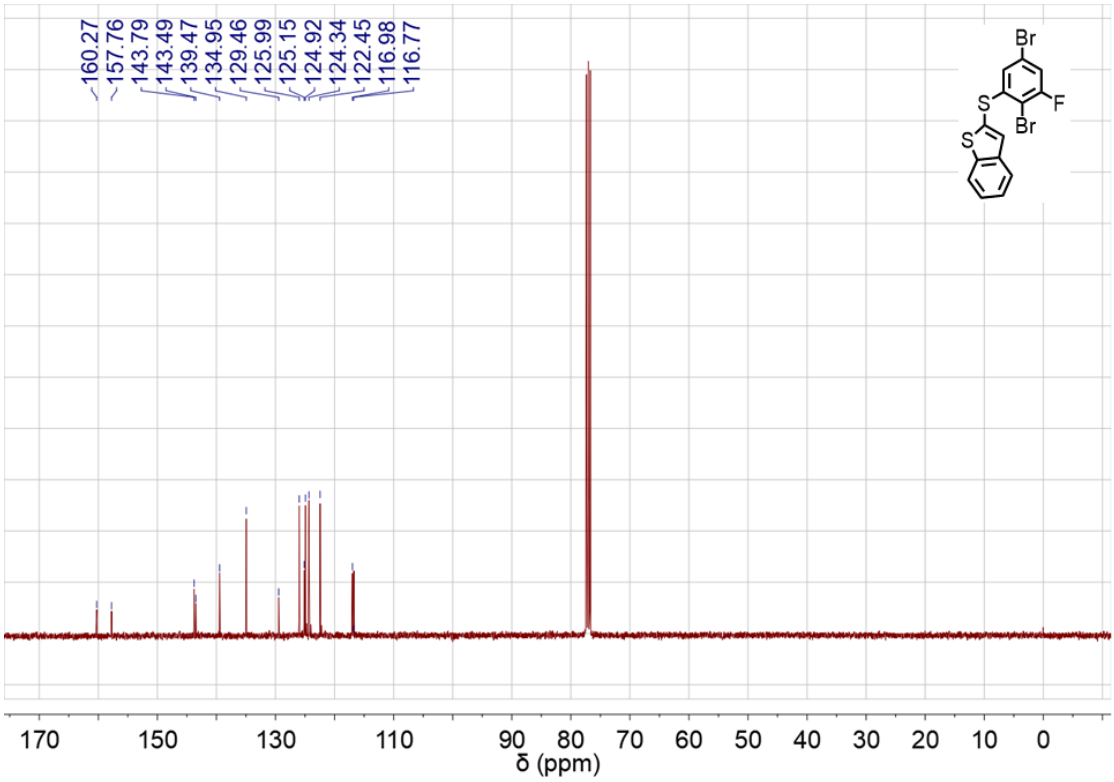


Figure S39. ^{13}C NMR spectrum of **7**.

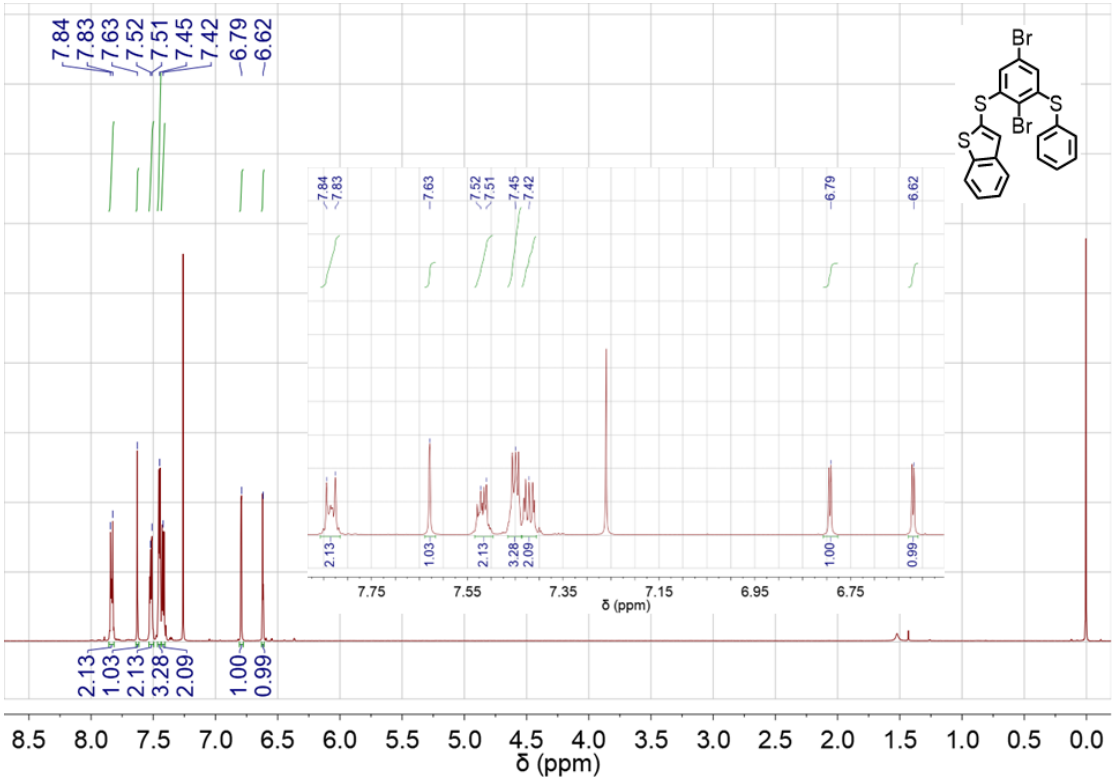


Figure S40. ^{1}H NMR spectrum of **8**.

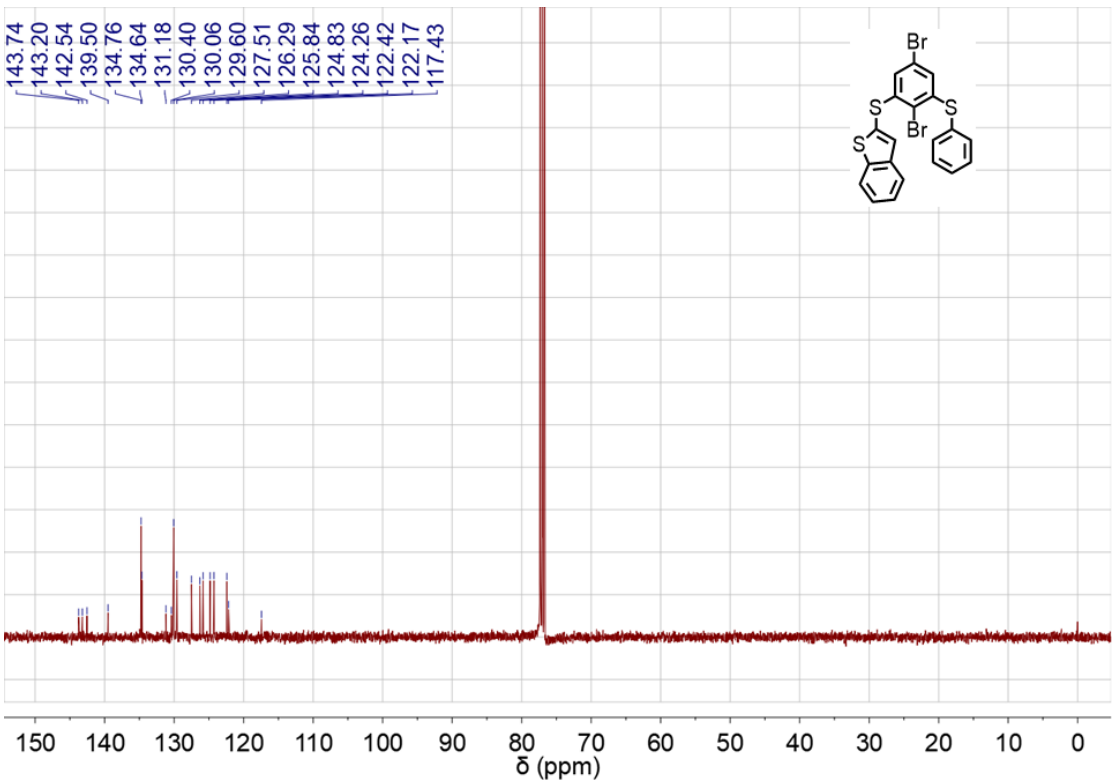


Figure S41. ^{13}C NMR spectrum of **8**.

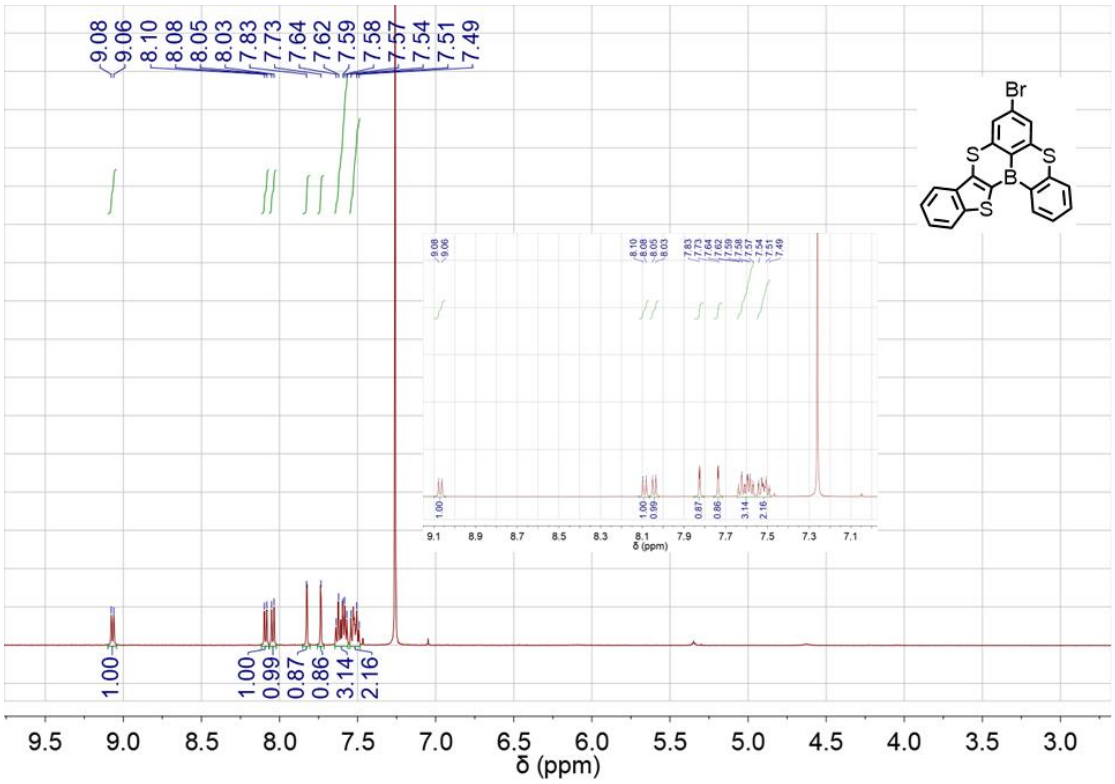


Figure S42. ^{1}H NMR spectrum of ***α*-ThBSS-Br**.

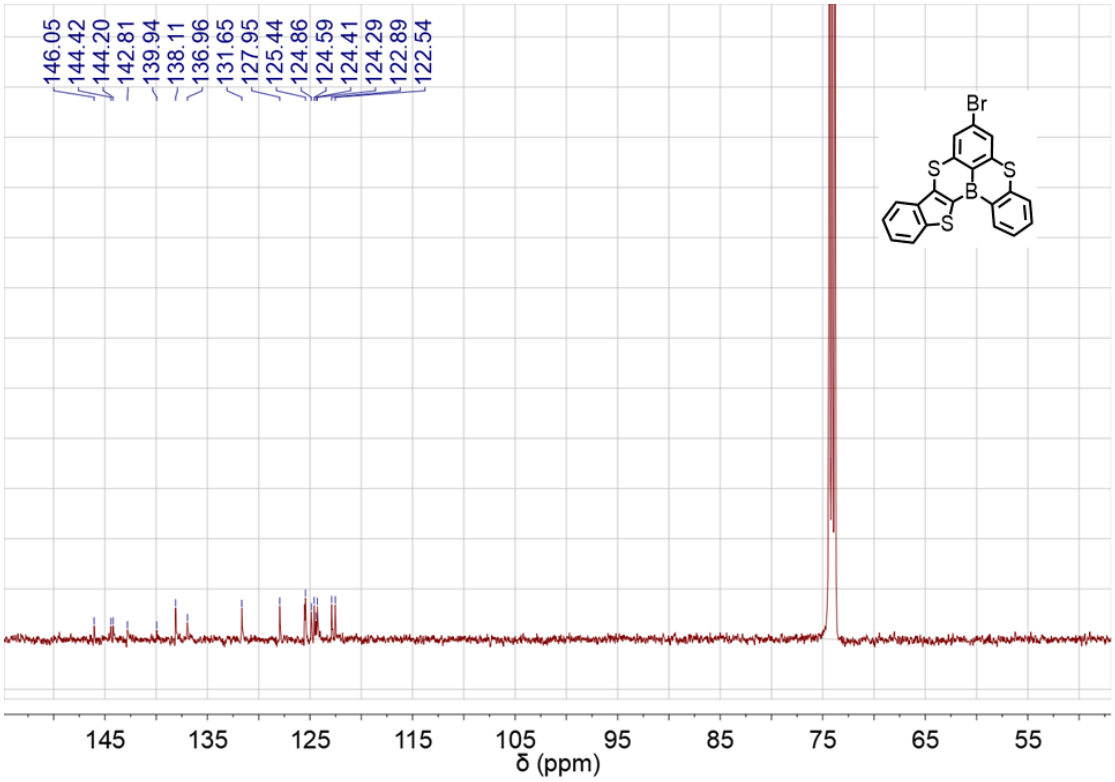


Figure S43. ^{13}C NMR spectrum of ***α*-ThBSS-Br**.

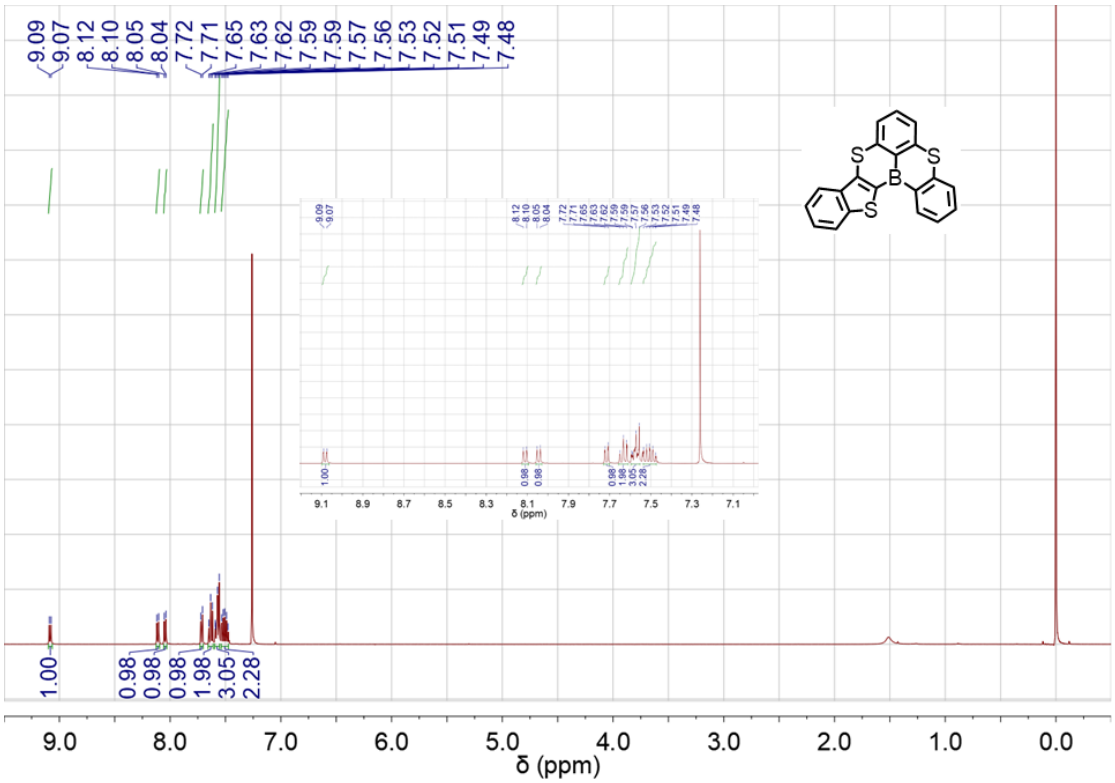


Figure S44. ^{1}H NMR spectrum of ***α*-ThBSS**.

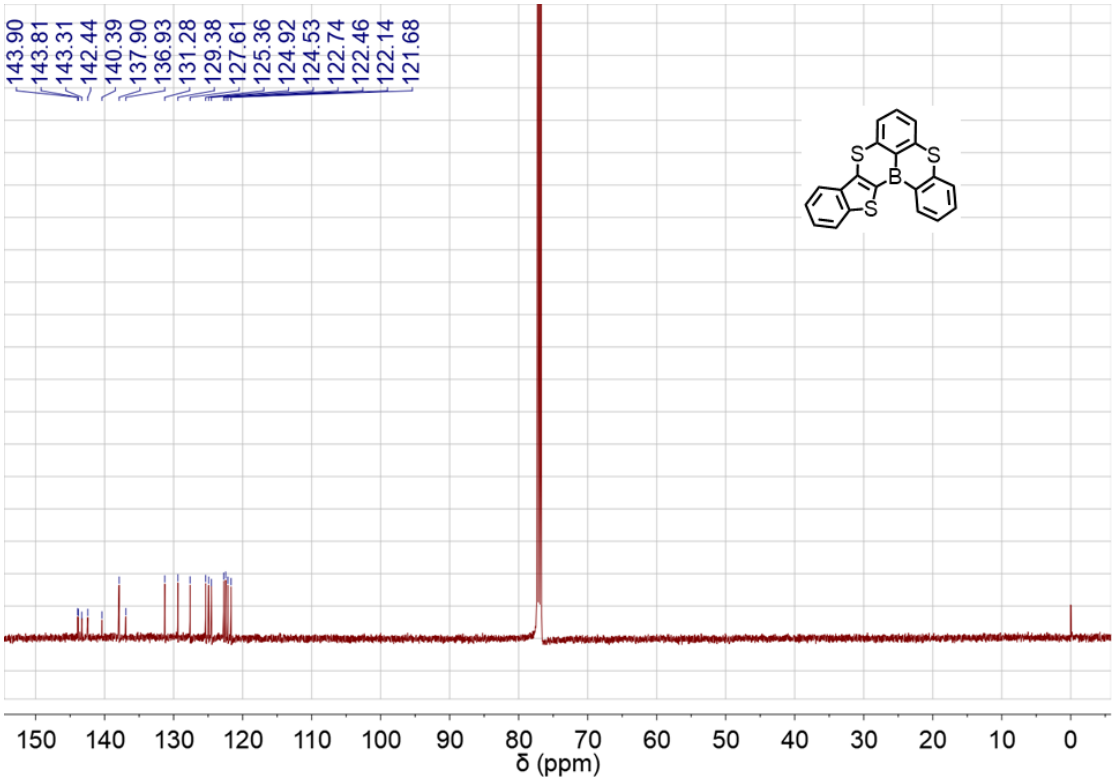


Figure S45. ^{13}C NMR spectrum of ***α*-ThBSS**.

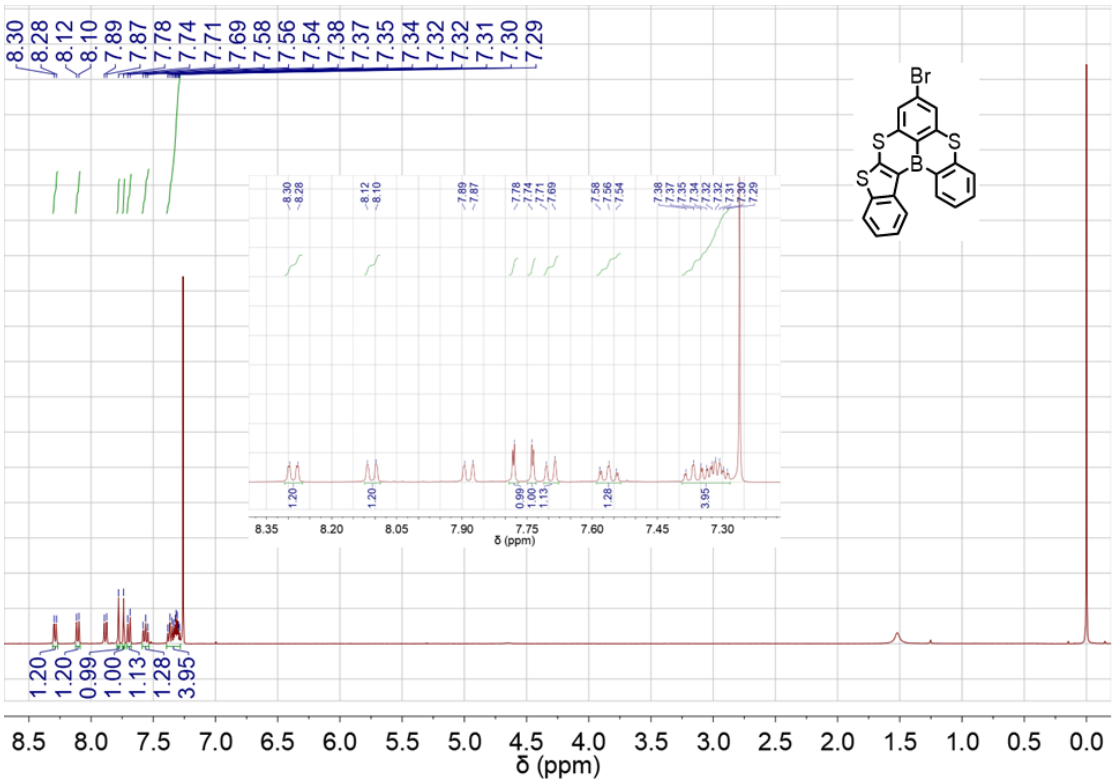


Figure S46. ^{1}H NMR spectrum of ***β*-ThBSS-Br**.

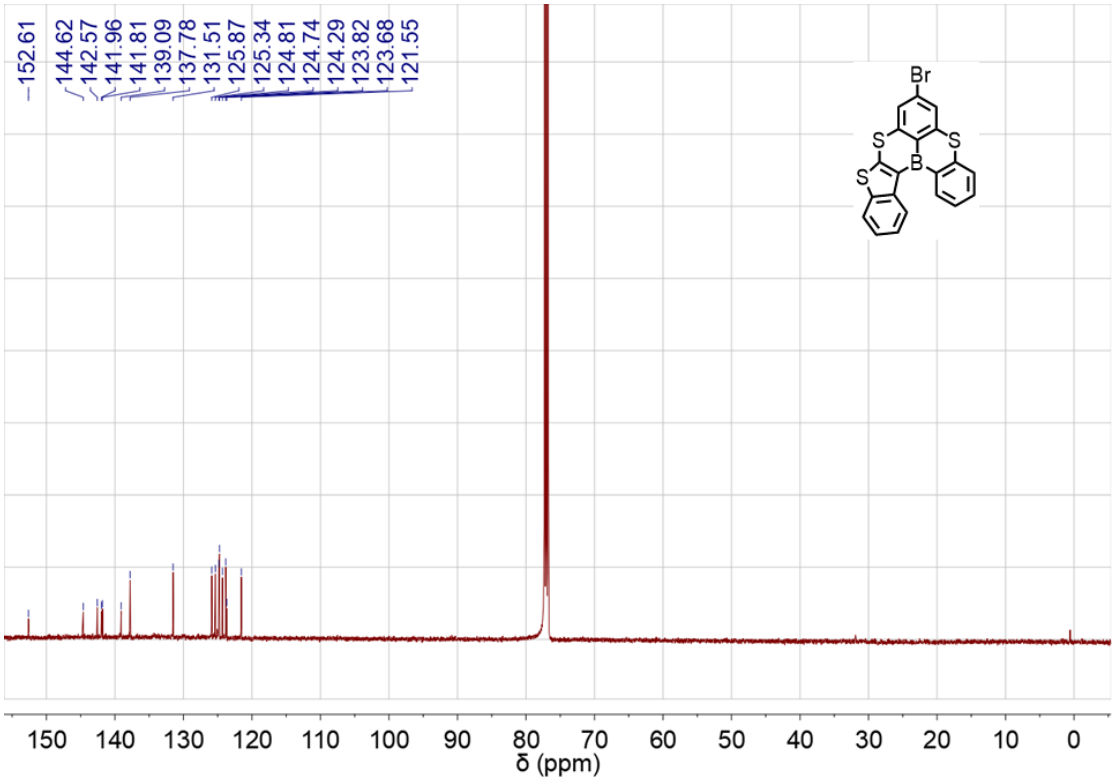


Figure S47. ^{13}C NMR spectrum of ***β*-ThBSS-Br**.

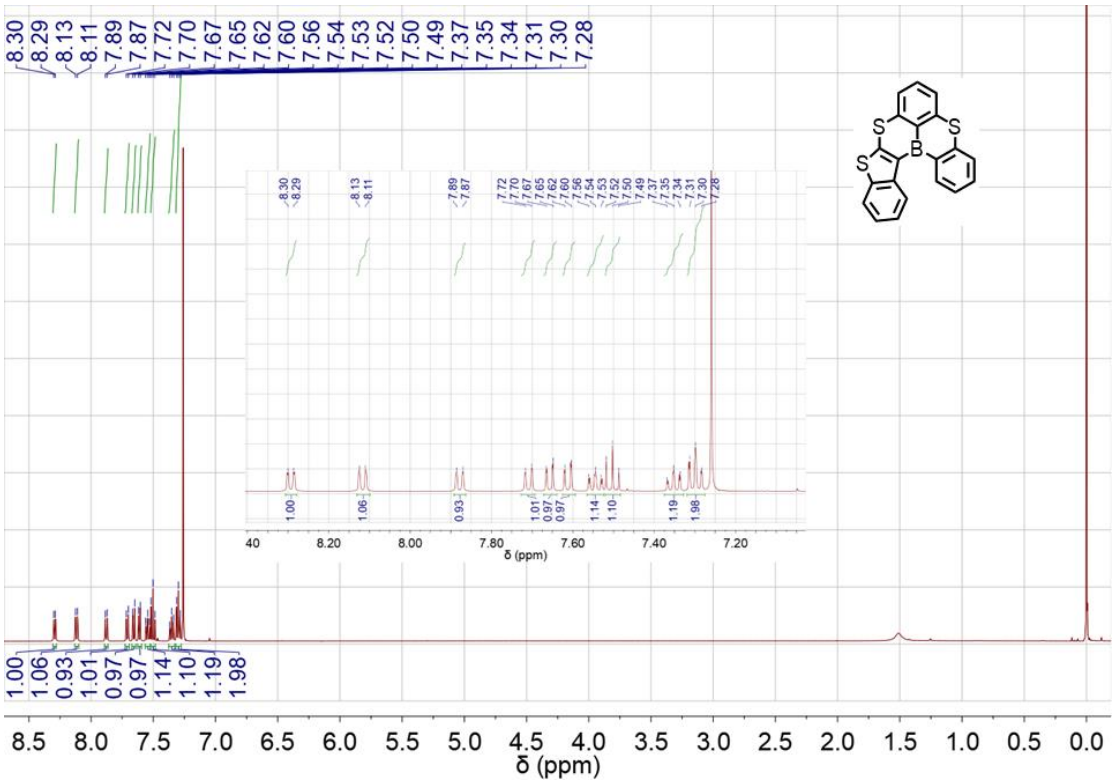


Figure S48. ^{1}H NMR spectrum of ***β*-ThBSS**.

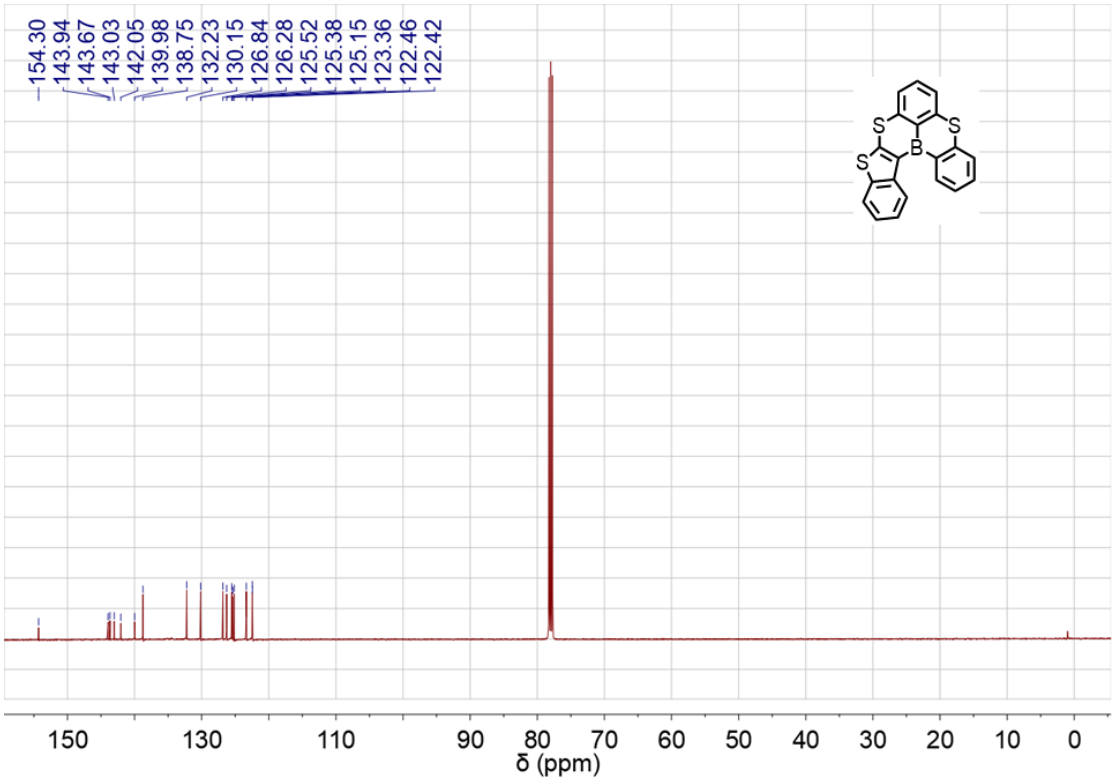


Figure S49. ^{13}C NMR spectrum of ***β*-ThBSS**.

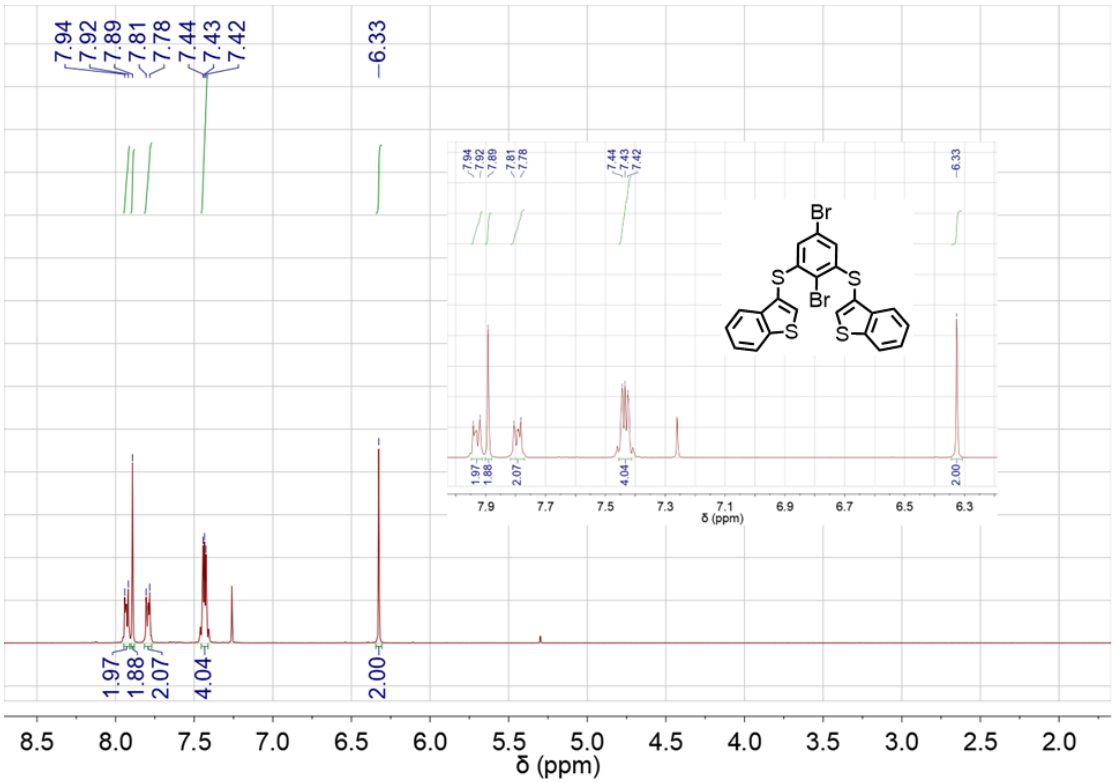


Figure S50. ^{1}H NMR spectrum of **9**.

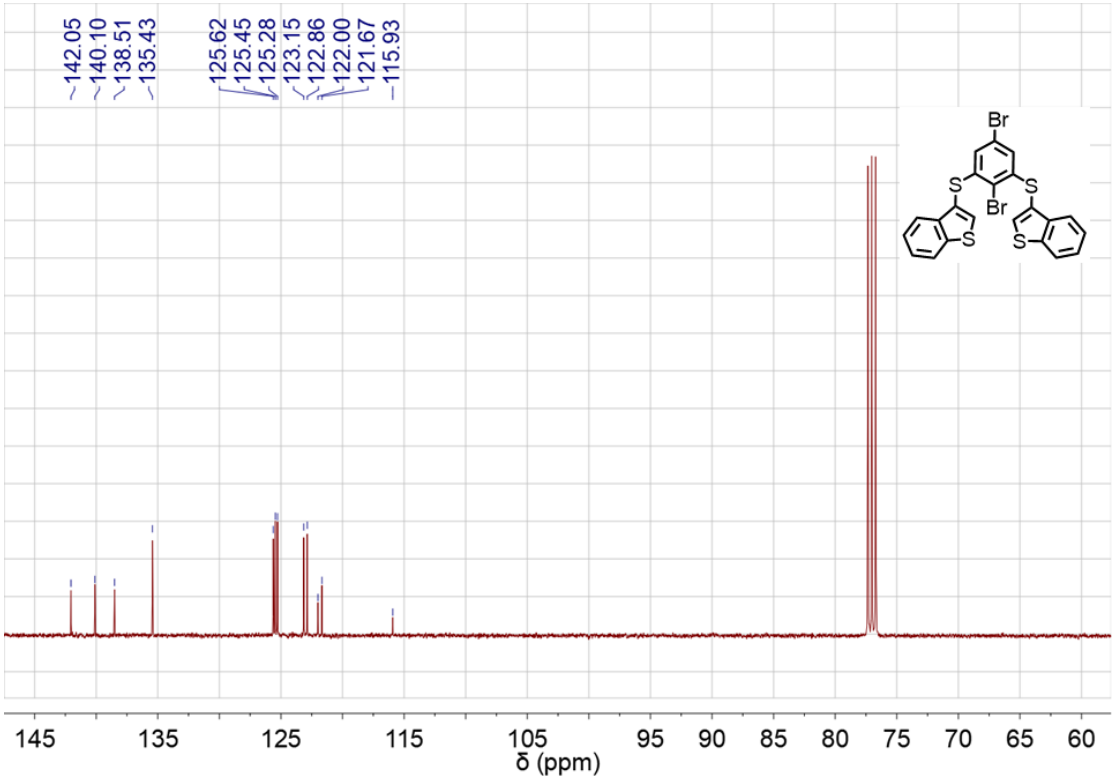


Figure S51. ^{13}C NMR spectrum of **9**.

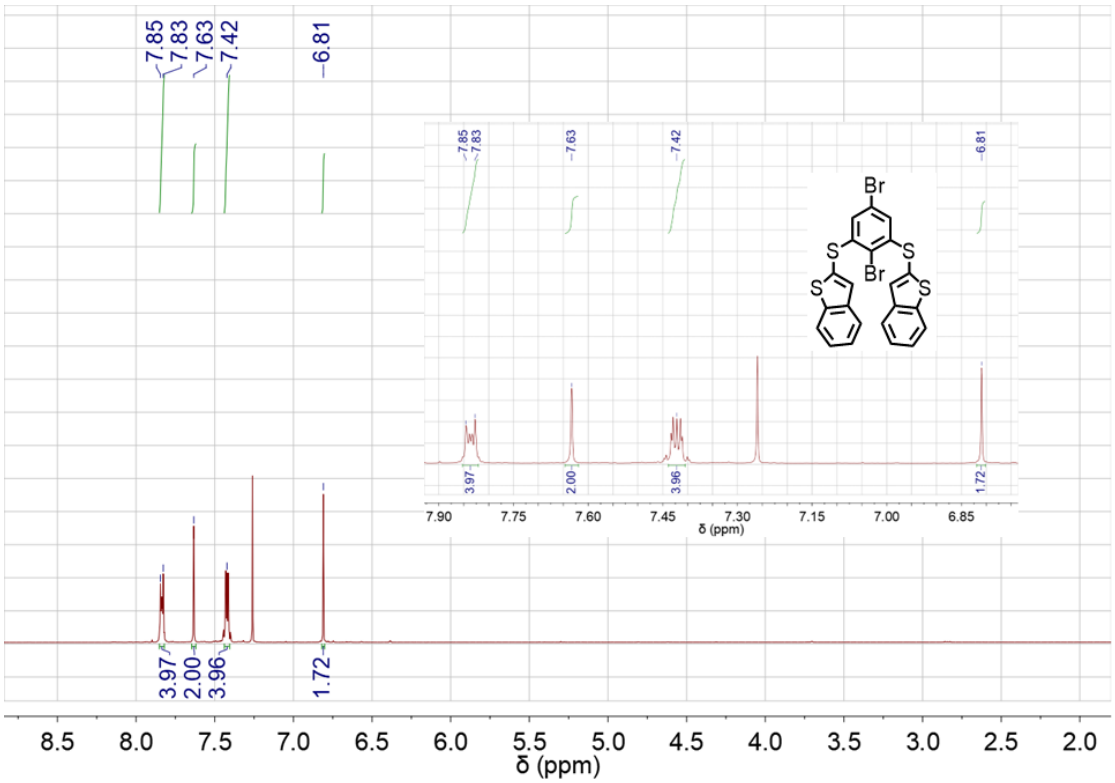


Figure S52. ^{1}H NMR spectrum of **10**.

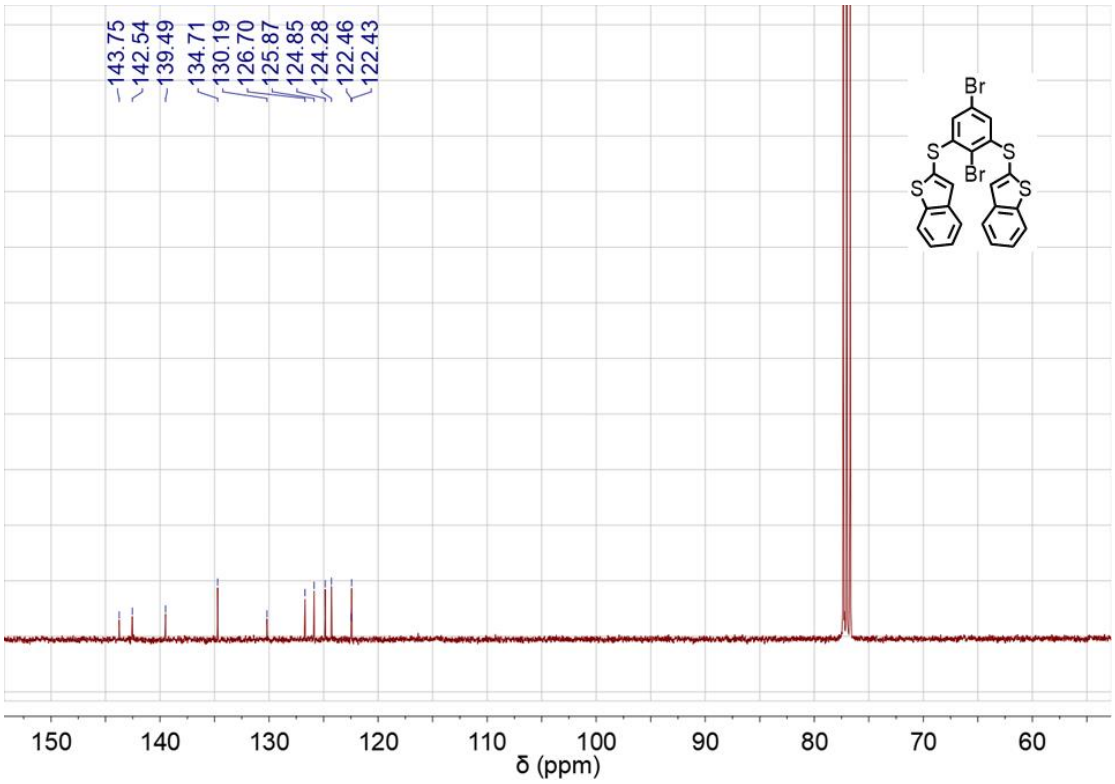


Figure S53. ^{13}C NMR spectrum of **10**.

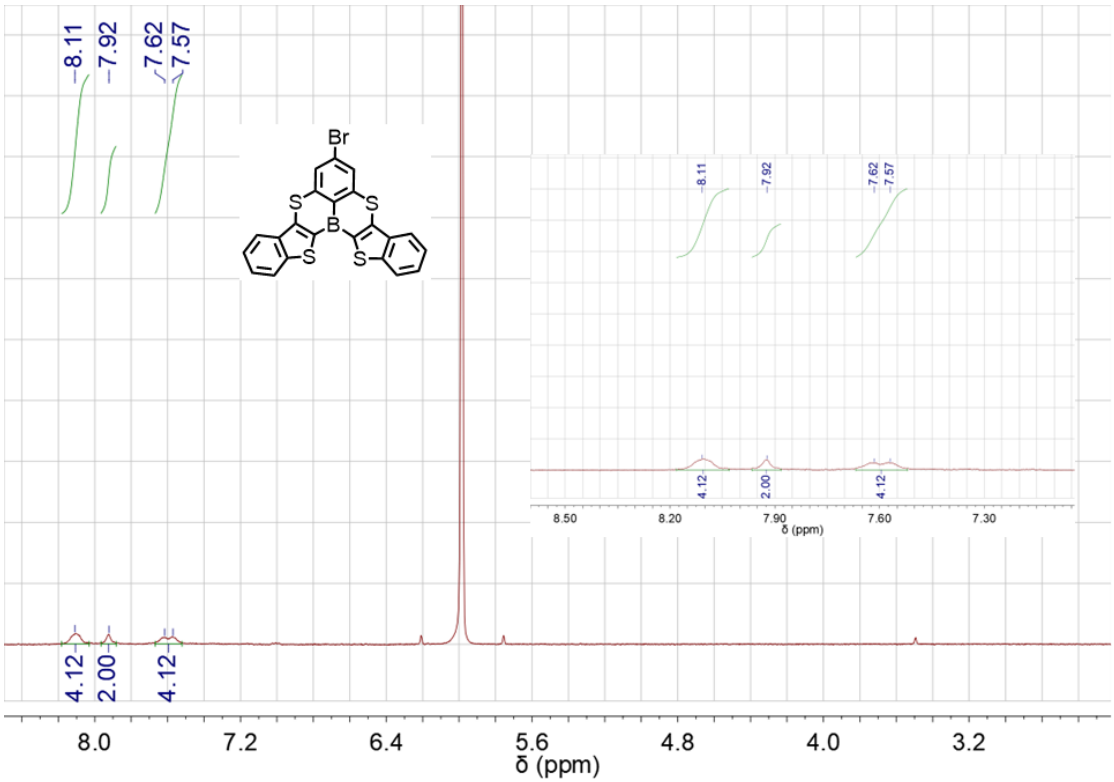


Figure S54. ^{1}H NMR spectrum of ***α*-DThBSS-Br**.

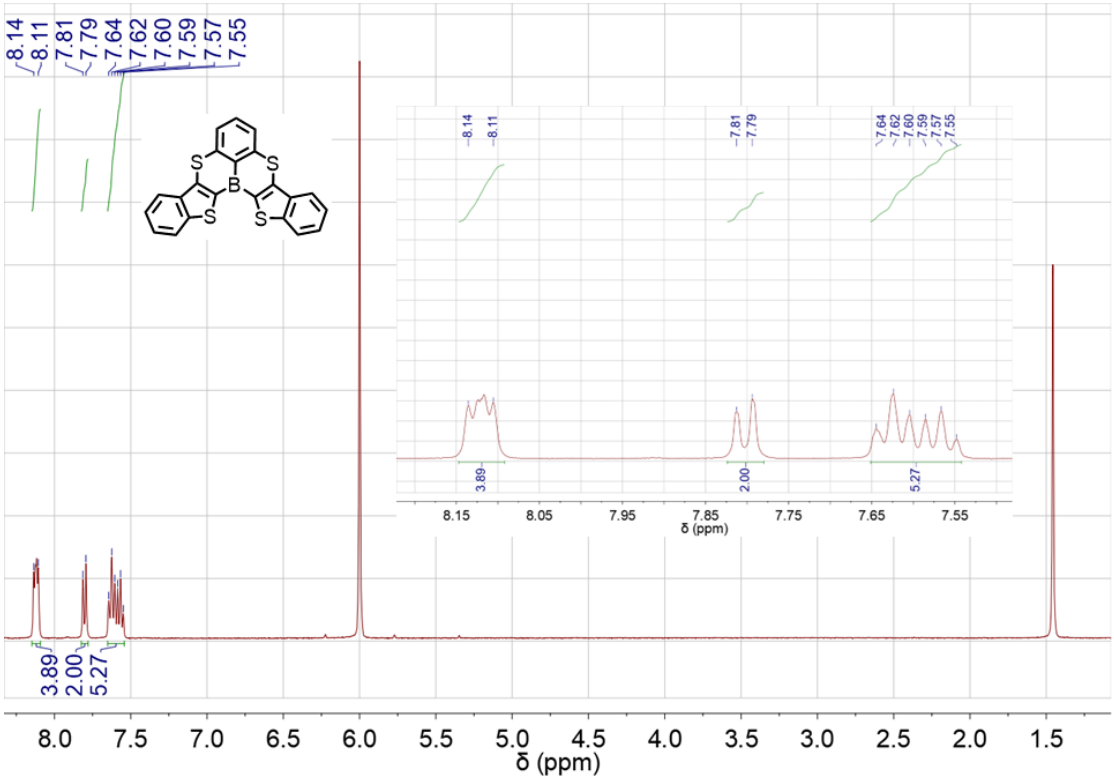


Figure S55. ^{1}H NMR spectrum of ***α*-DThBSS**.

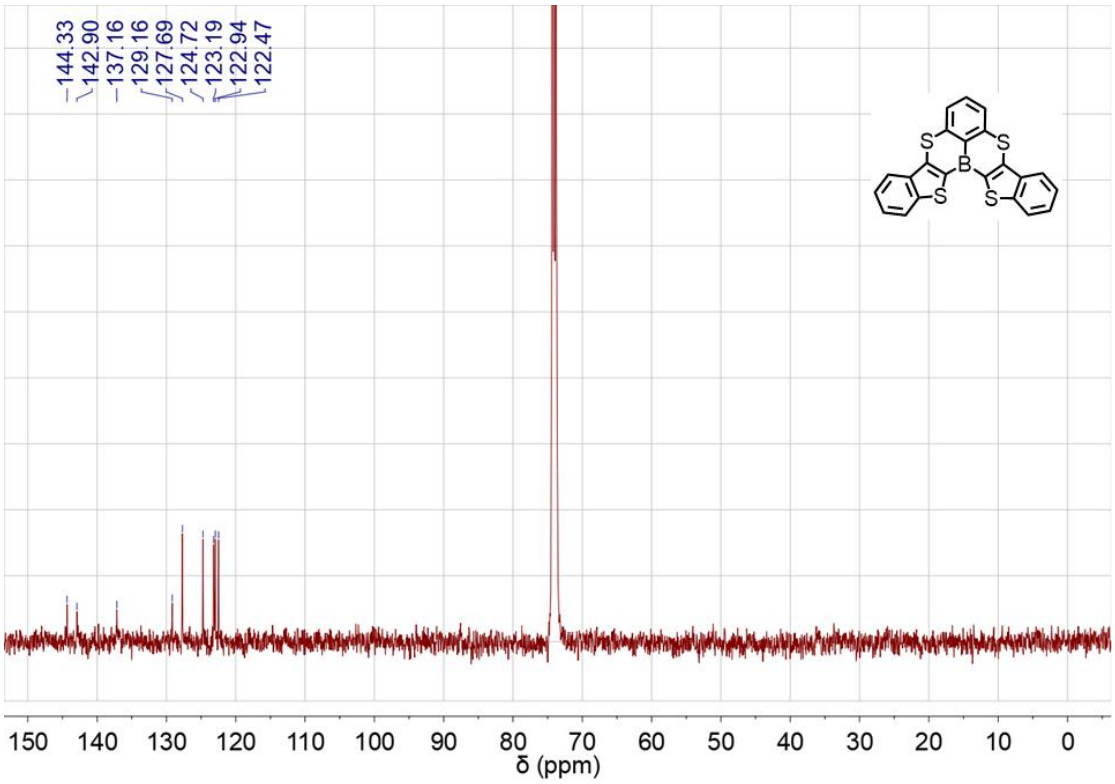


Figure S56. ^{13}C NMR spectrum of ***α*-DThBSS**.

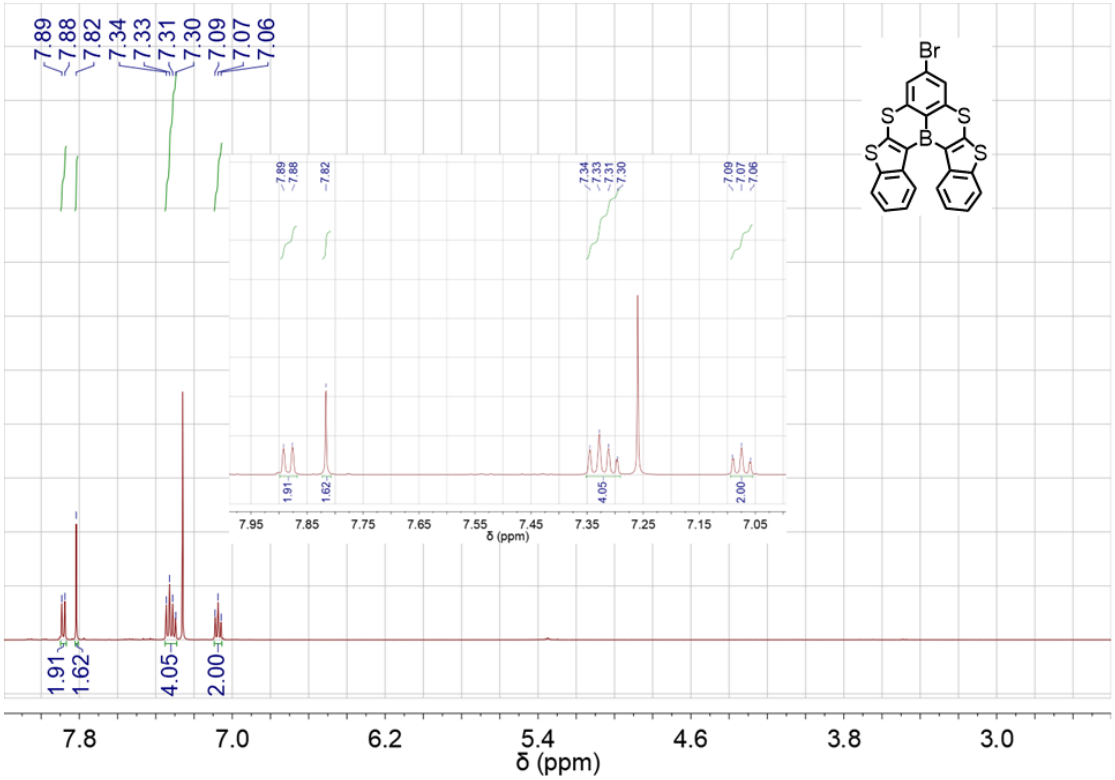


Figure S57. ^{1}H NMR spectrum of ***β*-DThBSS-Br**.

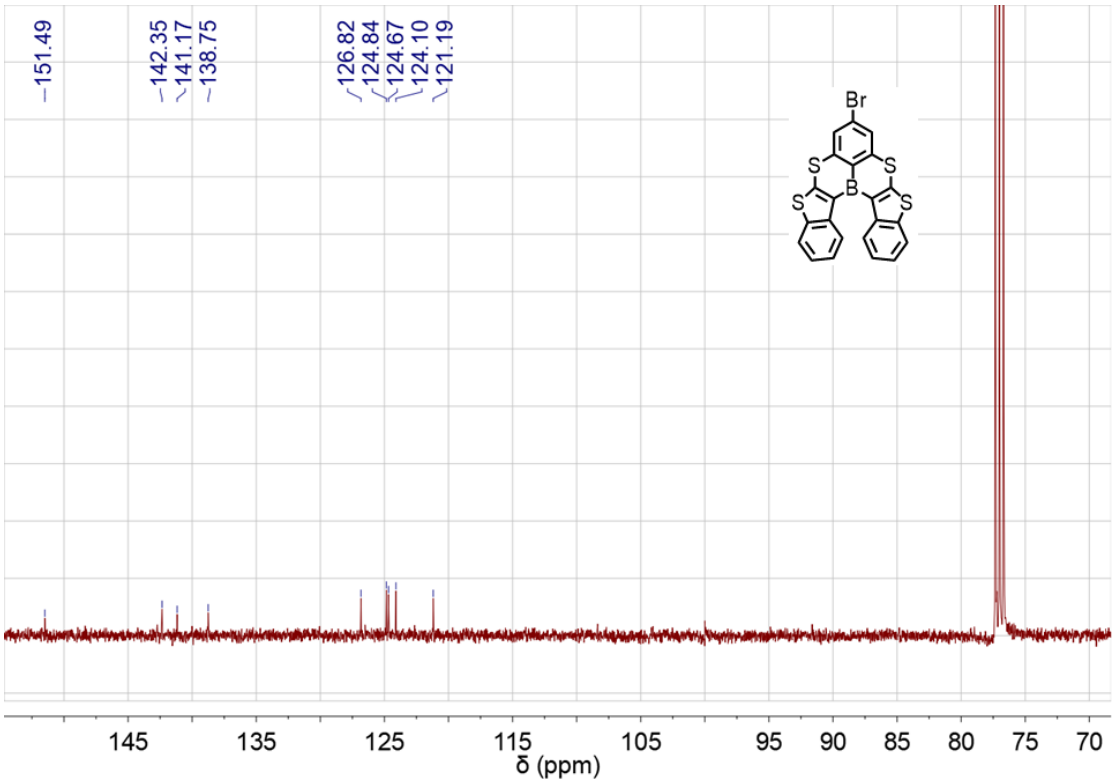


Figure S58. ^{13}C NMR spectrum of ***β*-DThBSS-Br**.

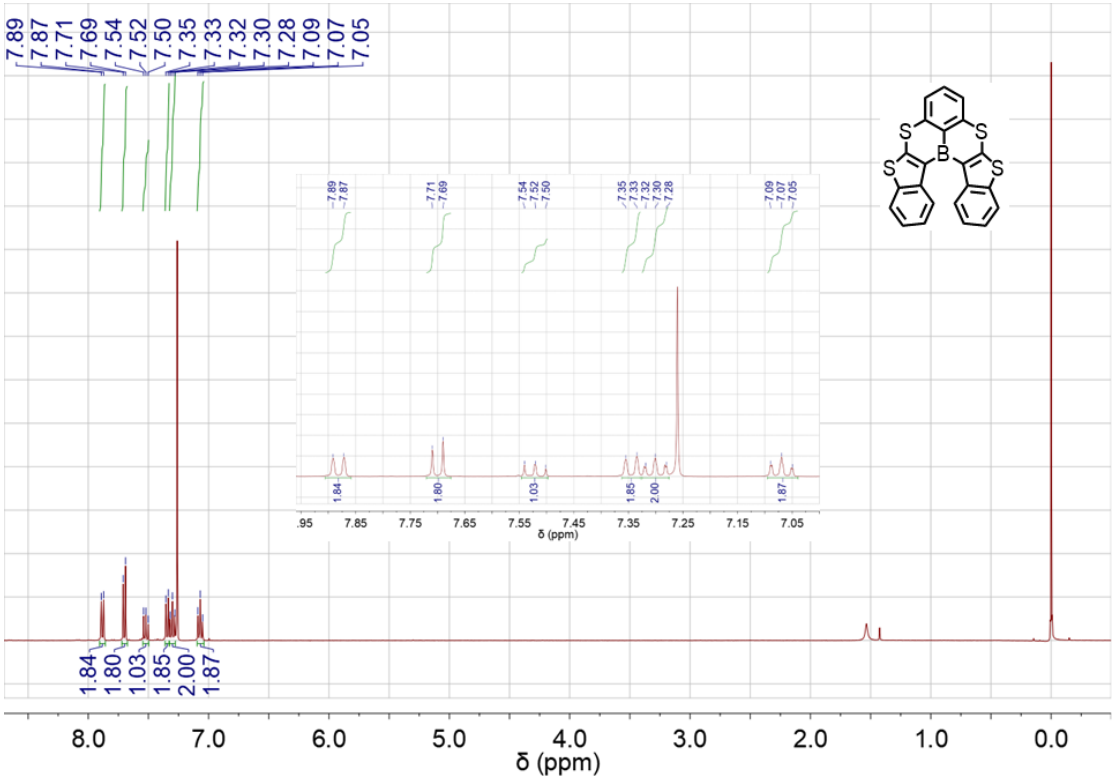


Figure S59. ^{1}H NMR spectrum of ***β*-DThBSS**.

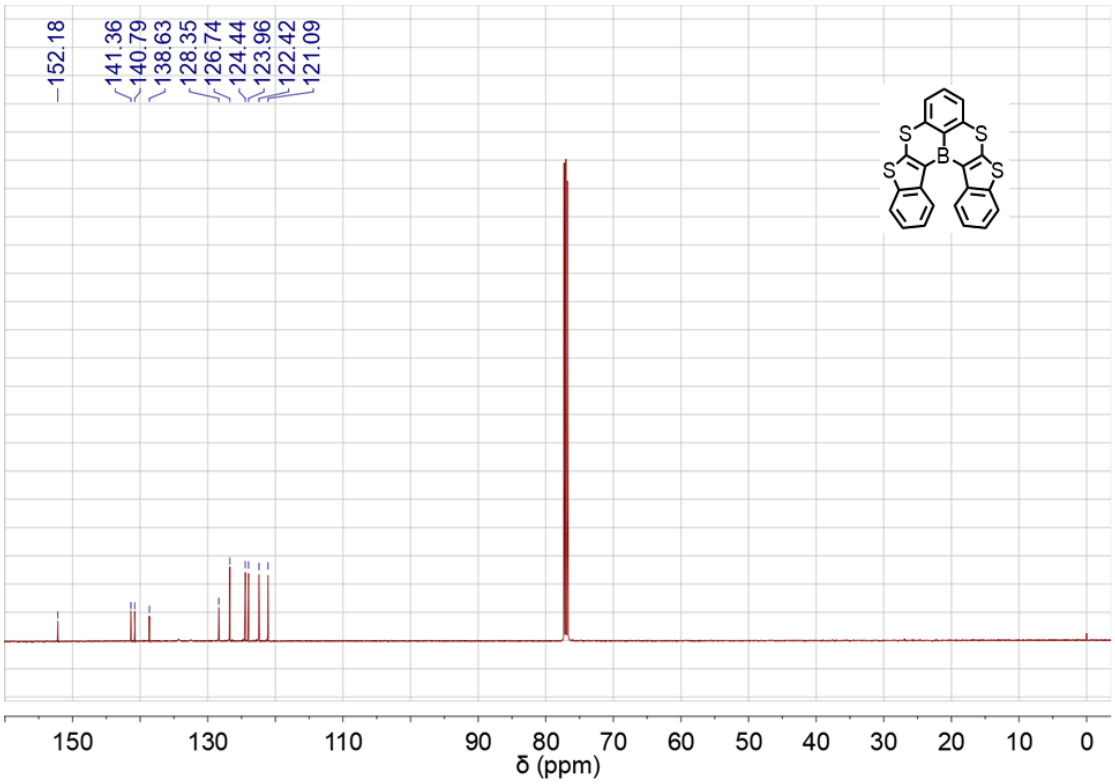


Figure S60. ^{13}C NMR spectrum of ***β*-DThBSS**.

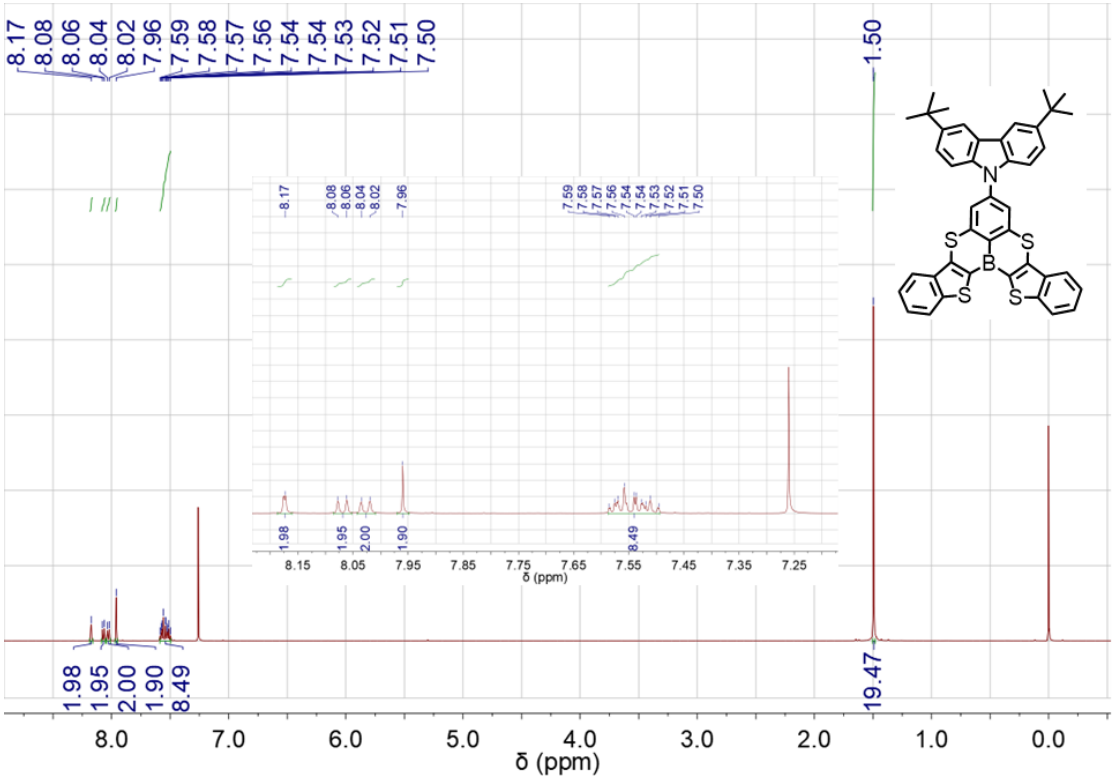


Figure S61. ^{1}H NMR spectrum of ***α*-DThBSS-Cz**.

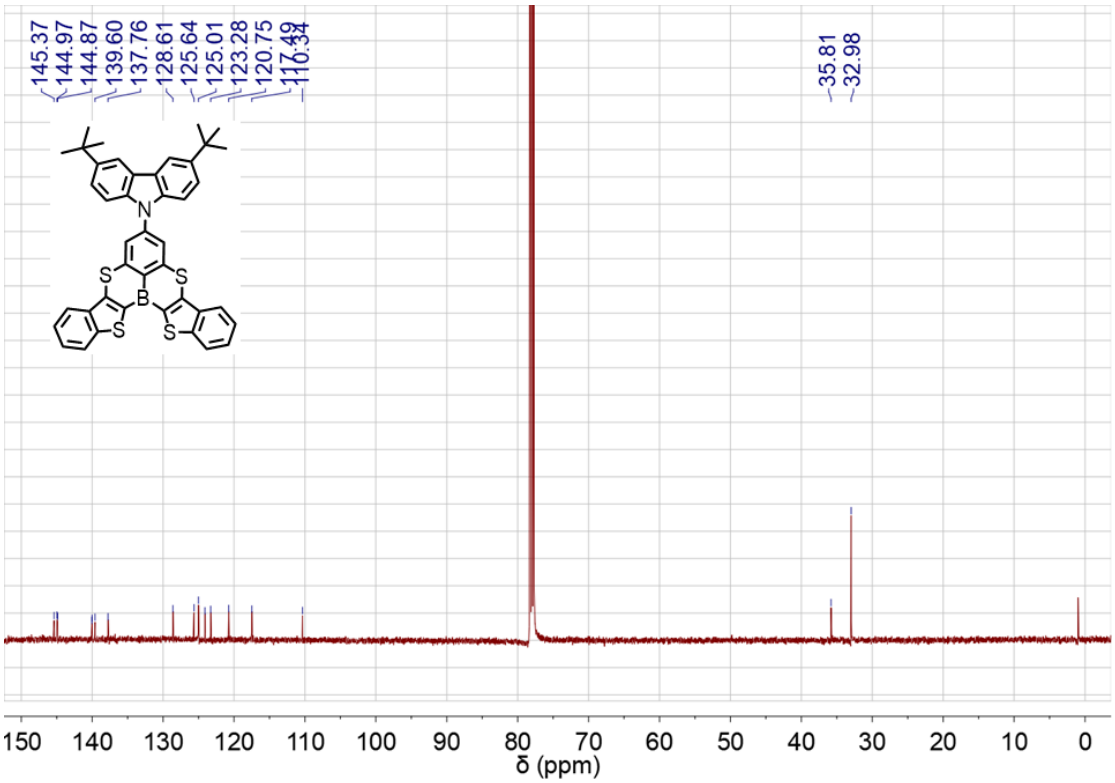


Figure S62. ^{13}C NMR spectrum of ***α*-DThBSS-Cz**.

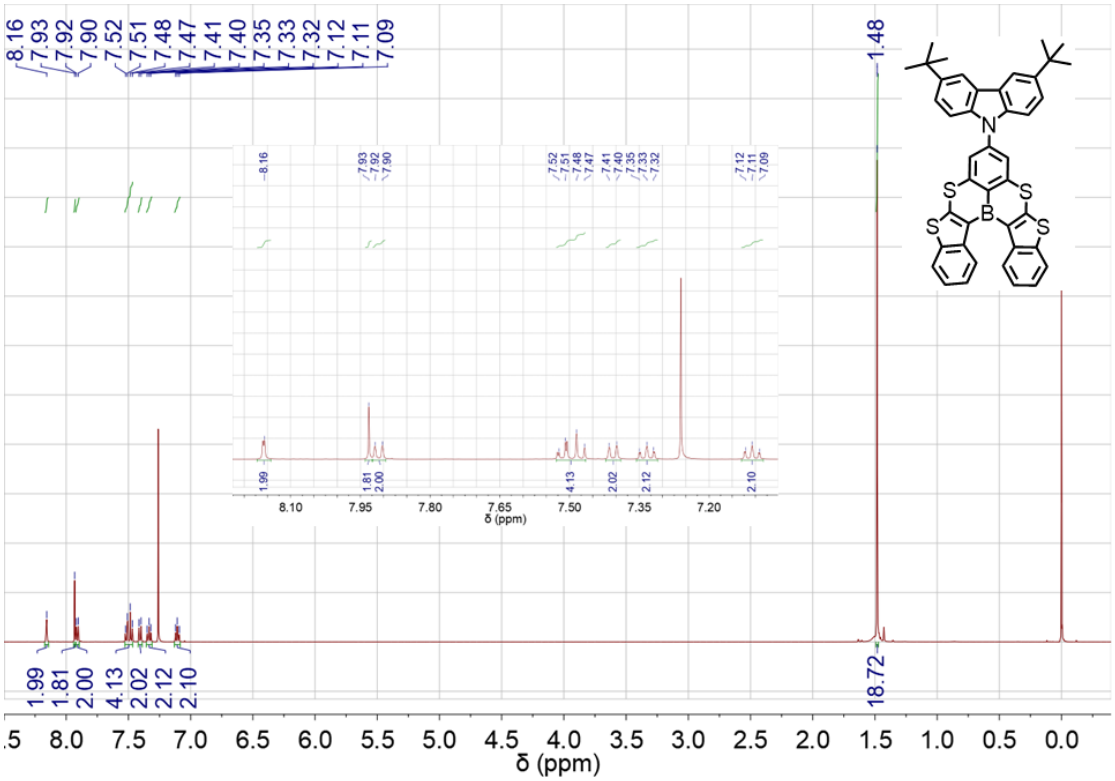


Figure S63. ^{1}H NMR spectrum of ***β*-DThBSS-Cz**.

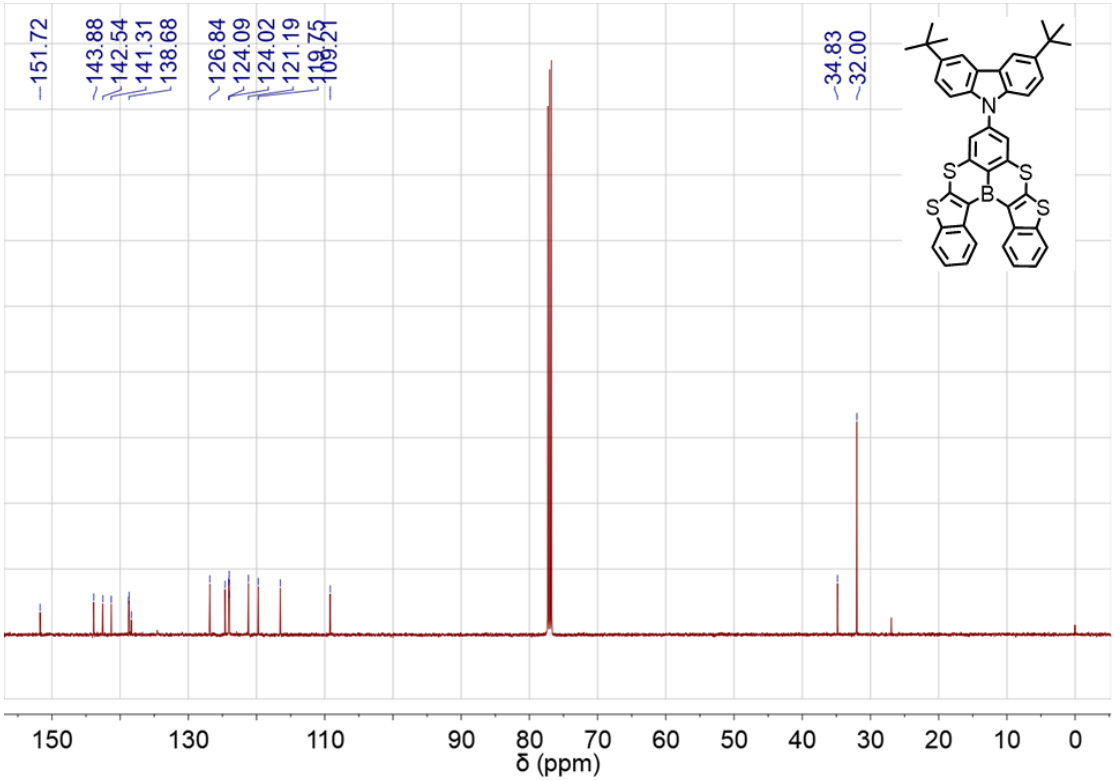


Figure S64. ^{13}C NMR spectrum of ***β*-DThBSS-Cz**.

High resolution mass spectrum

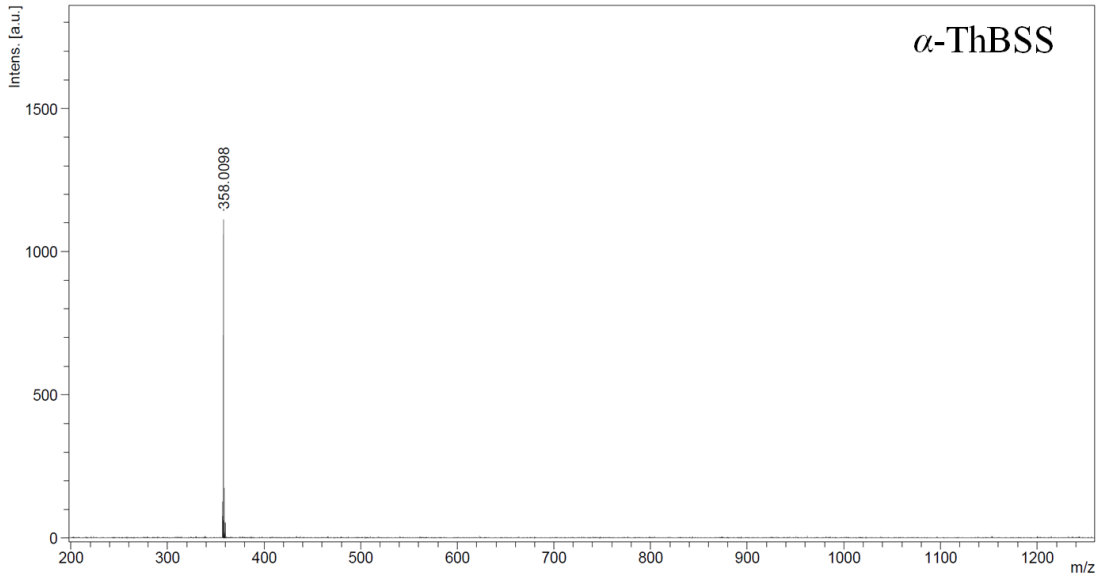


Figure S65. HRMS data of ***α*-ThBSS.**

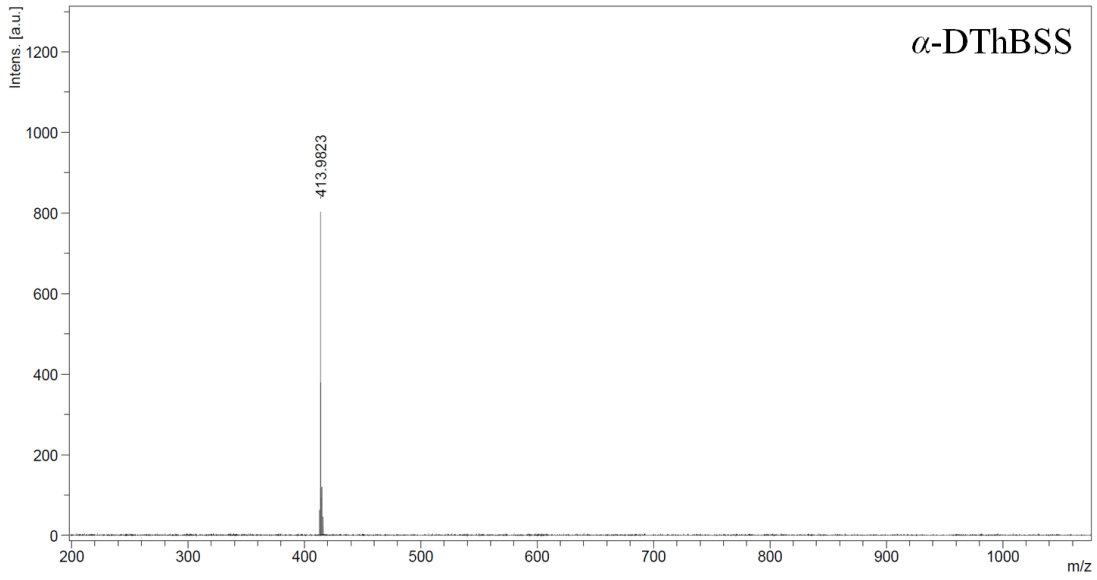


Figure S66. HRMS data of ***α*-DThBSS.**

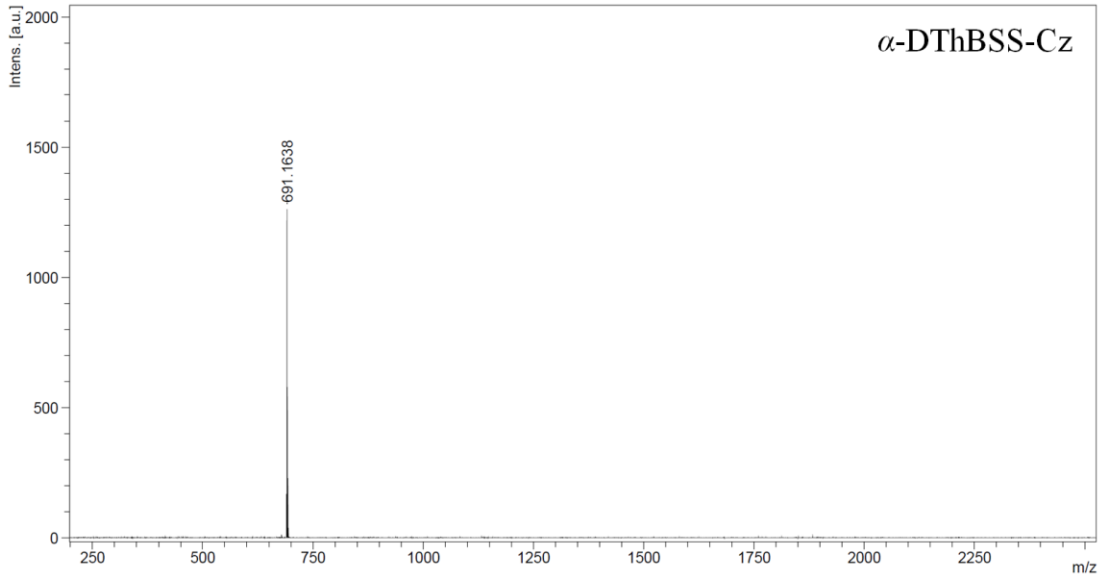


Figure S67. HRMS data of ***α*-DThBSS-Cz.**

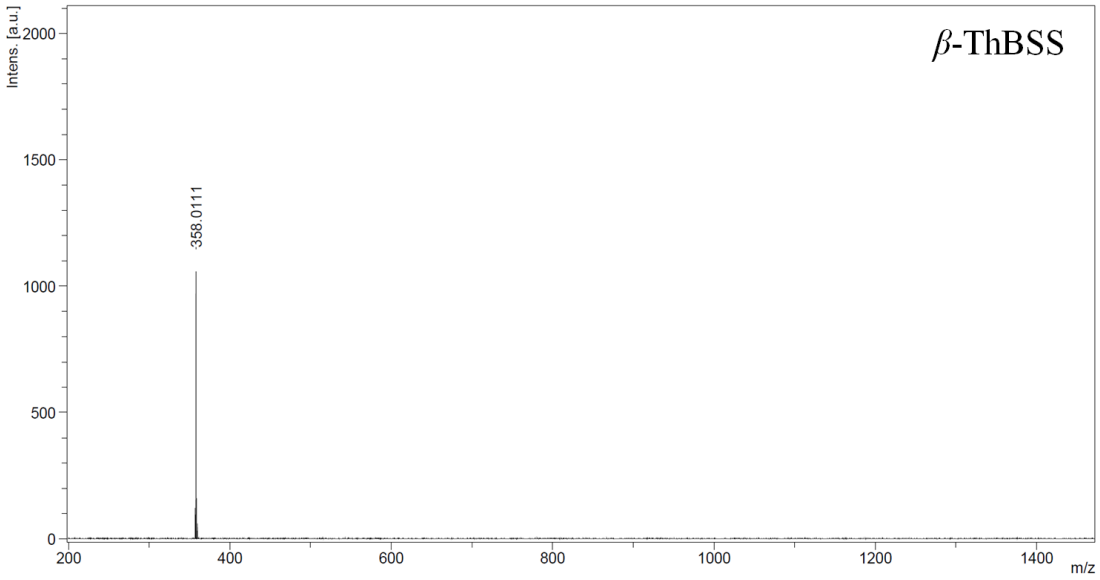


Figure S68. HRMS data of ***β*-ThBSS.**

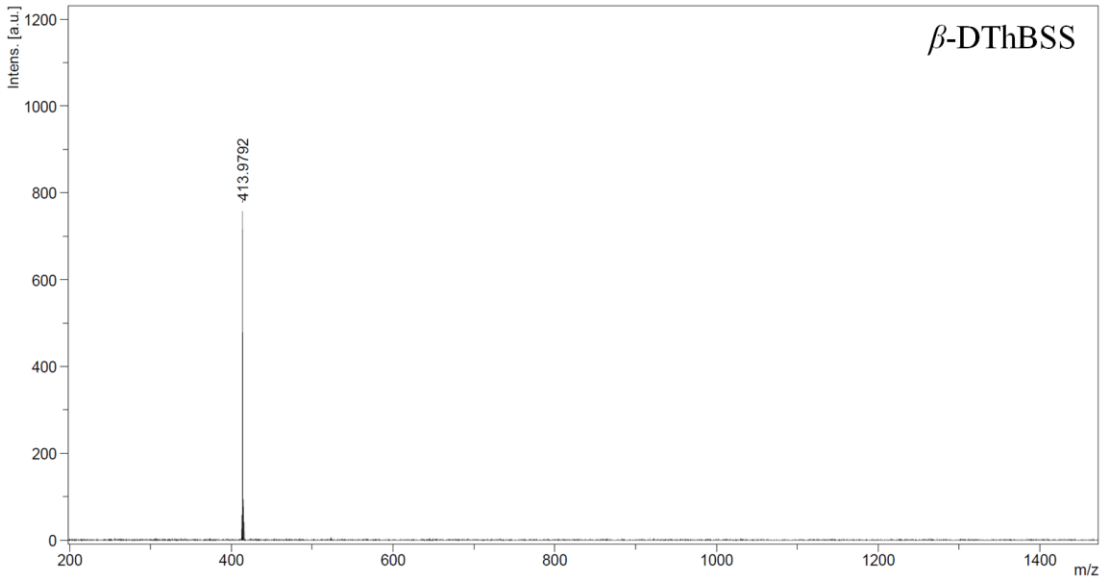


Figure S69. HRMS data of ***β*-DThBSS.**

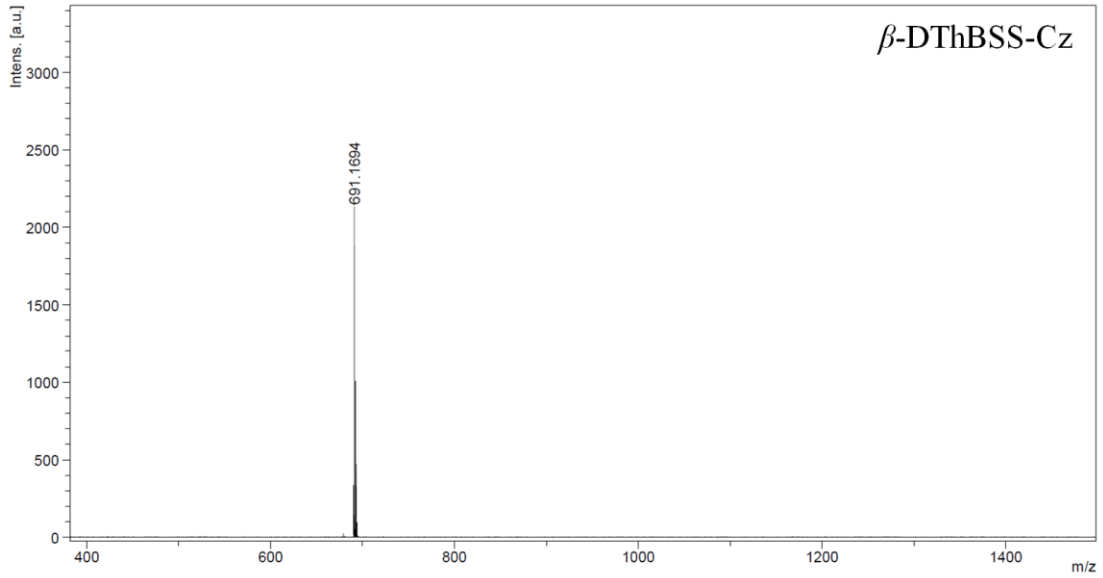


Figure S70. HRMS data of ***β*-DThBSS-Cz.**

Cartesian coordinates (Å) for optimized geometry

S_0 state of ***α*-ThBSS**

atom	X	Y	Z
C	3.077739	2.901718	-0.000115
C	2.609110	1.583172	-0.000074
C	1.222856	1.257725	0.000038
C	0.353016	2.384639	0.000106
C	0.817269	3.706018	0.000078
C	2.179946	3.959731	-0.000035
B	0.720237	-0.222454	0.000067
C	-0.824586	-0.427682	0.000027
C	-1.740767	0.605203	0.000096
S	-1.391580	2.295159	0.000227
C	-3.248405	-1.196533	-0.000099
H	4.152615	3.090713	-0.000204
H	0.101647	4.530039	0.000134
H	2.545545	4.987504	-0.000065
C	-3.130741	0.203892	0.000041
S	-1.697217	-1.962631	-0.000152
C	-4.504409	-1.819168	-0.000181
C	-4.290717	1.000399	0.000097
C	-5.634982	-1.018404	-0.000121
C	-5.530357	0.386062	0.000017
H	-4.210269	2.089308	0.000201
H	-6.435989	0.993554	0.000059
H	-6.621871	-1.483356	-0.000183
H	-4.585656	-2.906698	-0.000290
C	1.765021	-1.397756	0.000070
C	1.393037	-2.763726	0.000207
C	3.157729	-1.160227	-0.000062
C	2.306562	-3.805526	0.000186
H	0.343337	-3.040957	0.000357
C	4.096872	-2.207337	-0.000095
C	3.675741	-3.524237	0.000023
H	1.953800	-4.837303	0.000298
H	5.162933	-1.970689	-0.000206
H	4.409945	-4.331371	0.000000
S	3.906495	0.416458	-0.000179

S_1 state of ***α*-ThBSS**

atom	X	Y	Z
C	3.014933	2.922211	-0.308177
C	2.549830	1.588975	-0.238741
C	1.206470	1.256642	0.037158

C	0.357720	2.367561	0.232638
C	0.803764	3.697161	0.187143
C	2.143567	3.977186	-0.089141
B	0.720201	-0.229056	0.105258
C	-0.803327	-0.431235	0.053120
C	-1.760912	0.594199	0.180298
S	-1.358400	2.222494	0.580934
C	-3.221899	-1.192656	-0.234021
H	4.068449	3.110667	-0.524971
H	0.095720	4.509748	0.362951
H	2.497020	5.007287	-0.127687
C	-3.128408	0.194899	0.024681
S	-1.629824	-1.923116	-0.289934
C	-4.446376	-1.823380	-0.416768
C	-4.310366	0.956406	0.090676
C	-5.610154	-1.051792	-0.339987
C	-5.535707	0.324275	-0.090167
H	-4.261913	2.031275	0.275616
H	-6.453776	0.911428	-0.039658
H	-6.581612	-1.527232	-0.479116
H	-4.497036	-2.894390	-0.617633
C	1.762902	-1.375107	0.183235
C	1.438776	-2.699806	0.563675
C	3.138602	-1.157016	-0.102843
C	2.375737	-3.724470	0.599025
H	0.415131	-2.927705	0.862814
C	4.092882	-2.181967	-0.070787
C	3.712661	-3.474993	0.269017
H	2.066094	-4.728116	0.895190
H	5.135976	-1.957801	-0.305406
H	4.453035	-4.274957	0.294981
S	3.786833	0.405780	-0.559973

T_1 state of ***α*-ThBSS**

atom	X	Y	Z
C	3.001132	2.953668	0.039136
C	2.562725	1.615596	0.031773
C	1.200875	1.250479	-0.007059
C	0.323192	2.359371	-0.034392
C	0.742601	3.682298	-0.029963
C	2.100455	3.979317	0.007066
B	0.723270	-0.261182	-0.016556
C	-0.804199	-0.473927	-0.007924
C	-1.820617	0.601673	-0.024892
S	-1.440850	2.254479	-0.080413
C	-3.289673	-1.218723	0.033313

H	4.072237	3.161760	0.069239
H	0.005580	4.487185	-0.054345
H	2.438443	5.015387	0.010779
C	-3.180848	0.184851	-0.002917
S	-1.684238	-1.961662	0.038796
C	-4.501703	-1.869431	0.060142
C	-4.365256	0.947141	-0.010953
C	-5.679101	-1.092274	0.050926
C	-5.598244	0.294741	0.015819
H	-4.318137	2.037332	-0.036816
H	-6.513904	0.887777	0.009680
H	-6.650804	-1.585499	0.072305
H	-4.552464	-2.958695	0.088345
C	1.820489	-1.402594	-0.027800
C	1.538011	-2.792644	-0.088934
C	3.208725	-1.108936	0.018949
C	2.510881	-3.779015	-0.090258
H	0.517587	-3.135535	-0.146823
C	4.197227	-2.103077	0.019077
C	3.854834	-3.431218	-0.032393
H	2.216797	-4.828154	-0.139130
H	5.248513	-1.810456	0.058297
H	4.631310	-4.196684	-0.032308
S	3.897554	0.497666	0.083571

S_0 state of ***α*-DThBSS**

atom	X	Y	Z
C	-1.202590	4.069979	-0.000059
C	-1.201996	2.670528	-0.000034
C	0.000000	1.908720	-0.000025
C	1.201996	2.670528	-0.000042
C	1.202590	4.069979	-0.000069
C	0.000000	4.762824	-0.000076
B	0.000000	0.352858	-0.000001
C	1.363115	-0.369097	0.000035
C	2.579598	0.276113	0.000034
S	2.819340	1.990956	-0.000027
S	-2.819340	1.990956	-0.000004
C	-2.579598	0.276113	0.000056
C	-1.363115	-0.369097	0.000040
C	3.326228	-1.952470	0.000025
C	-3.326228	-1.952470	0.000021
H	-2.150280	4.611380	-0.000064
H	2.150280	4.611380	-0.000081
H	0.000000	5.853582	-0.000095
C	3.727140	-0.601763	-0.000002

S	1.598577	-2.110393	0.000177
C	4.273269	-2.986092	-0.000018
C	5.096831	-0.280793	-0.000075
C	5.617265	-2.649288	-0.000090
C	6.029493	-1.302411	-0.000118
H	5.414027	0.764222	-0.000101
H	7.093995	-1.065806	-0.000172
H	6.367870	-3.441013	-0.000115
H	3.955874	-4.029604	0.000022
C	-5.096831	-0.280793	-0.000078
C	-4.273269	-2.986092	-0.000045
C	-5.617265	-2.649288	-0.000128
C	-6.029493	-1.302412	-0.000144
C	-3.727140	-0.601763	0.000006
S	-1.598577	-2.110393	0.000218
H	-5.414027	0.764222	-0.000096
H	-7.093995	-1.065806	-0.000206
H	-6.367870	-3.441013	-0.000165
H	-3.955874	-4.029604	-0.000006

S_1 state of ***α*-DThBSS**

atom	X	Y	Z
C	1.197172	4.068962	0.000018
C	1.188408	2.660512	0.000013
C	0.000000	1.899413	0.000010
C	-1.188408	2.660512	0.000010
C	-1.197172	4.068962	0.000014
C	0.000000	4.773442	0.000018
B	0.000000	0.325271	0.000005
C	-1.356294	-0.376095	-0.000001
C	-2.601923	0.272245	-0.000002
S	-2.802708	1.985957	0.000004
S	2.802708	1.985957	0.000011
C	2.601923	0.272245	0.000004
C	1.356294	-0.376095	0.000003
C	-3.354002	-1.950207	-0.000012
C	3.354002	-1.950207	-0.000002
H	2.150325	4.601803	0.000020
H	-2.150325	4.601803	0.000014
H	0.000000	5.863284	0.000021
C	-3.746908	-0.591449	-0.000008
S	-1.608343	-2.098188	-0.000010
C	-4.287779	-2.980788	-0.000017
C	-5.119253	-0.277879	-0.000010
C	-5.644671	-2.649700	-0.000019
C	-6.051080	-1.308435	-0.000015

H	-5.445091	0.764320	-0.000007
H	-7.115586	-1.069989	-0.000017
H	-6.392165	-3.443666	-0.000024
H	-3.965987	-4.023153	-0.000021
C	5.119253	-0.277879	0.000005
C	4.287779	-2.980788	-0.000005
C	5.644671	-2.649700	-0.000002
C	6.051080	-1.308435	0.000003
C	3.746908	-0.591449	0.000002
S	1.608343	-2.098188	-0.000008
H	5.445091	0.764320	0.000008
H	7.115586	-1.069989	0.000005
H	6.392165	-3.443666	-0.000004
H	3.965987	-4.023153	-0.000009

T_1 state of ***α*-DThBSS**

atom	X	Y	Z
C	1.197958	4.068140	0.000017
C	1.189482	2.666996	0.000012
C	0.000000	1.902912	0.000007
C	-1.189482	2.666996	0.000008
C	-1.197958	4.068140	0.000013
C	0.000000	4.772100	0.000018
B	0.000000	0.333459	0.000002
C	-1.347723	-0.372356	-0.000002
C	-2.610388	0.280593	-0.000002
S	-2.816528	1.987821	0.000003
S	2.816528	1.987821	0.000011
C	2.610388	0.280593	0.000005
C	1.347723	-0.372356	0.000002
C	-3.347921	-1.948140	-0.000012
C	3.347921	-1.948140	-0.000002
H	2.149942	4.603180	0.000020
H	-2.149942	4.603180	0.000014
H	0.000000	5.862017	0.000022
C	-3.747531	-0.592575	-0.000008
S	-1.596922	-2.092744	-0.000006
C	-4.273998	-2.983104	-0.000018
C	-5.120902	-0.286785	-0.000012
C	-5.634734	-2.659734	-0.000021
C	-6.048686	-1.322431	-0.000018
H	-5.451020	0.754008	-0.000009
H	-7.114282	-1.089397	-0.000020
H	-6.376957	-3.458580	-0.000026
H	-3.946736	-4.023754	-0.000020
C	5.120902	-0.286785	0.000003

C	4.273998	-2.983104	-0.000006
C	5.634734	-2.659735	-0.000005
C	6.048686	-1.322431	0.000000
C	3.747532	-0.592575	0.000003
S	1.596922	-2.092744	0.000000
H	5.451020	0.754008	0.000007
H	7.114282	-1.089397	0.000000
H	6.376957	-3.458580	-0.000007
H	3.946736	-4.023754	-0.000008

S_0 state of ***α*-DThBSS-Cz**

atom	X	Y	Z
C	-0.318190	-1.136235	0.399502
C	1.078556	-1.136278	0.386832
C	1.843323	-0.000002	-0.000005
C	1.078556	1.136273	-0.386841
C	-0.318190	1.136231	-0.399510
C	-1.019356	-0.000002	-0.000004
B	3.396538	-0.000002	-0.000005
C	4.118721	1.291755	-0.435337
C	3.473291	2.440470	-0.834341
S	1.757571	2.666160	-0.915408
S	1.757571	-2.666164	0.915401
C	3.473291	-2.440473	0.834337
C	4.118721	-1.291758	0.435332
C	5.700786	3.151498	-1.063353
C	5.700786	-3.151499	1.063355
H	-0.869044	-2.016031	0.736487
H	-0.869044	2.016027	-0.736492
C	4.350208	3.527607	-1.204145
S	5.859292	1.519079	-0.499400
C	6.735044	4.049048	-1.363318
C	4.030013	4.821508	-1.653953
C	6.399018	5.318601	-1.804507
C	5.052370	5.705075	-1.950543
H	2.985552	5.119781	-1.766289
H	4.815850	6.710698	-2.299650
H	7.191088	6.030307	-2.041589
H	7.778241	3.751666	-1.250645
C	4.030013	-4.821509	1.653954
C	6.735044	-4.049048	1.363324
C	6.399018	-5.318601	1.804514
C	5.052370	-5.705075	1.950548
C	4.350208	-3.527609	1.204145
S	5.859292	-1.519080	0.499400
H	2.985552	-5.119783	1.766287

H	4.815850	-6.710698	2.299655
H	7.191088	-6.030306	2.041599
H	7.778241	-3.751665	1.250653
N	-2.425243	-0.000001	-0.000001
C	-3.242255	-0.988805	-0.553011
C	-3.242252	0.988804	0.553010
C	-2.905939	-2.146112	-1.254509
C	-4.594763	-0.633603	-0.355308
C	-2.905932	2.146113	1.254502
C	-4.594761	0.633602	0.355316
C	-3.942003	-2.949429	-1.725718
H	-1.867181	-2.416897	-1.443808
C	-5.609795	-1.458391	-0.839146
C	-3.941992	2.949432	1.725713
H	-1.867172	2.416899	1.443793
C	-5.609790	1.458390	0.839159
C	-5.300481	-2.635280	-1.527600
H	-3.671372	-3.851731	-2.272662
H	-6.651405	-1.171000	-0.677741
C	-5.300472	2.635281	1.527607
H	-3.671358	3.851737	2.272652
H	-6.651401	1.171000	0.677759
C	-6.436511	-3.524535	-2.048228
C	-6.436500	3.524540	2.048233
C	-7.319417	-3.966284	-0.869932
C	-7.285274	-2.728609	-3.052751
C	-5.909396	-4.778700	-2.750493
C	-7.285224	2.728645	3.052812
C	-7.319443	3.966229	0.869943
C	-5.909382	4.778742	2.750433
H	-7.769208	-3.104708	-0.356079
H	-8.137720	-4.610562	-1.226767
H	-6.730085	-4.530795	-0.132436
H	-7.722103	-1.831052	-2.591560
H	-6.673644	-2.405770	-3.908177
H	-8.111237	-3.350496	-3.431321
H	-5.298064	-4.524480	-3.629004
H	-5.302702	-5.397573	-2.072879
H	-6.755899	-5.390068	-3.095968
H	-8.111180	3.350538	3.431385
H	-7.722061	1.831067	2.591668
H	-6.673564	2.405842	3.908230
H	-8.137748	4.610507	1.226774
H	-6.730140	4.530721	0.132410
H	-7.769232	3.104624	0.356135
H	-5.298007	4.524566	3.628927
H	-5.302730	5.397604	2.072772

H	-6.755884	5.390104	3.095921

S_1 state of ***α*-DThBSS-Cz**

atom	X	Y	Z
C	-0.314937	-1.128067	0.407955
C	1.089526	-1.121825	0.388458
C	1.853656	0.000000	0.000000
C	1.089525	1.121825	-0.388458
C	-0.314938	1.128066	-0.407955
C	-1.026664	0.000000	0.000000
B	3.423870	0.000000	0.000000
C	4.126294	1.284522	-0.437262
C	3.478428	2.461190	-0.846398
S	1.765053	2.650135	-0.919732
S	1.765053	-2.650136	0.919731
C	3.478428	-2.461190	0.846398
C	4.126295	-1.284522	0.437262
C	5.701361	3.176349	-1.073537
C	5.701362	-3.176349	1.073537
H	-0.859583	-2.010556	0.750513
H	-0.859583	2.010556	-0.750513
C	4.343314	3.545681	-1.213056
S	5.847341	1.526226	-0.504555
C	6.733473	4.060468	-1.367826
C	4.031790	4.842137	-1.663154
C	6.404386	5.342777	-1.812666
C	5.063983	5.724813	-1.957780
H	2.990412	5.149106	-1.779236
H	4.826322	6.730747	-2.306359
H	7.199523	6.051059	-2.047501
H	7.775229	3.758223	-1.253034
C	4.031791	-4.842137	1.663154
C	6.733473	-4.060468	1.367826
C	6.404387	-5.342777	1.812666
C	5.063984	-5.724813	1.957780
C	4.343315	-3.545681	1.213056
S	5.847341	-1.526226	0.504554
H	2.990413	-5.149106	1.779236
H	4.826323	-6.730747	2.306359
H	7.199523	-6.051059	2.047501
H	7.775230	-3.758222	1.253034
N	-2.431669	0.000000	0.000000
C	-3.248249	-0.983537	-0.562534
C	-3.248249	0.983536	0.562534
C	-2.909956	-2.136384	-1.269765
C	-4.600725	-0.630738	-0.360691

C	-2.909956	2.136384	1.269765
C	-4.600725	0.630738	0.360691
C	-3.945140	-2.938217	-1.745636
H	-1.870793	-2.405771	-1.460732
C	-5.614607	-1.453818	-0.849778
C	-3.945139	2.938217	1.745636
H	-1.870793	2.405770	1.460733
C	-5.614607	1.453818	0.849779
C	-5.303821	-2.626119	-1.545711
H	-3.673886	-3.837277	-2.297541
H	-6.656639	-1.169348	-0.686215
C	-5.303821	2.626119	1.545711
H	-3.673885	3.837276	2.297541
H	-6.656639	1.169348	0.686215
C	-6.438835	-3.512973	-2.072572
C	-6.438835	3.512973	2.072572
C	-7.324305	-3.960241	-0.898302
C	-7.285200	-2.711971	-3.075138
C	-5.910262	-4.763923	-2.779477
C	-7.285199	2.711972	3.075139
C	-7.324305	3.960240	0.898302
C	-5.910262	4.763924	2.779475
H	-7.776127	-3.101408	-0.381658
H	-8.141321	-4.603195	-1.260293
H	-6.736718	-4.528067	-0.161956
H	-7.723642	-1.817002	-2.610409
H	-6.671545	-2.384551	-3.927351
H	-8.109886	-3.332184	-3.459052
H	-5.298157	-4.506089	-3.656386
H	-5.304280	-5.385529	-2.103704
H	-6.756146	-5.374098	-3.128414
H	-8.109885	3.332186	3.459053
H	-7.723641	1.817002	2.610412
H	-6.671543	2.384553	3.927352
H	-8.141321	4.603194	1.260293
H	-6.736719	4.528065	0.161955
H	-7.776127	3.101406	0.381659
H	-5.298156	4.506091	3.656384
H	-5.304281	5.385529	2.103701
H	-6.756145	5.374099	3.128412

T_1 state of ***α*-DThBSS-Cz**

atom	X	Y	Z
C	-0.314723	-1.128064	0.410352
C	1.083551	-1.121664	0.392552
C	1.849305	0.000000	-0.000001

C	1.083551	1.121663	-0.392553
C	-0.314723	1.128064	-0.410353
C	-1.024569	0.000000	-0.000001
B	3.417059	0.000000	-0.000001
C	4.123142	1.274175	-0.438877
C	3.469557	2.465627	-0.857992
S	1.762137	2.658496	-0.933982
S	1.762137	-2.658496	0.933981
C	3.469557	-2.465627	0.857992
C	4.123142	-1.274176	0.438876
C	5.698038	3.167591	-1.082923
C	5.698038	-3.167591	1.082924
H	-0.861959	-2.009266	0.752084
H	-0.861959	2.009266	-0.752085
C	4.342691	3.541731	-1.225811
S	5.842415	1.514504	-0.506414
C	6.733698	4.044217	-1.377887
C	4.037968	4.837622	-1.680712
C	6.411336	5.328394	-1.828468
C	5.074581	5.716088	-1.977163
H	2.997806	5.147644	-1.799123
H	4.841692	6.721662	-2.329675
H	7.210780	6.031395	-2.064365
H	7.773997	3.738005	-1.260444
C	4.037968	-4.837622	1.680712
C	6.733698	-4.044217	1.377888
C	6.411336	-5.328394	1.828469
C	5.074581	-5.716088	1.977164
C	4.342691	-3.541732	1.225811
S	5.842415	-1.514504	0.506414
H	2.997806	-5.147645	1.799123
H	4.841692	-6.721662	2.329677
H	7.210780	-6.031394	2.064366
H	7.773997	-3.738004	1.260445
N	-2.431386	0.000000	0.000000
C	-3.247452	-0.978593	-0.569507
C	-3.247452	0.978593	0.569507
C	-2.908738	-2.127051	-1.284048
C	-4.600433	-0.627883	-0.365398
C	-2.908737	2.127051	1.284047
C	-4.600433	0.627883	0.365399
C	-3.943463	-2.925879	-1.765496
H	-1.869128	-2.394501	-1.475046
C	-5.613914	-1.448003	-0.860596
C	-3.943462	2.925879	1.765496
H	-1.869127	2.394500	1.475045
C	-5.613913	1.448003	0.860597

C	-5.302509	-2.615403	-1.564278
H	-3.671785	-3.821487	-2.322847
H	-6.656128	-1.164952	-0.695517
C	-5.302507	2.615403	1.564279
H	-3.671783	3.821487	2.322847
H	-6.656128	1.164953	0.695518
C	-6.436951	-3.498560	-2.098624
C	-6.436949	3.498560	2.098625
C	-7.326552	-3.951267	-0.929619
C	-7.279683	-2.691673	-3.099574
C	-5.907733	-4.746541	-2.810333
C	-7.279681	2.691674	3.099576
C	-7.326551	3.951267	0.929620
C	-5.907731	4.746542	2.810332
H	-7.779280	-3.094826	-0.409843
H	-8.142992	-4.591581	-1.297664
H	-6.741737	-4.523468	-0.194442
H	-7.719063	-1.799092	-2.631134
H	-6.662851	-2.359612	-3.947681
H	-8.103384	-3.309226	-3.489944
H	-5.293789	-4.485114	-3.684872
H	-5.303234	-5.371357	-2.136185
H	-6.753292	-5.354711	-3.163628
H	-8.103381	3.309227	3.489946
H	-7.719061	1.799093	2.631136
H	-6.662848	2.359613	3.947682
H	-8.142992	4.591581	1.297665
H	-6.741737	4.523468	0.194442
H	-7.779280	3.094826	0.409844
H	-5.293786	4.485116	3.684872
H	-5.303232	5.371358	2.136184
H	-6.753290	5.354712	3.163628

S_0 state of ***β*-ThBSS**

atom	X	Y	Z
C	3.891413	-1.545522	-0.612784
C	2.876394	-0.596664	-0.454081
C	1.564488	-0.966945	-0.067282
C	1.344607	-2.344007	0.168052
C	2.359173	-3.296522	0.030790
C	3.626916	-2.888714	-0.366866
B	0.439146	0.092972	0.076697
C	-1.025247	-0.400046	0.030814
C	-1.308989	-1.710221	0.357746
S	-0.200986	-2.999254	0.702798
C	-2.262476	0.311313	-0.287167

C	-3.414592	-0.480416	-0.098420
H	4.891778	-1.226201	-0.909436
H	2.149908	-4.351077	0.217642
H	4.420906	-3.627660	-0.484155
S	-3.007638	-2.101172	0.406625
C	-4.704946	-0.003444	-0.344805
C	-2.438235	1.609550	-0.802793
C	-3.714513	2.087885	-1.059422
C	-4.846150	1.292727	-0.819658
H	-1.569095	2.232998	-1.012528
H	-3.839163	3.094413	-1.461018
H	-5.842345	1.687548	-1.023484
H	-5.575064	-0.640360	-0.180238
C	0.858311	1.573833	0.329338
C	2.128092	2.055619	-0.044050
C	0.016226	2.465978	1.026274
C	2.497897	3.390198	0.186334
C	0.382649	3.778676	1.284925
H	-0.953851	2.104340	1.373766
C	1.624032	4.246536	0.840022
H	3.484298	3.740137	-0.124481
H	-0.291391	4.440409	1.830042
H	1.921224	5.279808	1.027237
S	3.350922	1.058043	-0.823088

S_1 state of ***β*-ThBSS**

atom	X	Y	Z
C	3.785976	-1.719973	-0.703032
C	2.813239	-0.722758	-0.505770
C	1.492927	-1.002213	-0.082111
C	1.238670	-2.365248	0.178015
C	2.195339	-3.375811	-0.001972
C	3.476103	-3.055018	-0.457064
B	0.432076	0.115795	0.090376
C	-1.057207	-0.351697	0.104616
C	-1.402534	-1.658912	0.438085
S	-0.302293	-2.931328	0.832724
C	-2.254976	0.371231	-0.268519
C	-3.444400	-0.381174	-0.113085
H	4.783941	-1.436576	-1.043698
H	1.934775	-4.412925	0.220633
H	4.222549	-3.834817	-0.603969
S	-3.113668	-2.014583	0.410914
C	-4.699913	0.145693	-0.411729
C	-2.354886	1.673742	-0.801856
C	-3.600339	2.199242	-1.108616

C	-4.767368	1.446002	-0.902806
H	-1.446059	2.248983	-0.980607
H	-3.675955	3.205873	-1.521470
H	-5.739922	1.877142	-1.144893
H	-5.604089	-0.449152	-0.276577
C	0.918213	1.556786	0.363002
C	2.229841	1.973935	-0.009234
C	0.151905	2.531184	1.050002
C	2.711198	3.264986	0.223771
C	0.618729	3.819898	1.281009
H	-0.841258	2.252351	1.408595
C	1.898806	4.201808	0.860851
H	3.723954	3.531521	-0.085956
H	-0.017814	4.538547	1.800466
H	2.267542	5.211736	1.041486
S	3.324463	0.907043	-0.872841

T_1 state of ***β*-ThBSS**

atom	X	Y	Z
C	3.636104	-1.859875	-0.816052
C	2.734123	-0.813322	-0.547489
C	1.456629	-1.055122	-0.004807
C	1.155998	-2.405935	0.268595
C	2.029197	-3.454007	0.010354
C	3.284569	-3.171582	-0.543426
B	0.431559	0.106869	0.211824
C	-1.051769	-0.285948	0.174085
C	-1.458416	-1.672691	0.429576
S	-0.394354	-2.848090	1.054468
C	-2.223781	0.467634	-0.197416
C	-3.423001	-0.296714	-0.193918
H	4.619509	-1.628654	-1.230016
H	1.743320	-4.480868	0.245027
H	3.989026	-3.980106	-0.740959
S	-3.170723	-1.985779	0.240858
C	-4.642213	0.252563	-0.563982
C	-2.289274	1.805138	-0.643420
C	-3.508328	2.358516	-1.012415
C	-4.678544	1.592625	-0.961618
H	-1.373886	2.392428	-0.708980
H	-3.551825	3.393299	-1.352913
H	-5.631550	2.038259	-1.251034
H	-5.551358	-0.349721	-0.553803
C	0.997677	1.543049	0.417763
C	2.275780	1.899340	-0.068607
C	0.315932	2.528469	1.167201

C	2.801148	3.186165	0.117820
C	0.829113	3.802619	1.362099
H	-0.649528	2.268452	1.608846
C	2.074918	4.138827	0.819524
H	3.790539	3.428022	-0.275913
H	0.268256	4.536453	1.942751
H	2.490719	5.137015	0.965059
S	3.302816	0.793406	-0.982226

S_0 state of ***β*-DThBSS**

atom	X	Y	Z
C	4.353194	-1.119211	0.432231
C	2.955279	-1.119408	0.420936
C	2.202981	0.003316	0.000252
C	2.951825	1.128243	-0.420701
C	4.349736	1.132138	-0.432443
C	5.043025	0.007479	-0.000218
B	0.643902	0.000990	0.000531
C	-0.061857	1.376457	0.041237
C	0.585748	2.494527	-0.439257
S	2.217105	2.616904	-1.018749
S	2.225090	-2.610363	1.018798
C	0.593398	-2.492795	0.439344
C	-0.057672	-1.376579	-0.040754
C	-1.382934	1.742615	0.540687
C	-1.694144	3.101721	0.327822
C	-1.684554	-3.106817	-0.328127
C	-1.377562	-1.746666	-0.540460
H	4.896925	-2.007156	0.759355
H	4.890756	2.021672	-0.759741
H	6.133768	0.009092	-0.000392
S	-0.355527	-3.955518	0.424166
S	-0.367650	3.954320	-0.424507
C	-2.910200	3.663447	0.725958
C	-2.320322	0.949147	1.226187
C	-2.317393	-0.955848	-1.225678
C	-2.898829	-3.672175	-0.726537
C	-3.526375	1.500460	1.631903
C	-3.826477	2.848163	1.375943
C	-3.521709	-1.510756	-1.631637
C	-3.817623	-2.859494	-1.376234
H	-2.093686	-0.096407	1.436905
H	-4.249426	0.878998	2.161457
H	-4.780681	3.263288	1.703257
H	-3.125033	4.717197	0.543192
H	-2.094047	0.090517	-1.435926

H	-4.246682	-0.891322	-2.160938
H	-4.770529	-3.277448	-1.703725
H	-3.110381	-4.726652	-0.544141

S_1 state of ***β*-DThBSS**

atom	X	Y	Z
C	-4.288926	1.077324	0.513539
C	-2.887405	1.066675	0.508094
C	-2.120286	-0.004262	0.000179
C	-2.882949	-1.078268	-0.507971
C	-4.284408	-1.094748	-0.513555
C	-4.994756	-0.010197	-0.000004
B	-0.560472	-0.001092	0.000289
C	0.122521	-1.392248	-0.021678
C	-0.539969	-2.506154	-0.541184
S	-2.109719	-2.479437	-1.262603
S	-2.120079	2.471352	1.262298
C	-0.550367	2.504245	0.541021
C	0.116745	1.392881	0.021978
C	1.390022	-1.817292	0.540820
C	1.653386	-3.196221	0.367243
C	1.640206	3.202972	-0.367511
C	1.382489	1.822923	-0.540655
H	-4.821269	1.937348	0.925205
H	-4.813117	-1.956917	-0.925413
H	-6.084209	-0.012428	-0.000052
S	0.314201	4.018896	0.428356
S	0.330725	-4.017287	-0.429010
C	2.824856	-3.791140	0.837507
C	2.328849	-1.040878	1.247887
C	2.324443	1.050115	-1.247512
C	2.809308	3.802461	-0.837872
C	3.493259	-1.626029	1.719126
C	3.744367	-2.992420	1.508253
C	3.486517	1.639811	-1.718851
C	3.732083	3.007254	-1.508308
H	2.125076	0.017034	1.420776
H	4.219182	-1.023013	2.265540
H	4.666452	-3.437098	1.885615
H	3.009690	-4.855989	0.690199
H	2.124881	-0.008637	-1.420151
H	4.214929	1.039597	-2.265035
H	4.652387	3.455552	-1.885723
H	2.989881	4.868086	-0.690872

T_1 state of ***β*-DThBSS**

atom	X	Y	Z
C	-4.300053	1.090463	0.489263
C	-2.901570	1.081050	0.483808
C	-2.137879	-0.003201	0.000312
C	-2.898174	-1.089659	-0.483568
C	-4.296672	-1.103156	-0.489551
C	-5.003069	-0.007417	-0.000267
B	-0.570344	-0.000843	0.000484
C	0.108942	-1.379135	-0.015627
C	-0.567682	-2.522698	-0.505794
S	-2.143515	-2.527258	-1.198356
S	-2.151296	2.521037	1.198619
C	-0.575692	2.521464	0.505844
C	0.104604	1.379510	0.016175
C	1.390249	-1.794122	0.530543
C	1.656938	-3.173119	0.367380
C	1.646907	3.178185	-0.367723
C	1.384549	1.798231	-0.530130
H	-4.834547	1.959784	0.877720
H	-4.828437	-1.974027	-0.878280
H	-6.092855	-0.009022	-0.000436
S	0.317665	4.022373	0.402332
S	0.330271	-4.020855	-0.403129
C	2.835163	-3.758566	0.829717
C	2.329068	-1.012257	1.229764
C	2.325728	1.018884	-1.229016
C	2.823292	3.766966	-0.830420
C	3.503129	-1.587445	1.692156
C	3.760098	-2.951445	1.485090
C	3.498009	1.597430	-1.691749
C	3.750728	2.962308	-1.485366
H	2.119820	0.043237	1.407558
H	4.228367	-0.977008	2.231047
H	4.687555	-3.390172	1.856246
H	3.021355	-4.824116	0.689902
H	2.119653	-0.037317	-1.406286
H	4.225137	0.988972	-2.230323
H	4.676823	3.403711	-1.856743
H	3.006261	4.833154	-0.691203

S_0 state of ***β*-DThBSS-Cz**

atom	X	Y	Z
C	0.481828	1.084193	0.532346
C	-0.913608	1.076764	0.525626
C	-1.666650	0.000003	-0.000006
C	-0.913610	-1.076758	-0.525638

C	0.481826	-1.084191	-0.532358
C	1.181764	0.000000	-0.000007
B	-3.223137	0.000006	-0.000005
C	-3.925460	-0.916325	-1.029257
C	-3.274540	-2.029811	-1.514697
S	-1.644392	-2.536660	-1.194505
S	-1.644385	2.536665	1.194498
C	-3.274533	2.029816	1.514695
C	-3.925455	0.916332	1.029253
C	-5.242474	-0.800825	-1.645989
C	-5.547236	-1.883088	-2.497536
C	-5.547224	1.883090	2.497544
C	-5.242466	0.800830	1.645990
H	1.033766	1.910918	0.982661
H	1.033761	-1.910917	-0.982675
S	-4.218720	3.012705	2.601416
S	-4.218731	-3.012703	-2.601411
C	-6.759034	-1.974733	-3.187669
C	-6.180737	0.241507	-1.538576
C	-6.180730	-0.241501	1.538577
C	-6.759019	1.974733	3.187683
C	-7.382765	0.162148	-2.225593
C	-7.676844	-0.944016	-3.039109
C	-7.382755	-0.162145	2.225601
C	-7.676830	0.944016	3.039122
H	-5.956389	1.109001	-0.917478
H	-8.107398	0.972190	-2.135191
H	-8.627515	-0.989254	-3.572053
H	-6.970172	-2.825854	-3.836344
H	-5.956385	-1.108993	0.917474
H	-8.107389	-0.972187	2.135198
H	-8.627499	0.989252	3.572071
H	-6.970155	2.825851	3.836362
C	3.404043	-1.046933	0.432681
C	3.404046	1.046930	-0.432690
C	3.066145	-2.277444	0.993740
C	4.756625	-0.671623	0.277602
C	3.066151	2.277440	-0.993753
C	4.756627	0.671619	-0.277604
C	4.101017	-3.132577	1.366245
H	2.027170	-2.567022	1.150924
C	5.770564	-1.550431	0.658191
C	4.101026	3.132573	-1.366252
H	2.027178	2.567018	-1.150943
C	5.770568	1.550426	-0.658187
C	5.459595	-2.799831	1.203389
H	3.828751	-4.092407	1.803399

H	6.812583	-1.248547	0.529167
C	5.459603	2.799826	-1.203388
H	3.828763	4.092403	-1.803408
H	6.812587	1.248542	-0.529157
N	2.587059	-0.000002	-0.000008
C	6.594528	-3.751892	1.599850
C	6.594539	3.751886	-1.599843
C	7.500216	3.066741	-2.635419
H	8.322901	3.737732	-2.927244
H	7.944746	2.143775	-2.236481
H	6.929195	2.804332	-3.538356
C	7.419544	4.101451	-0.350357
H	8.243485	4.782919	-0.613138
H	6.789751	4.593223	0.405628
H	7.856894	3.202363	0.107479
C	6.067044	5.053269	-2.210320
H	5.479839	4.862502	-3.120914
H	5.436545	5.608557	-1.500310
H	6.912544	5.700753	-2.485334
C	7.419538	-4.101458	0.350366
H	7.856891	-3.202370	-0.107468
H	8.243476	-4.782927	0.613150
H	6.789747	-4.593228	-0.405621
C	7.500202	-3.066749	2.635429
H	7.944736	-2.143784	2.236493
H	6.929178	-2.804339	3.538364
H	8.322885	-3.737742	2.927257
C	6.067028	-5.053274	2.210324
H	5.479819	-4.862507	3.120915
H	5.436533	-5.608561	1.500311
H	6.912527	-5.700759	2.485342

S_1 state of ***β*-DThBSS-Cz**

atom	X	Y	Z
C	-0.450490	-1.066938	0.557939
C	0.947508	-1.060629	0.530096
C	1.716847	0.000000	0.000000
C	0.947508	1.060629	-0.530097
C	-0.450490	1.066937	-0.557939
C	-1.165150	0.000000	0.000000
B	3.272084	0.000000	0.000000
C	3.954297	0.889563	-1.073233
C	3.287020	1.989341	-1.617071
S	1.712615	2.529637	-1.154598
S	1.712615	-2.529637	1.154598
C	3.287020	-1.989341	1.617071

C	3.954297	-0.889563	1.073233
C	5.221761	0.721396	-1.757765
C	5.479600	1.722603	-2.724031
C	5.479599	-1.722603	2.724031
C	5.221761	-0.721396	1.757765
H	-0.992943	-1.898664	1.012394
H	-0.992943	1.898664	-1.012395
S	4.153814	-2.852417	2.863177
S	4.153815	2.852417	-2.863177
C	6.649042	1.735788	-3.484569
C	6.166660	-0.311891	-1.599297
C	6.166660	0.311891	1.599298
C	6.649041	-1.735788	3.484570
C	7.329313	-0.306200	-2.353671
C	7.573545	0.716164	-3.286363
C	7.329313	0.306199	2.353672
C	7.573544	-0.716164	3.286363
H	5.970112	-1.110946	-0.882888
H	8.060017	-1.105757	-2.227525
H	8.493723	0.706448	-3.872417
H	6.827319	2.519151	-4.222257
H	5.970112	1.110946	0.882888
H	8.060017	1.105757	2.227526
H	8.493722	-0.706448	3.872418
H	6.827318	-2.519151	4.222258
C	-3.388013	1.044432	0.434004
C	-3.388013	-1.044432	-0.434004
C	-3.047700	2.277083	0.989423
C	-4.741801	0.672184	0.275786
C	-3.047700	-2.277083	-0.989423
C	-4.741801	-0.672184	-0.275786
C	-4.080673	3.138432	1.352024
H	-2.007733	2.563004	1.148691
C	-5.753633	1.557461	0.647316
C	-4.080674	-3.138432	-1.352024
H	-2.007734	-2.563004	-1.148692
C	-5.753633	-1.557461	-0.647315
C	-5.440027	2.809702	1.184591
H	-3.806867	4.100283	1.783819
H	-6.796481	1.259658	0.515048
C	-5.440027	-2.809702	-1.184591
H	-3.806868	-4.100283	-1.783819
H	-6.796481	-1.259658	-0.515047
N	-2.571927	0.000000	0.000000
C	-6.573064	3.770481	1.565246
C	-6.573064	-3.770481	-1.565246
C	-7.488557	-3.099781	-2.601646

H	-8.310374	-3.777031	-2.881309
H	-7.934062	-2.174683	-2.208774
H	-6.924494	-2.843920	-3.510800
C	-7.388953	-4.112143	-0.307546
H	-8.211522	-4.799688	-0.558790
H	-6.752173	-4.593986	0.449031
H	-7.827288	-3.210723	0.144713
C	-6.043618	-5.075580	-2.166181
H	-5.462664	-4.891413	-3.082111
H	-5.406416	-5.620911	-1.454422
H	-6.887884	-5.729462	-2.429752
C	-7.388953	4.112144	0.307546
H	-7.827287	3.210724	-0.144712
H	-8.211522	4.799688	0.558791
H	-6.752173	4.593987	-0.449030
C	-7.488557	3.099782	2.601647
H	-7.934061	2.174683	2.208775
H	-6.924493	2.843920	3.510800
H	-8.310373	3.777032	2.881309
C	-6.043617	5.075580	2.166182
H	-5.462664	4.891413	3.082112
H	-5.406415	5.620912	1.454422
H	-6.887883	5.729462	2.429752

T_1 state of ***β*-DThBSS-Cz**

atom	X	Y	Z
C	-0.452627	-1.067129	0.556096
C	0.943246	-1.059640	0.534212
C	1.707095	-0.000004	-0.000005
C	0.943248	1.059634	-0.534222
C	-0.452626	1.067127	-0.556102
C	-1.162784	0.000000	-0.000003
B	3.275212	-0.000006	-0.000005
C	3.950987	0.884490	-1.059441
C	3.266054	1.984706	-1.636491
S	1.693038	2.526742	-1.193572
S	1.693035	-2.526751	1.193560
C	3.266044	-1.984714	1.636493
C	3.950983	-0.884498	1.059436
C	5.230286	0.728498	-1.731094
C	5.485006	1.725083	-2.702231
C	5.484992	-1.725082	2.702240
C	5.230277	-0.728504	1.731093
H	-0.997472	-1.895958	1.012595
H	-0.997469	1.895956	-1.012601
S	4.151544	-2.849452	2.870570

S	4.151559	2.849453	-2.870558
C	6.657805	1.743035	-3.455363
C	6.178204	-0.300235	-1.570275
C	6.178197	0.300228	1.570272
C	6.657786	-1.743028	3.455378
C	7.348026	-0.288662	-2.315662
C	7.591723	0.732223	-3.247001
C	7.348015	0.288661	2.315665
C	7.591706	-0.732217	3.247013
H	5.980493	-1.104490	-0.860842
H	8.080759	-1.085378	-2.183911
H	8.515047	0.727741	-3.828136
H	6.832383	2.523270	-4.197165
H	5.980490	1.104477	0.860831
H	8.080750	1.085375	2.183912
H	8.515027	-0.727731	3.828153
H	6.832359	-2.523256	4.197187
C	-3.386327	1.044098	0.435738
C	-3.386328	-1.044095	-0.435742
C	-3.046529	2.275585	0.993942
C	-4.739870	0.671393	0.277730
C	-3.046532	-2.275582	-0.993947
C	-4.739870	-0.671389	-0.277731
C	-4.079910	3.134774	1.360529
H	-2.006765	2.562526	1.152217
C	-5.752185	1.554643	0.652968
C	-4.079914	-3.134771	-1.360532
H	-2.006768	-2.562524	-1.152224
C	-5.752187	-1.554638	-0.652967
C	-5.439141	2.805244	1.194104
H	-3.806430	4.095610	1.794771
H	-6.794867	1.256208	0.520880
C	-5.439145	-2.805240	-1.194105
H	-3.806435	-4.095607	-1.794775
H	-6.794869	-1.256203	-0.520879
N	-2.570466	0.000001	-0.000002
C	-6.572593	3.763309	1.580394
C	-6.572598	-3.763304	-1.580394
C	-7.485200	-3.087543	-2.616039
H	-8.307268	-3.762724	-2.899948
H	-7.930398	-2.163402	-2.220568
H	-6.919022	-2.828912	-3.523100
C	-7.391281	-4.108639	-0.325533
H	-8.214117	-4.794331	-0.580885
H	-6.756534	-4.593959	0.430516
H	-7.829536	-3.208403	0.129157
C	-6.043489	-5.066697	-2.185266

H	-5.460578	-4.879646	-3.099373
H	-5.408255	-5.615503	-1.474422
H	-6.888009	-5.718584	-2.452922
C	-7.391278	4.108644	0.325534
H	-7.829534	3.208408	-0.129154
H	-8.214113	4.794336	0.580888
H	-6.756532	4.593964	-0.430515
C	-7.485194	3.087549	2.616041
H	-7.930393	2.163408	2.220571
H	-6.919015	2.828918	3.523101
H	-8.307261	3.762730	2.899951
C	-6.043483	5.066702	2.185266
H	-5.460571	4.879651	3.099372
H	-5.408250	5.615507	1.474421
H	-6.888002	5.718590	2.452923