Supporting Information

Pentacyclic Ladder-Heteraborin Emitters Exhibiting High-Efficiency Blue Thermally Activated Delayed Fluorescence with an Ultrashort Emission Lifetime

Tomohiro Agou,*[,†] Kyohei Matsuo,[‡] Rei Kawano,[†] In Seob Park,[‡] Takaaki Hosoya,[†] Hiroki Fukumoto,[†] Toshio Kubota,[†] Yoshiyuki Mizuhata,[‖] Norihiro Tokitoh,[‖] and Takuma Yasuda*[,‡]

[†]Department of Quantum Beam Science, Graduate School of Science and Engineering, Ibaraki University, 4-12-1 Nakanarusawa, Hitachi, Ibaraki 316-8511, Japan

[‡]INAMORI Frontier Research Center (IFRC), Kyushu University, 744 Motooka, Nishi-ku, Fukuoka 819-0395, Japan

[‖]Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan

E-mail: tomohiro.agou.mountain@vc.ibaraki.ac.jp (T.A.)

E-mail: yasuda@ifrc.kyushu-u.ac.jp (T.Y.)

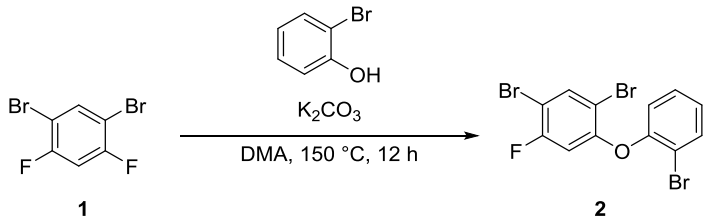
Table of Contents:

General remarks

All the manipulations were performed under a dry N_2 atmosphere using Schlenk techniques. Commercially available materials and reagents were used as received. Solvents (THF, Et_2O, and toluene) were purified by the Ultimate Solvent System, Glass Contour Company.[S1] ^{1}H, ^{19}F, and ^{13}C NMR spectra were recorded on a Bruker Avance III 400 NMR spectrometer. High resolution mass spectra were collected on a JEOL JMS-700 MStation mass spectrometer (EI or FAB), Bruker micrOTOF mass spectrometer (APCI, APPI, or ESI), or Bruker solariX ion-cyclotron Fourier transform mass spectrometer (ESI or APCI). Thermogravimetric analysis (TGA) was performed on a Rigaku Thermo Plus EVO TG-DTA under Ar atmosphere with a heating rate of 10 °C min^{-1}. Elemental analysis was performed at the Microanalytical Laboratory, Institute for Chemical Research, Kyoto University. 1,3-Dibromo-4,6-diiodobenzene (**4**),[S2] TipB(OMe)$_2$,[S3] and 1,3,6,8-tetramethylcarbazole[S4] were prepared according to the literature.

Synthesis and characterization

*1,5-Dibromo-2-(3-bromophenoxy)-4-fluorobenzene (**2**)*



A mixture of 1,5-dibromo-2,4-difluorobenzene (**1**, 1.8 g, 6.6 mmol), 2-bromophenol (1.1 g, 6.6 mmol), K_2CO_3(0.91 g, 6.6 mmol), and DMA (10 mL) was stirred at 150 °C for 12 h. The reaction was quenched with aq. NH_4Cl, and the mixture was extracted with CH_2Cl_2. The organic layer was dried with $MgSO_4$, and the solvents were evaporated. The crude product was separated by column chromatography (SiO_2, eluent: hexane/$CHCl_3$ = 9:1, v/v) to give **2** as a colorless oil (1.8 g, 4.2 mmol, 65%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.50 (d, $^3J_{HF}$ = 9.2 Hz, 1H), 7.00 (dd, J = 8.0, 1.5 Hz, 1H), 7.13 (td, J = 8.0, 1.5 Hz, 1H), 7.34 (td, J = 8.0, 1.5 Hz, 1H), 7.67 (dd, J = 8.0, 1.5 Hz, 1H), 7.82 (d, $^4J_{HF}$ = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 103.01 (d, J = 22.6 Hz), 106.35 (d, J = 26.8 Hz), 108.29 (d, J = 3.6 Hz), 115.18 (s), 121.25 (s), 126.31 (s), 129.07 (s), 134.33 (s), 136.73 (d, J = 1.5 Hz), 152.03 (s), 154.10 (d, J = 8.8 Hz), 158.65 (d, J = 247.4 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ −104.90; HRMS (EI$^+$) m/z 421.7956 (M$^+$, $C_{12}H_6O^{79}Br_3F$, calcd 421.7953), 423.7935 (M$^+$, $C_{12}H_6O^{79}Br_2{}^{81}BrF$, calcd 423.7933), 425.7915 (M$^+$, $C_{12}H_6O^{79}Br^{81}Br_2F$, calcd 425.7913), 427.7894 (M$^+$, $C_{12}H_6O^{81}Br_3F$, calcd 427.7894).

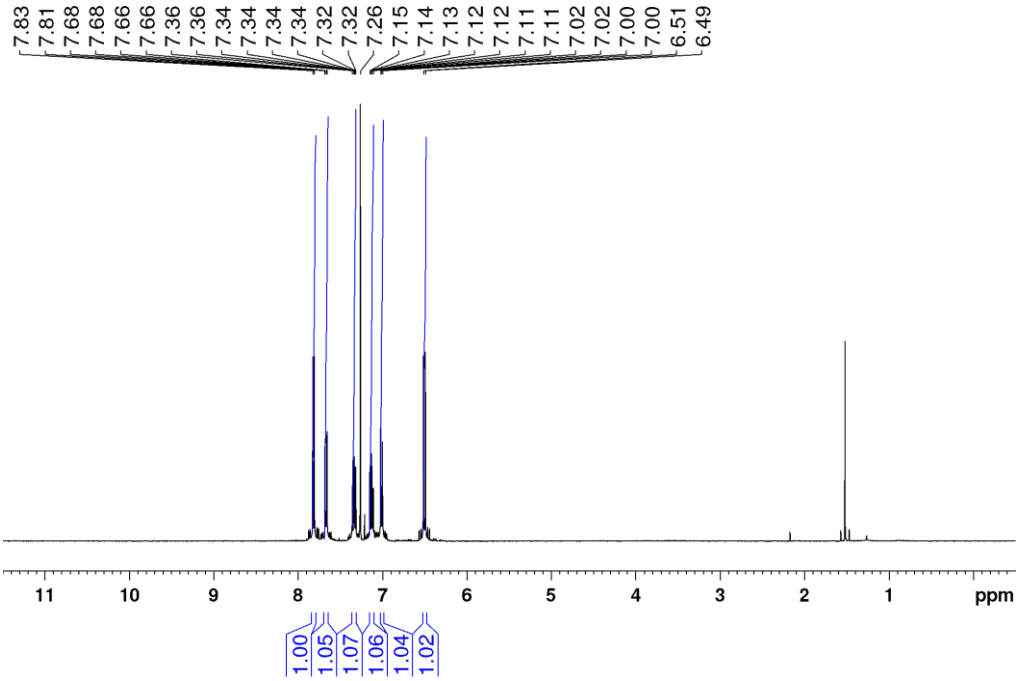


Figure S1. ^{1}H NMR spectrum of **2** in $CDCl_3$.

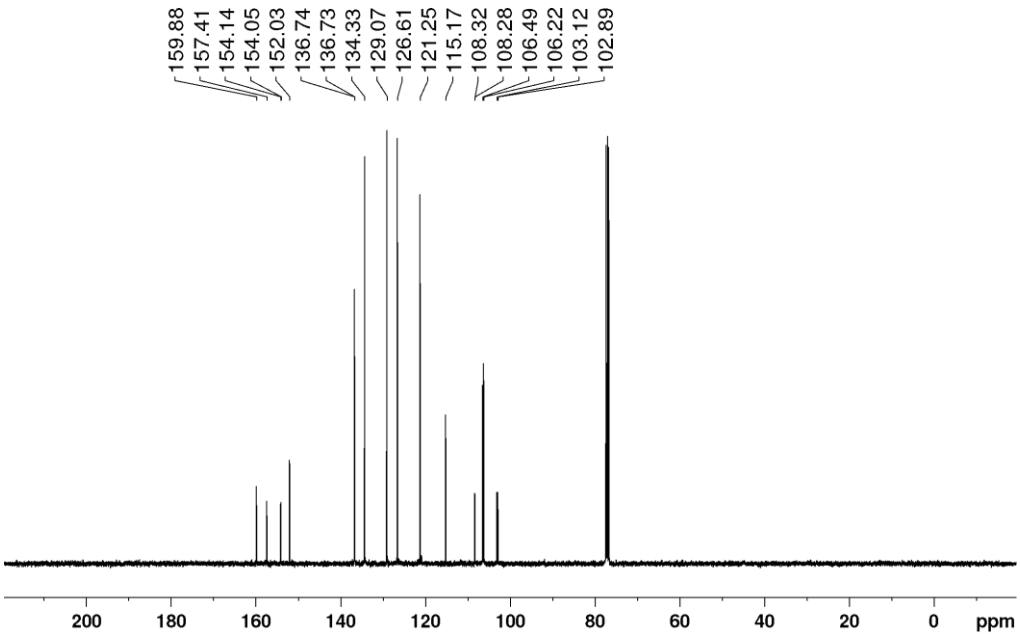
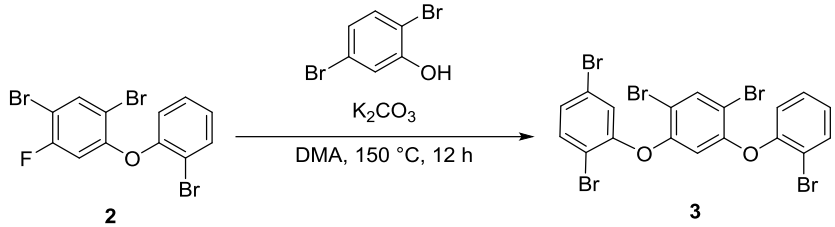


Figure S2. ^{13}C NMR spectrum of **2** in $CDCl_3$.

*1,5-Dibromo-2-(2-bromophenoxy)-4-(2,5-dibromophenoxy)benzene (**3**)*



A mixture of **2** (1.8 g, 4.2 mmol), 2,5-dibromophenol (1.1 g, 4.3 mmol), K_2CO_3(0.59g, 4.3 mmol), and DMA (10 mL) was stirred at 150 °C for 12 h. The reaction was quenched with aq. NH_4Cl, and the mixture was extracted with CH_2Cl_2. The organic layer was dried with $MgSO_4$, and the solvents were evaporated. The crude product was separated by column chromatography (SiO_2, eluent: hexane/$CHCl_3$ = 9:1, v/v) to give **3** as a white solid (2.0 g, 3.1 mmol, 73%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.37 (s, 1H), 6.86 (d, J = 2.1 Hz, 1H), 6.91 (dd, J = 8.1, 1.4 Hz, 1H), 7.05 (dt, J = 7.9, 1.4 Hz, 1H), 7.01 (dd, J = 8.5, 2.1 Hz, 1H), 7.28 (td, J = 8.1, 1.6 Hz, 1H), 7.43 (d, J = 8.5 Hz, 1H), 7.62 (dd, J = 8.0, 1.5 Hz, 1H), 7.92 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 108.98, 109.65, 110.83, 112.30, 114.44, 120.13, 121.39, 121.56, 126.05, 134.24, 134.87, 137.61, 152.26, 152.32, 153.51, 153.71; HRMS (EI$^+$) *m/z* 651.6520 (M^+, $C_{18}H_9{}^{79}Br_5O_2$, calcd 651.6519), 653.6495 (M^+, $C_{18}H_9{}^{79}Br_4{}^{81}BrO_2$, calcd 653.6499), 655.6480 (M^+, $C_{18}H_9{}^{79}Br_3{}^{81}Br_2O_2$, calcd 655.6479), 657.6459 (M^+, $C_{18}H_9{}^{79}Br_2{}^{81}Br_3O_2$, calcd 657.6460), 659.6439 (M^+, $C_{18}H_9{}^{79}Br^{81}Br_4O_2$, calcd 659.6441), 661.6426 (M^+, $C_{18}H_9{}^{81}Br_5O_2$, calcd 661.6426).

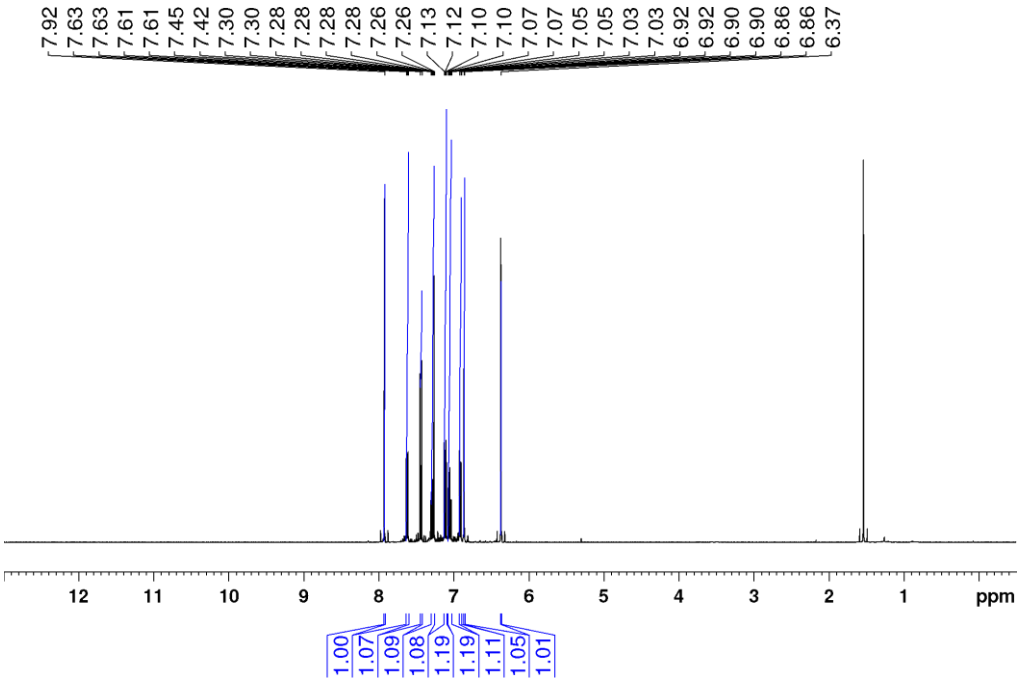


Figure S3. ^{1}H NMR spectrum of **3** in $CDCl_3$.

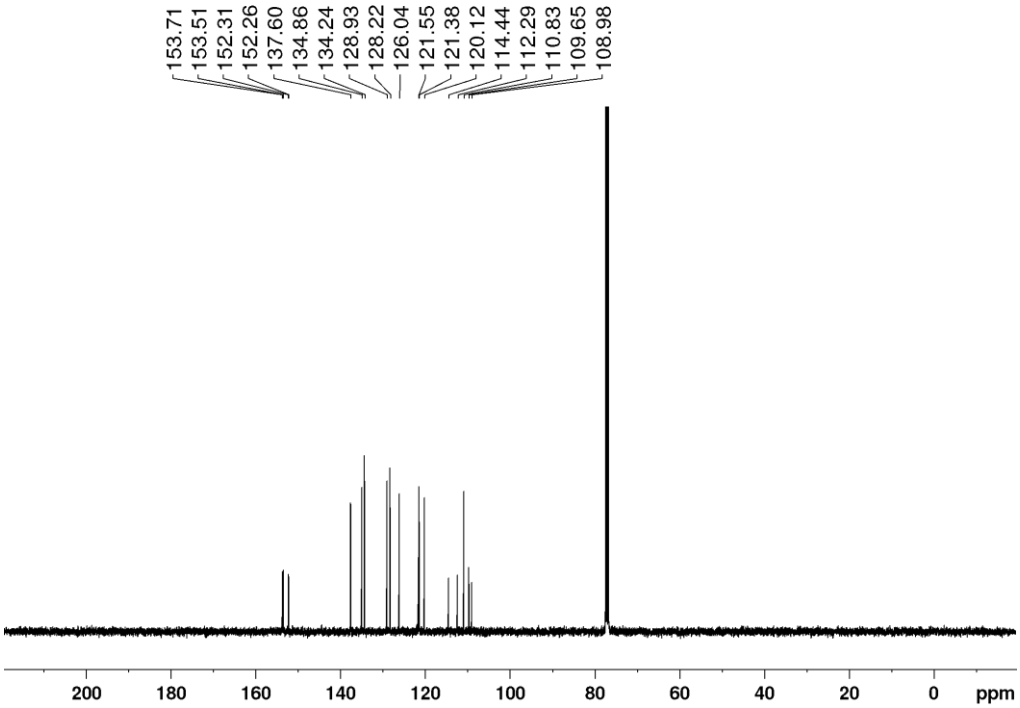
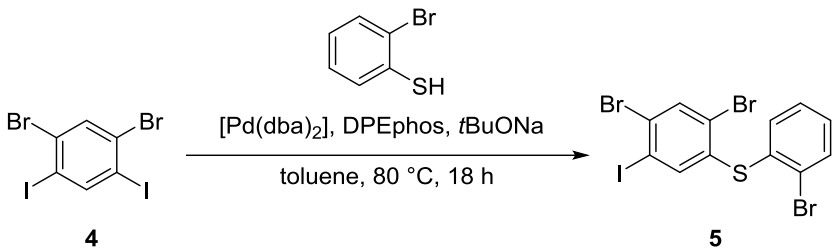


Figure S4. ^{13}C NMR spectrum of **3** in $CDCl_3$.

*(2-Bromophenyl)(2,4-dibromo-5-iodophenyl)sulfane (**5**)*



A mixture of 1,4-dibromo-2,5-diiodobenzene (**4**, 5.4 g, 11 mmol), 2-bromobenzenethiol (1.9 g, 10 mmol), [Pd(dba)$_2$] (0.29 g, 0.50 mmol), DPEphos (0.27 g, 0.50 mmol), *t*BuONa(1.4 g, 15 mmol), and toluene (30 mL) was stirred at 80 °C for 18 h. The reaction was quenched with aq. NH_4Cl, and the mixture was extracted with $CHCl_3$. The organic layer was dried with $MgSO_4$, and the solvents were evaporated. The crude product was separated by column chromatography (SiO_2, eluent: hexane/$CHCl_3$ = 9:1, v/v) followed by recrystallization from $CHCl_3$ to give **5** as a white solid (1.3 g, 2.4 mmol, 24%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21-7.33 (m, 3H), 7.43 (s, 1H), 7.68 (d, J = 7.9 Hz, 1H), 7.84 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 100.24, 125.13, 126.66, 128.50, 128.83, 129.78, 133.37, 133.89, 134.03, 136.10, 137.23, 141.47; HRMS (EI$^+$) *m*/*z* 545.6790 (M$^+$, $C_{12}H_6{}^{79}Br_3SI$, calcd 545.6785), 547.6766 (M$^+$, $C_{12}H_6{}^{79}Br_2{}^{81}BrSI$, calcd 547.6765), 549.6746 (M$^+$, $C_{12}H_6{}^{79}Br^{81}Br_2SI$, calcd 549.6744), 551.6722 (M$^+$, $C_{12}H_6{}^{81}Br_3SI$, calcd 551.6723).

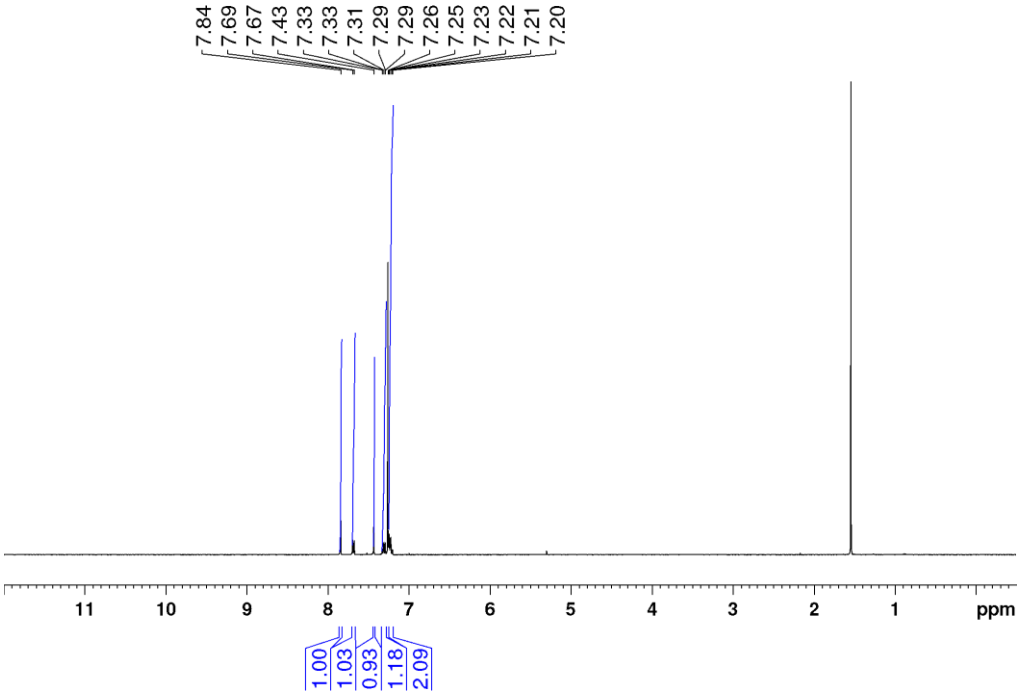


Figure S5. ^{1}H NMR spectrum of **5** in $CDCl_3$.

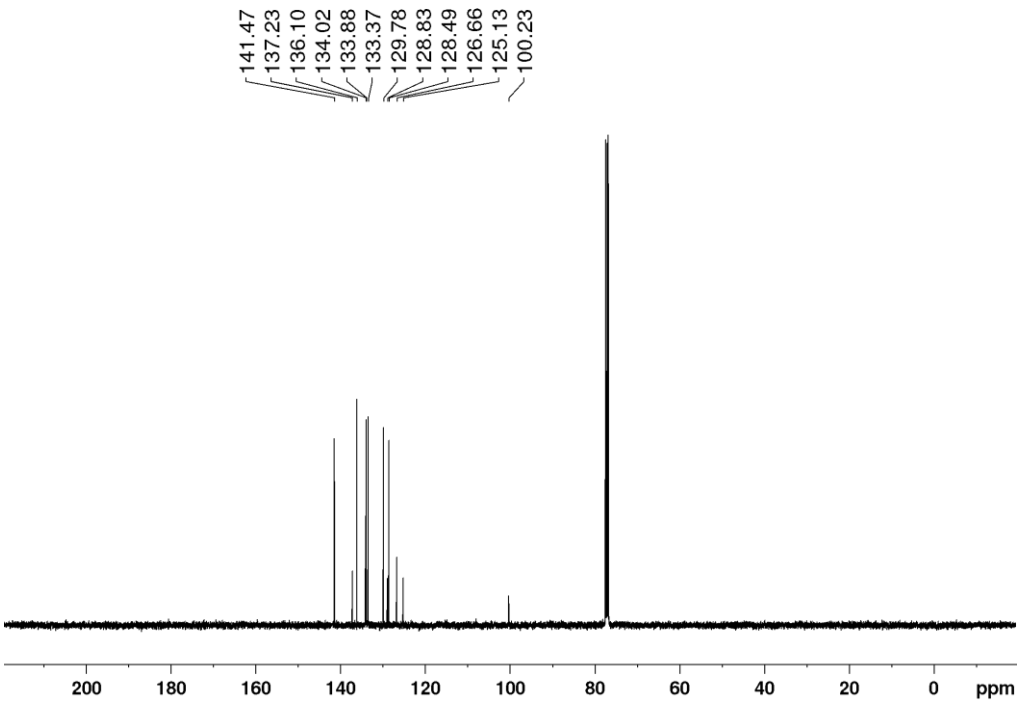
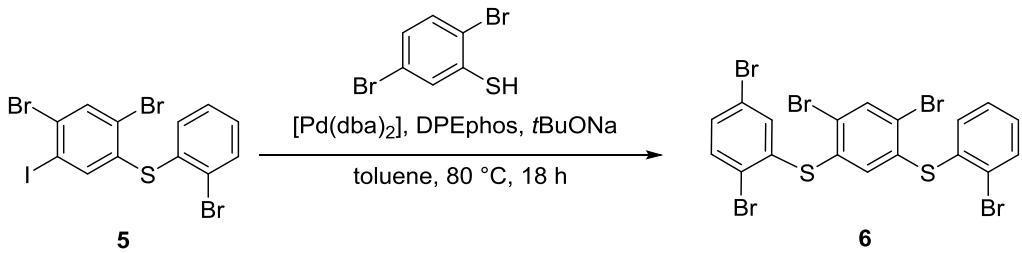


Figure S6. ^{13}C NMR spectrum of **5** in $CDCl_3$.

*(2-Bromophenyl){2,4-dibromo-5-[(2,5-dibromophenyl)thio]phenyl}sulfane (**6**)*



A mixture of **5** (2.3 g, 4.2 mmol), 2,5-dibromobenzenethiol (1.1 g, 4.0 mmol), $[Pd(dba)_2]$ (0.24 g, 0.42 mmol), DPEphos (0.23 g, 0.42 mmol), *t*BuONa(0.81 g, 8.4 mmol), and toluene (16 mL) was stirred at 80 °C for 18 h. The reaction was quenched with aq. NH_4Cl, and the mixture was extracted with $CHCl_3$. The organic layer was dried with $MgSO_4$, and the solvents were evaporated. The crude product was separated by column chromatography (SiO_2, eluent: hexane/$CHCl_3$ = 8/2) followed by recrystallization from $CHCl_3$ to give **6** as a colorless solid (1.4 g, 2.1 mmol, 51%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.13 (s, 1H), 7.19-7.29 (m, 3H), 7.34-7.39 (m, 3H), 7.57 (dd, J = 7.8, 1.4 Hz, 1H), 7.79 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 120.53, 120.68, 121.73, 126.69, 128.47, 129,16, 130.74, 132.51, 133.06, 133.98, 134.90, 135.65, 135.91, 136.39, 136.43, 136.86, 138.29 (One signal could not be observed probably because of the overlapping); HRMS (EI$^+$) *m*/*z* 683.6063 (M^+, $C_{18}H_9{}^{79}Br_5S_2$, calcd 683.6062), 685.6047 (M^+, $C_{18}H_9{}^{79}Br_4{}^{81}BrS_2$, calcd 685.6042), 687.6026 (M^+, $C_{18}H_9{}^{79}Br_3{}^{81}Br_2S_2$, calcd 687.6022), 689.6002 (M^+, $C_{18}H_9{}^{79}Br_2{}^{81}Br_3S_2$, calcd 689.6001), 691.5980 (M^+, $C_{18}H_9{}^{79}Br^{81}Br_4S_2$, calcd 691.5981), 693.5960 (M^+, $C_{18}H_9{}^{81}Br_5S_2$, calcd 693.5960).

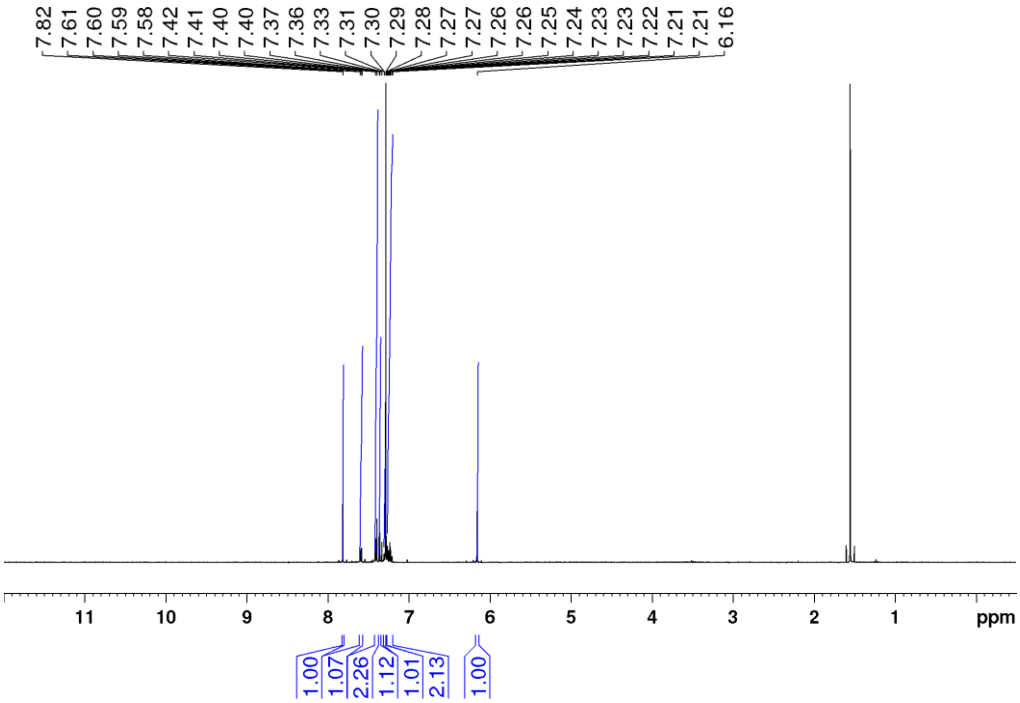


Figure S7. ^{1}H NMR spectrum of **6** in $CDCl_3$.

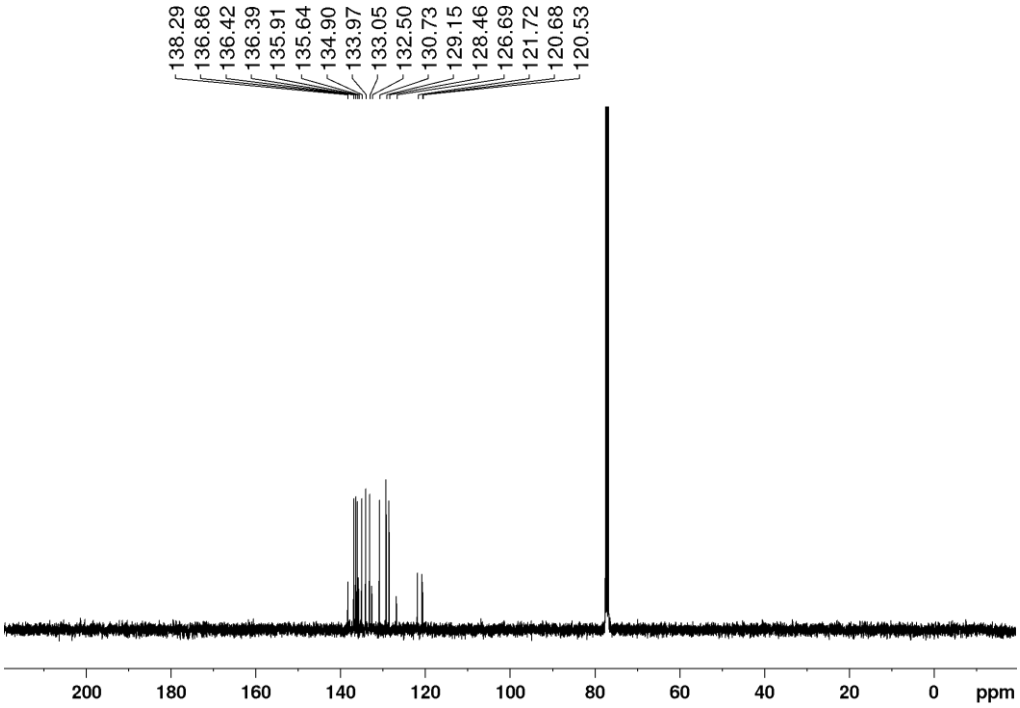
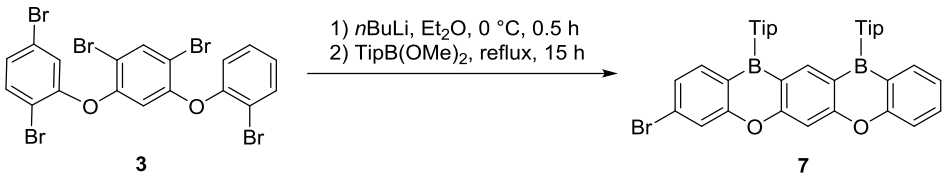


Figure S8. ^{13}C NMR spectrum of **6** in $CDCl_3$.

Br-BOBO (7)



To a Et_2O solution (70 mL) of **3** (0.54 g, 0.81 mmol) was added *n*BuLi (1.57 M in hexane, 2.3 mL, 3.6 mmol) at 0 °C, and the mixture was stirred for 30 min at 0 °C. To this mixture was added $TipB(OMe)_2$ (0.74 mL, 2.4 mmol). This mixture was refluxed for 15 h. The reaction was quenched with aq. NH_4Cl, and the mixture was extracted with $CHCl_3$. The organic layer was dried with $MgSO_4$, and the solvents were evaporated. The crude product was separated by column chromatography (SiO_2, eluent: hexane/$CHCl_3$ = 8:2, v/v) followed by recrystallization from $CHCl_3/CH_3OH$ to give **7** as a white solid (0.12 g, 0.16 mmol, 19%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 0.70 (d, J = 6.7 Hz, 12H), 0.93 (d, J = 6.9 Hz, 6H), 0.94 (d, J = 6.9 Hz, 6H), 1.29 (d, J = 7.0 Hz, 12H), 2.21-2.30 (m, 4H), 2.90 (sept, J = 7.0 Hz, 2H), 6.91 (s, 4H), 7.22-7.27 (m, 1H), 7.36 (dd, J = 8.2, 2.5 Hz, 1H), 7.59 (s, 1H), 7.59 (d, J = 8.0 Hz, 1H), 7.69 (d, J = 8.1 Hz, 1H), 7.27 (td, J = 7.1, 1.8 Hz, 1H), 7.80 (d, J = 1.7 Hz, 1H), 7.84 (dd, J = 7.5, 1.6 Hz, 1H), 8.09 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.90, 24.22, 24.23, 24.85, 34.51, 34.98, 35.02, 103.53, 117.32, 119.75, 119.83, 120.59, 121.97, 122.54, 122.84, 125.11, 126.30, 126.40, 128.80, 134.59, 134.67, 135.06, 137.04, 138.05, 148.56, 148.74, 149.26, 149.94, 149.97, 158.81, 158.97, 162.43, 162.93 (Three aliphatic signals could not be observed probably because of overlapping); HRMS (ESI$^+$) *m*/*z* 763.34858 ([M–H]$^+$, calcd 763.3488).

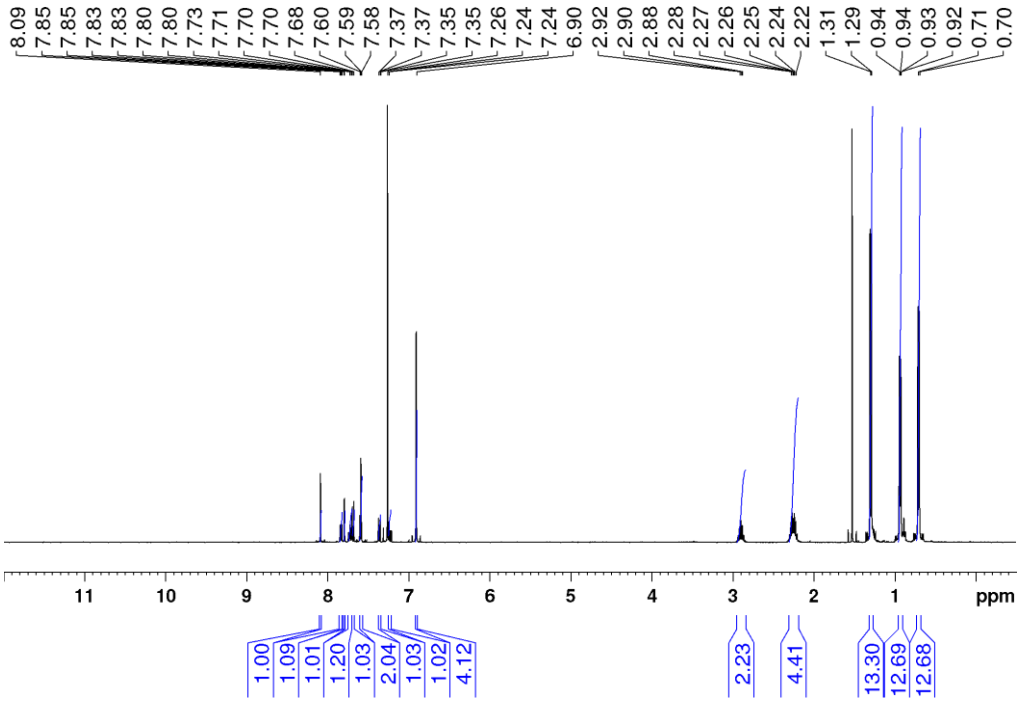


Figure S9. ^{1}H NMR spectrum of **7** in $CDCl_3$.

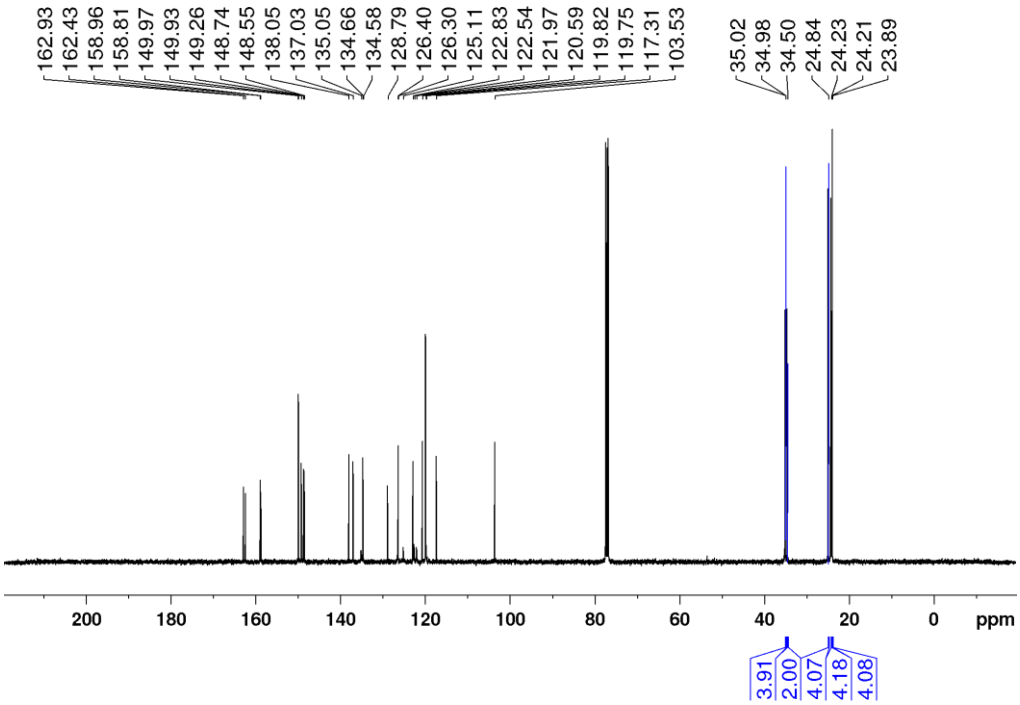


Figure S10. ^{13}C NMR spectrum of **7** in $CDCl_3$.

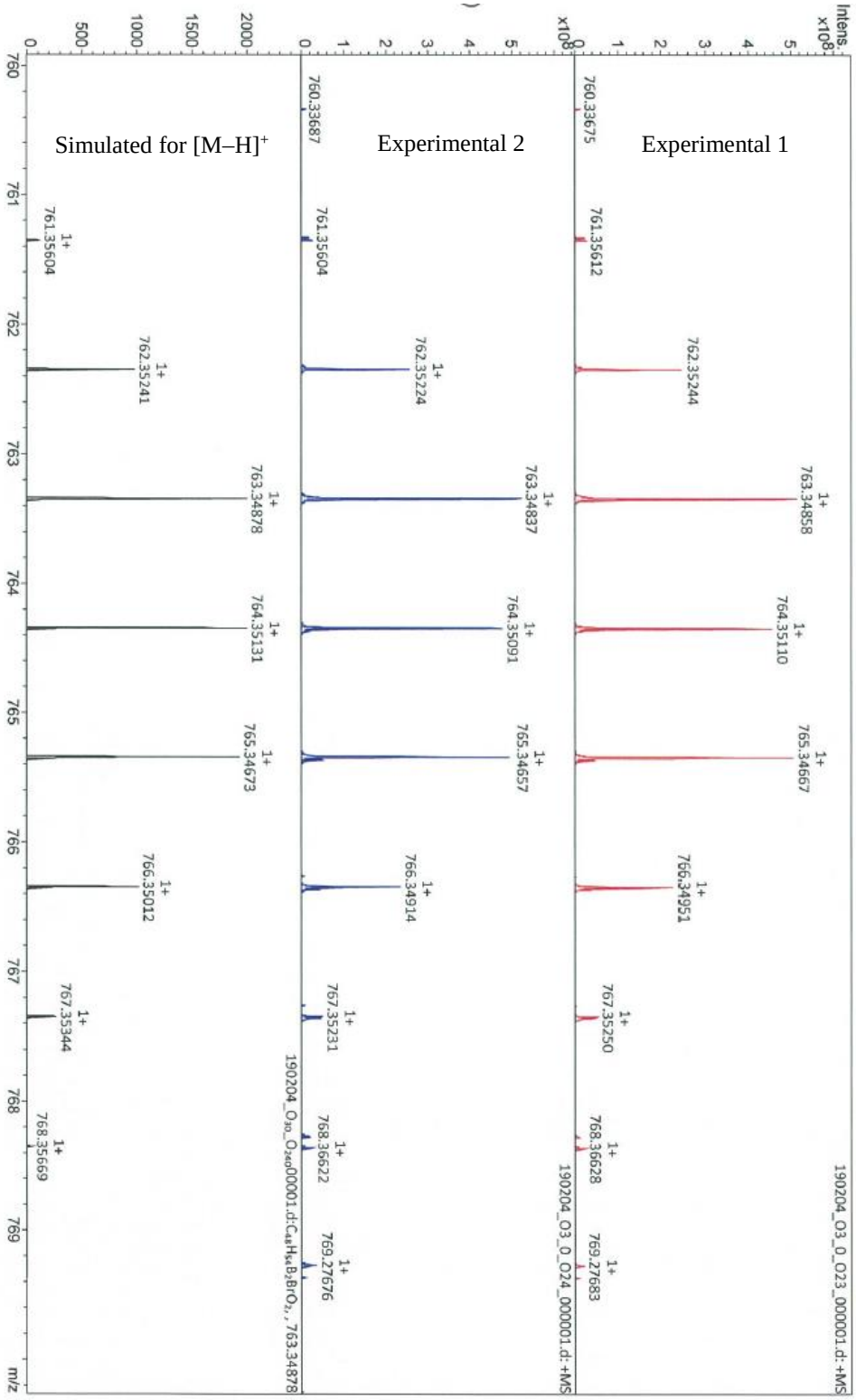
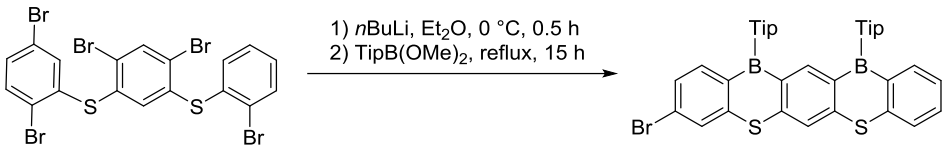


Figure S11. HRMS of **7** (ESI^+). Results of two independent measurements (experimental 1 and 2) are shown.

*Br-BSBS (**8**)*



6 **8**

To a Et_2O solution (70 mL) of **6** (0.80 g, 1.2 mmol) was added *n*BuLi (1.57 M in hexane, 3.3 mL, 5.1 mmol) at 0 °C, and the mixture was stirred for 30 min at 0 °C. To this mixture was added $TipB(OMe)_2$ (1.1 mL, 3.5 mmol). This mixture was refluxed for 15 h. The reaction was quenched with aq. NH_4Cl, and the mixture was extracted with $CHCl_3$. The organic layer was dried with $MgSO_4$, and the solvents were evaporated. The crude product was separated by column chromatography (SiO_2, eluent: hexane/$CHCl_3$ = 8:2, v/v) followed by recrystallization from $CHCl_3/CH_3OH$ to give **8** as a white solid (0.27 g, 0.34 mmol, 29%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 0.59 (d, J = 6.7 Hz, 12H), 0.86 (d, J = 6.7 Hz, 12H), 1.33 (d, J = 6.9 Hz, 12H), 2.05-2.14 (m, 4H), 2.91 (sept, J = 6.7 Hz, 2H), 6.87 (s, 4H), 7.25-7.31 (m, 2H), 7.37 (dd, J = 8.4, 1.8 Hz, 1H), 7.59 (td, J = 7.6, 1.6 Hz, 1H), 7.71 (t, J = 7.4 Hz, 1H), 7.86 (d, J = 1.7 Hz, 1H), 7.88 (dd, J = 7.7, 1.3 Hz, 1H), 7.98 (s, 1H), 8.53 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.03, 24.05, 24.28, 24.30, 24.62, 24.63, 34.44, 35.21, 35.23, 119.73, 120.06, 120.14, 124.73, 124.89, 127.30, 127.45, 128.01, 130.53, 131.11, 132.33, 133.98, 135.45, 136.92, 137.37, 140.31, 141.42, 141.66, 143.55, 145.73, 147.10, 148.20, 148.38, 149.39, 149.43, 152.94 (One aliphatic signal could not be observed probably because of overlapping); HRMS (ESI$^+$) m/z 795.30327 ([M–H]$^+$, calcd 795.3031).

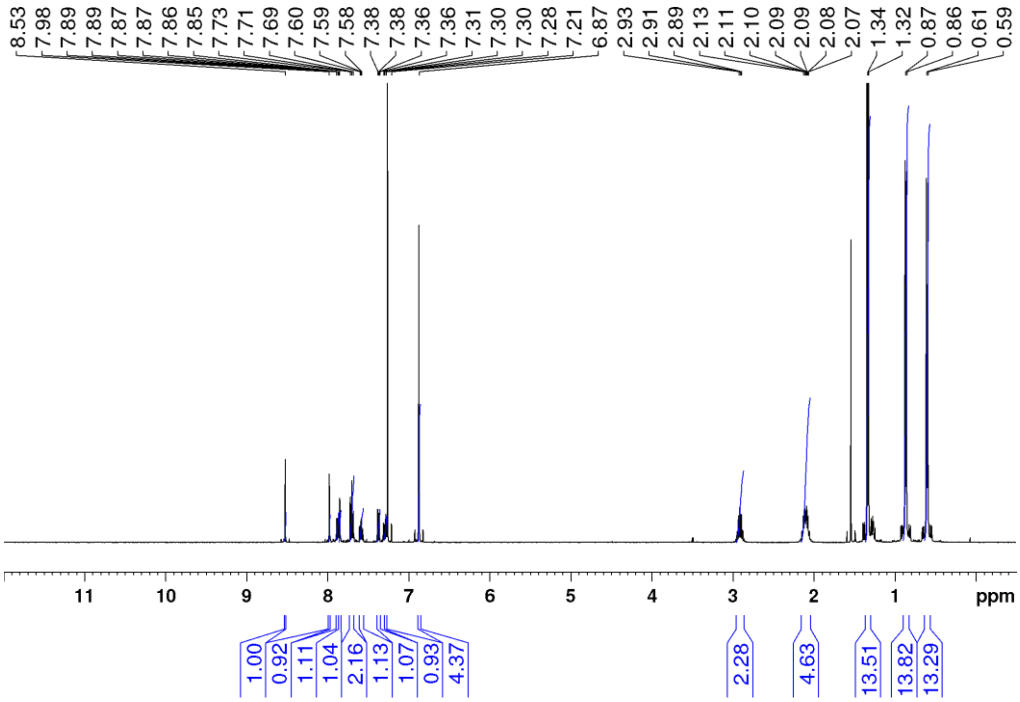


Figure S12. ^{1}H NMR spectrum of **8** in $CDCl_3$.

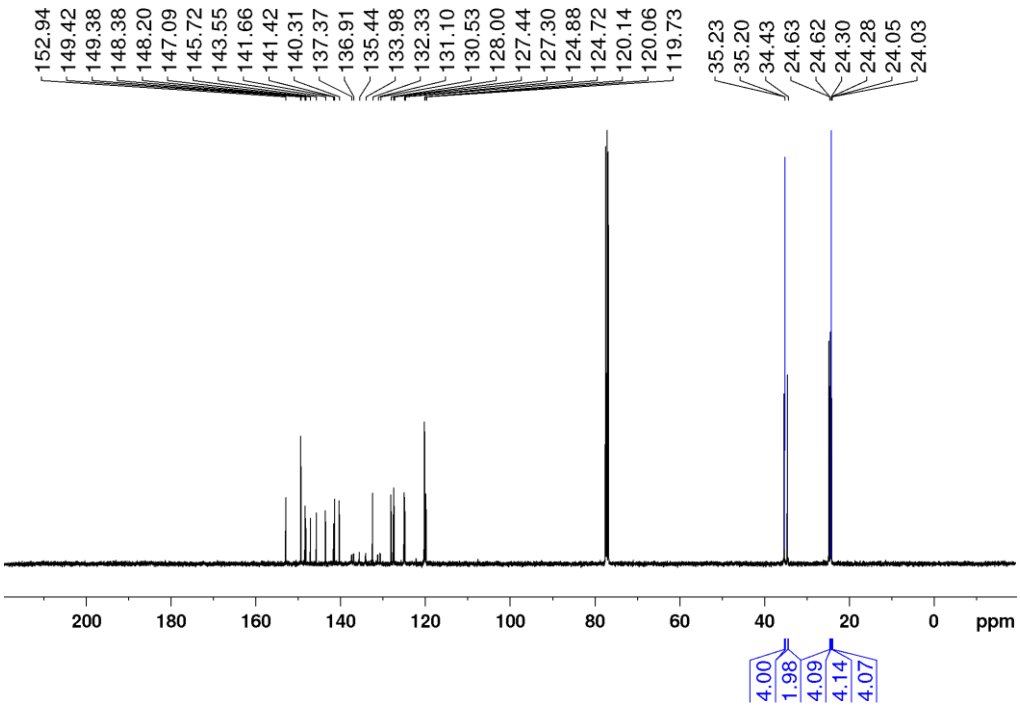


Figure S13. ^{13}C NMR spectrum of **8** in $CDCl_3$.

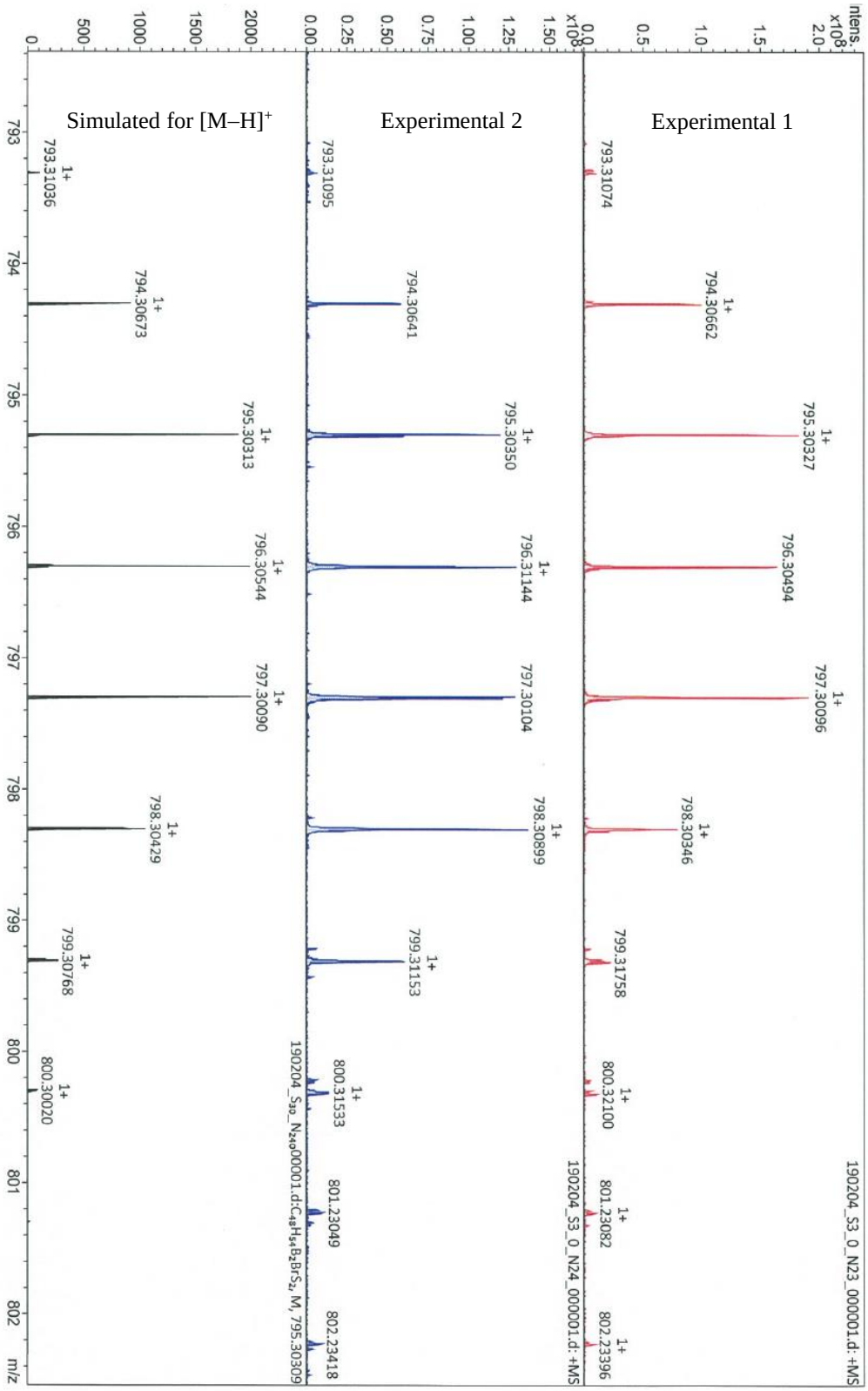
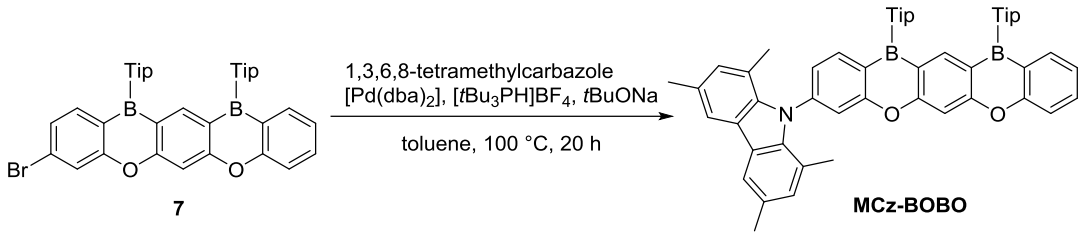


Figure S14. HRMS of **8** (ESI^+). Results of two independent measurements (experimental 1 and 2) are shown.

MCz-BOBO



A mixture of **7** (0.62 g, 0.81 mmol), 1,3,6,8-tetramethylcarbazole (0.22 g, 0.97 mmol), $[Pd(dba)_2]$ (47 mg, 0.081 mmol), $[t\mathrm{Bu}_3\mathrm{PH}]\mathrm{BF}_4$ (24 mg, 0.081 mmol), *t*BuONa(0.12 g, 1.2 mmol), and toluene (8 mL) was stirred at 100 °C for 20 h. The reaction was quenched with aq. NH_4Cl, and the mixture was extracted with $CHCl_3$. The organic layer was dried with $MgSO_4$, and the solvents were evaporated. The crude product was separated by column chromatography (SiO_2, eluent: hexane/$CHCl_3$ = 7:3, v/v) followed by recrystallization from $CHCl_3/CH_3OH$ to give **MCz-BOBO** as a light-yellow solid (0.58 g, 0.64 mmol, 79%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 0.73 (d, *J* = 6.8 Hz, 6H), 0.95 (d, *J* = 6.8 Hz, 6H), 0.95 (d, *J* = 6.7 Hz, 12H), 1.30 (d, *J* = 6.8 Hz, 6H), 1.31 (d, *J* = 6.9 Hz, 6H), 1.92 (s, 6H), 2.24-2.37 (m, 4H), 2.48 (s, 6H), 2.86-2.96 (m, 2H), 6.92 (d, *J* = 0.8 Hz, 2H), 6.93 (s, 4H), 7.23-7.27 (m, 2H), 7.32 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.60 (s, 1H), 7.71-7.76 (m, 3H), 7.85-7.87 (m, 2H), 8.18 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.43, 21.17, 23.84, 24.00, 24.30, 24.32, 24.90, 34.58, 35.09, 35.26, 103.63, 117.44, 117.92, 119.84, 119.93, 120.09, 121,38, 122.12, 122.61, 122.92, 124.52, 126.14, 126.42, 126.67, 129.35, 130.38, 134.76, 134.94, 135.12, 136.81, 137.10, 139.62, 148.27, 148.64, 148.84, 149.41, 149.92, 150.04, 158.33, 158.91, 162.84, 163.01 (two aliphatic signals could not be observed probably due to overlapping); HRMS (ESI$^+$) *m*/*z* 907.56540 (M^+, calcd 907.5665); Anal. calcd (%) for $C_{64}H_{71}B_2NO_2$: C 84.67, H 7.88, N 1.54; found: C 84.73, H 8.13, N 1.45 (averaged values of two independent measurements).

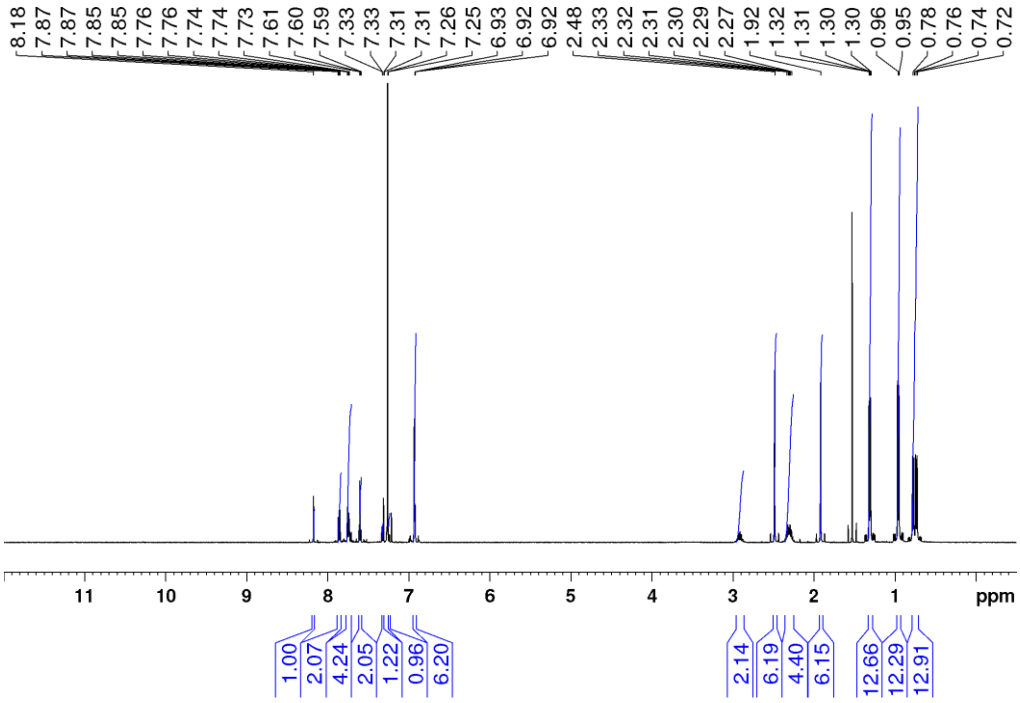


Figure S15. ^{1}H NMR spectrum of **MCz-BOBO** in $CDCl_3$.

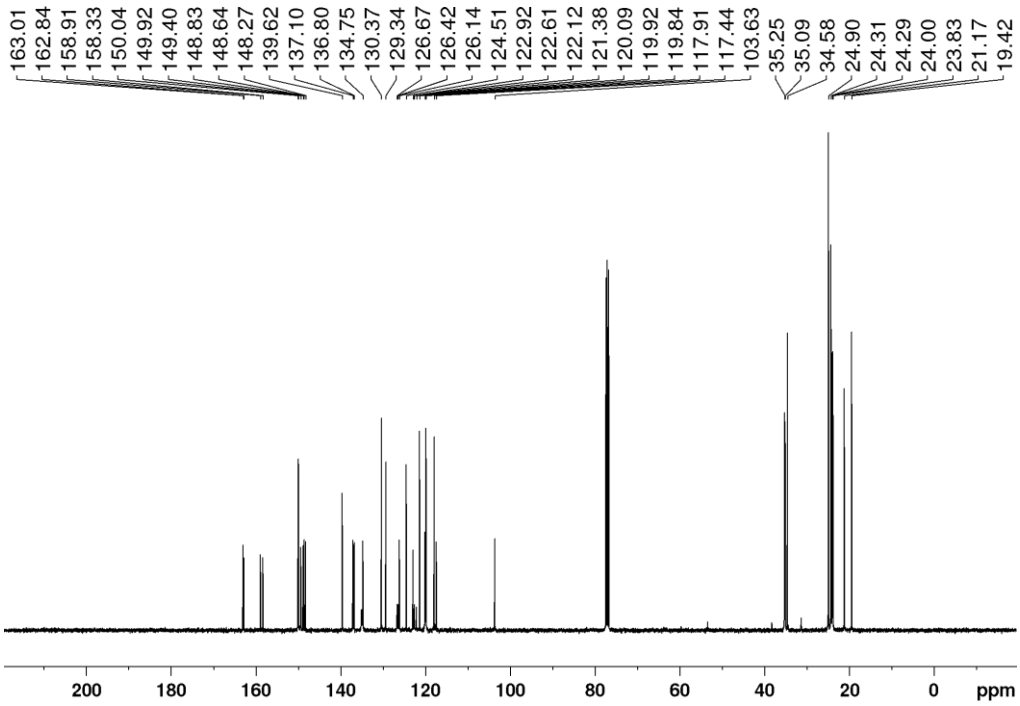


Figure S16. ^{13}C NMR spectrum of **MCz-BOBO** in $CDCl_3$.

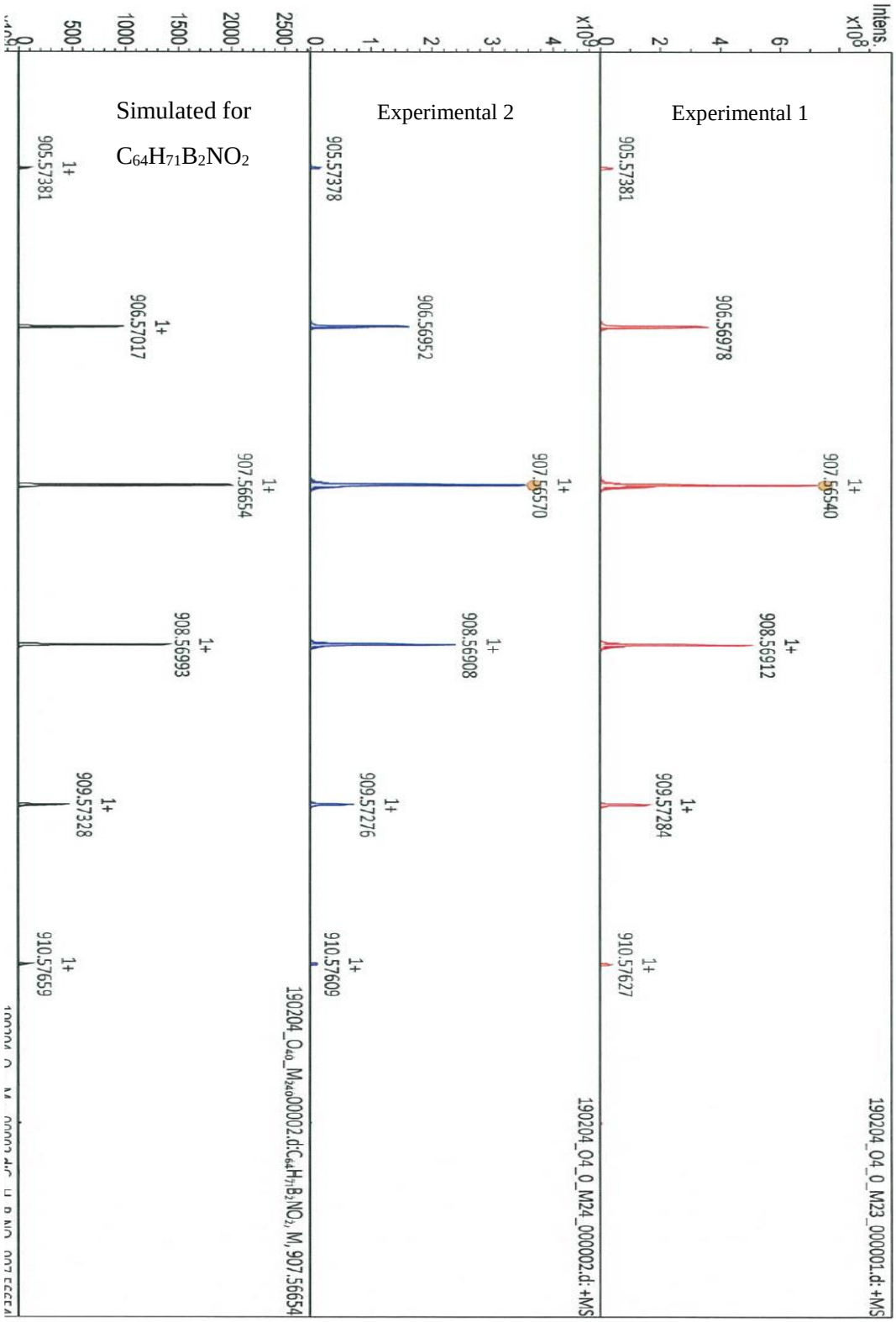
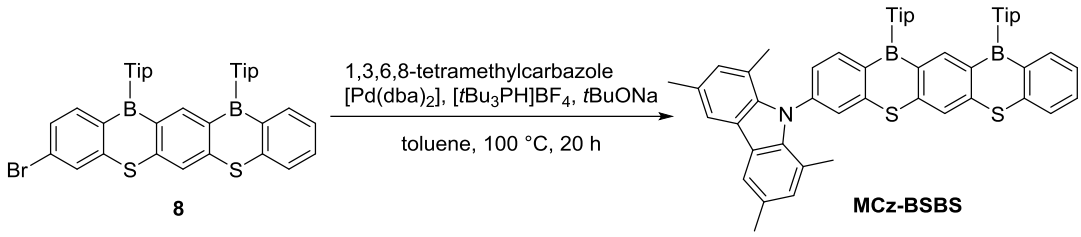


Figure S17. HRMS of **MCz-BOBO** (ESI^+). Results of two independent measurements (experimental 1 and 2) are shown.

MCz-BSBS



A mixture of **8** (0.50 g, 0.63 mmol), 1,3,6,8-tetramethylcarbazole (0.17 g, 0.76 mmol), [Pd(dba)$_2$] (36 mg, 0.063 mmol), [*t*Bu$_3$PH]BF$_4$ (18 mg, 0.063 mmol), *t*BuONa (0.090 g, 0.94 mmol), and toluene (5 mL) was stirred at 100 °C for 20 h. The reaction was quenched with aq. NH_4Cl, and the mixture was extracted with $CHCl_3$. The organic layer was dried with $MgSO_4$, and the solvents were evaporated. The crude product was separated by column chromatography (SiO_2, eluent: hexane/$CHCl_3$ = 8:2, v/v) followed by recrystallization from $CHCl_3$/CH_3OH to give **MCz-BSBS** as a light-yellow solid (0.36 g, 0.38 mmol, 61%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 0.64 (d, J = 6.7 Hz, 6H), 0.67 (d, J = 6.7 Hz, 6H), 0.88 (d, J = 6.6 Hz, 6H), 0.90 (d, J = 6.6 Hz, 6H), 1.34 (d, J = 7.0 Hz, 6H), 1.35 (d, J = 6.9 Hz, 6H), 1.87 (s, 6H), 2.08-2.23 (m, 4H), 2.47 (s, 6H), 2.87-2.98 (m, 2H), 6.89 (d, J = 1.9 Hz, 2H), 6.90 (s, 4H), 7.26-7.31 (m, 1H), 7.40 (dd, J = 8.0, 1.9 Hz, 1H), 7.59 (td, J = 7.5, 1.5 Hz, 1H), 7.70-7.74 (m, 3H), 7.78 (d, J = 1.8 Hz, 1H), 7.90 (dd, J = 7.9, 1.4 Hz, 1H), 7.94 (d, J = 8.0 Hz, 1H), 8.02 (s, 1H), 8.62 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.49, 21.15, 23.10, 24.14, 24.36, 24.38, 24.62, 24.67, 34.52, 35.29, 35.43, 117.96, 119.84, 120.16, 120.25, 121.25, 124.49, 124.68, 124.79, 124.95, 127.15, 127.73, 129.35, 130.40, 130.77, 131.21, 132.40, 135.53, 137.35, 137.47, 139.49, 140.23, 140.36, 141.79, 141.86, 146.04, 146.28, 147.21, 148.30, 148.53, 149.40, 149.52, 153.11 (one aliphatic signal could not be observed probably because of overlapping); HRMS (ESI$^+$) m/z 939.52015 (M$^+$, calcd 939.5227); Anal. calcd (%) for $C_{64}H_{71}B_2NS_2$: C 81.78, H 7.61, N 1.49; found: C 81.65, H 7.70, N 1.57 (averaged values of two independent measurements).

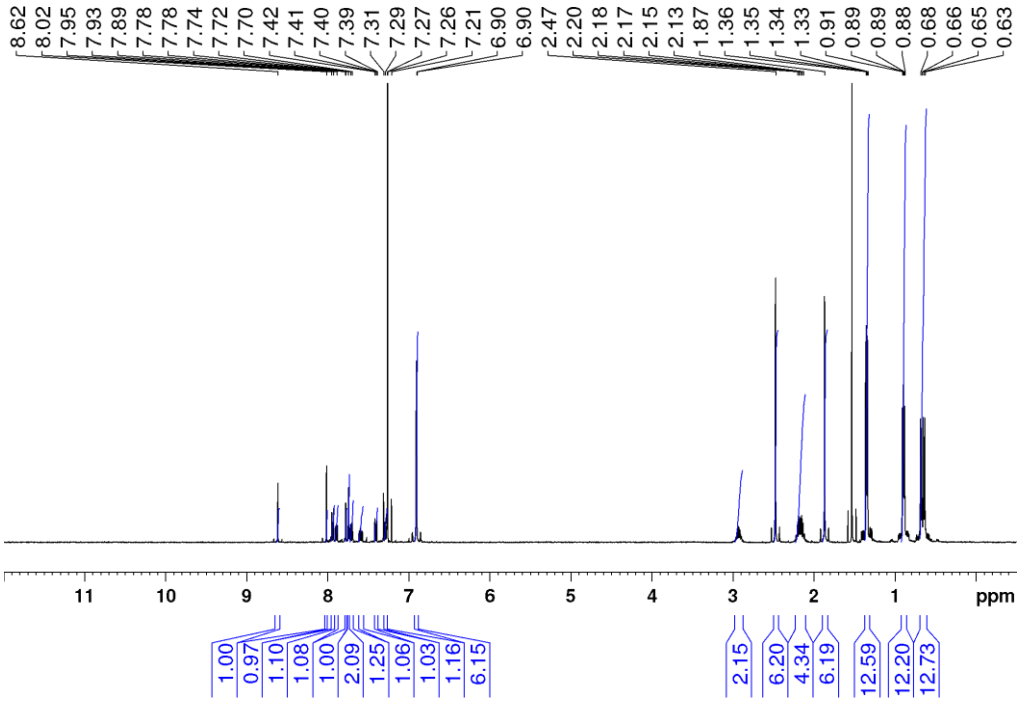


Figure S18. ^{1}H NMR spectrum of **MCz-BSBS** in $CDCl_3$.

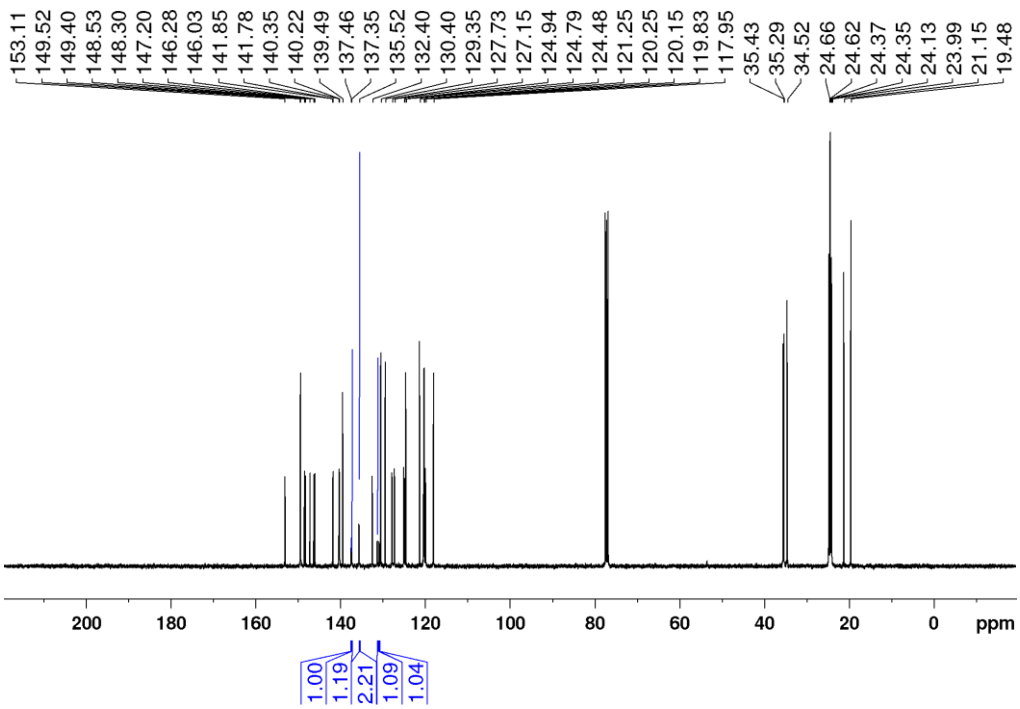


Figure S19. ^{13}C NMR spectrum of **MCz-BSBS** in $CDCl_3$.

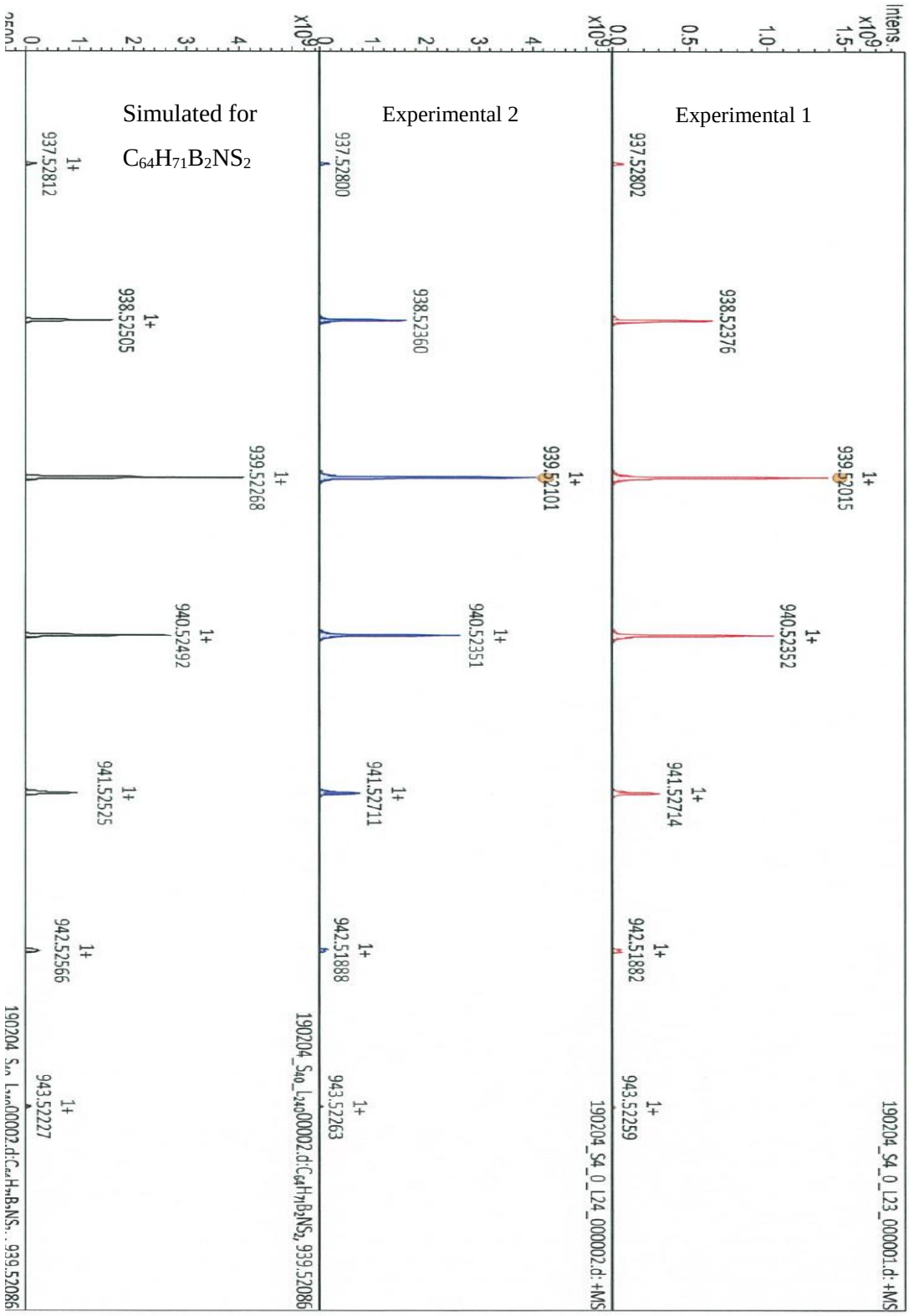
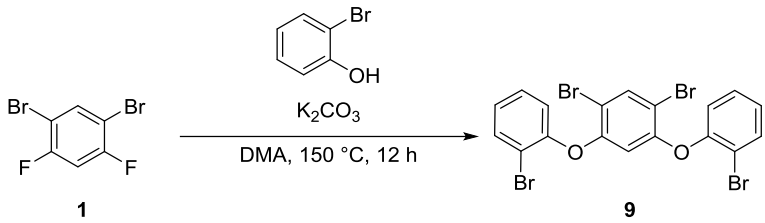


Figure S20. HRMS of **MCz-BSBS** (ESI$^+$). Results of two independent measurements (experimental 1 and 2) are shown.

*2,2'-[(4,6-dibromo-1,3-phenylene)bis(oxy)]bis(bromobenzene) (**9**)*



A mixture of 1,5-dibromo-2,4-difluorobenzene (**1**, 0.90 g, 3.3 mmol), 2-bromophenol (1.2 g, 7.0 mmol), K_2CO_3 (0.97 g, 7.0 mmol), and DMA (5 mL) was stirred at 150 °C for 12 h. The reaction was quenched with aq. NH_4Cl and the mixture was extracted with CH_2Cl_2. The organic layer was dried with $MgSO_4$, and the solvents were evaporated. The crude product was separated by column chromatography (SiO_2, eluent: hexane/$CHCl_3$ = 8:2, v/v) followed by recrystallization from $CHCl_3$ to give **9** as a white solid (1.7 g, 2.9 mmol, 90%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.32 (s, 1H), 6.92 (dd, J = 8.0, 1.5 Hz, 2H), 7.01 (td, J = 8.0, 1.5 Hz, 2H), 7.24 (td, J = 8.0, 1.5 Hz, 2H), 7.58 (dd, J = 8.0, 1.5 Hz, 2H), 7.90 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 108.83, 110.47, 114.07, 119.42, 125.64, 128.80, 134.09, 137.36, 152.54, 153.31; HRMS (EI$^+$) *m*/*z* 573.7414 (M^+, $C_{18}H_{10}O_2{}^{79}Br_4$, calcd 573.7414), 575.7392 (M^+, $C_{18}H_{10}O_2{}^{79}Br_3{}^{81}Br$, calcd 575.7394), 577.7375 (M^+, $C_{18}H_{10}O_2{}^{79}Br_2{}^{81}Br_2$, calcd 577.7375), 579.7355 (M^+, $C_{18}H_{10}O_2{}^{79}Br^{81}Br_3$, calcd 579.7356), 581.7338 (M^+, $C_{18}H_{10}O_2{}^{81}Br_4$, calcd 581.7340).

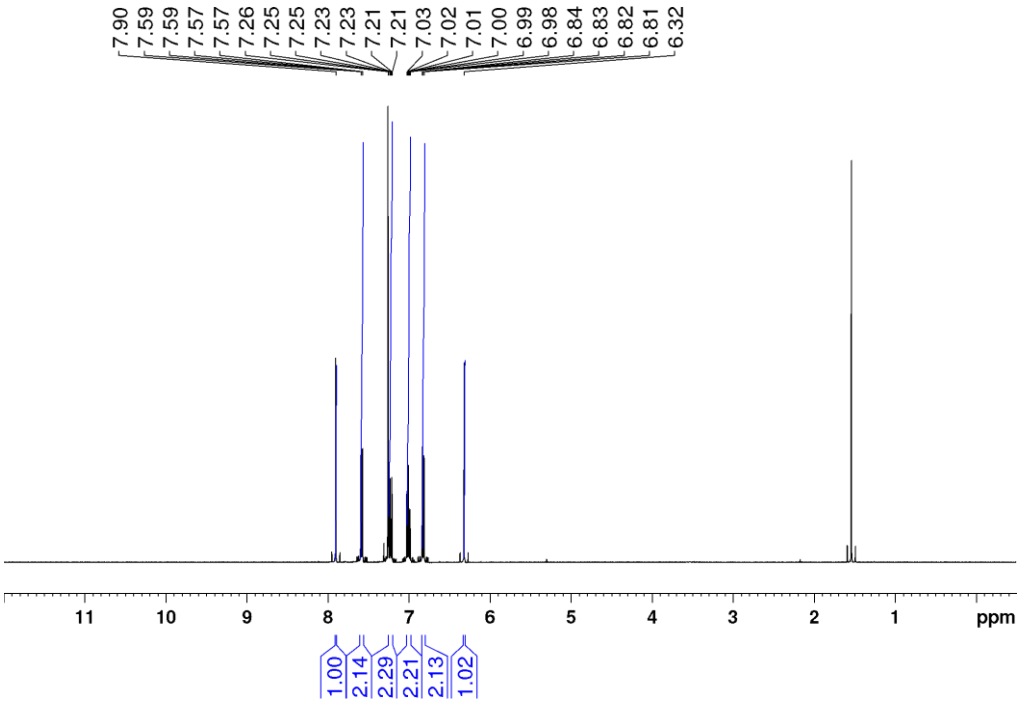


Figure S21. ^{1}H NMR spectrum of **9** in $CDCl_3$.

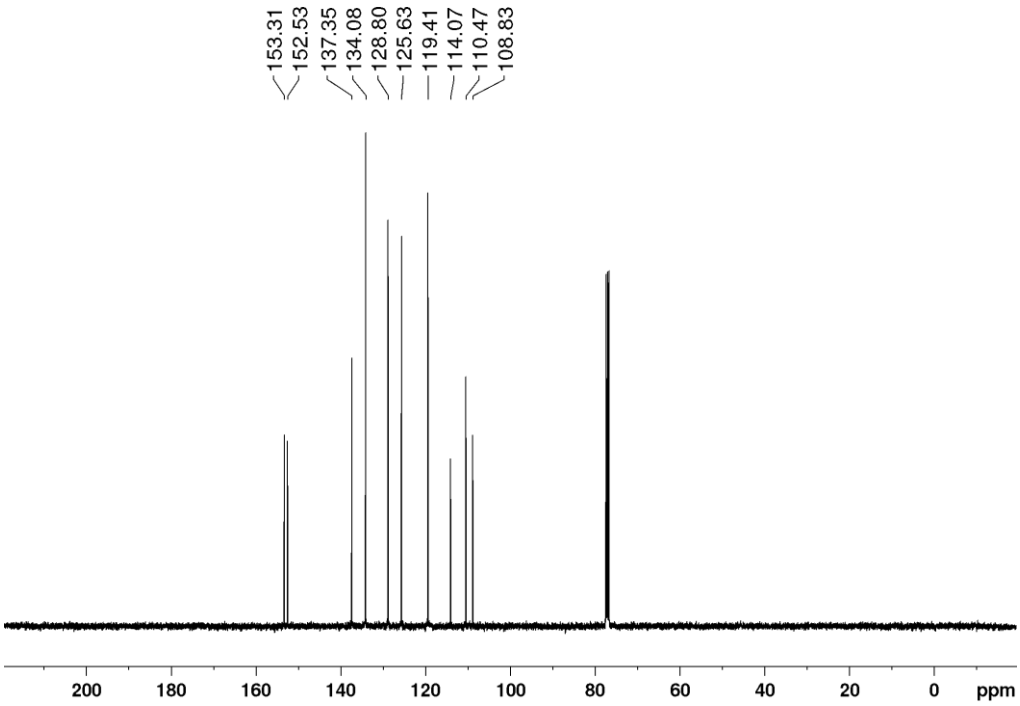
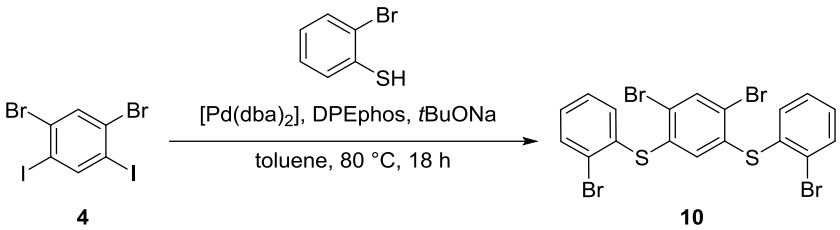


Figure S22. ^{13}C NMR spectrum of **9** in $CDCl_3$.

*2,2'-[(4,6-dibromo-1,3-phenylene)bis(oxy)]bis(bromobenzene) (**10**)*



A mixture of 1,5-dibromo-2,4-difluorobenzene (**4**, 2.9 mmol, 6 mmol), 2-bromobenzenethiol (1.9 g, 10 mmol), $[Pd(dba)_2]$ (0.29 g, 0.50 mmol), DPEphos (0.27 g, 0.50 mmol), *t*BuONa (1.4 g, 15 mmol), and toluene (20 mL) was stirred at 80 °C for 18 h. The reaction was quenched with aq. NH_4Cl and the mixture was extracted with CH_2Cl_2. The organic layer was dried with $MgSO_4$, and the solvents were evaporated. The crude product was separated by column chromatography (SiO_2, eluent: hexane/$CHCl_3$ = 7:3, v/v) followed by recrystallization from $CHCl_3$ to give **10** as a white solid (2.0 g, 4.7 mmol, 81%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.14 (s, 1H), 7.13-7.22 (m, 4H), 7.30 (dd, J = 7.7, 1.6 Hz, 2H), 7.51 (dd, J = 7.7, 1.5 Hz, 2H), 7.77 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 120.10, 128.42, 128.71, 128.76, 130.36, 132.84, 133.92, 135.44, 136.23, 137.66; HRMS (EI$^+$) *m*/*z* 605.6958 (M^+, $C_{18}H_{10}S_2{}^{79}Br_4$, calcd 605.6977), 607.6937 (M^+, $C_{18}H_{10}S_2{}^{79}Br_3{}^{81}Br$, calcd 607.6937), 609.6915 (M^+, $C_{18}H_{10}S_2{}^{79}Br_2{}^{81}Br_2$, calcd 609.6916), 611.6896 (M^+, $C_{18}H_{10}S_2{}^{79}Br^{81}Br_3$, calcd 611.6896), 613.6874 (M^+, $C_{18}H_{10}S_2{}^{81}Br_4$, calcd 613.6875).

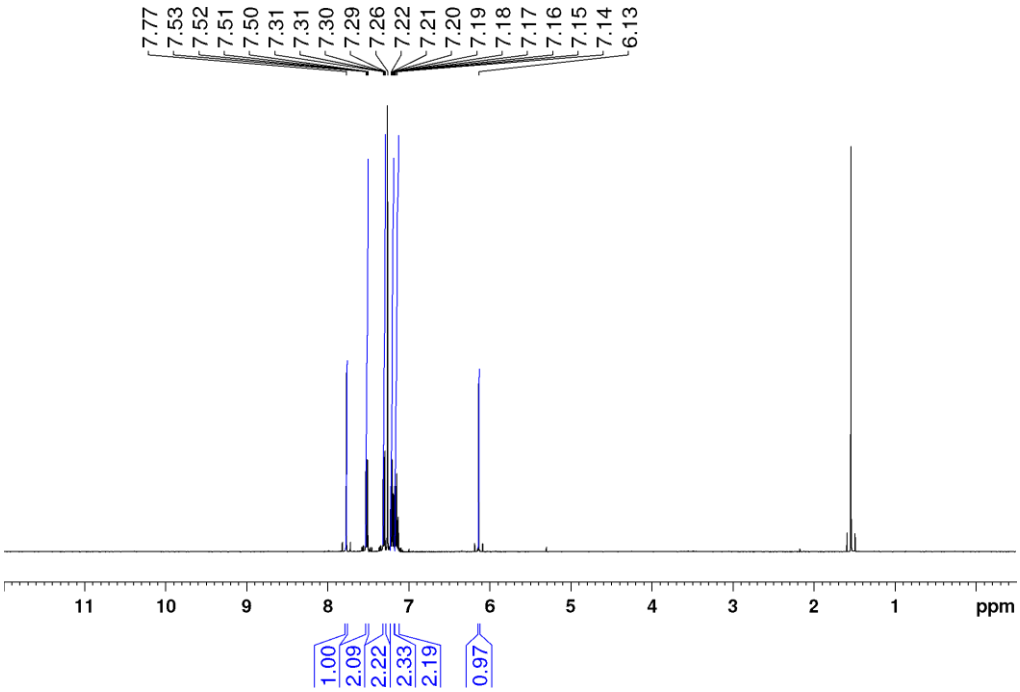


Figure S23. ^{1}H NMR spectrum of **10** in $CDCl_3$.

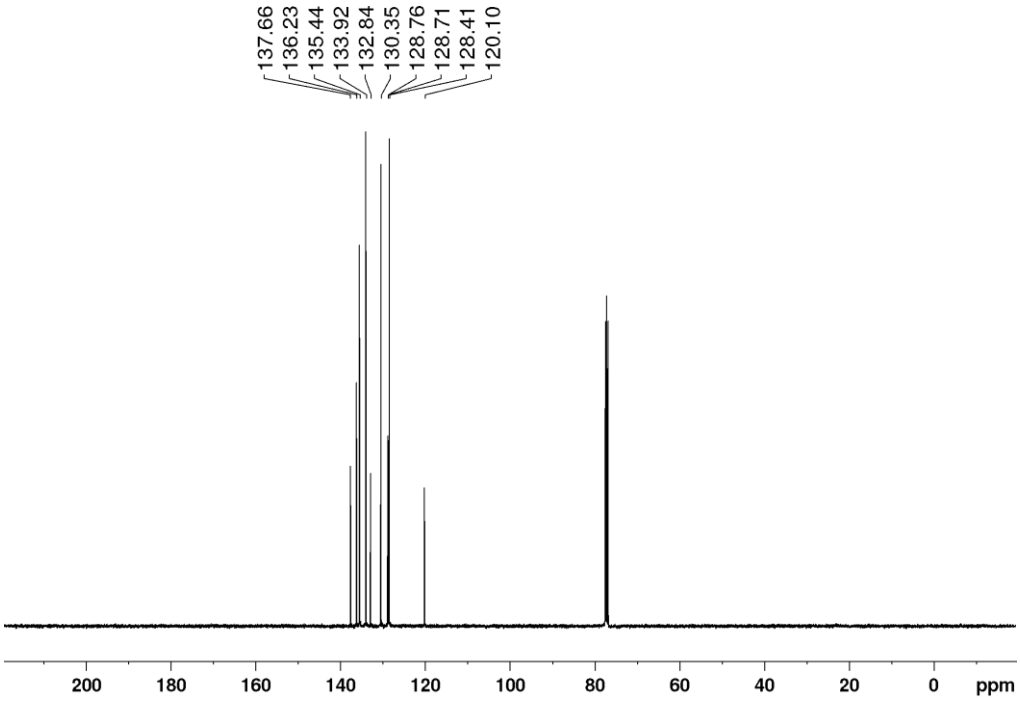
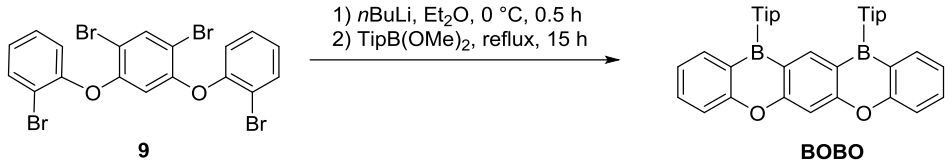


Figure S24. ^{13}C NMR spectrum of **10** in $CDCl_3$.

BOBO



To a Et_2O solution (100 mL) of **9** (0.80 g, 1.4 mmol) was added *n*BuLi (1.57 M in hexane, 3.9 mL, 6.1 mmol) at 0 °C, and the mixture was stirred for 30 min at 0 °C. To this mixture was added $TipB(OMe)_2$ (1.3 mL, 4.1 mmol). This mixture was refluxed for 15 h. The reaction was quenched with aq. NH_4Cl, and the mixture was extracted with $CHCl_3$. The organic layer was dried with $MgSO_4$, and the solvents were evaporated. The crude product was separated by column chromatography (SiO_2, eluent; hexane/$CHCl_3$ = 8:2, v/v) followed by recrystallization from $CHCl_3$/CH_3OH to give **BOBO** as a colorless solid (0.33 g, 0.48 mmol, 34%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 0.70 (d, J = 6.8 Hz, 12H), 0.93 (d, J = 6.9 Hz, 12H), 1.30 (d, J = 7.0 Hz, 12H), 2.28 (sept, J = 6.9 Hz, 4H), 2.90 (sept, J = 6.9 Hz, 2H), 6.91 (s, 4H), 7.23 (td, J =7.3, 1.0 Hz, 2H), 7.59 (d, J = 7.8 Hz, 2H), 7.60 (s, 1H), 7.72 (td, J = 7.1, 1.8 Hz, 2H), 7.84 (dd, J = 7.5, 1.7 Hz, 2H), 8.10 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.90, 24.24, 24.84, 34.50, 34.95, 103.36, 117.30, 119.72, 122.20, 122.71, 126.43, 134.55, 135.20, 137.02, 148.47, 149.24, 149.94, 158.85, 162.79; HRMS (ESI$^+$) *m*/*z* 686.44616 (M^+, calcd 686.4461).

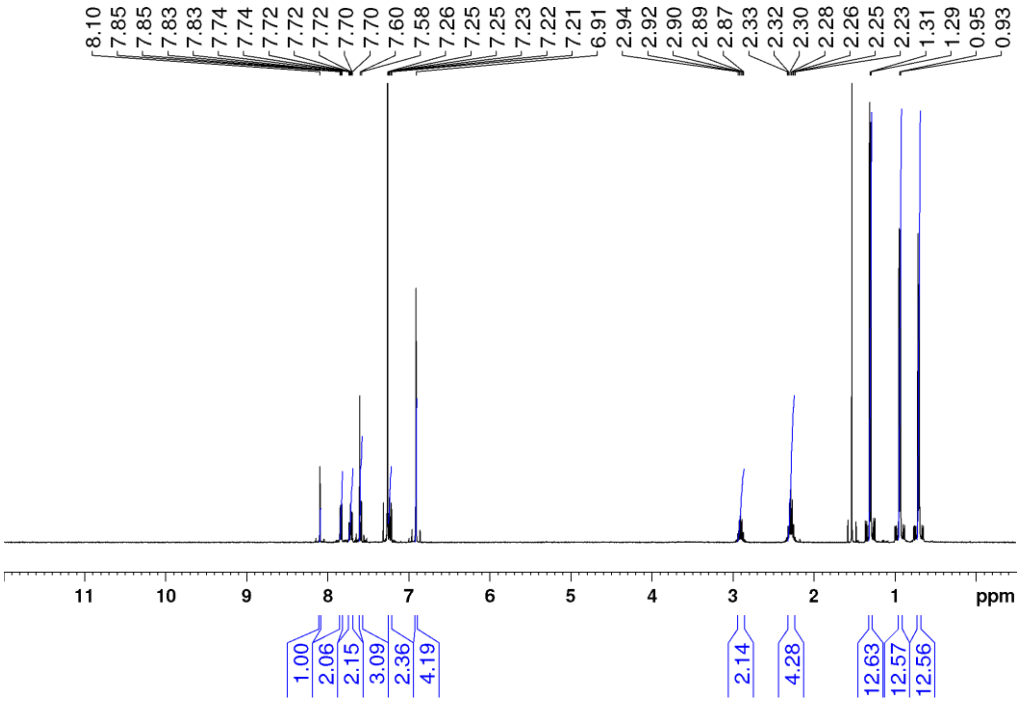


Figure S25. ^{1}H NMR spectrum of **BOBO** in $CDCl_3$.

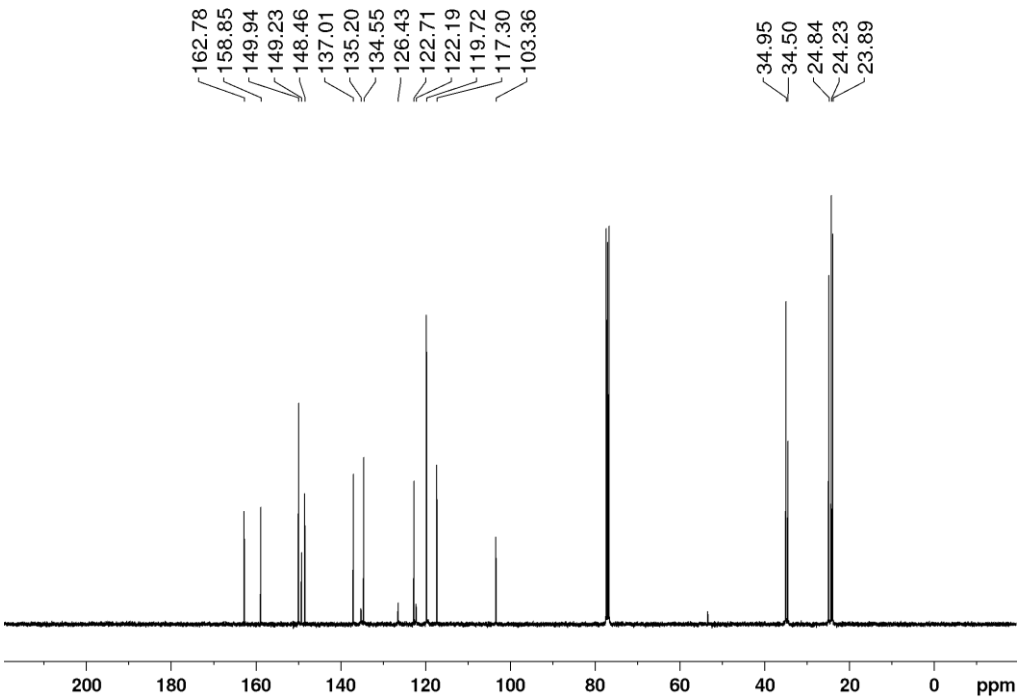


Figure S26. ^{13}C NMR spectrum of **BOBO** in $CDCl_3$.

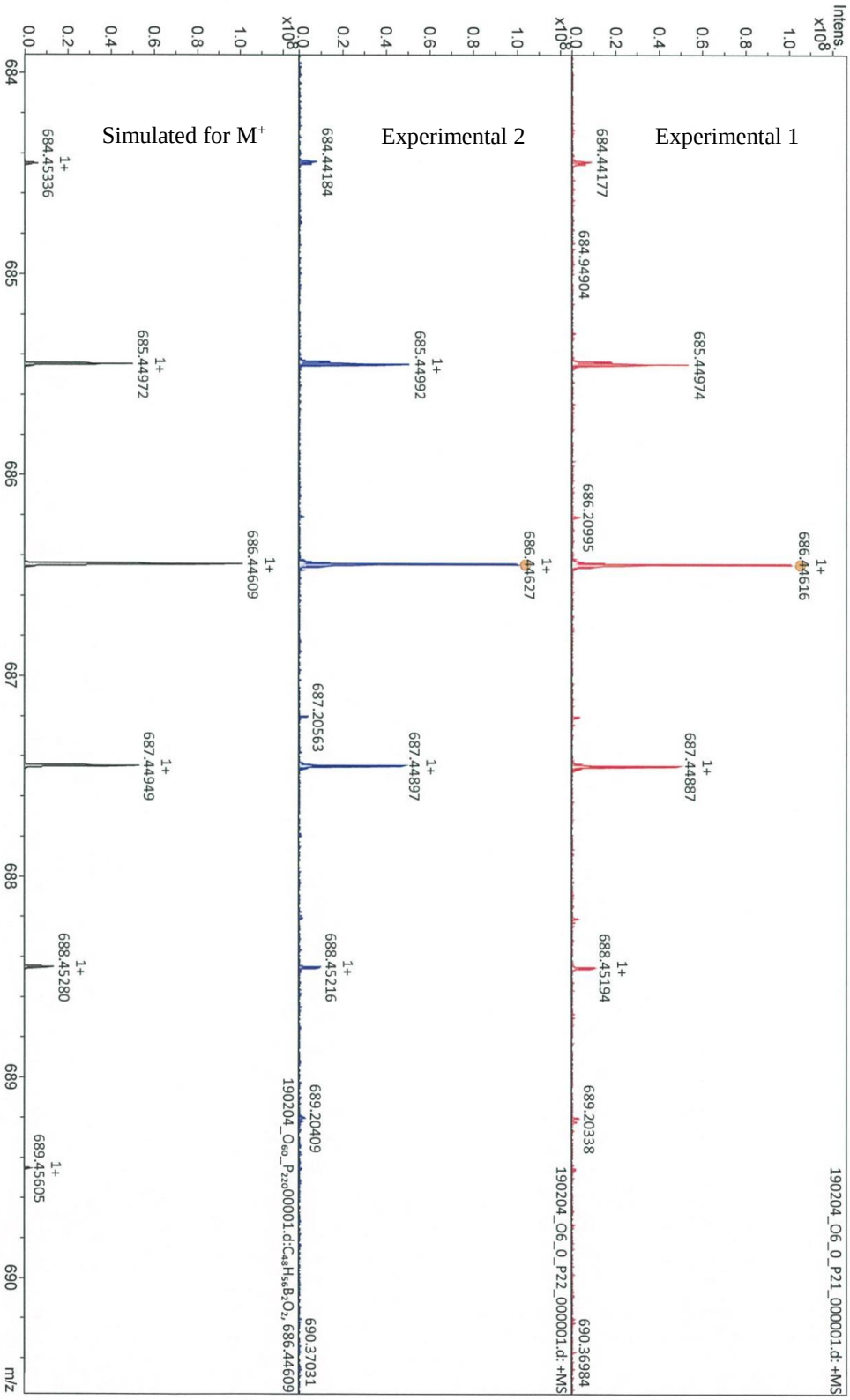
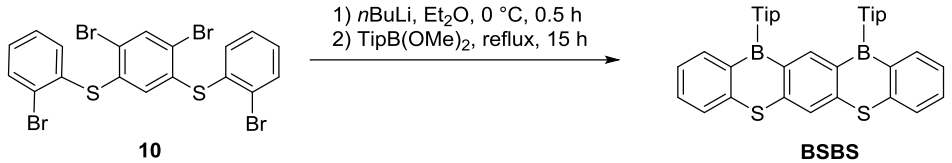


Figure S27. HRMS of **BOBO** (ESI^+). Results of two independent measurements (experimental 1 and 2) are shown.

BSBS



To a Et_2O solution (120 mL) of **10** (1.0 g, 1.6 mmol) was added *n*BuLi (1.57 M in hexane, 4.6 mL, 7.2 mmol) at 0 °C, and the mixture was stirred for 30 min at 0 °C. To this mixture was added $TipB(OMe)_2$ (1.5 mL, 4.9 mmol). This mixture was refluxed for 15 h. The reaction was quenched with aq. NH_4Cl, and the mixture was extracted with $CHCl_3$. The organic layer was dried with $MgSO_4$, and the solvents were evaporated. The crude product was separated by column chromatography (SiO_2, eluent: hexane/$CHCl_3$ = 8:2, v/v) followed by recrystallization from $CHCl_3/CH_3OH$ to give **BSBS** as a colorless solid (0.61 g, 0.85 mmol, 52%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 0.61 (d, J = 6.9 Hz, 12H), 0.87 (d, J = 6.9 Hz, 12H), 1.34 (d, J = 7.0 Hz, 12H), 2.13 (sept, J = 6.9 Hz, 4H), 2.92 (sept, J = 6.9 Hz, 2H), 6.88 (s, 4H), 7.27 (td, J =7.8, 1.3 Hz, 2H), 7.57 (td, J = 7.8, 1.3 Hz, 2H), 7.70 (d, J = 7.8 Hz, 2H), 7.88 (dd, J = 7.8, 1.3 Hz, 2H), 8.01 (s, 1H), 8.55 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.06, 24.30, 24.61, 34.44, 35.19, 119.70, 120.04, 124.62, 124.86, 130.82, 132.23, 135.51, 137.52, 140.27, 141.77, 146.66, 148.13, 149.40, 152.93; HRMS (ESI$^+$) *m*/*z* 718.40044 (M^+, calcd 718.4005).

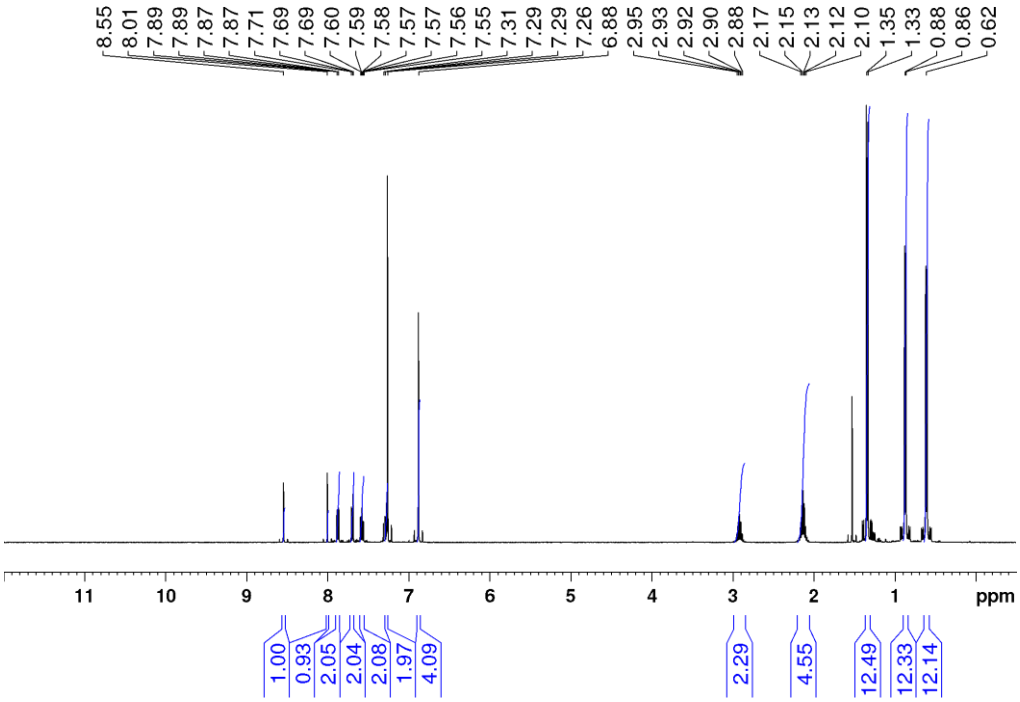


Figure S28 ^{1}H NMR spectrum of **BSBS** in $CDCl_3$.

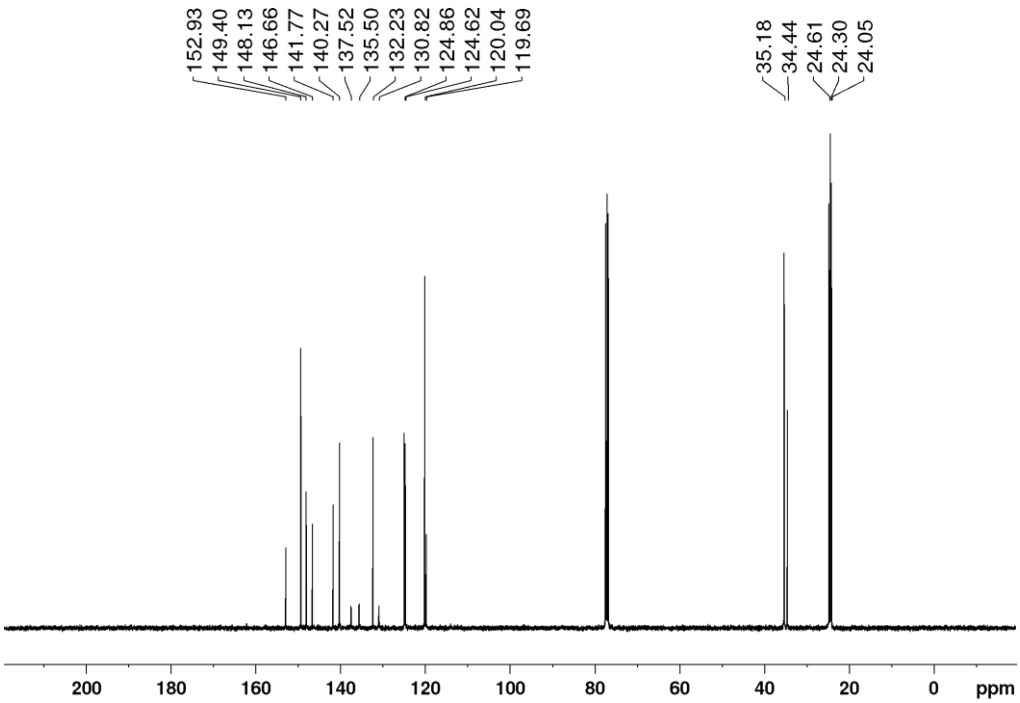


Figure S29. ^{13}C NMR spectrum of **BSBS** in $CDCl_3$.

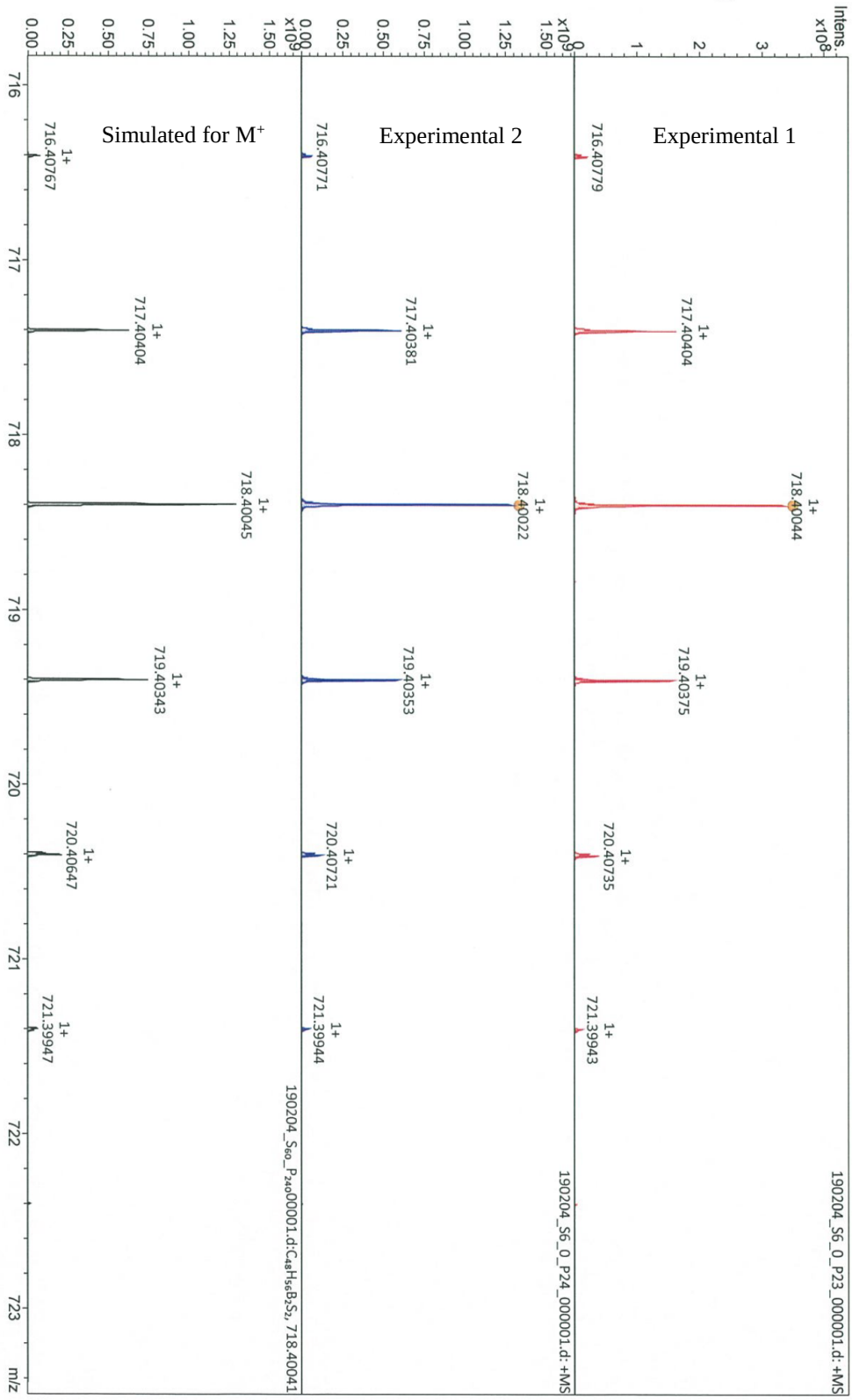


Figure S30. HRMS of **BSBS** (ESI^+). Results of two independent measurements (experimental 1 and 2) are shown.

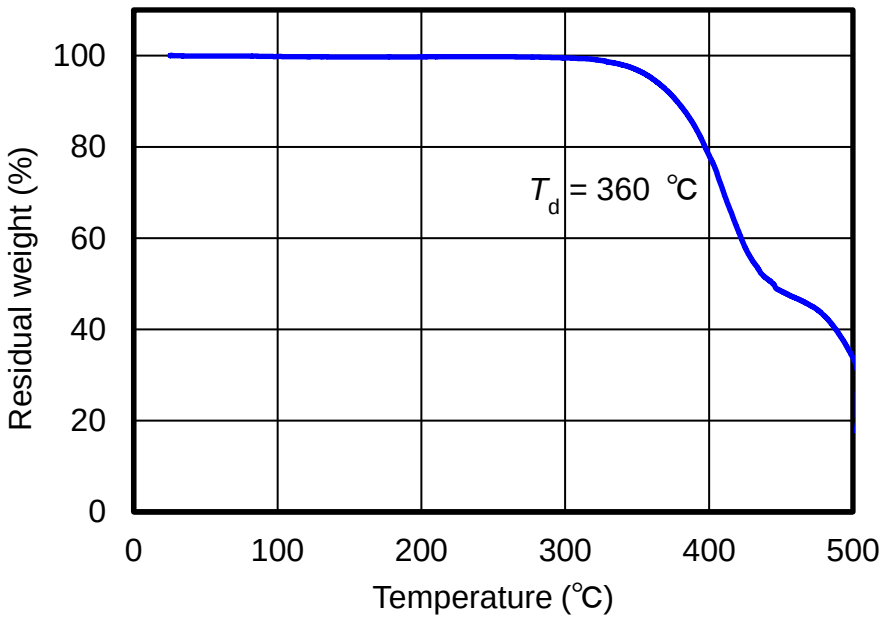


Figure S31. TGA curve of MCz-BOBO.

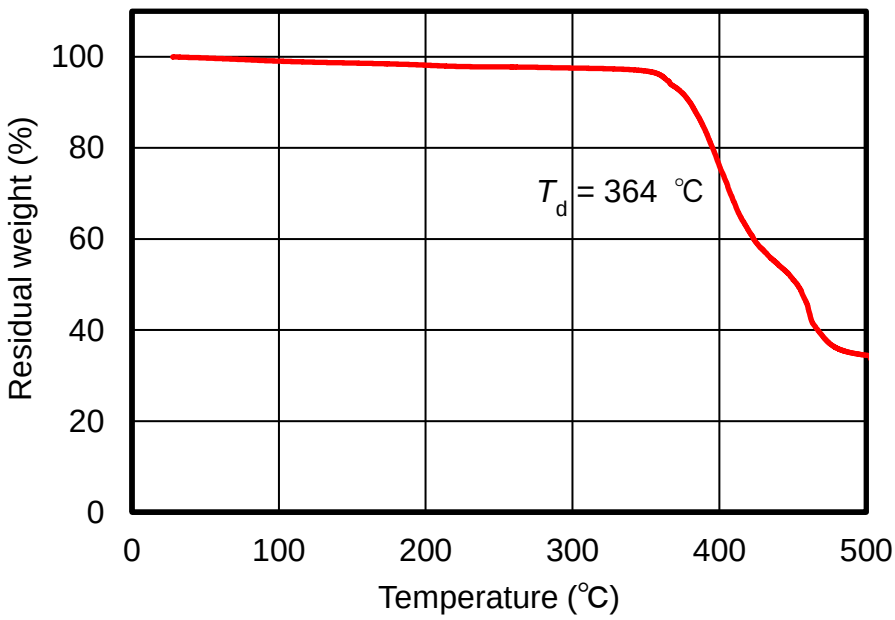


Figure S32. TGA curve of MCz-BSBS.

X-ray crystallography

Single crystals suitable for the X-ray analysis were obtained by recrystallization from $CHCl_3$. The single crystals were immersed in cryo-oil, mounted on a MicroMounts™, and measured at a temperature of 173 K (MCz-BOBO) or 103 K (MCz-BSBS). X-Ray diffraction data were recorded on a Rigaku XtaLabMini CCD diffractometer (MCz-BOBO) or on a Rigaku Saturn 724 CCD diffractometer equipped with a Rigaku VariMax optic system (MCz-BSBS) using Mo-*Kα* radiation (λ = 0.71075 Å). The reflection data were integrated, scaled and averaged by using the *CrysAlisPro* (ver. 1.171.38.46) (MCz-BOBO) or the *HKL-2000* (MCz-BSBS).[S5] Empirical absorption corrections were applied using the *SCALE3 ABSPACK* scaling algorithm (*CrysAlisPro*). The structures were solved by a direct method (*SHELXT-2014/5*) and refined by full-matrix least square method on F^2 for all reflections (*SHELXL-2016/6 or SHELXL-2014/7*)[S6] All hydrogen atoms were placed using AFIX instructions, while all the other atoms were refined anisotropically.

The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication materials. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

Table S1. Crystallographic data for MCz-BOBO-$(CHCl_3)_3$ and MCz-BSBS.

	MCz-BOBO-$(CHCl_3)_3$	MCz-BSBS
Empirical formula	$C_{67}H_{74}B_2Cl_9NO_2$	$C_{64}H_{71}B_2NS_2$
FW	1265.94	939.95
Temperature (K)	173	103
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	C_2/c
a (Å)	20.879(1)	46.427(2)
b (Å)	10.1453(6)	22.725(1)
c (Å)	32.428(2)	10.8682(5)
β (°)	105.291(7)	103.413(4)
V (Å^3)	6625.8(7)	11153.6(9)
Z	4	8
D_{calcd} (g cm^{-3})	1.269	1.120
μ (mm^{-1})	0.424	0.135
F(000)	2648	4032
Crystal size (mm)	0.41 x 0.21 x 0.17	0.15 x 0.10 x 0.05
θ_{range} (°)	1.847 to 25.499	1.804 to 25.249
Reflection collected	49235	63791
Independent reflections	12344	10080
R_{int}	0.1054	0.1478
Completeness to θ_{max}	100.0%	100.0%
Data/restraints/parameters	12344/0/746	10080/1/654
GOF on F^2	1.029	1.031
R_1 (I>2σ(I))	0.0729	0.0687
wR_2 (all data)	0.2251	0.1540
Largest diff. peak and hole (e Å^{-3})	0.739, –0.887	0.506, –0.329
CCDC	1935681	1935682

Photophysical measurements

Organic thin films for photophysical measurements were deposited under high vacuum (~7 × 10^{-5} Pa) onto quartz substrates using an ALS E-200 vacuum evaporation system. UV/Vis absorption and PL spectra were measured with a JASCO V-670 spectrometer and a JASCO FP-8600 spectrophotometer, respectively. The absolute PL quantum yields were determined using a JASCO ILF-835 integrating sphere system. The transient PL decay curves for the toluene solutions and thin films were measured using a Hamamatsu Photonics C11367 Quantaurus-tau fluorescence lifetime spectrometer (λ = 340 nm, pulse width = 100 ps, repetition rate = 20 Hz) under N_2. The ionization potentials (IP) of materials in neat films were determined using a Riken-Keiki AC-2 ultraviolet photoelectron spectrometer. The electron affinities (EA) were estimated by subtracting the optical energy gaps (E_g) from the measured IP values.

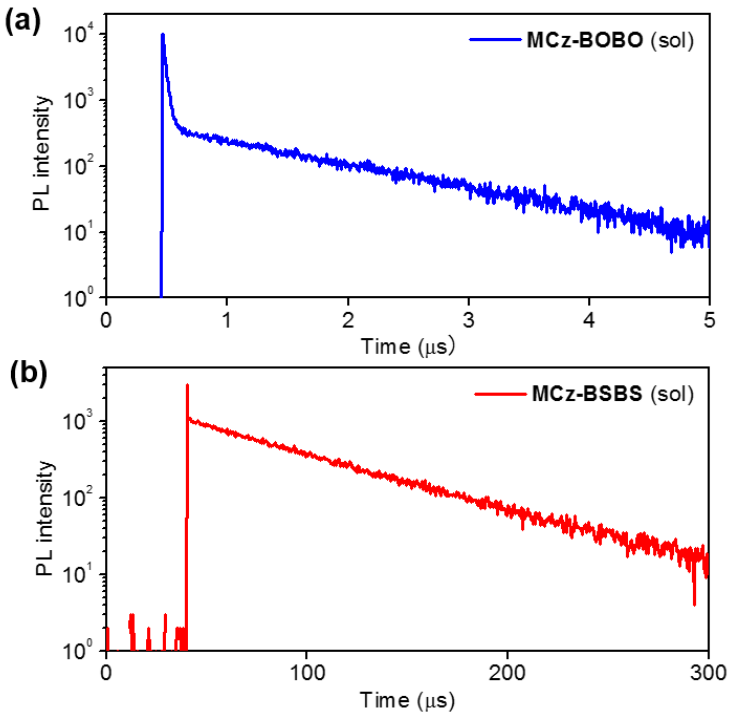


Figure S33. Transient PL decay profiles of (a) MCz-BOBO and (b) MCz-BSBS in deoxygenated toluene solutions.

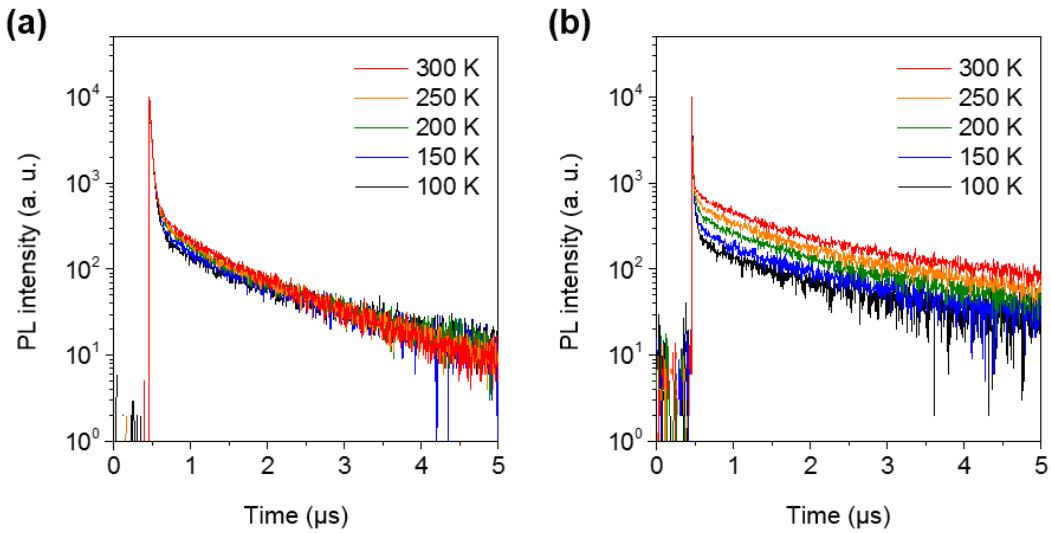


Figure S34. Temperature dependence of transient PL decays for (a) MCz-BOBO and (b) MCz-BSBS in the doped films in the PPF host in the temperature range of 100–300 K.

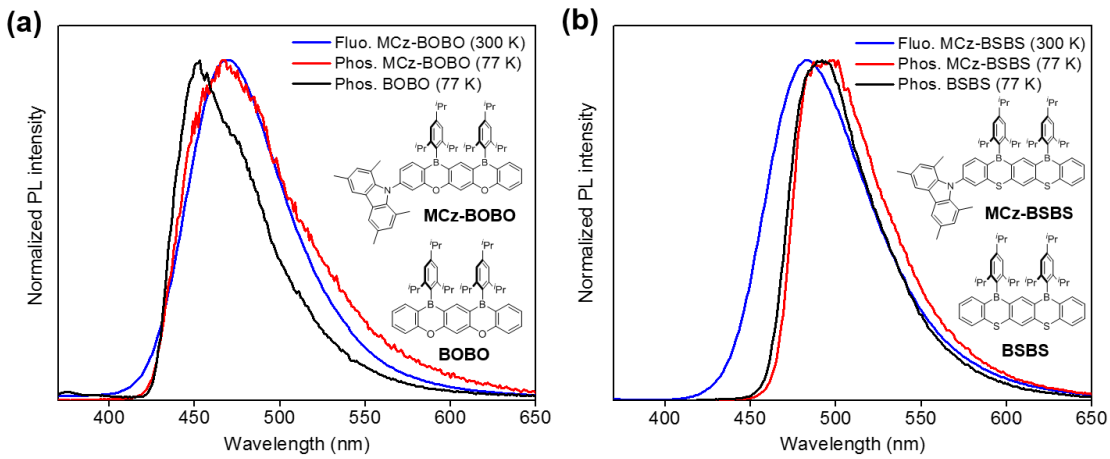


Figure S35. Fluorescence (blue) and phosphorescence (red) spectra of (a) MCz-BOBO and (b) MCz-BSBS in the doped films in the PPF host. Reference phosphorescence spectra (black) of BOBO and BSBS are also included. The lowest triplet (^{3}LE) energies of BOBO and BSBS can be estimated to be 2.92 and 2.69 eV, respectively.

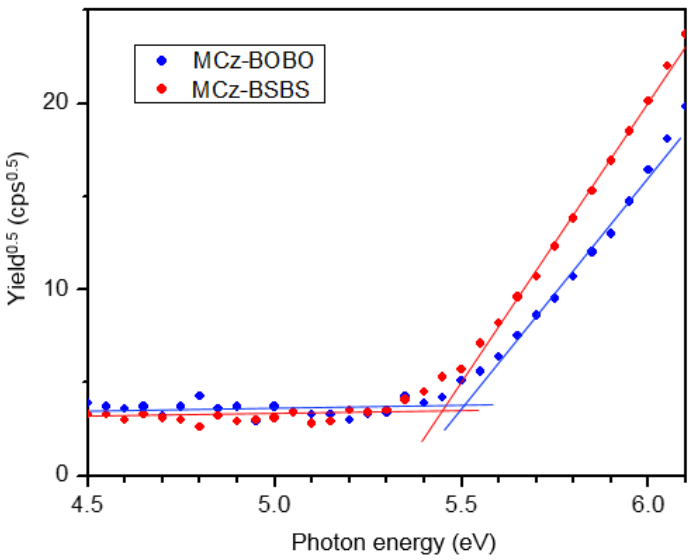


Figure S36. Photoelectron yield spectra of MCz-BOBO and MCz-BSBS in neat films measured in air.

OLED fabrication and evaluation

ITO-coated glass substrates were cleaned with detergent, deionized water, acetone, and isopropanol. The substrates were then subjected to UV-ozone treatment for 0.5 h before being loaded into an ALS E-200 vacuum evaporation system. The organic layers and a cathode Al layer were thermally evaporated on the substrates under vacuum with a deposition rate of <0.3 nm s^{-1} through a shadow mask, defining a pixel size of 0.04 cm^2. The thickness and deposition rate were monitored in situ during deposition by an oscillating quartz thickness monitor. The *J*–*V*–*L* characteristics of the fabricated OLED devices were measured using a Keithley 2400 source meter and a Konica Minolta CS-2000 spectroradiometer.

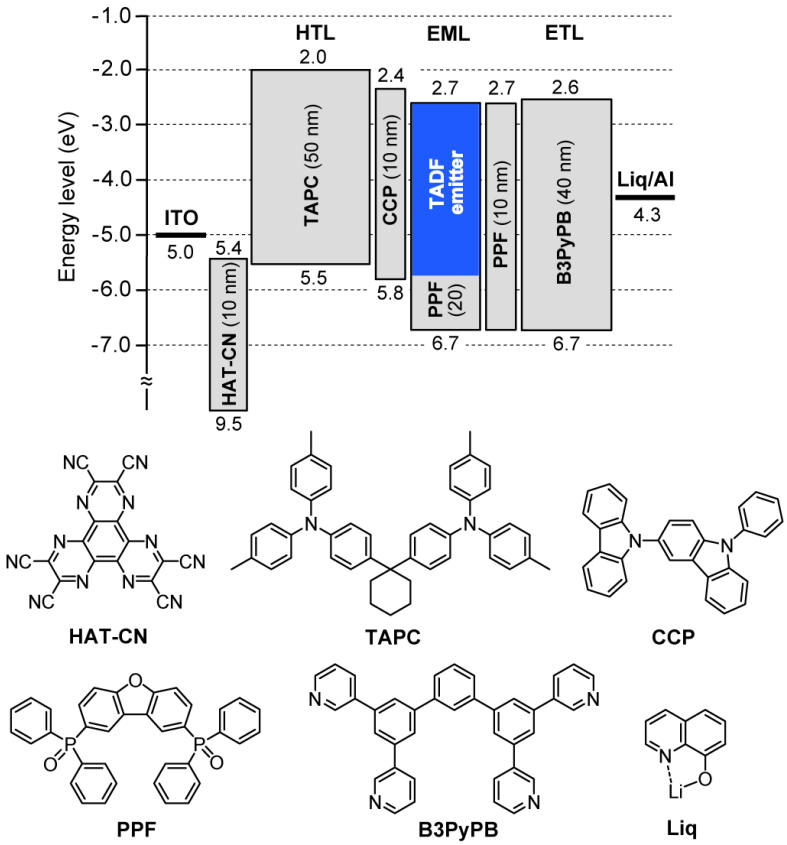


Figure S37. Energy level diagram and chemical structures of the materials for the TADF-OLEDs based on MCz-BOBO and MCz-BSBS as emitters.

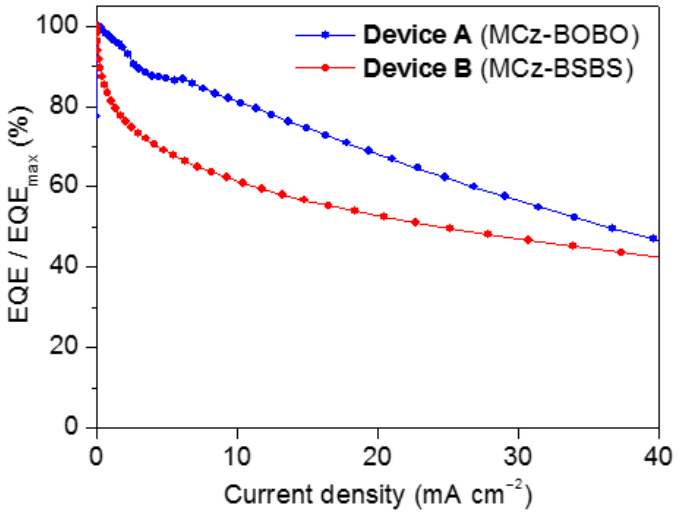


Figure S38. Efficiency roll-off behavior of devices A and B.

Quantum chemical calculations

Geometry optimizations in the S_0 states for MCz-BOBO and MCz-BSBS were performed using the PBE0 functional with the 6-31G(d) basis set in the gas phase, implemented in the Gaussian 16 program package. TD-DFT vertical excitation calculations were performed using the optimized geometry in the S_0 state at the same level of theory. Geometry optimization in the S_1 and T_1 states were performed using the optimized geometry in the S_0 state as initial geometry with TD-DFT method at the same level of theory. The T_2 states were simulated using the optimized T_1 geometries. The computational geometry data for MCz-BOBO and MCz-BSBS were provided in pages S40–S55.

The spin-orbit coupling (SOC) matrix elements $\langle S_n|H_{\mathrm{SOC}}|T_m\rangle$ at the optimized T_1 geometries were calculated by using a scalar relativistic TD-DFT with the two-component zeroth-order regular approximation (ZORA)[S7] and the PBE0 functional and the DZP basis set, implemented in the ADF2017 program package.[S8] The contributions of the three degenerate triplet states ($T_{m,x}$, $T_{m,y}$, and $T_{m,z}$) were taken into account by calculating the root sum square of the real and imaginary parts (Re and Im) of the matrix elements, as expressed by the following equation:[S9]

$$\langle S_n|H_{\mathrm{SOC}}|T_m\rangle = \left\{ \sum_{a=x,y,z} \left(\mathrm{Re}^2\langle S_n|H_{\mathrm{SOC}}|T_{m,a}\rangle + \mathrm{Im}^2\langle S_n|H_{\mathrm{SOC}}|T_{m,a}\rangle\right) \right\}^{1/2}$$

Geometry data for MCz-BOBO (S_0 optimization: unit Å)

C	2.738899	–2.981400	1.773100
C	1.680599	–2.222000	1.268400
C	1.886999	–1.040500	0.538600
C	3.224800	–0.646200	0.334699
C	4.289600	–1.378600	0.827700
C	4.038900	–2.555299	1.548899
O	0.445100	–2.728500	1.530900
C	–0.692900	–2.087599	1.162300
C	–0.683399	–0.860900	0.457400
B	0.661300	–0.264299	0.008499
C	–1.867199	–2.738400	1.517200
C	–3.077600	–2.134800	1.195599
C	–3.153799	–0.873300	0.559299
C	–1.934900	–0.287700	0.195700
O	–4.176200	–2.841100	1.551300
C	–5.441300	–2.394900	1.304000
C	–5.713100	–1.143599	0.727999
B	–4.535000	–0.228100	0.338700
C	–6.454500	–3.277999	1.684000
C	–7.774000	–2.909400	1.482899
C	–8.090999	–1.670500	0.911399
C	–7.071100	–0.808999	0.547499
C	0.779699	0.970999	–0.963600
C	–4.715300	1.255800	–0.163899
C	0.983100	0.739500	–2.341000
C	1.051000	1.818300	–3.222500
C	0.938700	3.136499	–2.778999
C	0.758600	3.352699	–1.414600
C	0.670200	2.297800	–0.503900
C	–4.638600	1.596299	–1.531000
C	–4.766100	2.929199	–1.920100
C	–4.956599	3.952300	–0.989900
C	–5.039400	3.603299	0.355700
C	–4.929699	2.277600	0.782300
C	0.990299	4.301300	–3.747100
C	2.302100	4.339100	–4.534800
C	–0.216799	4.293000	–4.689899
C	–5.058299	5.400699	–1.423900
C	–3.758300	5.883000	–2.074500
C	–6.255099	5.637999	–2.348600
C	–5.029300	1.963300	2.267600
C	–4.473000	0.511600	–2.583200
C	–5.825800	0.149500	–3.206300
C	–3.457100	0.870700	–3.668899
C	–3.884300	2.592299	3.065099
C	–6.389200	2.365900	2.843600
C	1.119200	–0.675799	–2.883599
C	–0.016099	–1.035599	–3.844700
C	2.486000	–0.905700	–3.533700
C	0.511000	2.589200	0.979300
C	1.853700	2.986600	1.602500
C	–0.555800	3.644900	1.275399

N	5.124800	–3.321000	2.050899
C	5.753500	–4.372299	1.376899
C	6.840299	–4.811999	2.162399
C	6.873100	–3.991700	3.343999
C	5.804200	–3.075600	3.247799
C	7.723300	–3.981700	4.452199
C	7.512800	–3.060700	5.466100
C	6.435299	–2.164200	5.345200
C	5.557199	–2.134199	4.265500
C	5.462199	–4.971200	0.135999
C	6.302100	–6.013300	–0.246300
C	7.387600	–6.478499	0.518299
C	7.651800	–5.864400	1.732299
C	4.331800	–4.565599	–0.770500
C	4.429800	–1.137900	4.257699
C	8.403600	–3.007899	6.677199
C	8.231900	–7.616300	0.012899
H	2.542200	–3.890200	2.332500
H	3.406900	0.263800	–0.232099
H	5.317499	–1.068600	0.665099
H	–1.841200	–3.692500	2.031599
H	–1.961000	0.670000	–0.321000
H	–6.188200	–4.232300	2.127499
H	–8.568000	–3.592100	1.773900
H	–9.129700	–1.391900	0.758900
H	–7.302100	0.158200	0.107100
H	1.192900	1.625499	–4.284699
H	0.679199	4.377799	–1.057199
H	–4.708800	3.180699	–2.977100
H	–5.190400	4.392000	1.091799
H	0.936299	5.221099	–3.148100
H	2.338199	5.221700	–5.184000
H	3.167000	4.371900	–3.863800
H	2.408499	3.454400	–5.173400
H	–0.201899	5.168700	–5.349500
H	–1.156599	4.302199	–4.127099
H	–0.215799	3.397500	–5.322599
H	–5.216600	5.999400	–0.515999
H	–3.820500	6.948499	–2.325199
H	–2.903099	5.735600	–1.406199
H	–3.554200	5.334000	–3.001599
H	–6.341399	6.700099	–2.606500
H	–7.190800	5.323300	–1.874500
H	–6.149999	5.076900	–3.284499
H	–4.942000	0.874300	2.386400
H	–4.096899	–0.386800	–2.071900
H	–5.713699	–0.655299	–3.942600
H	–6.538700	–0.183499	–2.444500
H	–6.260000	1.017700	–3.716800
H	–3.284399	0.011100	–4.326699
H	–2.495200	1.172100	–3.240199
H	–3.814100	1.692100	–4.301200
H	–3.962200	2.328200	4.126400
H	–2.912600	2.247200	2.697300

H	–3.900800	3.686000	2.990500
H	–6.457100	2.089600	3.902399
H	–7.207100	1.870499	2.309600
H	–6.548100	3.448200	2.771100
H	1.049300	–1.368900	–2.033300
H	0.089000	–2.068600	–4.196900
H	–0.991000	–0.938000	–3.356500
H	–0.015800	–0.381300	–4.724499
H	2.582599	–1.943400	–3.874099
H	3.299499	–0.701200	–2.829300
H	2.627100	–0.255100	–4.404699
H	0.187200	1.656300	1.464399
H	1.746700	3.166200	2.679000
H	2.605999	2.203100	1.461500
H	2.236200	3.905699	1.142499
H	–0.712900	3.733899	2.356499
H	–1.515099	3.392599	0.810700
H	–0.256100	4.634300	0.910800
H	8.544200	–4.692500	4.517400
H	6.269899	–1.447099	6.148099
H	6.101499	–6.496300	–1.201700
H	8.486499	–6.196399	2.345799
H	4.377799	–3.507099	–1.048599
H	4.367300	–5.154299	–1.692100
H	3.351599	–4.729899	–0.309000
H	3.450200	–1.623099	4.188200
H	4.446200	–0.552300	5.181700
H	4.496299	–0.437500	3.417900
H	7.834999	–3.161800	7.602500
H	9.179600	–3.778299	6.632500
H	8.905000	–2.036200	6.766200
H	8.681899	–7.382800	–0.959800
H	9.045099	–7.845899	0.708299
H	7.639300	–8.530100	–0.118499

Geometry data for MCz–BOBO (S_1 optimization: unit Å)

C	2.738899	–2.981400	1.773100
C	1.680599	–2.222000	1.268400
C	1.886999	–1.040500	0.538600
C	3.224800	–0.646200	0.334699
C	4.289600	–1.378600	0.827700
C	4.038900	–2.555299	1.548899
O	0.445100	–2.728500	1.530900
C	–0.692900	–2.087599	1.162300
C	–0.683399	–0.860900	0.457400
B	0.661300	–0.264299	0.008499
C	–1.867199	–2.738400	1.517200
C	–3.077600	–2.134800	1.195599
C	–3.153799	–0.873300	0.559299
C	–1.934900	–0.287700	0.195700
O	–4.176200	–2.841100	1.551300
C	–5.441300	–2.394900	1.304000

C	–5.713100	–1.143599	0.727999
B	–4.535000	–0.228100	0.338700
C	–6.454500	–3.277999	1.684000
C	–7.774000	–2.909400	1.482899
C	–8.090999	–1.670500	0.911399
C	–7.071100	–0.808999	0.547499
C	0.779699	0.970999	–0.963600
C	–4.715300	1.255800	–0.163899
C	0.983100	0.739500	–2.341000
C	1.051000	1.818300	–3.222500
C	0.938700	3.136499	–2.778999
C	0.758600	3.352699	–1.414600
C	0.670200	2.297800	–0.503900
C	–4.638600	1.596299	–1.531000
C	–4.766100	2.929199	–1.920100
C	–4.956599	3.952300	–0.989900
C	–5.039400	3.603299	0.355700
C	–4.929699	2.277600	0.782300
C	0.990299	4.301300	–3.747100
C	2.302100	4.339100	–4.534800
C	–0.216799	4.293000	–4.689899
C	–5.058299	5.400699	–1.423900
C	–3.758300	5.883000	–2.074500
C	–6.255099	5.637999	–2.348600
C	–5.029300	1.963300	2.267600
C	–4.473000	0.511600	–2.583200
C	–5.825800	0.149500	–3.206300
C	–3.457100	0.870700	–3.668899
C	–3.884300	2.592299	3.065099
C	–6.389200	2.365900	2.843600
C	1.119200	–0.675799	–2.883599
C	–0.016099	–1.035599	–3.844700
C	2.486000	–0.905700	–3.533700
C	0.511000	2.589200	0.979300
C	1.853700	2.986600	1.602500
C	–0.555800	3.644900	1.275399
N	5.124800	–3.321000	2.050899
C	5.753500	–4.372299	1.376899
C	6.840299	–4.811999	2.162399
C	6.873100	–3.991700	3.343999
C	5.804200	–3.075600	3.247799
C	7.723300	–3.981700	4.452199
C	7.512800	–3.060700	5.466100
C	6.435299	–2.164200	5.345200
C	5.557199	–2.134199	4.265500
C	5.462199	–4.971200	0.135999
C	6.302100	–6.013300	–0.246300
C	7.387600	–6.478499	0.518299
C	7.651800	–5.864400	1.732299
C	4.331800	–4.565599	–0.770500
C	4.429800	–1.137900	4.257699
C	8.403600	–3.007899	6.677199
C	8.231900	–7.616300	0.012899
H	2.542200	–3.890200	2.332500

H	3.406900	0.263800	–0.232099
H	5.317499	–1.068600	0.665099
H	–1.841200	–3.692500	2.031599
H	–1.961000	0.670000	–0.321000
H	–6.188200	–4.232300	2.127499
H	–8.568000	–3.592100	1.773900
H	–9.129700	–1.391900	0.758900
H	–7.302100	0.158200	0.107100
H	1.192900	1.625499	–4.284699
H	0.679199	4.377799	–1.057199
H	–4.708800	3.180699	–2.977100
H	–5.190400	4.392000	1.091799
H	0.936299	5.221099	–3.148100
H	2.338199	5.221700	–5.184000
H	3.167000	4.371900	–3.863800
H	2.408499	3.454400	–5.173400
H	–0.201899	5.168700	–5.349500
H	–1.156599	4.302199	–4.127099
H	–0.215799	3.397500	–5.322599
H	–5.216600	5.999400	–0.515999
H	–3.820500	6.948499	–2.325199
H	–2.903099	5.735600	–1.406199
H	–3.554200	5.334000	–3.001599
H	–6.341399	6.700099	–2.606500
H	–7.190800	5.323300	–1.874500
H	–6.149999	5.076900	–3.284499
H	–4.942000	0.874300	2.386400
H	–4.096899	–0.386800	–2.071900
H	–5.713699	–0.655299	–3.942600
H	–6.538700	–0.183499	–2.444500
H	–6.260000	1.017700	–3.716800
H	–3.284399	0.011100	–4.326699
H	–2.495200	1.172100	–3.240199
H	–3.814100	1.692100	–4.301200
H	–3.962200	2.328200	4.126400
H	–2.912600	2.247200	2.697300
H	–3.900800	3.686000	2.990500
H	–6.457100	2.089600	3.902399
H	–7.207100	1.870499	2.309600
H	–6.548100	3.448200	2.771100
H	1.049300	–1.368900	–2.033300
H	0.089000	–2.068600	–4.196900
H	–0.991000	–0.938000	–3.356500
H	–0.015800	–0.381300	–4.724499
H	2.582599	–1.943400	–3.874099
H	3.299499	–0.701200	–2.829300
H	2.627100	–0.255100	–4.404699
H	0.187200	1.656300	1.464399
H	1.746700	3.166200	2.679000
H	2.605999	2.203100	1.461500
H	2.236200	3.905699	1.142499
H	–0.712900	3.733899	2.356499
H	–1.515099	3.392599	0.810700
H	–0.256100	4.634300	0.910800

H	8.544200	–4.692500	4.517400
H	6.269899	–1.447099	6.148099
H	6.101499	–6.496300	–1.201700
H	8.486499	–6.196399	2.345799
H	4.377799	–3.507099	–1.048599
H	4.367300	–5.154299	–1.692100
H	3.351599	–4.729899	–0.309000
H	3.450200	–1.623099	4.188200
H	4.446200	–0.552300	5.181700
H	4.496299	–0.437500	3.417900
H	7.834999	–3.161800	7.602500
H	9.179600	–3.778299	6.632500
H	8.905000	–2.036200	6.766200
H	8.681899	–7.382800	–0.959800
H	9.045099	–7.845899	0.708299
H	7.639300	–8.530100	–0.118499

Geometry data for MCz–BOBO (T_1 optimization: unit Å)

C	2.783600	–2.953400	1.766300
C	1.737699	–2.193000	1.269999
C	1.925699	–1.010300	0.505399
C	3.287400	–0.651600	0.264900
C	4.354300	–1.386899	0.745800
C	4.099999	–2.538099	1.498600
O	0.499100	–2.682000	1.559499
C	–0.647700	–2.041700	1.188099
C	–0.640900	–0.823600	0.464500
B	0.711499	–0.243700	0.007000
C	–1.810199	–2.692300	1.568400
C	–3.036500	–2.102600	1.254899
C	–3.126500	–0.858599	0.601599
C	–1.903300	–0.266300	0.215300
O	–4.122000	–2.821500	1.644899
C	–5.391600	–2.391600	1.421000
C	–5.680700	–1.151099	0.826700
B	–4.512599	–0.242100	0.394600
C	–6.393500	–3.272400	1.838900
C	–7.719800	–2.916500	1.662700
C	–8.053700	–1.688300	1.075499
C	–7.046599	–0.829600	0.672400
C	0.818399	1.007599	–0.966100
C	–4.727699	1.227799	–0.149899
C	1.047900	0.815299	–2.347400
C	1.097600	1.909800	–3.213199
C	0.938200	3.216200	–2.754600
C	0.729300	3.403399	–1.389999
C	0.660899	2.330699	–0.498400
C	–4.665400	1.527600	–1.527700
C	–4.825200	2.843100	–1.961900
C	–5.031900	3.893100	–1.065999
C	–5.096700	3.587800	0.290600
C	–4.956499	2.278999	0.760099

C	0.965000	4.397900	–3.703499
C	2.285600	4.492900	–4.471599
C	–0.226699	4.367600	–4.665200
C	–5.167600	5.323699	–1.547599
C	–3.884899	5.811400	–2.227700
C	–6.377800	5.505700	–2.467400
C	–5.024499	2.017699	2.257100
C	–4.473899	0.413000	–2.543599
C	–5.821200	–0.019700	–3.132500
C	–3.485599	0.768100	–3.655500
C	–3.841600	2.649600	2.994899
C	–6.357499	2.467300	2.859800
C	1.220900	–0.581500	–2.925799
C	0.073700	–0.953000	–3.868300
C	2.576500	–0.753200	–3.615999
C	0.468800	2.593199	0.986899
C	1.821500	2.829599	1.668300
C	–0.493900	3.741200	1.292699
N	5.195000	–3.315200	2.008600
C	5.805000	–4.356300	1.341800
C	6.850500	–4.865500	2.157799
C	6.846999	–4.072400	3.373500
C	5.799600	–3.122900	3.232000
C	7.621500	–4.103299	4.510499
C	7.360999	–3.173800	5.539899
C	6.324900	–2.249400	5.376599
C	5.509699	–2.175900	4.243499
C	5.521300	–4.901399	0.066699
C	6.340900	–5.965800	–0.319300
C	7.375600	–6.484799	0.464800
C	7.629700	–5.916600	1.731000
C	4.439199	–4.426700	–0.851899
C	4.425800	–1.146300	4.173900
C	8.192100	–3.188100	6.785800
C	8.211900	–7.628500	–0.021100
H	2.573699	–3.850399	2.341200
H	3.477799	0.244200	–0.320799
H	5.379200	–1.082299	0.546600
H	–1.770299	–3.638000	2.097499
H	–1.946299	0.683000	–0.314700
H	–6.110199	–4.217100	2.293200
H	–8.503799	–3.597599	1.983800
H	–9.097000	–1.415899	0.941000
H	–7.294500	0.127700	0.218600
H	1.256900	1.736400	–4.277099
H	0.606600	4.419799	–1.020100
H	–4.777700	3.059500	–3.027399
H	–5.255799	4.397999	1.001600
H	0.872200	5.305900	–3.090900
H	2.302400	5.385000	–5.109500
H	3.138500	4.544500	–3.786400
H	2.431000	3.619900	–5.118800
H	–0.231200	5.253000	–5.312800
H	–1.173700	4.337599	–4.115600

H	–0.188300	3.480999	–5.309300
H	–5.329900	5.949600	–0.658599
H	–3.971200	6.866500	–2.514700
H	–3.020600	5.703700	–1.563699
H	–3.677900	5.234299	–3.136900
H	–6.488700	6.556000	–2.762899
H	–7.301900	5.188699	–1.972299
H	–6.270500	4.912399	–3.383100
H	–4.954700	0.932400	2.407800
H	–4.057999	–0.449500	–2.004300
H	–5.690700	–0.846900	–3.841100
H	–6.509400	–0.350000	–2.347099
H	–6.294300	0.813199	–3.667300
H	–3.289100	–0.109500	–4.282599
H	–2.530599	1.117300	–3.248799
H	–3.878499	1.552200	–4.313999
H	–3.889100	2.425200	4.067699
H	–2.891800	2.268099	2.606600
H	–3.837499	3.740299	2.879800
H	–6.399799	2.222699	3.928000
H	–7.200199	1.973099	2.364600
H	–6.498200	3.550399	2.761699
H	1.191600	–1.284900	–2.084000
H	0.198399	–1.974100	–4.250299
H	–0.888699	–0.898000	–3.349800
H	0.028600	–0.276700	–4.730699
H	2.697899	–1.781400	–3.979900
H	3.399300	–0.535200	–2.926200
H	2.677700	–0.084099	–4.479299
H	0.039899	1.679399	1.419700
H	1.694900	2.983199	2.747599
H	2.490699	1.975199	1.519800
H	2.311600	3.720100	1.254600
H	–0.694800	3.789700	2.369400
H	–1.450700	3.612799	0.775100
H	–0.077900	4.713100	1.000199
H	8.423500	–4.828300	4.624200
H	6.136400	–1.540800	6.178600
H	6.157300	–6.415000	–1.291599
H	8.430299	–6.310300	2.352000
H	4.570700	–3.375199	–1.123199
H	4.435400	–5.027300	–1.765100
H	3.453700	–4.495299	–0.381900
H	3.441600	–1.605899	4.044300
H	4.417599	–0.550699	5.090300
H	4.559400	–0.476099	3.319800
H	7.869500	–2.423400	7.496200
H	8.133600	–4.163000	7.284600
H	9.249400	–3.012100	6.553099
H	7.894300	–7.971000	–1.008799
H	9.268599	–7.341699	–0.084099
H	8.152899	–8.478300	0.669499

Geometry data for MCz–BSBS (S_0 optimization: unit Å)

C	2.839300	–3.143700	1.859799
C	1.655200	–2.555299	1.395000
C	1.673099	–1.364300	0.640499
C	2.941700	–0.806400	0.372000
C	4.118700	–1.375799	0.824400
C	4.062600	–2.556499	1.574000
S	0.198000	–3.440700	1.800399
C	–1.139100	–2.473900	1.218000
C	–0.995599	–1.239799	0.533299
B	0.383099	–0.675500	0.114500
C	–2.394200	–3.023900	1.468500
C	–3.547500	–2.338199	1.089599
C	–3.479999	–1.052700	0.493599
C	–2.190100	–0.570099	0.220400
S	–5.035499	–3.190399	1.426599
C	–6.334600	–2.156200	0.861500
C	–6.144200	–0.854199	0.354800
B	–4.743200	–0.206500	0.194299
C	–7.615200	–2.715099	0.979599
C	–8.725500	–1.982100	0.595400
C	–8.576099	–0.685599	0.095300
C	–7.307200	–0.143299	–0.013799
C	0.510500	0.533399	–0.896900
C	–4.630100	1.322400	–0.195800
C	0.702300	0.241200	–2.264600
C	0.835200	1.280699	–3.184800
C	0.798999	2.618800	–2.788899
C	0.624800	2.893700	–1.434600
C	0.475800	1.879299	–0.485400
C	–4.439600	1.757400	–1.523500
C	–4.365200	3.123000	–1.799199
C	–4.466199	4.084400	–0.792699
C	–4.661699	3.642700	0.513999
C	–4.751399	2.284299	0.826800
C	0.936399	3.743699	–3.795299
C	2.266700	3.679000	–4.550000
C	–0.245700	3.771400	–4.768400
C	–4.364200	5.564100	–1.104600
C	–2.992899	5.925599	–1.682499
C	–5.489600	6.028900	–2.032699
C	–4.982900	1.862099	2.270299
C	–4.364599	0.752300	–2.662299
C	–5.690300	0.688899	–3.428800
C	–3.204300	1.021599	–3.622000
C	–3.819099	2.257399	3.181899
C	–6.313000	2.394100	2.809900
C	0.772500	–1.200500	–2.747699
C	–0.381300	–1.552300	–3.689200
C	2.125699	–1.518900	–3.388600
C	0.329099	2.238100	0.984899
C	1.677199	2.642799	1.591400
C	–0.716099	3.327599	1.231600

N	5.258600	–3.163100	2.038999
C	5.961199	–4.177300	1.380399
C	7.136299	–4.446500	2.113900
C	7.146500	–3.558999	3.246400
C	5.976000	–2.774500	3.174499
C	8.054000	–3.391499	4.294900
C	7.798800	–2.444600	5.274199
C	6.618200	–1.684899	5.181399
C	5.680099	–1.814499	4.161300
C	5.669900	–4.872600	0.190800
C	6.599700	–5.835600	–0.191600
C	7.773300	–6.133700	0.524400
C	8.036500	–5.424900	1.685899
C	4.453199	–4.643900	–0.664600
C	4.443399	–0.957700	4.182199
C	8.747899	–2.223799	6.420199
C	8.710700	–7.198500	0.024100
H	2.817999	–4.058999	2.445700
H	2.979400	0.104000	–0.220500
H	5.085299	–0.932500	0.603900
H	–2.475200	–3.990999	1.960600
H	–2.109199	0.397299	–0.271600
H	–7.735300	–3.722099	1.371900
H	–9.714800	–2.422699	0.687600
H	–9.448100	–0.110099	–0.201899
H	–7.182400	0.867099	–0.394700
H	0.972200	1.041500	–4.238299
H	0.604000	3.933900	–1.114399
H	–4.222700	3.448200	–2.827799
H	–4.745400	4.382500	1.309300
H	0.921099	4.685599	–3.229599
H	2.368699	4.533700	–5.228799
H	3.115899	3.687499	–3.858500
H	2.337199	2.766600	–5.153800
H	–0.163600	4.621100	–5.456499
H	–1.196300	3.854200	–4.230400
H	–0.283000	2.855799	–5.370600
H	–4.475100	6.102699	–0.152999
H	–2.910699	7.007500	–1.840299
H	–2.185999	5.612700	–1.011300
H	–2.829699	5.434899	–2.649499
H	–5.430100	7.110199	–2.203800
H	–6.473099	5.802900	–1.607300
H	–5.426800	5.534200	–3.009099
H	–5.046299	0.764300	2.292100
H	–4.194999	–0.239000	–2.215299
H	–5.638099	–0.053400	–4.234099
H	–6.522200	0.417200	–2.770900
H	–5.921400	1.661199	–3.880500
H	–3.122200	0.211499	–4.355800
H	–2.248900	1.102499	–3.093499
H	–3.355799	1.950800	–4.184000
H	–4.001599	1.919000	4.208700
H	–2.880000	1.812399	2.837299

H	–3.685199	3.345300	3.206899
H	–6.483300	2.040800	3.833600
H	–7.152300	2.060699	2.190399
H	–6.324099	3.490200	2.829599
H	0.674999	–1.853600	–1.867900
H	–0.317700	–2.601100	–4.002000
H	–1.348899	–1.399200	–3.200600
H	–0.360399	–0.931700	–4.592800
H	2.176299	–2.574400	–3.680500
H	2.949499	–1.316599	–2.695600
H	2.291100	–0.916300	–4.289400
H	–0.011799	1.333899	1.511700
H	1.568299	2.880000	2.656400
H	2.418000	1.841900	1.496899
H	2.076300	3.531200	1.087200
H	–0.865300	3.474799	2.307400
H	–1.682499	3.073500	0.784300
H	–0.396000	4.290400	0.815600
H	8.953300	–4.001799	4.341899
H	6.416999	–0.949700	5.959300
H	6.401300	–6.389999	–1.107899
H	8.938899	–5.625299	2.259299
H	4.350400	–3.598600	–0.975099
H	4.517300	–5.255599	–1.569500
H	3.525100	–4.913600	–0.147699
H	3.525600	–1.555000	4.162699
H	4.427399	–0.352600	5.093500
H	4.393600	–0.273500	3.327699
H	8.254900	–2.380800	7.387300
H	9.599999	–2.908499	6.366800
H	9.143700	–1.200700	6.423700
H	9.066399	–6.978000	–0.989800
H	9.588500	–7.290100	0.671300
H	8.221999	–8.180000	–0.013300

Geometry data for MCz–BSBS (S_1 optimization: unit Å)

C	2.774400	–2.751899	0.868500
C	1.605200	–2.191000	0.374400
C	1.594500	–1.003700	–0.423600
C	2.890800	–0.475500	–0.726000
C	4.067300	–1.024699	–0.261000
C	4.007299	–2.164800	0.552100
S	0.141299	–3.102700	0.730600
C	–1.214400	–2.093299	0.230899
C	–1.065500	–0.864300	–0.465299
B	0.319200	–0.328800	–0.917300
C	–2.457900	–2.627600	0.539100
C	–3.625799	–1.935800	0.195000
C	–3.562199	–0.660000	–0.407199
C	–2.269199	–0.184800	–0.723000
S	–5.105499	–2.783399	0.590100
C	–6.417200	–1.744900	0.080699

C	–6.230400	–0.445899	–0.439100
B	–4.828700	0.184399	–0.656900
C	–7.700700	–2.287599	0.251399
C	–8.817200	–1.545300	–0.090300
C	–8.671500	–0.251299	–0.602399
C	–7.402300	0.274900	–0.764200
C	0.424800	0.894199	–1.935800
C	–4.728300	1.714600	–1.060900
C	0.609300	0.640000	–3.314699
C	0.710000	1.697300	–4.221300
C	0.645000	3.027299	–3.807299
C	0.476500	3.274500	–2.447200
C	0.361599	2.240199	–1.514700
C	–4.562600	2.136100	–2.396400
C	–4.494000	3.498100	–2.691499
C	–4.574399	4.471900	–1.695300
C	–4.742500	4.045700	–0.379999
C	–4.826400	2.690900	–0.049399
C	0.740899	4.171199	–4.797400
C	2.067500	4.160599	–5.561100
C	–0.446300	4.178400	–5.764399
C	–4.475300	5.947900	–2.025999
C	–3.113200	6.300800	–2.630300
C	–5.614600	6.404999	–2.940999
C	–5.013200	2.288699	1.405999
C	–4.505400	1.116400	–3.522900
C	–5.850500	1.029900	–4.252399
C	–3.371500	1.381499	–4.514500
C	–3.801500	2.664100	2.262100
C	–6.306200	2.858100	1.994699
C	0.700600	–0.785500	–3.840100
C	–0.464800	–1.133100	–4.768699
C	2.045400	–1.056199	–4.520099
C	0.219700	2.577099	–0.038300
C	1.588599	2.871700	0.585600
C	–0.747800	3.729599	0.234700
N	5.216200	–2.744700	1.066999
C	5.962600	–3.714599	0.432200
C	7.084700	–4.026499	1.245800
C	6.983800	–3.186900	2.425400
C	5.805900	–2.408399	2.266099
C	7.772200	–3.051099	3.544899
C	7.393600	–2.123199	4.538499
C	6.230500	–1.368600	4.358099
C	5.395600	–1.467699	3.241700
C	5.741400	–4.354999	–0.810600
C	6.702800	–5.304600	–1.167900
C	7.815300	–5.629200	–0.385599
C	8.003300	–4.971000	0.847899
C	4.585999	–4.089299	–1.724500
C	4.171900	–0.610900	3.151599
C	8.236100	–1.959500	5.766100
C	8.801999	–6.660800	–0.839099
H	2.741099	–3.647900	1.484899

H	2.935499	0.408700	–1.356399
H	5.028799	–0.583400	–0.513899
H	–2.526900	–3.588600	1.045299
H	–2.202000	0.783899	–1.213799
H	–7.814300	–3.292099	0.652500
H	–9.807300	–1.974100	0.042500
H	–9.547700	0.333599	–0.868600
H	–7.282600	1.282099	–1.155599
H	0.838999	1.476299	–5.280400
H	0.429200	4.309200	–2.111299
H	–4.369600	3.809900	–3.726900
H	–4.806200	4.795000	0.408600
H	0.699799	5.104000	–4.217400
H	2.138900	5.025300	–6.232000
H	2.919499	4.188300	–4.873299
H	2.163700	3.256299	–6.173700
H	–0.396600	5.040799	–6.440500
H	–1.395199	4.221099	–5.218999
H	–0.458600	3.270599	–6.379299
H	–4.569999	6.497600	–1.078899
H	–3.031000	7.380900	–2.802799
H	–2.296500	5.992800	–1.968799
H	–2.966400	5.797200	–3.593100
H	–5.555999	7.484099	–3.127500
H	–6.591200	6.185899	–2.496300
H	–5.569199	5.896900	–3.911600
H	–5.101399	1.194100	1.440100
H	–4.313999	0.135200	–3.065000
H	–5.814099	0.274500	–5.047000
H	–6.661099	0.762000	–3.566599
H	–6.102599	1.992900	–4.713399
H	–3.302000	0.561900	–5.239300
H	–2.404500	1.472600	–4.009299
H	–3.541599	2.302499	–5.085199
H	–3.945800	2.338600	3.299400
H	–2.891399	2.192000	1.877999
H	–3.640400	3.748899	2.269500
H	–6.442799	2.517000	3.027900
H	–7.177399	2.538500	1.413200
H	–6.292100	3.954600	2.005599
H	0.635400	–1.453200	–2.971199
H	–0.390699	–2.172500	–5.111999
H	–1.422499	–1.012500	–4.252900
H	–0.477800	–0.487800	–5.655900
H	2.112900	–2.103400	–4.840899
H	2.877700	–0.852500	–3.837200
H	2.180900	–0.428499	–5.409600
H	–0.180600	1.682100	0.457400
H	1.490499	3.086100	1.657600
H	2.268800	2.021600	0.467100
H	2.050899	3.744799	0.107799
H	–0.903999	3.845900	1.313700
H	–1.723100	3.558200	–0.232600
H	–0.357100	4.684900	–0.137600

H	8.674299	–3.644299	3.671800
H	5.952900	–0.658300	5.132200
H	6.571800	–5.820900	–2.115100
H	8.863399	–5.213300	1.467100
H	4.544999	–3.040900	–2.033699
H	4.665400	–4.715500	–2.616800
H	3.629600	–4.296499	–1.235599
H	3.261999	–1.213600	3.077400
H	4.098100	0.027500	4.035800
H	4.185800	0.023300	2.260499
H	7.826000	–1.204199	6.440500
H	8.310900	–2.904199	6.318200
H	9.258400	–1.662400	5.502800
H	8.529799	–7.081700	–1.809900
H	9.807300	–6.230900	–0.924299
H	8.867400	–7.484099	–0.117599

Geometry data for MCz–BSBS (T_1 optimization: unit Å)

C	2.878900	–3.150499	1.800800
C	1.710000	–2.589600	1.306599
C	1.699300	–1.402999	0.507399
C	2.996099	–0.875699	0.203799
C	4.172499	–1.425300	0.668000
C	4.112600	–2.564700	1.482600
S	0.245999	–3.500900	1.663600
C	–1.109600	–2.491300	1.164199
C	–0.960600	–1.263000	0.467000
B	0.424500	–0.728200	0.013999
C	–2.353200	–3.024700	1.473600
C	–3.520800	–2.332500	1.129799
C	–3.456900	–1.057199	0.526400
C	–2.163900	–0.583099	0.209399
S	–5.000899	–3.178599	1.526800
C	–6.312199	–2.139699	1.017100
C	–6.125000	–0.841399	0.495900
B	–4.722900	–0.212100	0.276600
C	–7.595900	–2.681400	1.189199
C	–8.712199	–1.938799	0.847200
C	–8.566000	–0.645500	0.333599
C	–7.296500	–0.120200	0.170700
C	0.529500	0.493700	–1.005900
C	–4.621899	1.317499	–0.129200
C	0.712699	0.237900	–2.384699
C	0.813099	1.294100	–3.292500
C	0.749200	2.624599	–2.879900
C	0.582099	2.873400	–1.520000
C	0.467499	1.840100	–0.586100
C	–4.456800	1.737599	–1.465300
C	–4.387499	3.099300	–1.761699
C	–4.466700	4.074099	–0.766300
C	–4.634200	3.649200	0.549499
C	–4.718700	2.294700	0.881400

C	0.844800	3.767399	–3.871300
C	2.170899	3.755299	–4.635899
C	–0.343000	3.774100	–4.837599
C	–4.366899	5.549599	–1.098499
C	–3.004799	5.901200	–1.703900
C	–5.506399	6.006499	–2.013299
C	–4.904799	1.894100	2.337399
C	–4.401100	0.716700	–2.590800
C	–5.746900	0.630300	–3.319199
C	–3.267900	0.980200	–3.583599
C	–3.692400	2.269700	3.192300
C	–6.197200	2.464599	2.926300
C	0.803000	–1.188200	–2.908499
C	–0.363200	–1.536400	–3.836000
C	2.147099	–1.460199	–3.589299
C	0.327199	2.178700	0.890100
C	1.696899	2.473100	1.512500
C	–0.639399	3.331999	1.162800
N	5.320699	–3.144199	1.997400
C	6.072100	–4.108000	1.358499
C	7.194799	–4.418799	2.171400
C	7.088899	–3.585899	3.355500
C	5.907800	–2.811900	3.199199
C	7.876000	–3.451999	4.476300
C	7.492799	–2.530399	5.473899
C	6.327199	–1.779300	5.295699
C	5.493499	–1.876700	4.178000
C	5.853600	–4.744600	0.113500
C	6.819600	–5.688100	–0.247900
C	7.933599	–6.010500	0.533100
C	8.117900	–5.357399	1.769900
C	4.695900	–4.481700	–0.798400
C	4.267200	–1.023400	4.090000
C	8.333500	–2.369100	6.702900
C	8.925999	–7.034699	0.074700
H	2.845500	–4.045999	2.418000
H	3.041000	0.008100	–0.427399
H	5.134000	–0.984899	0.414100
H	–2.422399	–3.985300	1.980699
H	–2.096399	0.385100	–0.282400
H	–7.709999	–3.685500	1.591300
H	–9.702500	–2.366800	0.981100
H	–9.442000	–0.060299	0.067500
H	–7.176299	0.886499	–0.222000
H	0.941100	1.071900	–4.351599
H	0.535599	3.908400	–1.185100
H	–4.263500	3.409899	–2.797399
H	–4.696900	4.399299	1.337400
H	0.804499	4.700800	–3.292199
H	2.242299	4.619300	–5.307799
H	3.023400	3.783399	–3.948699
H	2.266300	2.850299	–5.247600
H	–0.293400	4.635699	–5.514600
H	–1.291599	3.817700	–4.291600

H	–0.356099	2.865599	–5.451399
H	–4.460699	6.100299	–0.151800
H	–2.922100	6.981000	–1.877500
H	–2.187900	5.593300	–1.042600
H	–2.858899	5.396600	–2.666400
H	–5.447300	7.085499	–2.200700
H	–6.482899	5.788500	–1.567800
H	–5.461899	5.497599	–2.983400
H	–4.993399	0.799500	2.372500
H	–4.209900	–0.264200	–2.132099
H	–5.711499	–0.125800	–4.112999
H	–6.557000	0.363500	–2.632500
H	–5.998700	1.593099	–3.780900
H	–3.199500	0.159900	–4.307700
H	–2.300399	1.071399	–3.079399
H	–3.437999	1.900699	–4.155199
H	–3.836200	1.945299	4.230200
H	–2.782700	1.796900	2.808299
H	–3.530799	3.354400	3.198700
H	–6.333300	2.124599	3.960000
H	–7.068900	2.144799	2.345600
H	–6.182499	3.561099	2.936200
H	0.738200	–1.855000	–2.038999
H	–0.289800	–2.576200	–4.178200
H	–1.320600	–1.414799	–3.319500
H	–0.376599	–0.892099	–4.723700
H	2.214099	–2.507799	–3.908899
H	2.979999	–1.256099	–2.907100
H	2.282299	–0.833699	–4.479600
H	–0.073199	1.284400	1.387000
H	1.599900	2.688700	2.584200
H	2.376400	1.622400	1.394199
H	2.159199	3.345400	1.033300
H	–0.794500	3.449500	2.241800
H	–1.615300	3.160800	0.696599
H	–0.248399	4.286600	0.789299
H	8.780600	–4.041900	4.601000
H	6.046299	–1.073200	6.072499
H	6.690900	–6.201300	–1.197000
H	8.978400	–5.599199	2.388700
H	4.652600	–3.433800	–1.108800
H	4.774400	–5.108899	–1.690099
H	3.740800	–4.689799	–0.307200
H	3.358700	–1.628699	4.019500
H	4.194099	–0.383800	4.973400
H	4.276800	–0.390799	3.197700
H	7.920499	–1.617699	7.380000
H	8.410500	–3.315799	7.251300
H	9.355300	–2.067900	6.442100
H	8.651000	–7.459199	–0.893800
H	9.926900	–6.596099	–0.017900
H	9.003400	–7.856100	0.796999

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