# Supporting Information

## Extended conjugated borenium dimers via late stage functionalization of air-stable borepinium ions

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## ***Experimental***

*General*

All reactions were carried out under nitrogen using Schlenk techniques or an inert-atmosphere glovebox. THF and ether were distilled from Na/benzophenone prior to use. Dichloromethane and fluorobenzene were distilled from $CaH_2$. Hexane and toluene were purified using a solvent purification system (alumina/copper) and stored over Na/K alloy. All chemicals were purchased from commercial sources and directly used. 1,2-Bis(2-bromo-3-thienyl)benzene,[S1] 1,2-bis(2-bromo-3-thienyl)-4,5-difluorobenzene,[S1] and 1,3-di-*tert*-butyl-4,5-dimethyl-2-(trimethylsilyl)-1*H*-imidazol-3-ium trifluoromethanesulfonate[S2] were prepared according to literature.

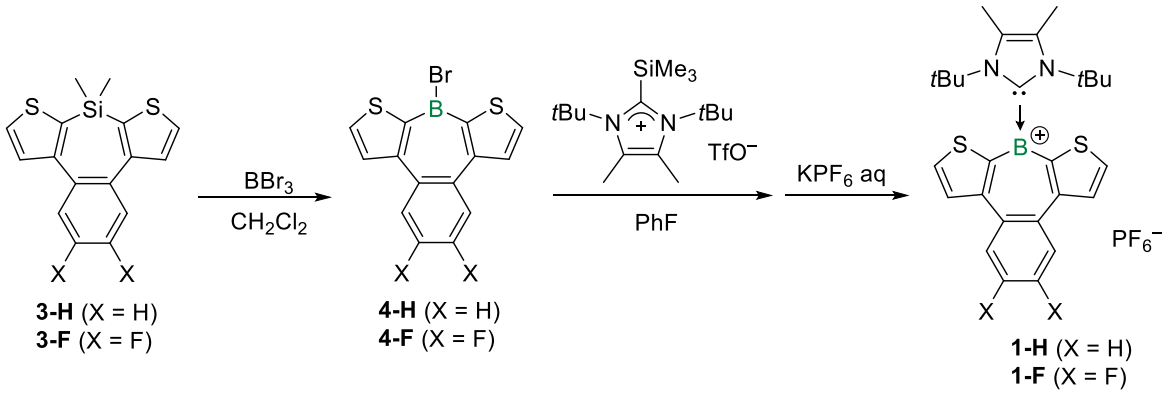
NMR data were acquired at room temperature. 160 MHz $^{11}$B and 470 MHz $^{19}$F NMR data were recorded on a 500 MHz Bruker AVANCE spectrometer; 500 MHz $^{1}$H and 126 MHz $^{13}$C NMR data were recorded on a 500 MHz Bruker Auto AVANCE spectrometer. $^{11}$B NMR spectra were acquired with boron-free quartz NMR tubes on the 500 MHz Bruker AVANCE with a 5 mm PH SEX 500S1 $^{11}$B-H/F-D probe. Abbreviations Bz and Th used for the following NMR assignments stand for fused benzene and thiophene ring, respectively.

MALDI-TOF MS measurements were performed on a Bruker Ultraflextreme in reflectron mode with delayed extraction. Compounds were dissolved in DCM (10 mg/mL), mixed with a matrix solution of *trans*-2[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene]malononitrile in DCM (10 mg/mL), and then spotted on the wells of a target plate. Red phosphorous was used for calibration. High-resolution ESI and APCI mass spectra were obtained on a Thermo Fisher Scientific LTQ Orbitrap XL spectrometer at N-BARD, Hiroshima University. Single crystal X-ray diffraction data was collected at 123K on a Rigaku R-AXIS RAPID diffractometer using graphite-monochromated MoKα radiation. The structure was solved by Direct Method (SIR92) and expanded using Fourier techniques. Since the solvent (dichloromethane) in the crystal of **1-F** was highly disordered, the SQUEEZE subroutine of the PLATON[S3] software suite was used to remove the scattering contributions from the highly disordered solvent molecules. The resulting new HKL file was used to further refine the structure. Non-hydrogen atoms were refined anisotropically, whereas hydrogen atoms were refined using the riding model by the full-matrix least-squares method. Graphical crystal structures were generated using Mercury 3.10.3 (Cambridge Crystallographic Data Centre). All other calculations

were performed using the Olex2 program. UV-visible absorption data were acquired on a Varian Cary 5000 UV-Vis/NIR spectrophotometer. The fluorescence data and lifetimes were measured using a Horiba Fluorolog-3 spectrofluorometer equipped with a 350 nm nanoLED and a FluoroHub R-928 detector. Absolute quantum yields ($\Phi$) were measured on the HORIBA Fluorolog-3 using a pre-calibrated Quanta-φ integrating sphere. Light from the sample compartment is directed into the sphere via a fiber-optic cable and an F-3000 Fiber-Optic Adapter, and then returned to the sample compartment (and to the emission monochromator) via a second fiber-optic cable and an F-3000 Fiber-Optic Adapter. Cyclic voltammetry (CV) experiments were carried out on a BASI CV-50 W analyzer. The three-electrode system consisted of a platinum disk as working electrode, a Pt wire as secondary electrode, and an Ag wire as the pseudo-reference electrode. The voltammograms were recorded with ca. 1.0 mM solutions in acetonitrile containing *n*Bu$_4$N[PF$_6$] (0.1 M) as the supporting electrolyte. The scans were referenced after the addition of a small amount of ferrocene as internal standard. The potentials are reported relative to the ferrocene/ferrocenium couple.

Geometry optimization and TD-DFT calculations were performed with the Gaussian09 program using the hybrid density functional B3LYP with a 6-31G(d,p) basis set. NICS calculations were carried out using the GIAO method at the B3LYP/6-31+G(d,p) level of theory.

*Synthesis*




**3-H** (X = H)
**3-F** (X = F)

**4-H** (X = H)
**4-F** (X = F)

**1-H** (X = H)
**1-F** (X = F)

**Synthesis of 3-H.**

To a solution of 1,2-bis(2-bromo-3-thienyl)benzene (4.30 g, 10.7 mmol) in a mixture of 8 mL of diethyl ether and 40 mL of toluene were slowly added 13.5 mL (21.6 mmol) of 1.6 mol/L *n*BuLi in hexane at –78 °C and

the mixture was stirred for 1 h. Dimethyldichlorosilane (1.47 g, 11.4 mmol) was slowly added at –78 °C. The mixture was warmed to room temperature and then stirred overnight. The resulting mixture was hydrolyzed with water, and the organic layer was washed twice with water and then once with brine. After drying over anhydrous sodium sulfate, the solvent was evaporated. The crude product was purified by silica gel chromatography using hexanes as the eluent to give 2.31 g (7.73 mmol, 72% yield) of **3-H** as a white solid. $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.62 (dd, $J$ = 5.8, 3.4 Hz, 2H, Bz), 7.52 (d, $J$ = 4.7 Hz, 2H, Th), 7.38–7.35 (m, 4H, Bz and Th), 0.81 (br s, 3H, $SiMe_2$), 0.06 (br s, 3H, $SiMe_2$). $^{13}$C NMR (126 MHz, $CDCl_3$) δ: 148.1, 135.1, 135.0, 131.8, 131.1, 128.9, 126.6. Two signals for Si−C were not detected, probably due to their low intensities. HRMS (APCI, positive) Calcd for $C_{16}H_{14}S_2Si$: $M^+$: 298.03062, Found 298.03024.

**Synthesis of 3-F.**

Compound **3-F** was prepared from 3.00 g (6.88 mmol) of 1,2-bis(2-bromo-3-thienyl)-4,5-difluorobenzene, 8.6 mL (13.8 mmol) of 1.6 mol/L *n*BuLi in hexane, and 1.08 g (8.37 mmol) of dimethyldichlorosilane in a mixture of 8 mL of diethyl ether and 40 mL of toluene in a manner similar to that above. The crude product was purified by silica gel chromatography using hexanes as the eluent to give 1.43 g (4.27 mmol, 62% yield) of **3-F** as a white solid. $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.53 (d, $J$ = 4.7 Hz, 2H, Th), 7.42 (t, $J$ = 10.0 Hz, 2H, Bz), 7.29 (d, $J$ = 4.7 Hz, 2H, Th), 0.82 (br s, 3H, $SiMe_2$), 0.09 (br s, 3H, $SiMe_2$). $^{13}$C NMR (126 MHz, $CDCl_3$) δ: 148.4 (dd, $J_{C\text{-}F}$ = 15, 251 Hz), 146.1, 135.8, 132.1 (t, $J_{C\text{-}F}$ = 4.6 Hz), 131.5, 129.5, 119.4 (dd, $J_{C\text{-}H}$ = 6, 12 Hz). Two signals for Si−C were not detected, probably due to their low intensities. $^{19}$F NMR (470 MHz, $CDCl_3$) δ: –139.9 (t, $J$ = 10.0 Hz). HRMS (APCI, positive) Calcd for $C_{16}H_{12}F_2S_2Si$: $M^+$: 334.01177, Found 334.01163.

**Synthesis of 4-H.**

A solution of **3-H** (599 mg, 2.01 mmol) in 8 mL of dichloromethane was pre-cooled to –40 °C in a freezer. The solution was taken out from the freezer and immediately 1.02 g (4.07 mmol) of boron tribromide were added over three min. The mixture was stirred overnight at room temperature. All volatiles were removed in vacuum, and the resulting solid was washed twice with hexanes. The residue was dried in vacuum to give

**4-H** as an air-sensitive yellowish solid in quantitative yield. $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 8.19 (dd, $J$ = 6.1, 3.5 Hz, 2H, Bz), 8.05 (d, $J$ = 5.0 Hz, 2H, Th), 7.98 (d, $J$ = 5.0 Hz, 2H, Th), 7.55 (dd, $J$ = 6.2, 3.4 Hz, 1H, Bz). $^{13}$C NMR (126 MHz, $CDCl_3$) δ: 150.8, 135.9, 132.6, 131.8, 131.5, 127.9. One signal for B−C was not detected, probably due to its low intensity as a result of quadrupolar broadening. $^{11}$B NMR (160 MHz, $CDCl_3$) δ: 45.6.

**Synthesis of 4-F.**

A solution of **3-F** (668 mg, 2.00 mmol) in 8 mL of dichloromethane was pre-cooled to –40 °C in a freezer. The solution was taken out from the freezer and immediately 1.02 g (4.07 mmol) of boron tribromide were added over three min. The mixture was stirred overnight at room temperature. Hexanes (3 mL) were added and the solution was cooled in a freezer to –40 °C, resulting in formation of a solid. The liquid layer was carefully removed by decantation and the remaining solid was washed with cold hexanes. The solid was collected by filtration and dried in vacuum to give 686 mg (1.87 mmol, 94% yield) of **4-F** as an air-sensitive colorless solid. $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, $J$ = 5.0 Hz, 2H, Th), 8.00 (t, $J$ = 10.4 Hz, 2H, Bz), 7.96 (d, $J$ = 5.0 Hz, 2H, Th). $^{13}$C NMR (126 MHz, $CDCl_3$) δ: 149.0 (dd, $J_{C\text{-}F}$ = 16 and 253 Hz), 148.7, 136.6, 131.7, 130.0 (t, $J_{C\text{-}F}$ = 5 Hz), 119.7 (dd, $J_{C\text{-}F}$ = 7 and 13 Hz). One signal for B−C was not detected, probably due to its low intensity as a result of quadrupolar broadening. $^{11}$B NMR (160 MHz, $CDCl_3$) δ: 45.9. $^{19}$F NMR (470 MHz, $CDCl_3$) δ: –136.6 (t, $J$ = 9.4 Hz).

**Synthesis of 1-H.**

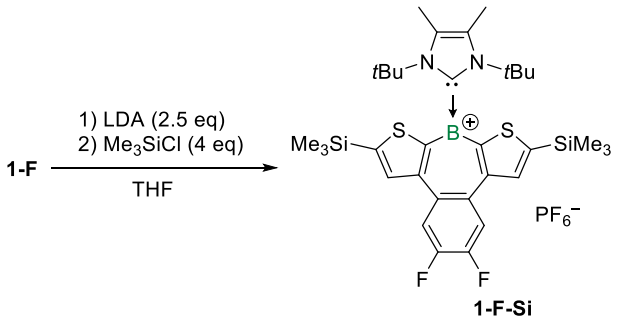
A solution of **4-H** (663 mg, 2.00 mmol) in 12 mL of fluorobenzene was pre-cooled to –40 °C in a freezer. To the solution was added a solution of 873 mg (2.03 mmol) of 1,3-di-*tert*-butyl-4,5-dimethyl-2-(trimethylsilyl)-1*H*-imidazol-3-ium trifluoromethanesulfonate in 3 mL of fluorobenzene at room temperature. The mixture was stirred for 3 hours, then all volatiles were removed in vacuum. The resulting solid was dissolved in dichloromethane and washed three times with saturated $KPF_6$ solution, then four times with deionized water. After drying over anhydrous sodium sulfate, the solvent was evaporated. The resulting viscous oil was reprecipitated from $CH_2Cl_2$/$Et_2O$ to give 1.07 g (1.76 mmol, 88% yield) of **1-H** as light yellowish powder.

$^{1}$H NMR (500 MHz, $CD_2Cl_2$) δ: 8.52 (dd, *J* = 6.2, 3.5 Hz, 2H, Bz), 8.30 (d, *J* = 5.2 Hz, 2H, Th), 8.23 (d, *J* = 5.1 Hz, 2H, Th), 7.73 (dd, *J* = 6.3, 3.4 Hz, 2H, Bz), 2.64 (s, 6H, Me), 1.56 (s, 18H, *t*Bu). $^{11}$B NMR (160 MHz, $CD_2Cl_2$) δ: 41.8. $^{13}$C NMR (126 MHz, $CD_2Cl_2$) δ: 153.8 (Th), 147.1 (br, NHC), 142.3 (br, Th), 137.7 (Th), 132.9 (Bz), 132.6 (Th), 132.5 (Bz), 131.9 (NHC), 129.5 (Bz), 64.6 (C-$Me_3$), 31.8 (C-$Me_3$), 14.5 (Me). $^{19}$F NMR (470 MHz, $CD_2Cl_2$) δ: –73.4 (d, *J* = 711 Hz). HRMS (ESI, positive) Calcd for $C_{27}H_{32}BN_2S_2$: $M^+$: 459.20945, Found 459.20972.

**Synthesis of 1-F.**

Compound **1-F** was prepared from 686 mg (1.87 mmol) of **4-F** and 805 mg (1.87 mmol) of 1,3-di-*tert*-butyl-4,5-dimethyl-2-(trimethylsilyl)-1*H*-imidazol-3-ium trifluoromethanesulfonate in 15 mL of fluorobenzene in a manner similar to that above. The product was obtained as a white powder (1.10 g, 1.71 mmol, 91% yield). This powder was recrystallized from dichloromethane by vapor diffusion with hexane as the precipitant to give single crystals for XRD analysis. $^{1}$H NMR (500 MHz, $CD_2Cl_2$) δ: 8.30 (t, *J* = 10.7 Hz, 2H, Bz), 8.25 (d, *J* = 5.1 Hz, 2H, Th), 8.15 (d, *J* = 5.2 Hz, 2H, Th), 2.64 (s, 6H, Me), 1.56 (s, 18H, *t*Bu). $^{11}$B NMR (160 MHz, $CD_2Cl_2$) δ: 44.0. $^{13}$C NMR (126 MHz, $CD_2Cl_2$) δ 151.7 (Th), 150.0 (dd, *J* = 254.4, 15.3 Hz, Bz), 146.6 (br, NHC), 142.6 (br, Th), 138.4, (Th), 132.6 (Th), 132.1 (NHC), 130.6 (t, *J* = 4.5 Hz, Bz), 120.7 (dd, *J* = 13.1, 7.1 Hz, Bz), 64.7 (C-$Me_3$), 31.8 (C-$Me_3$), 14.5 (Me). $^{19}$F NMR (470 MHz, $CDCl_3$) δ –71.5 (d, *J* = 710 Hz), –133.4 (t, *J* = 11 Hz). HRMS (ESI, positive) Calcd for $C_{27}H_{30}BF_2N_2S_2$: $M^+$: 495.19060, Found 495.19104.

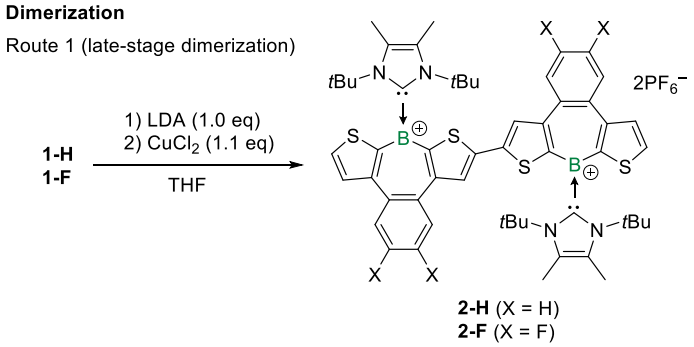
*Derivatization of borepinium ions*




**Synthesis of 1-F-Si.**

To a solution of **1-F** (101 mg, 0.157 mmol) in 5 mL of THF were slowly added 0.44 mL (0.40 mmol) of 0.9

mol/L LDA in hexanes/THF at –78 °C, and the mixture was stirred for 40 min at that temperature. Trimethylsilyl chloride (70 mg, 0.64 mmol) was added. The mixture was immediately warmed to room temperature and then stirred for 3h. All volatiles were removed in vacuum, and the residue was dissolved in dichloromethane. The solution was washed with saturated $KPF_6$ solution, then twice with deionized water. After drying over anhydrous sodium sulfate, the solvent was evaporated. The residue was dissolved in $CH_2Cl_2$ and the solution added dropwise to ether. The suspension was filtered with Celite and the filtrate was concentrated. The residue was again dissolved in $CH_2Cl_2$ and precipitated into hexanes. The precipitate was collected by filtration to give 83.9 mg (0.107 mmol, 68% yield) of **1-F-Si** as a light brown solid. $^1$H NMR (500 MHz, $CDCl_3$) δ: 8.24 (t, $J$ = 10.5 Hz, 2H, Bz), 8.09 (s, 2H, Th), 2.68 (s, 6H, Me), 1.55 (s, 18H, *t*Bu), 0.45 (s, 18H, $SiMe_3$). $^{11}$B NMR (160 MHz, $CDCl_3$) δ: 40.9. $^{13}$C NMR (126 MHz, $CDCl_3$) δ: 156.3 (Th), 151.6 (Th), 149.5 (dd, $J$ = 254.9, 15.2 Hz, Bz), 137.9 (Th), 131.7 (NHC), 130.1 (t, $J$ = 4.4 Hz, Bz), 120.2 (dd, $J$ = 12.9, 6.8 Hz, Bz), 64.0 (C-$Me_3$), 31.6 (C-$Me_3$), 14.2 (NHC-Me), –0.29 ($SiMe_3$). $^{19}$F NMR (470 MHz, $CDCl_3$) δ: –73.4 (d, $J$ = 713 Hz), –134.8 (t, $J$ = 11 Hz). Two signals for B–C were not detected, probably due to their low intensity as a result of quadrupolar broadening. HRMS (ESI, positive) Calcd for $C_{33}H_{46}BF_2N_2S_2Si_2$: $M^+$: 639.26966, Found 639.27106.



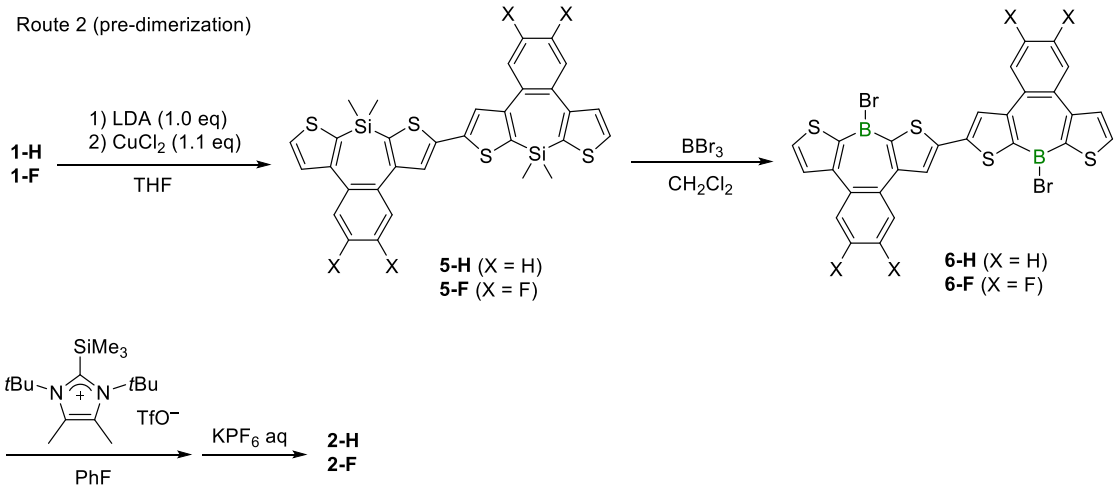

**Synthesis of 2-H via route 1.**

To a solution of **1-H** (100 mg, 0.165 mmol) in 10 mL of THF were slowly added 0.17 mL (0.15 mmol) of 0.9 mol/L LDA in hexanes/THF at –78 °C and the mixture was stirred for 40 min at that temperature. $CuCl_2$ (28.3 mg, 0.21 mmol) was added as a solid. The mixture was gradually warmed to room temperature over 3h, and then stirred for 3h at room temperature. All volatiles were removed in vacuum, and the residue was

dispersed in 100 mL of dichloromethane. The mixture was filtered through Celite and the filtrate was concentrated. The residue was reprecipitated from acetonitrile/saturated $KPF_6$ solution. The precipitate was again dissolved in dichloromethane and dried over anhydrous sodium sulfate. The residue was dispersed in 5 mL of chloroform and sonicated for 20 min. The precipitate was collected to give 46.4 mg (38.4 μmol, 47% yield) of **2-H** as a yellowish powder. NMR spectral data matched those of compound **2-H** prepared via route 2 (see below).

**Synthesis of 2-F via route 1.**

Compound **2-F** was prepared from 101 mg (0.158 mmol) of **1-F**, 0.16 mL (0.144 mmol) of 0.9 mol/L LDA in hexane/THF, and 26.8 mg (0.199 mmol) of $CuCl_2$ in 5 mL of THF in a manner similar to that above. The product was obtained as light reddish powder (53.9 mg, 42.2 μmol, 53% yield). NMR spectral data matched those of compound **2-F** prepared via route 2 (see below).




**Synthesis of 5-H.**

To a solution of **3-H** (251 mg, 0.839 mmol) in 5 mL of diethyl ether were slowly added 0.53 mL (0.848 mmol) of 1.6 mol/L *n*BuLi in hexane at 0 °C and the mixture was stirred for 1 h at the temperature. The mixture was cooled to –78 °C, then $CuCl_2$ (128 mg, 0.952 mmol) was added as a solid. The mixture was slowly warmed to room temperature and stirred overnight. Dichloromethane was added and the organic components were washed twice with water, then once with brine. After drying over anhydrous sodium sulfate, the solvent

was evaporated. The crude product was purified by silica gel chromatography using a 9:1 mixture of hexanes/dichloromethane to give 103 mg (0.174 mmol, 41% yield) of **5-H** as a white solid. $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.67–7.59 (m, 4H, Bz), 7.50 (d, $J$ = 4.6 Hz, 2H, Th), 7.44 (s, 2H, Th), 7.38–7.33 (m, 6H, Bz and Th), 0.82 (br s, 6H, $SiMe_2$), 0.08 (br s, 6H, $SiMe_2$). $^{13}$C NMR (126 MHz, $CDCl_3$) δ: 148.7, 148.1, 140.3, 135.1, 134.92, 134.88, 134.7, 131.9, 131.2, 131.0, 129.1, 128.9, 126.8, 126.7, –2.3 (br s), –3.7 (br s). HRMS (MALDI-TOF, positive) Calcd for $C_{32}H_{26}S_4Si_2$: $M^+$: 594.0450, Found 594.0478.

**Synthesis of 5-F.**

Compound **5-F** was prepared from 248.1 mg (0.742 mmol) of **3-F**, 0.47 mL (0.75 mmol) of 1.6 mol/L *n*BuLi in hexane, and 111 g (0.826 mmol) of $CuCl_2$ in 5 mL of diethyl ether in a manner similar to that above. The crude product was purified by silica gel chromatography using a 9:1 mixture of hexanes/dichloromethane as the eluent to give 95.3 mg (0.143 mmol, 39% yield) of **5-F** as a white solid. $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 7.56 (d, $J$ = 4.7 Hz, 2H, Th), 7.47–7.40 (m, 4H, Bz), 7.34 (s, 2H, Th), 7.31 (d, $J$ = 4.7 Hz, 2H, Th), 0.81 (br s, 6H, $SiMe_2$), 0.11 (br s, 6H, $SiMe_2$). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 148.5 (dd, $J$ = 254.3, 17.1 Hz), 148.4 (dd, $J$ = 245.3, 8.4 Hz), 146.6, 146.1, 140.4, 135.6, 135.5, 132.2 (dd, $J$ = 5.6, 3.5 Hz), 131.6 (dd, $J$ = 5.6, 3.5 Hz), 131.5, 129.7, 128.5, 119.4 (dd, $J$ = 30.4, 17.3 Hz), –2.33 (br s), –3.92 (br s). $^{19}$F NMR (470 MHz, $CDCl_3$) δ: –139.2 – –139.6 (m). HRMS (MALDI-TOF, positive) Calcd for $C_{32}H_{22}F_4S_4Si_2$: $M^+$: 666.0074, Found 666.0104.

**Synthesis of 6-H.**

To a solution of **5-H** (109 mg, 0.183 mmol) in 3 mL of dichloromethane were slowly added 185 mg (0.738 mmol) of boron tribromide at room temperature and the mixture was stirred overnight. All volatiles were removed in vacuum, and the resulting solid was washed twice with hexanes. The residue was dried in vacuum to give 112 mg (0.169 mmol, 93% yield) of **6-H** as an air-sensitive yellowish solid. $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 8.38 (s, 2H, Th), 8.34–8.29 (m, 2H, Bz), 8.27–8.23 (m, 2H, Bz), 8.10 (d, $J$ = 5.0 Hz, 2H, Th), 8.04 (d, $J$ = 4.9 Hz, 2H, Th), 7.66 – 7.60 (m, 4H, Bz). $^{11}$B NMR (160 MHz, $CDCl_3$) δ: 44.6. $^{13}$C NMR could not be recorded due to the low solubility of the sample.

**Synthesis of 6-F.**

To a solution of **5-F** (50.0 mg, 75.0 μmol) in 10 mL of dichloromethane were slowly added 75.3 mg (0.301 mmol) of boron tribromide at room temperature and the mixture was stirred for 1 day. All volatiles were removed in vacuum, and the resulting solid was washed twice with hexanes. The residue was dried in vacuum to give 39.1 mg (53.4 μmol, 71% yield) of **6-F** as an air-sensitive yellowish solid. The $^{1}$H and $^{19}$F NMR spectra indicate the presence of unidentified byproducts. Further analysis and purification could not be performed due to the low solubility and air sensitivity of the sample. $^{1}$H NMR (500 MHz, $CDCl_3$) δ: 8.21 (br s, 2H), 8.08–7.94 (m, 8H). $^{11}$B NMR (160 MHz, $CDCl_3$) δ: 45.0. $^{19}$F NMR (470 MHz, $CDCl_3$) δ –135.6 – –136.2 (m). $^{13}$C NMR could not be recorded due to the low solubility of the sample.

**Synthesis of 2-H via route 2.**

To a solution of **6-H** (112 mg, 0.169 mmol) in 4 mL of fluorobenzene was slowly added a solution of 1,3-di-*tert*-butyl-4,5-dimethyl-2-(trimethylsilyl)-1*H*-imidazol-3-ium trifluoromethanesulfonate (146 mg, 0.339 mmol) in 4 mL of fluorobenzene at room temperature. The mixture was stirred for 1 day, then all volatiles were removed in vacuum. The resulting solid was dissolved in dichloromethane and washed three times with saturated $KPF_6$ solution, then four times with deionized water. After drying over anhydrous sodium sulfate, the solvent was evaporated. The residue was dispersed in 5 mL of chloroform and sonicated for 20 min. The solid was collected by filtration and dried in vacuum to give 46.4 mg (38.4 μmol, 23% yield) of **2-H** as a yellowish powder. $^{1}$H NMR (500 MHz, $CD_3CN$) δ: 8.75 (s, 2H, Th), 8.72–8.65 (m, 2H, Bz), 8.65–8.58 (m, 2H, Bz), 8.44–8.32 (m, 4H, Th), 7.90–7.72 (m, 4H, Bz), 2.65 (s, 12H, Me), 1.59 (s, 36H, *t*Bu). $^{11}$B NMR (160 MHz, $CD_3CN$) δ: 42.0. $^{13}$C NMR (126 MHz, $CD_3CN$) δ: 154.8 (Th), 154.3 (Th), 146.5 (br, NHC), 146.2 (Th), 144.2 (br, Th), 143.4 (br, Th), 139.4 (Th), 133.7 (Bz), 133.39 (Bz), 133.35 (Th), 133.28 (Bz), 132.90 (NHC), 132.88 (Bz), 132.1 (Th), 130.6 (Bz), 130.2 (Bz), 65.1 (<u>C</u>-$Me_3$), 31.9 (C-<u>$Me_3$</u>), 14.6 (Me). $^{19}$F NMR (470 MHz, $CD_3CN$) δ: –72.9 (d, $J$ = 707 Hz). HRMS (ESI, positive) Calcd for $C_{54}H_{62}B_2N_4S_4$: $[M]^{2+}$: 458.20162, Found 458.20386.

**Synthesis of 2-F via route 2.**

Compound **2-F** was prepared from 39.1 mg (53.4 μmol) of **6-F** and 48.5 mg (0.113 mmol) of 1,3-di-*tert*-butyl-4,5-dimethyl-2-(trimethylsilyl)-1*H*-imidazol-3-ium trifluoromethanesulfonate in 2 mL of fluorobenzene in a manner similar to that above. The product was obtained as a yellowish powder (7.8 mg, 6.1 μmol, 11% yield). $^{1}$H NMR (500 MHz, $CD_3CN$) δ: 8.64 (s, 2H, Th), 8.59 (dd, *J* = 13.4, 8.5 Hz, 2H, Bz), 8.50 (dd, *J* = 13.4, 8.5 Hz, 2H, Bz), 8.40 (d, *J* = 5.1 Hz, 2H, Th), 8.30 (d, *J* = 5.2 Hz, 2H, Th), 2.65 (s, 12H, Me), 1.58 (s, 36H, *t*Bu). $^{11}$B NMR (160 MHz, $CD_3CN$) δ: 41.8. $^{13}$C NMR (126 MHz, $CD_3CN$) δ: 152.7, 152.3, 150.8 (dd, *J* = 251, 12.9 Hz), 150.5 (dd, *J* = 250, 13.2 Hz), 146.4, 146.1 (br), 144.5 (br), 143.7 (br), 139.9, 133.6, 133.0, 132.4, 131.7 (dd, *J* = 5.9, 3.0 Hz), 130.7 (dd, *J* = 5.9, 2.9 Hz), 121.6 (t, *J* = 18.3 Hz), 65.1, 31.9, 14.6. $^{19}$F NMR (470 MHz, $CD_3CN$) δ: –72.9 (d, *J* = 706 Hz), –136.3 – –137.3 (m). HRMS (ESI, positive) Calcd for $C_{54}H_{58}B_2F_4N_4S_4$: $[M]^{2+}$: 494.18278, Found 494.18405.

**References**

[S1] Y. Adachi and J. Ohshita, *Organometallics*, 2018, **37**, 869−881.

[S2] M. F. Silva Valverde, E. Theuergarten, T. Bannenberg, M. Freytag, P. G. Jones and M. Tamm, *Dalton Trans.*, 2015, **44**, 9400−9408.

[S3] A. L. Spek, Structure validation in chemical crystallography. *Acta Crystallogr.*, 2009, **D65**, 148–155.

***Water-stability test***

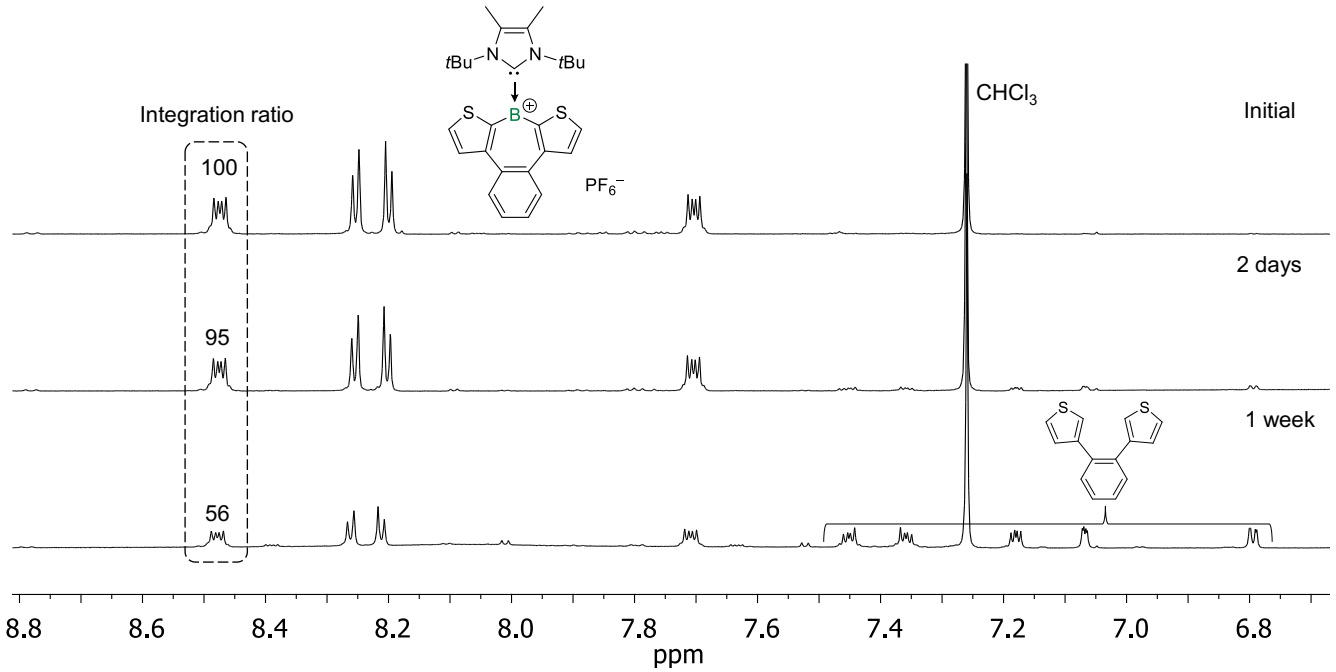



**Figure S1** $^{1}$H NMR spectral changes of **1-H**; initial, after two days, and after one week in water-saturated $CDCl_3$. The integration ratio is given relative to the initial signal. The residual $CHCl_3$ peak was used as the integration standard.

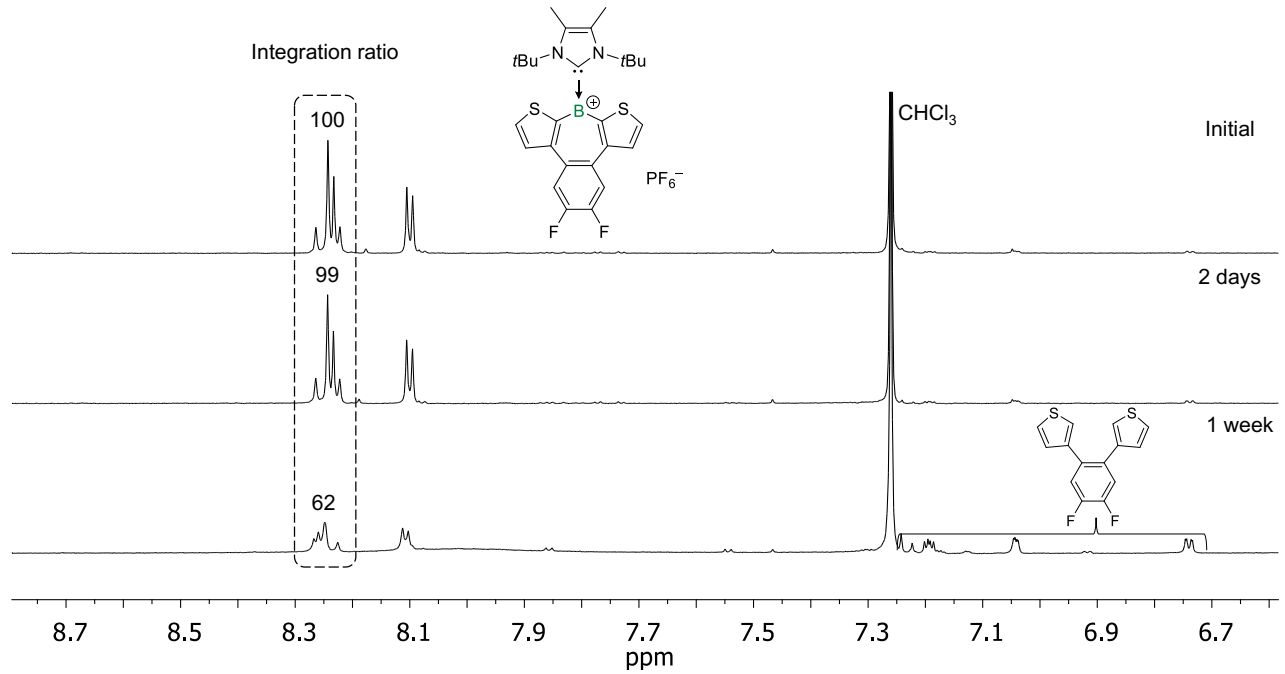



**Figure S2** $^{1}$H NMR spectral changes of **1-F**; initial, after two days, and after one week in water-saturated $CDCl_3$. The integration ratio is given relative to the initial signal. The residual $CHCl_3$ peak was used as the integration standard.

## *[1]H NMR spectral changes upon lithiation*

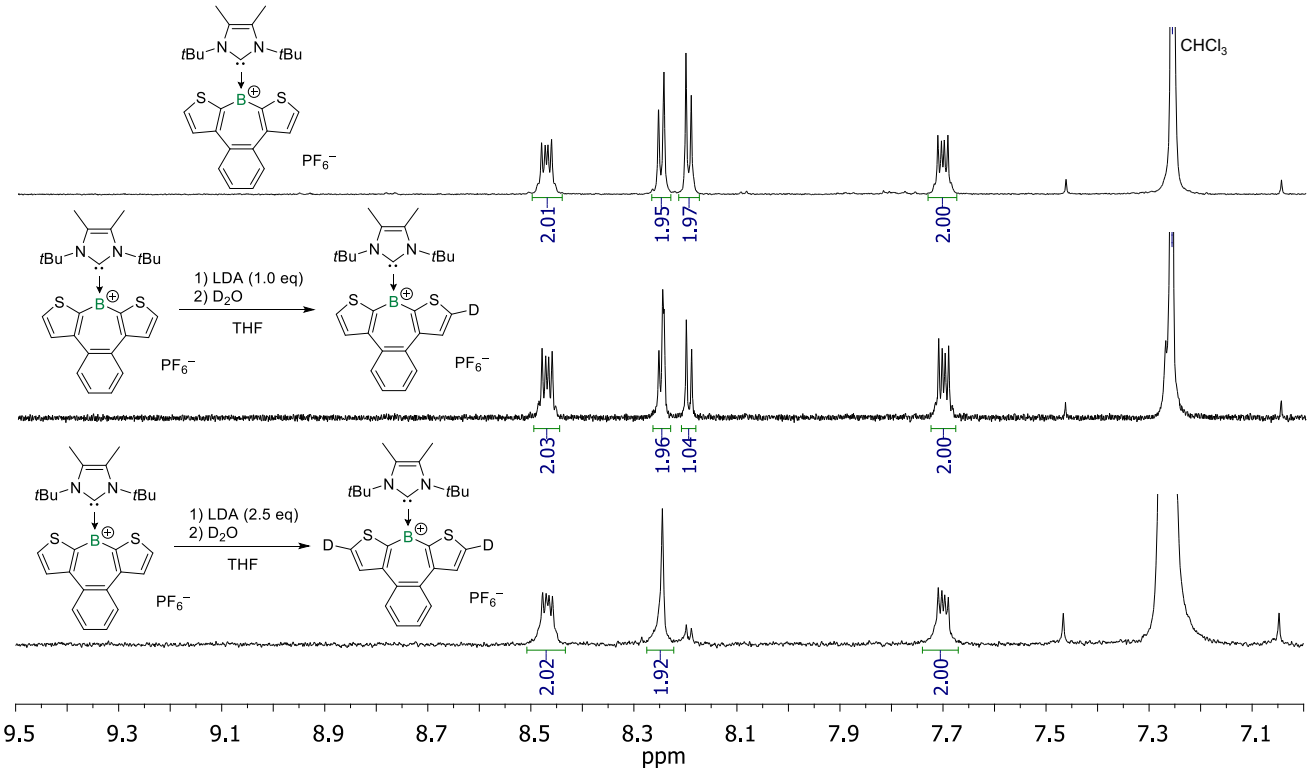



**Figure S3** [1]H NMR spectral changes of **1-H** after lithiation with LDA, then quenching with $D_2O$.

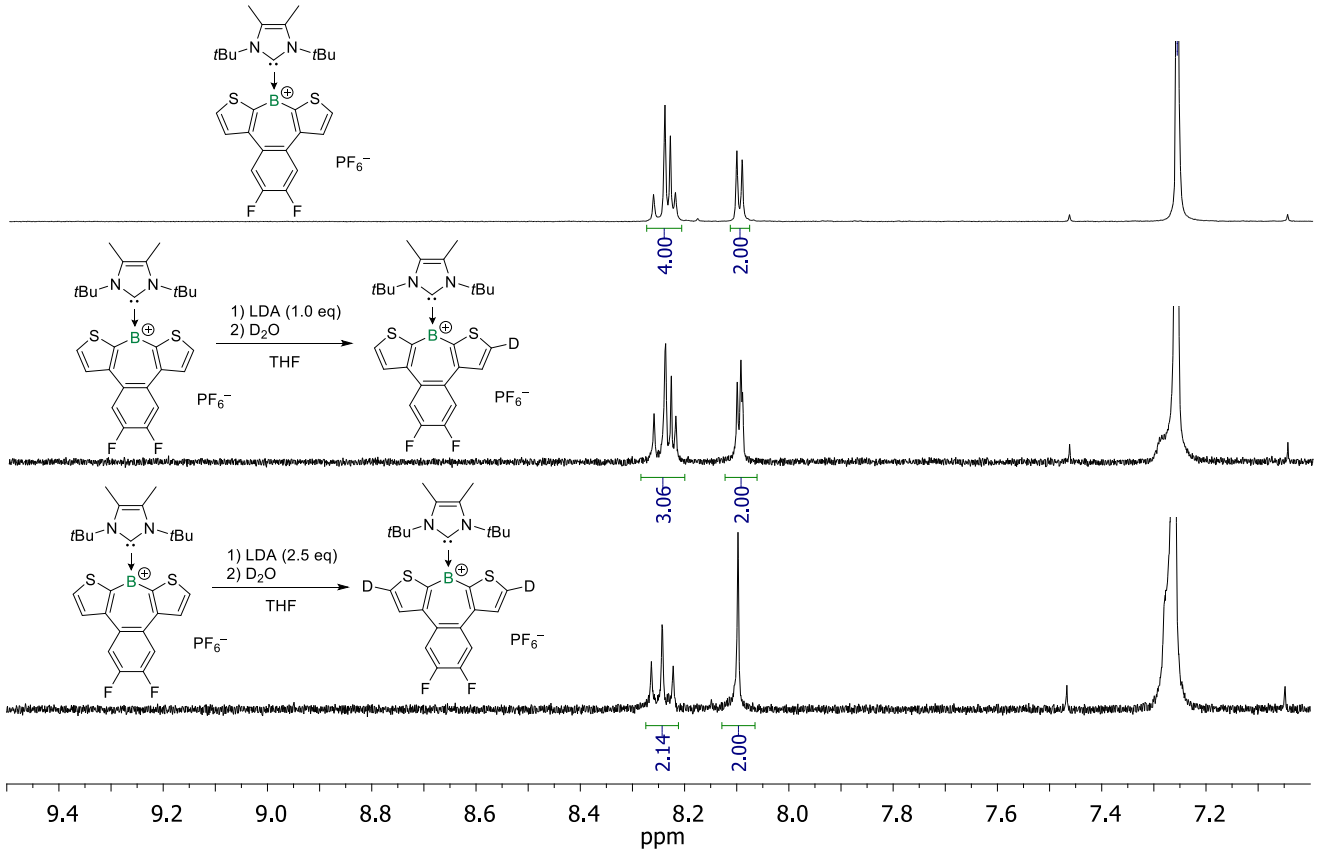



**Figure S4** [1]H NMR spectral changes of **1-F** after lithiation with LDA, then quenching with $D_2O$.

## *[1]H NMR spectral comparison of 2-H and 2-F*

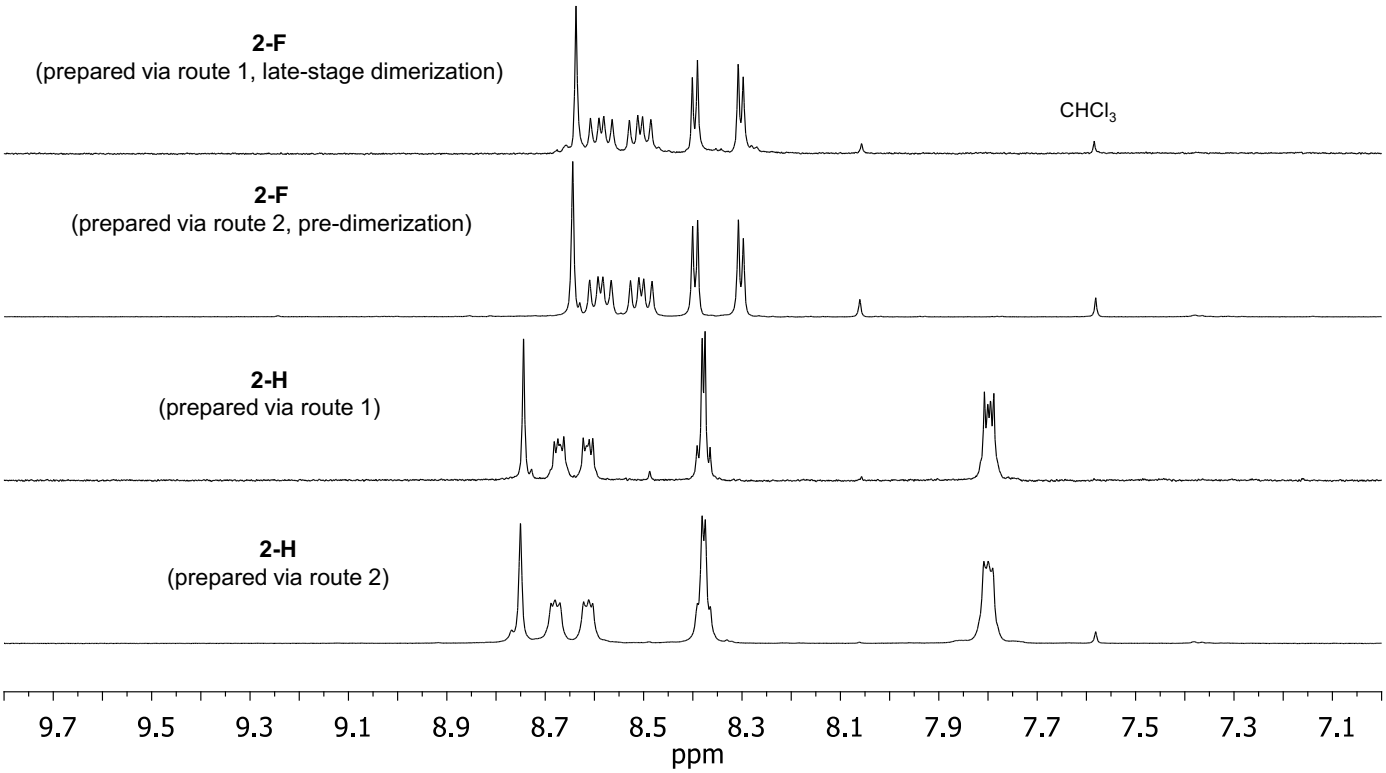



**Figure S5** $^{1}$H NMR spectra of **2-H** and **2-F** prepared by the two difference routes in $CD_3CN$.

## *Crystal structures of 1-F*

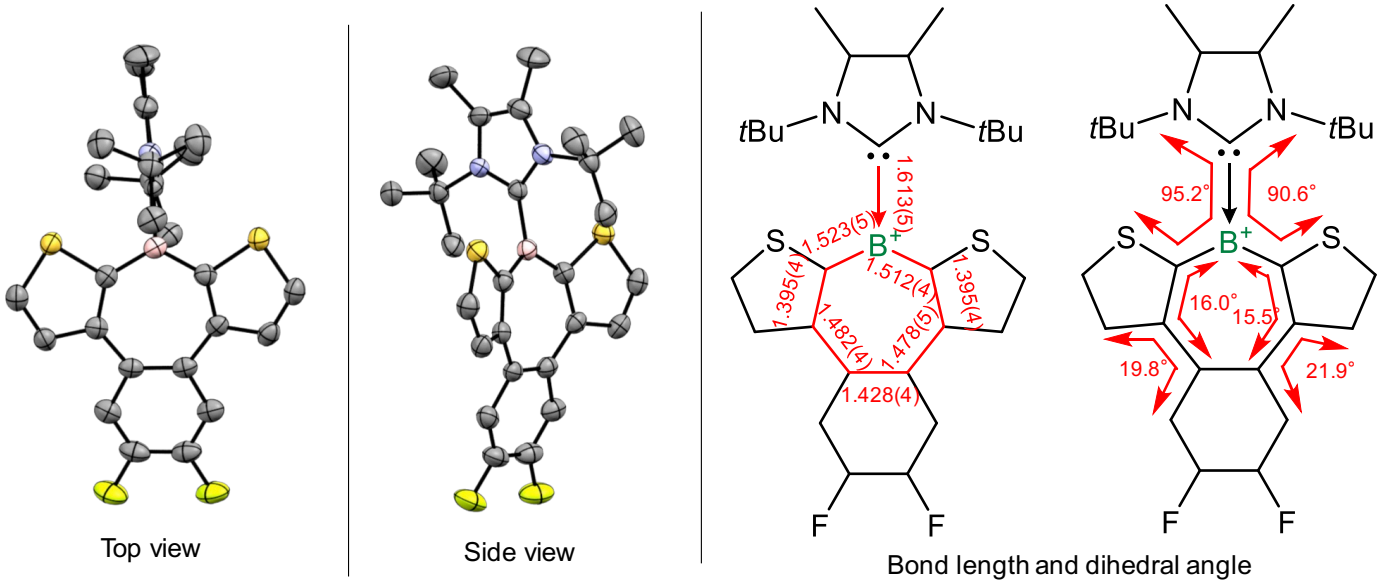



**Figure S6** Crystal structure of **1-F** obtained at 123 K. Thermal ellipsoids are at the 50% probability level. Hydrogen atoms and $PF_6^-$ anion are omitted for clarity.

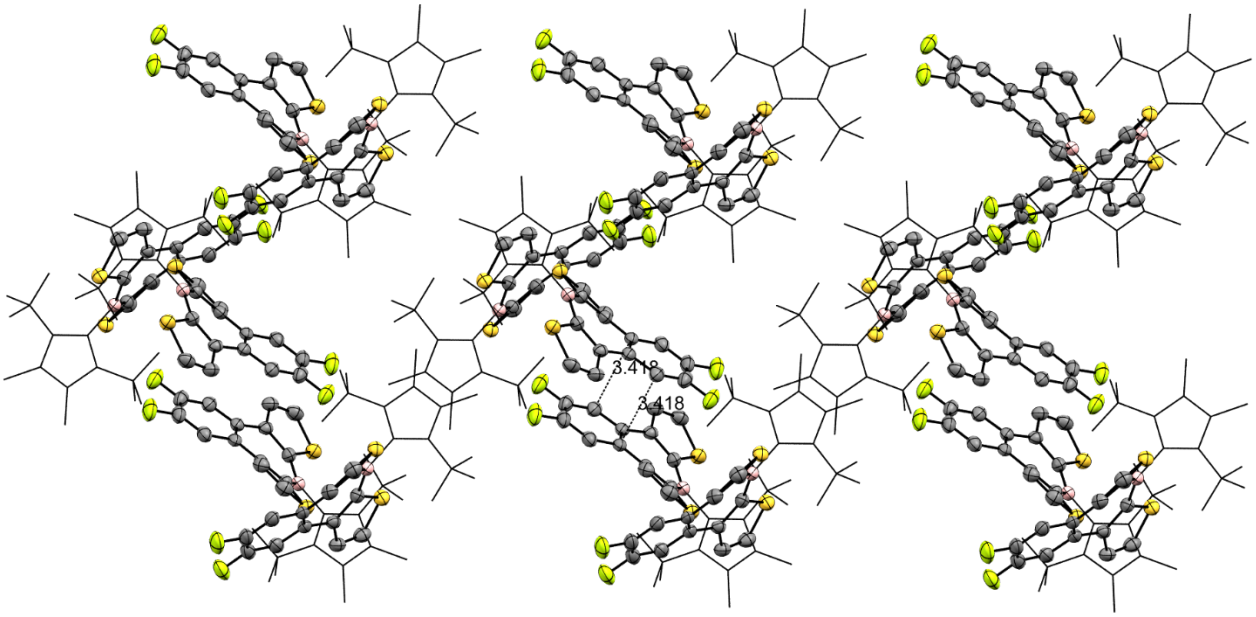



**Figure S7** Crystal packing structure of **1-F** obtained at 123 K. Thermal ellipsoids are at the 50% probability level. $PF_6^-$ and hydrogen atoms are omitted for clarity. NHC ligands are shown in wireframe style.

***Absorption and fluorescence data***

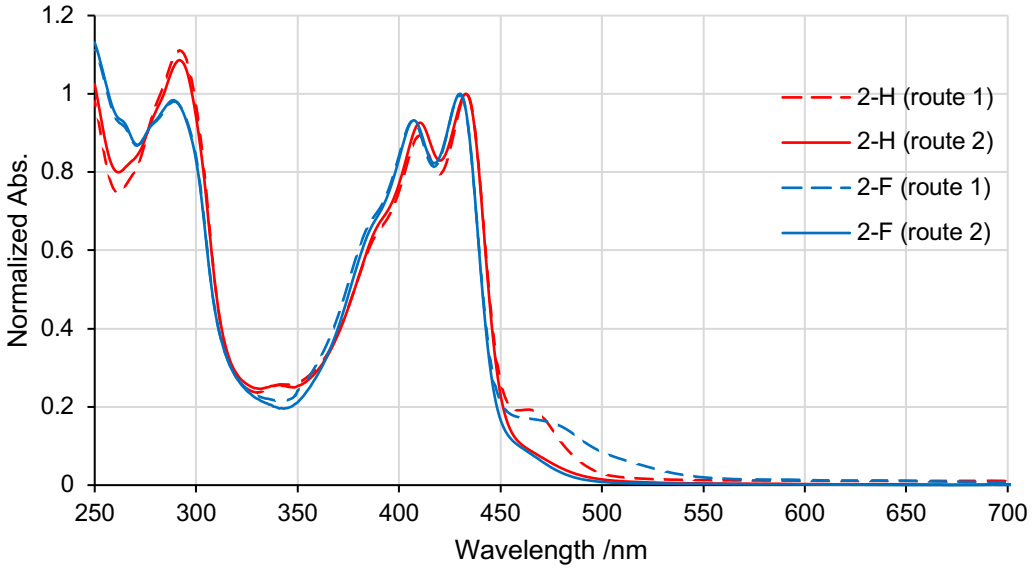



**Figure S8** Absorption spectra of dimers prepared via two different synthetic routes in $CH_2Cl_2$.

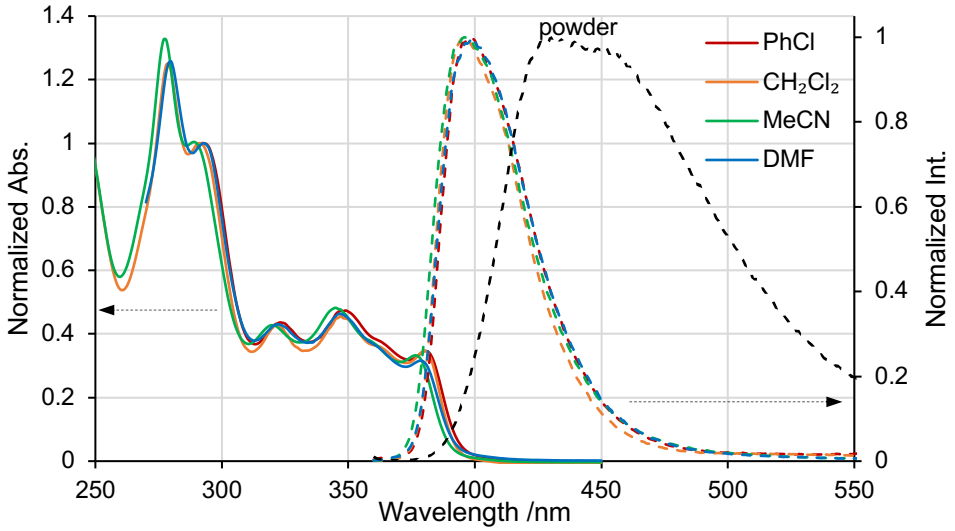



**Figure S9** Absorption (solid lines) and fluorescence spectra (dashed lines) of **1-H** in various solvents.

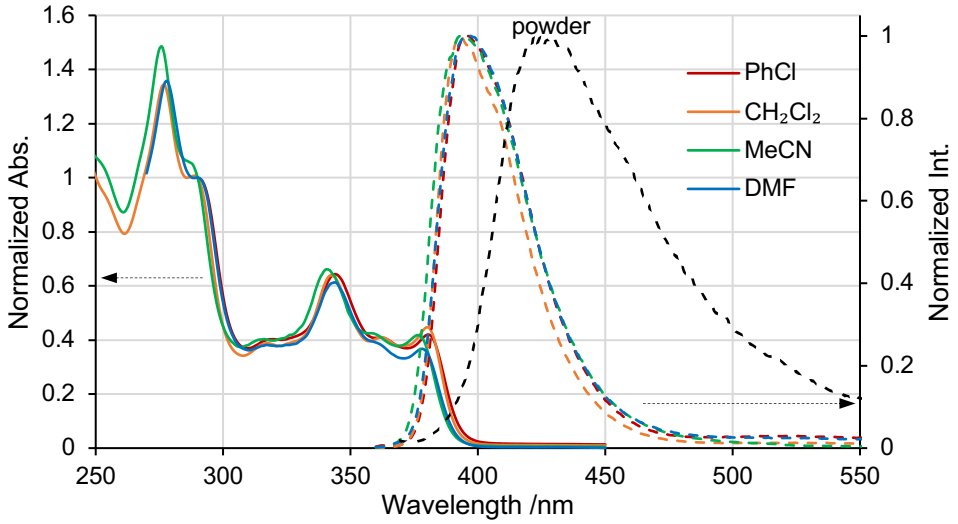



**Figure S10** Absorption (solid lines) and fluorescence spectra (dashed lines) of **1-F** in various solvents.

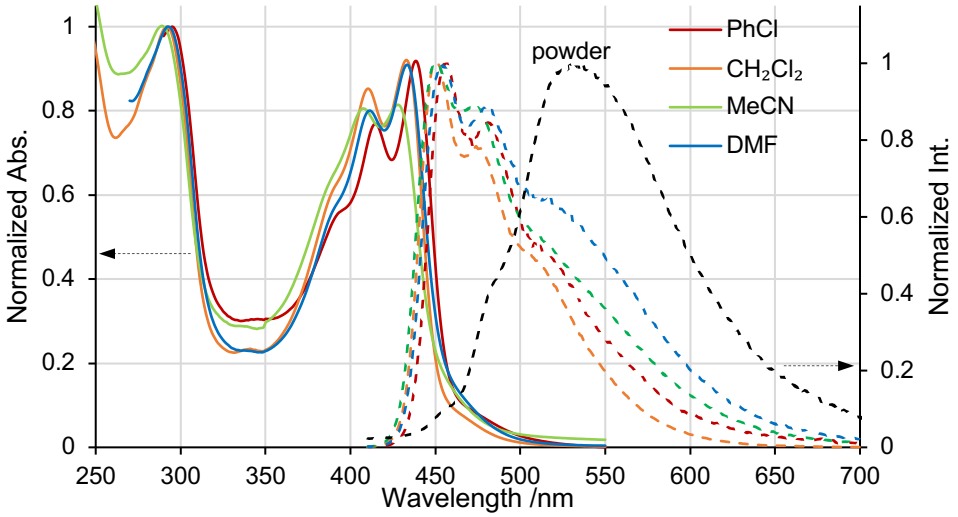



**Figure S11** Absorption (solid lines) and fluorescence spectra (dashed lines) of **2-H** in various solvents.

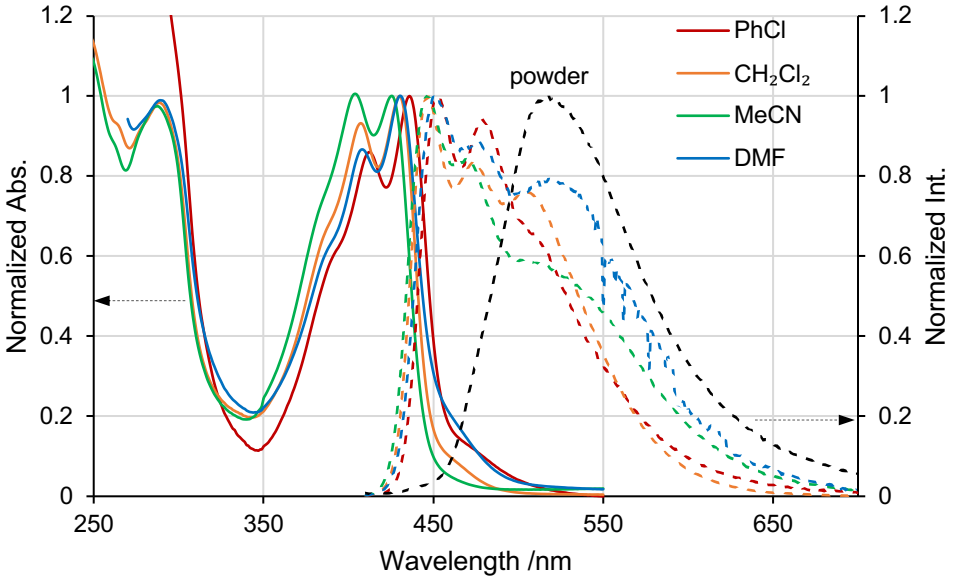



**Figure S12** Absorption (solid lines) and fluorescence spectra (dashed lines) of **2-F** in various solvents.

**Table S1** Optical data of borepinium ions in various solvents.

| | Solvent | $\lambda_{Abs}^{max}$ | $\lambda_{Abs}^{onset}$ | $\lambda_{Em}^{max}$ | $\Phi$ /% | $\tau$ (ampl.)/ns |
|---|---|---|---|---|---|---|
| **1-H** | PhCl | 323, 347, 380 | 394 | 398 | 1.8 | 0.40 (1.0) |
| | DCM | 279, 322, 347, 380 | 393 | 397 | 1.4 | 0.41 (1.0) |
| | ACN | 277, 320, 345, 377 | 390 | 396 | 1.6 | 0.40 (1.0) |
| | DMF | 280, 322, 347, 379 | 394 | 399 | 1.5 | 0.44 (1.0) |
| | Powder | - | - | 430 | 0.5 | 0.33 (0.90), 3.72 (0.10) |
| **1-F** | PhCl | 344, 381 | 394 | 396 | 1.7 | 0.37 (1.0) |
| | DCM | 276, 341, 376 | 392 | 393 | 1.9 | 0.37 (1.0) |
| | ACN | 277, 342, 380 | 390 | 393 | 1.2 | 0.37 (1.0) |
| | DMF | 278, 344, 378 | 392 | 397 | 1.4 | 0.29 (0.90), 1.66 (0.10) |
| | Powder | - | - | 425 | 0.4 | 0.36 (0.91), 4.02 (0.09) |
| **2-H** | PhCl | 295, 415, 438 | 461 | 457 | 7.1 | 0.22 (1.0) |
| | DCM | 292, 410, 433 | 454 | 451 | 5.7 | 0.21 (1.0) |
| | ACN | 290, 408, 428 | 455 | 450 | 5.0 | 0.21 (1.0) |
| | DMF | 293, 411, 433 | 457 | 453 | 3.6 | 0.23 (1.0) |
| | Powder | - | - | 482 | 2.8 | 0.51 (0.73), 3.08 (0.19), 18.09 (0.08) |
| **2-F** | PhCl | 412, 436 | 458 | 452 | 8.8 | 0.22 (1.0) |
| | DCM | 289, 407, 430 | 450 | 447 | 7.3 | 0.21 (1.0) |
| | ACN | 288, 404, 425 | 447 | 446 | 5.5 | 0.22 (1.0) |
| | DMF | 289, 408, 430 | 450 | 450 | 9.6 | 0.25 (1.0) |
| | Powder | - | - | 466 | 6.2 | 0.49 (0.53), 2.59 (0.35), 16.14 (0.12) |

**Table S2** Summary of electrochemical data of borepinium ions.

| | $E_{1/2}^{red1}$ [a] /V($Fc^{0/+}$) | $E_{1/2}^{red2}$ [a] /V($Fc^{0/+}$) | LUMO[b] /eV | $E_g^{opt}$ [c] /eV | HOMO[d] /eV | $E_g^{calc}$ [e] /eV |
|---|---|---|---|---|---|---|
| **1-H** | −1.86 | - | −2.94 | 3.18 | −6.12 | 3.90 |
| **1-F** | −1.79 | - | −3.01 | 3.18 | −6.19 | 3.80 |
| **2-H** | −1.39 | −1.76 | −3.41 | 2.73 | −6.14 | 3.20 |
| **2-F** | −1.36 | −1.59 | −3.44 | 2.77 | −6.21 | 3.25 |

[a] $E_{red} = 0.5\ (E_{pc} + E_{pa})$; [b] Determined as $-(4.8 - E_{red}^{1})$; [c] Obtained from the absorption onset in acetonitrile; [d] Determined as LUMO − $E_g^{opt}$; [e] Estimated from DFT calculations (B3LYP/6-31g(d,p)) for compounds without $PF_6^-$.

***DFT results***

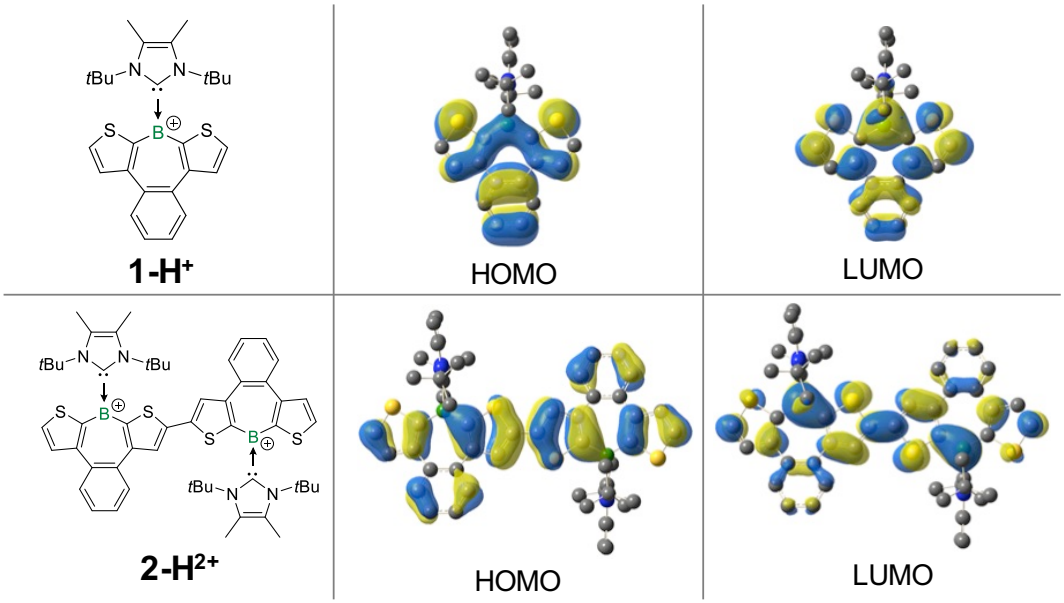
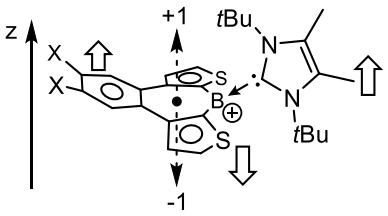



**Figure S13** HOMO/LUMO frontier orbitals of **1-H**$^+$ and **2-H**$^{2+}$ from DFT calculations at the B3LYP/6-31G(d,p) level of theory.

**Table S3** Calculated NICS values of borepinium cations.

| | NICS(0) | NICS(+1) | NICS(-1) |
|---|---|---|---|
| **B** | 0.97 | −1.69 | −2.72 |
| **1-H**$^+$ | 0.65 | −2.10 | −2.57 |
| **1-F**$^+$ | 0.20 | −2.45 | −2.92 |



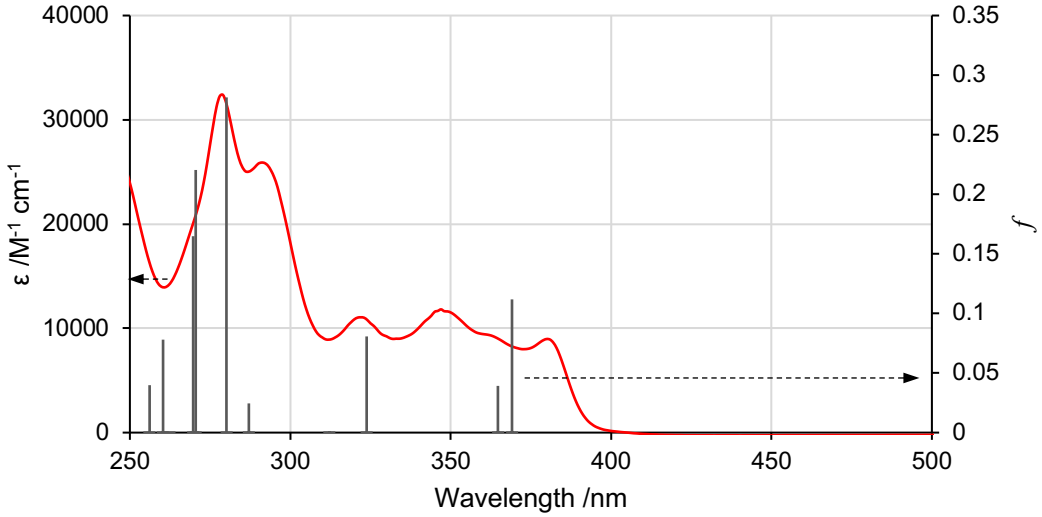



**Figure S14** Experimental absorption spectrum of **1-H** in $CH_2Cl_2$ and TD-DFT results of **1-H**$^+$ at B3LYP/6-31G(d,p) level.

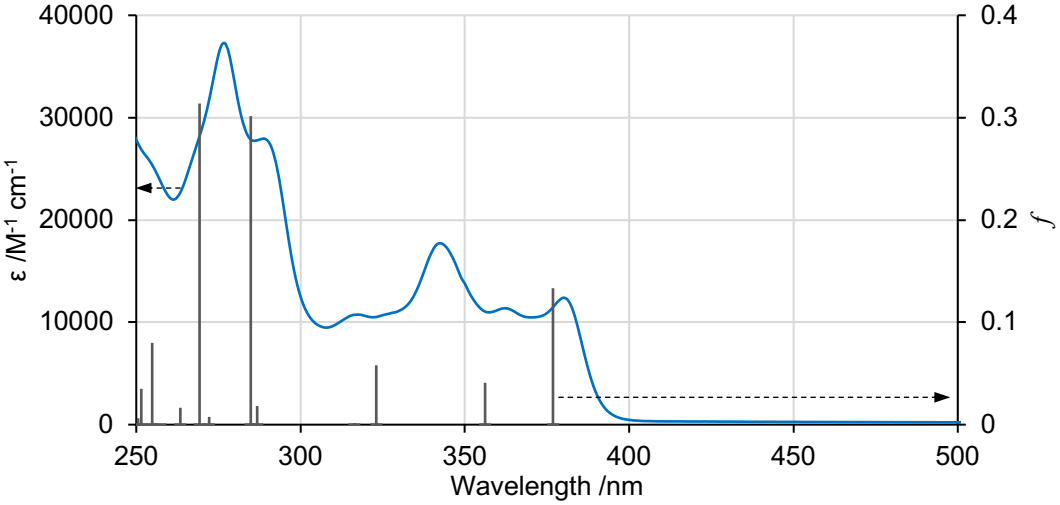



**Figure S15** Experimental absorption spectrum of **1-F** in $CH_2Cl_2$ and TD-DFT results of **1-H**$^+$ at B3LYP/6-31G(d,p) level.

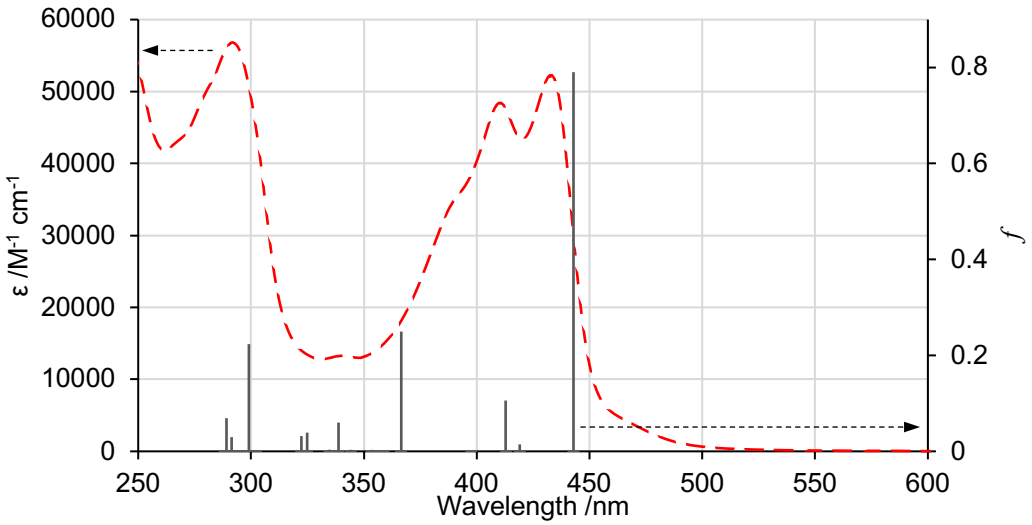



**Figure S16** Experimental absorption spectrum of **2-H** in $CH_2Cl_2$ and TD-DFT results of **2-H**$^{2+}$ at B3LYP/6-31G(d,p) level.

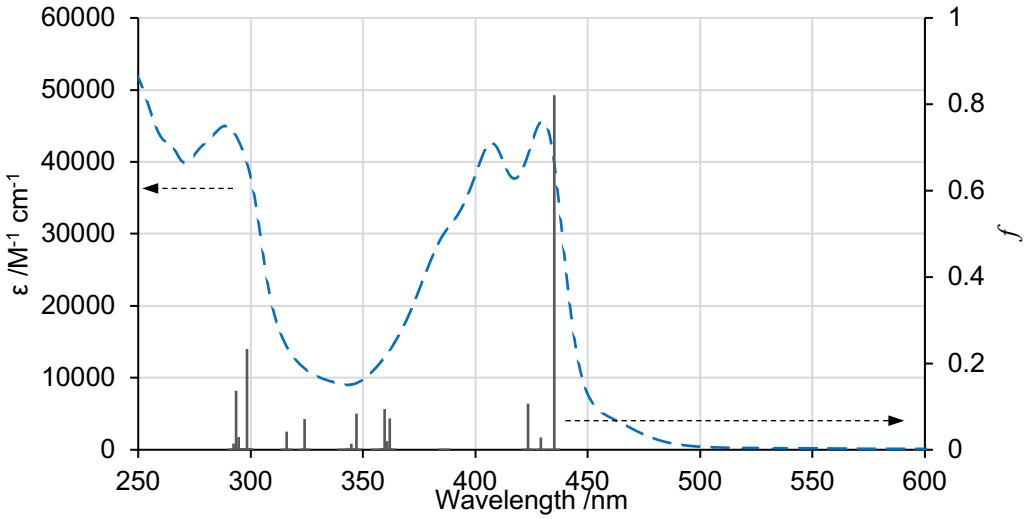



**Figure S17** Experimental absorption spectrum of **2-F** in $CH_2Cl_2$ and TD-DFT results of **2-F**$^{2+}$ at B3LYP/6-31G(d,p) level.

***NMR and MS spectra***

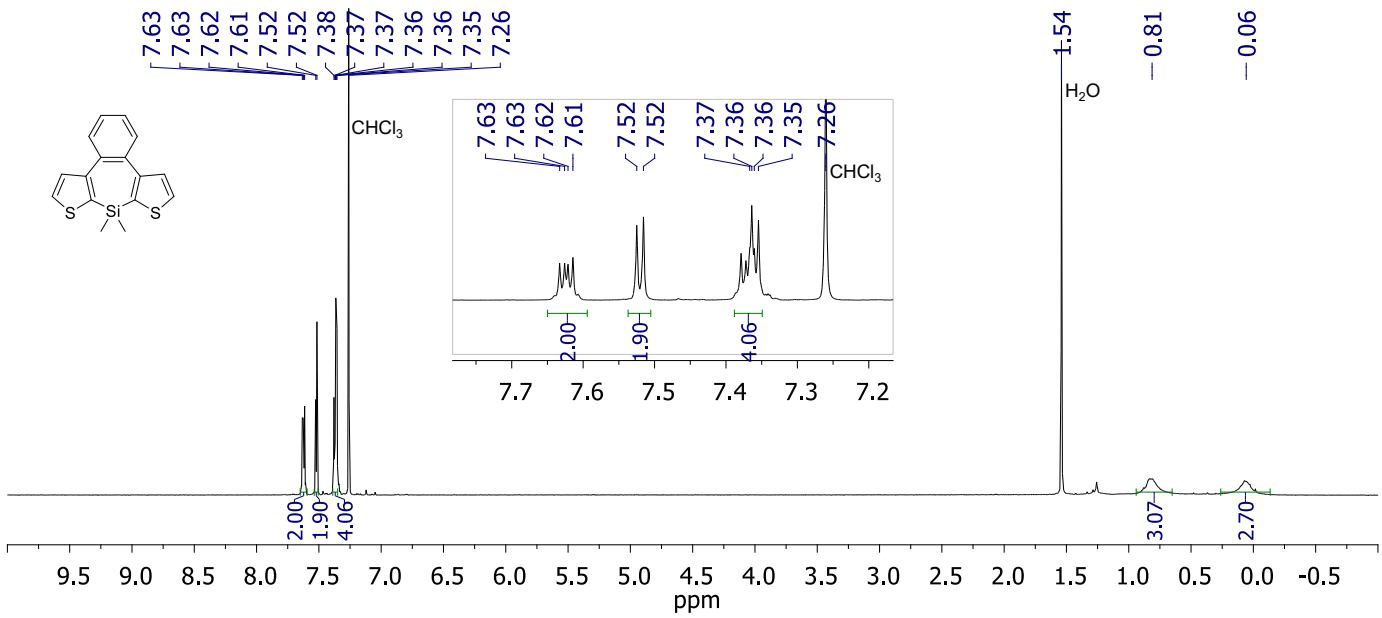



**Fig. S18** $^{1}$H NMR spectrum of **3-H** in $CDCl_3$ at room temperature.

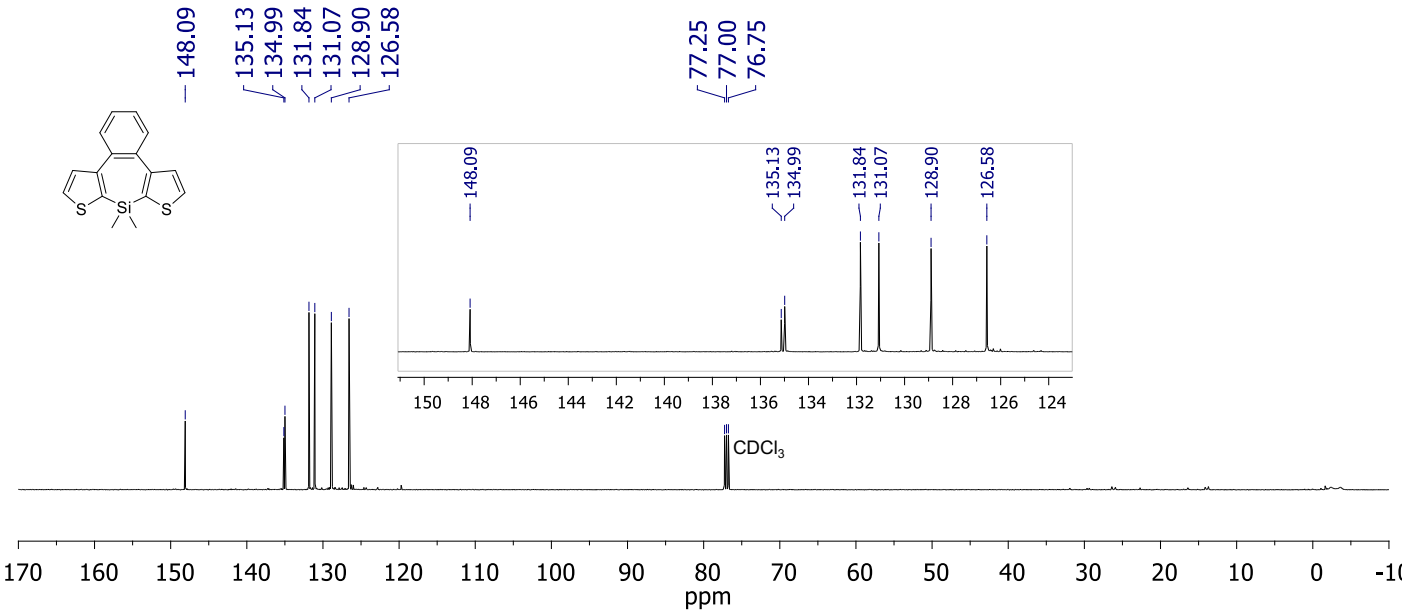



**Fig. S19** $^{13}$C NMR spectrum of **3-H** in $CDCl_3$ at room temperature.

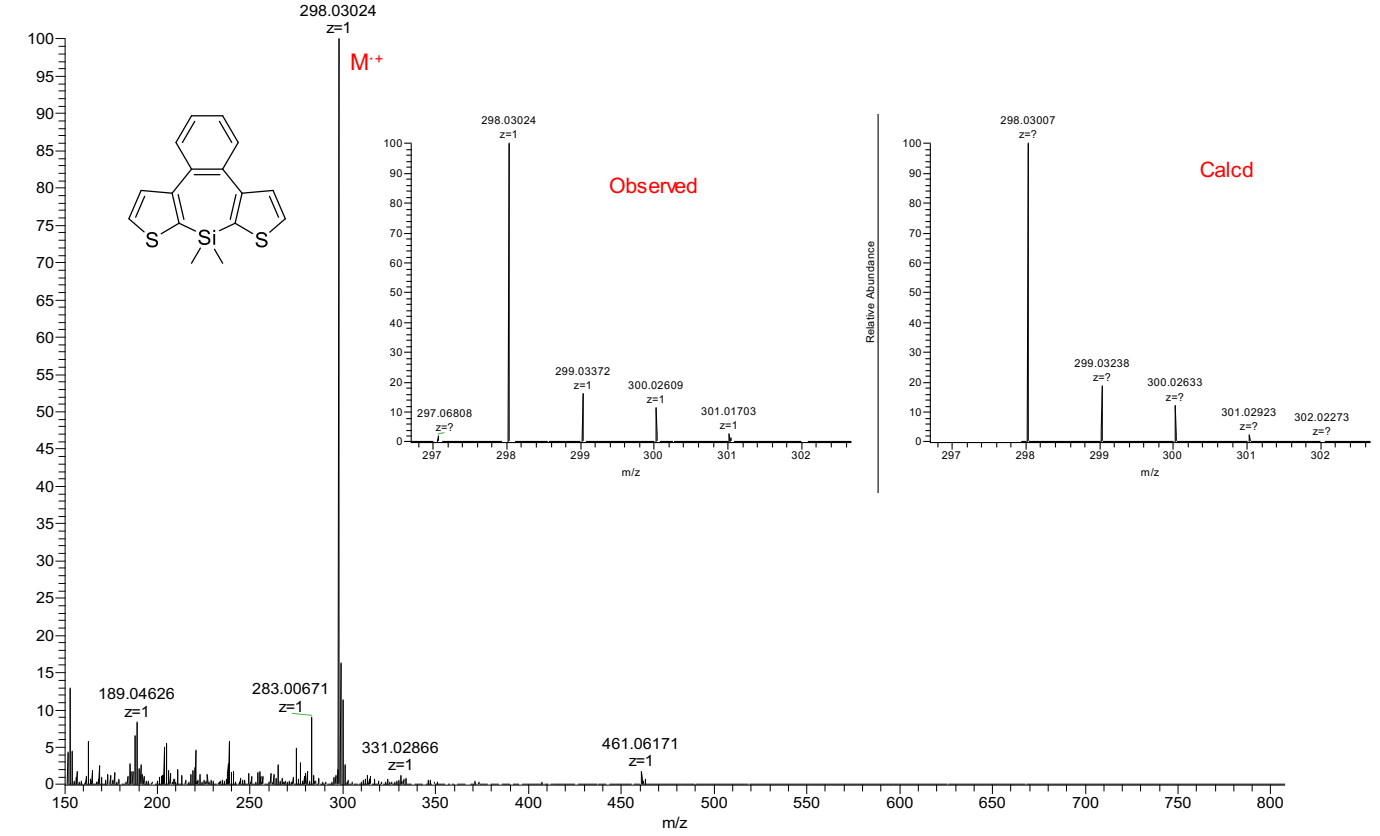



**Fig. S20** APCI mass spectrum of **3-H** (positive mode).

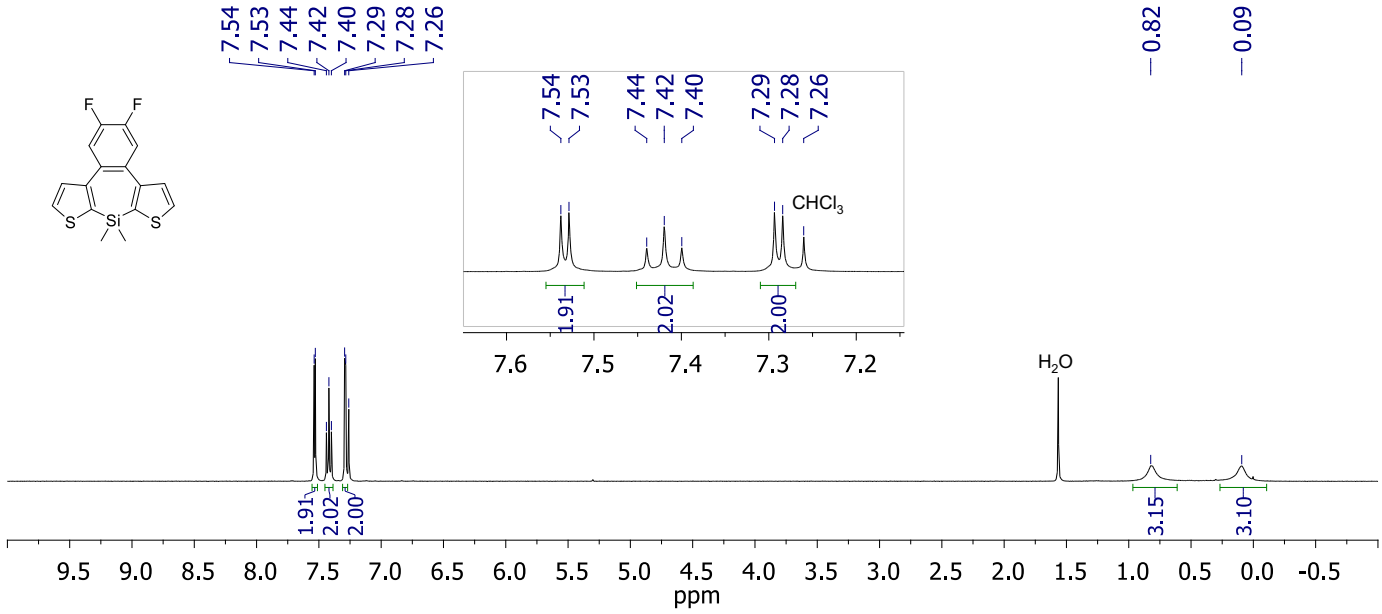



**Fig. S21** $^{1}$H NMR spectrum of **3-F** in $CDCl_3$ at room temperature.

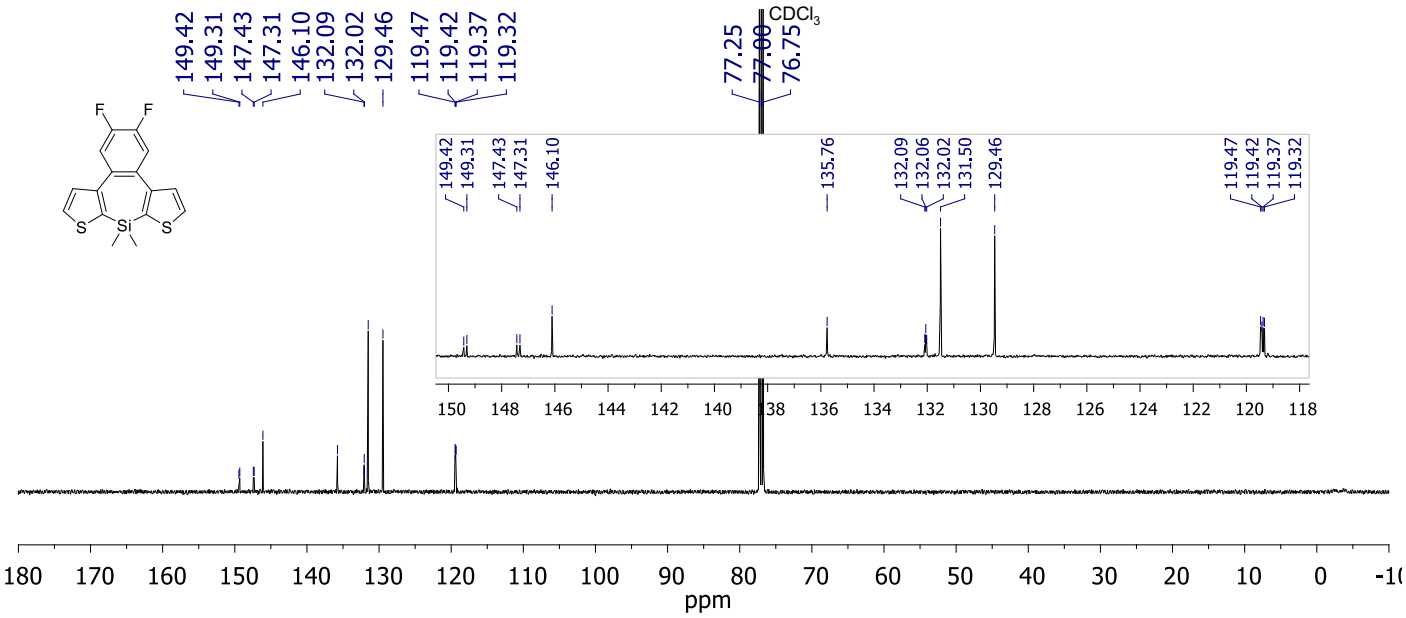



**Fig. S22** $^{13}C$ NMR spectrum of **3-F** in $CDCl_3$ at room temperature.

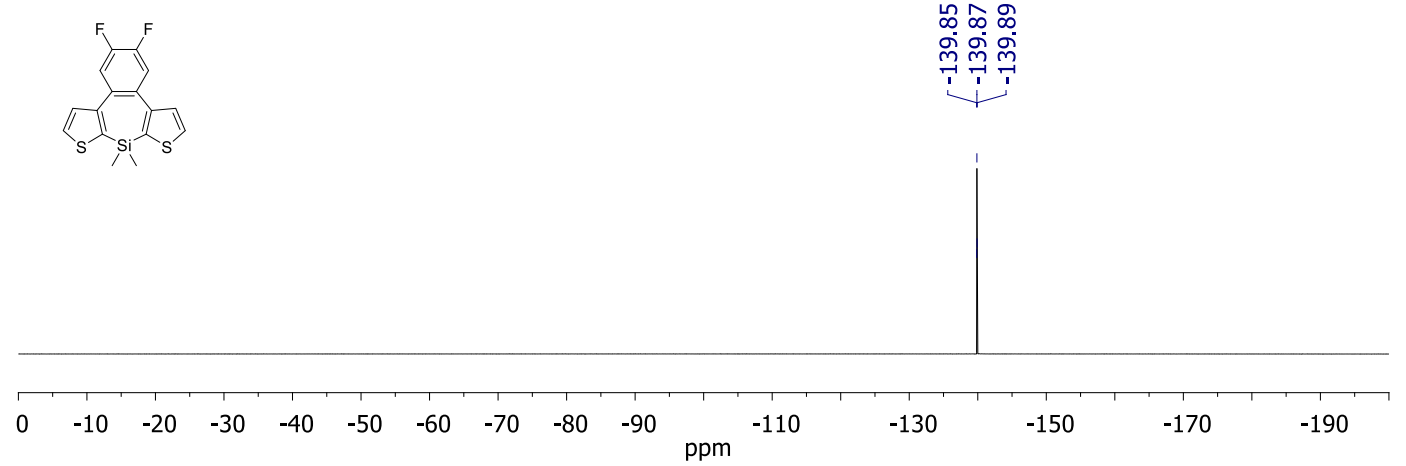



**Fig. S23** $^{19}F$ NMR spectrum of **3-F** in $CDCl_3$ at room temperature.

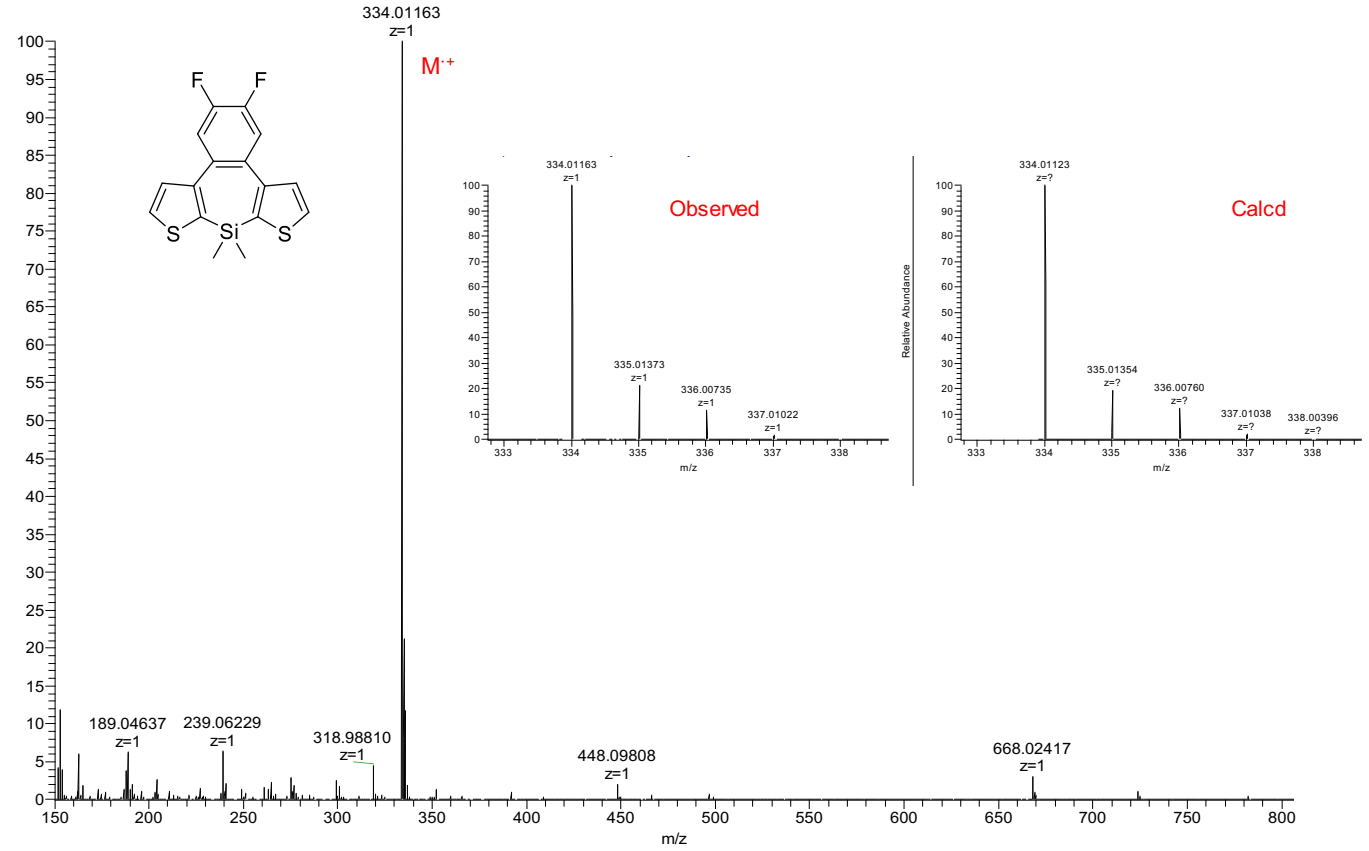



**Fig. S24** APCI mass spectrum of **3-H** (positive mode).

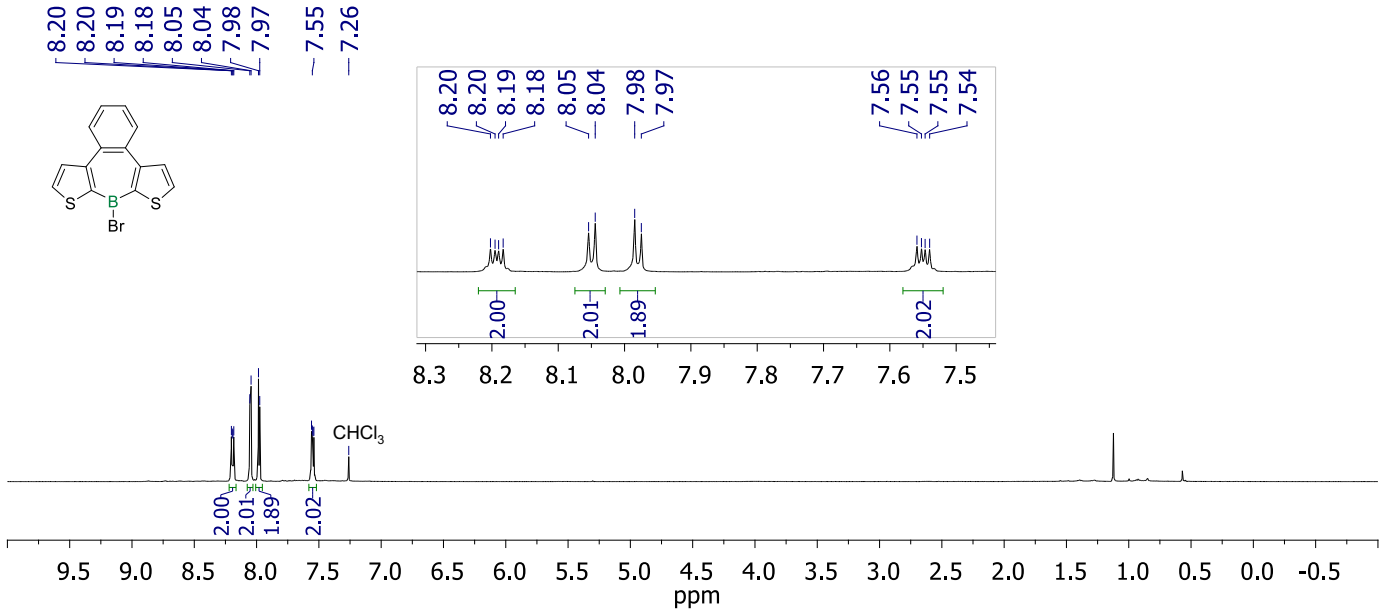



**Fig. S25** $^{1}$H NMR spectrum of **4-H** in $CDCl_3$ at room temperature.

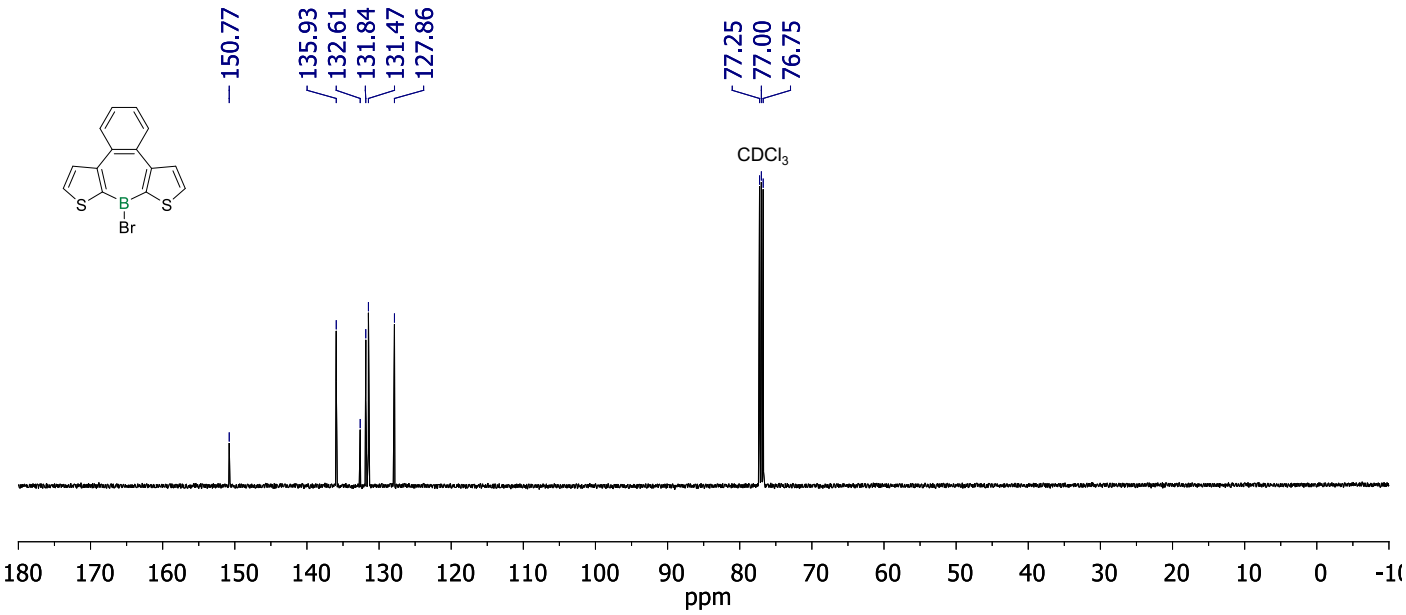



**Fig. S26** $^{13}$C NMR spectrum of **4-H** in $CDCl_3$ at room temperature.

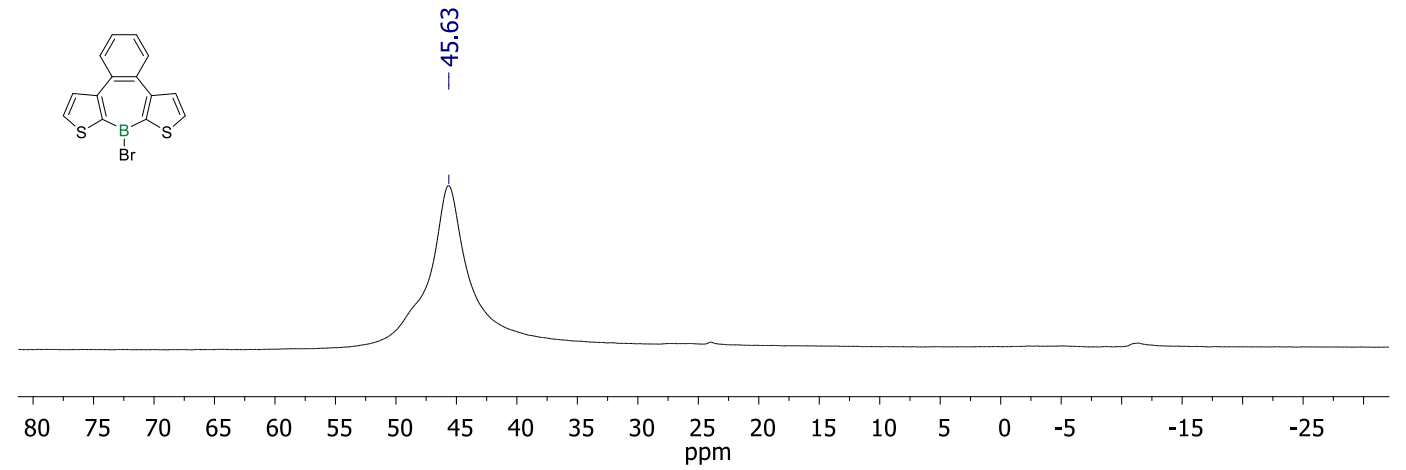



**Fig. S27** $^{11}$B NMR spectrum of **4-H** in $CDCl_3$ at room temperature.

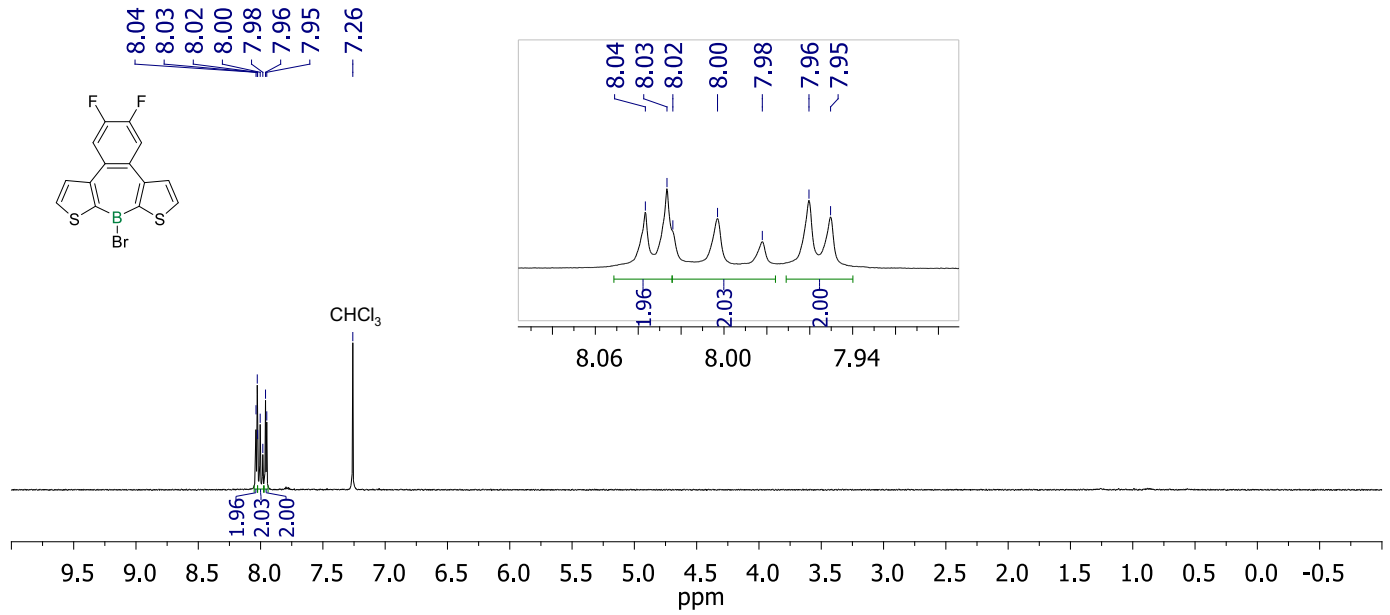



**Fig. S28** $^{1}$H NMR spectrum of **4-F** in $CDCl_3$ at room temperature.

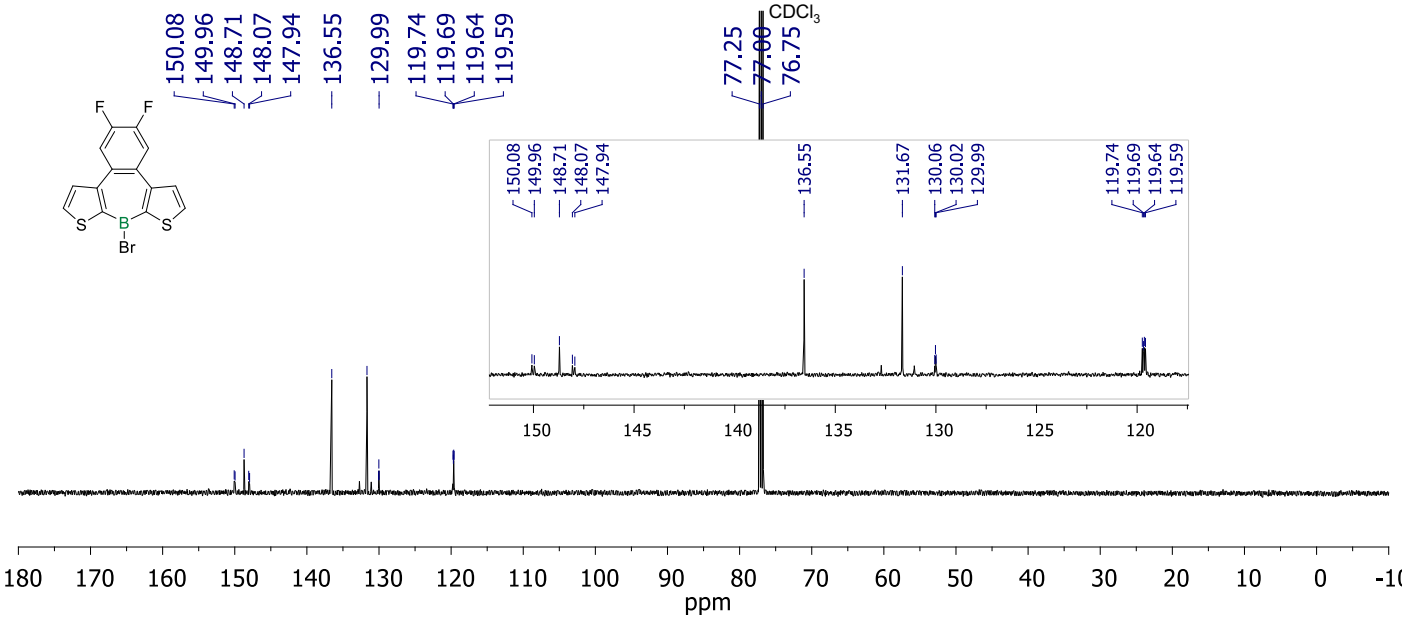



**Fig. S29** $^{13}$C NMR spectrum of **4-F** in $CDCl_3$ at room temperature.

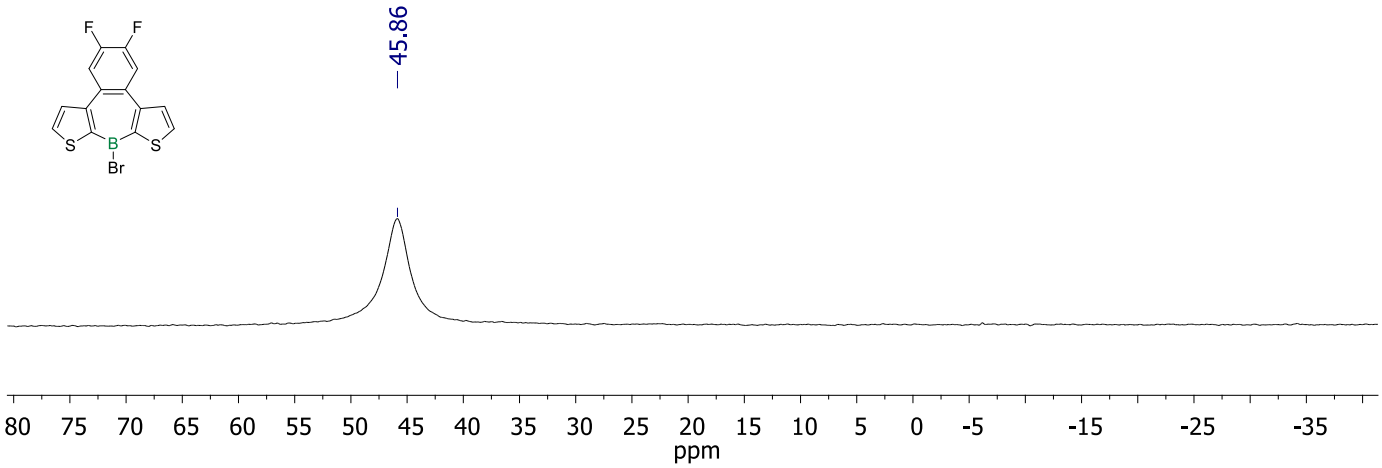



**Fig. S30** $^{11}$B NMR spectrum of **4-F** in $CDCl_3$ at room temperature.

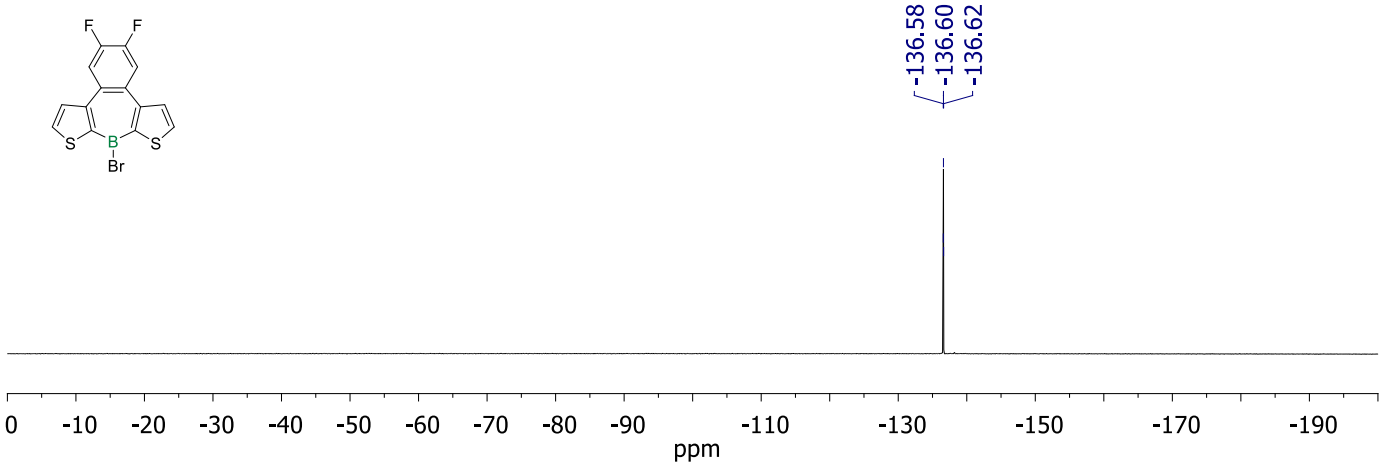



**Fig. S31** $^{19}$F NMR spectrum of **4-F** in $CDCl_3$ at room temperature.

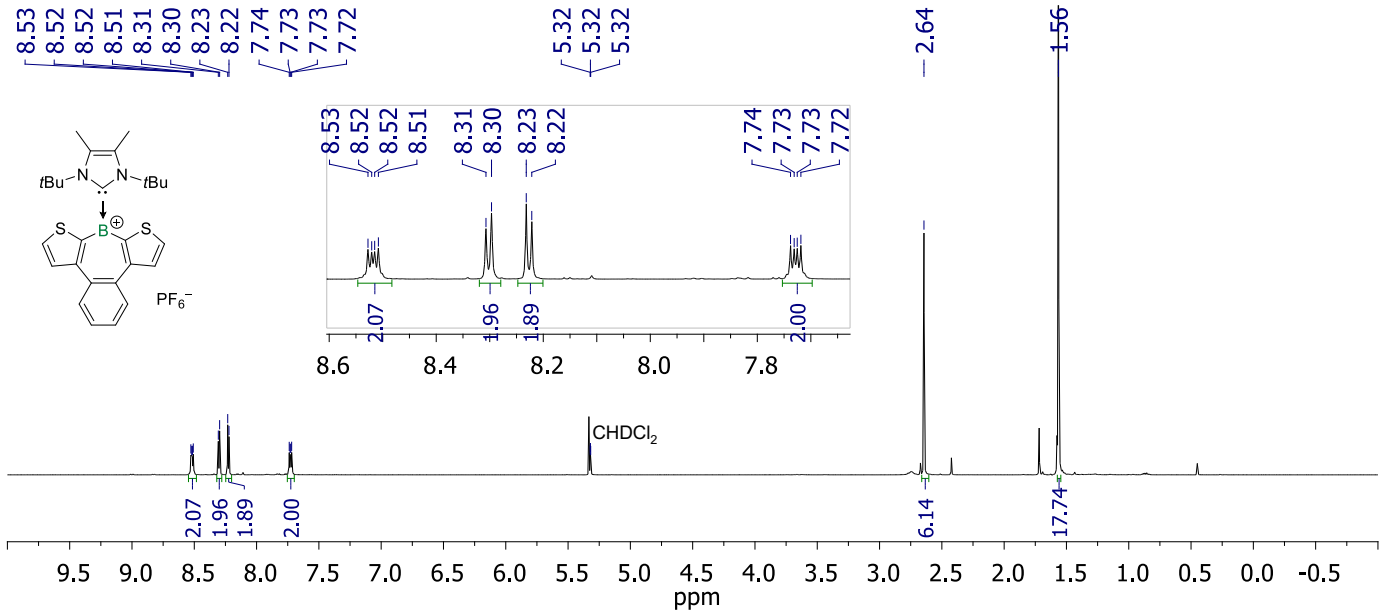



**Fig. S32** $^{1}$H NMR spectrum of **1-H** in $CD_2Cl_2$ at room temperature.

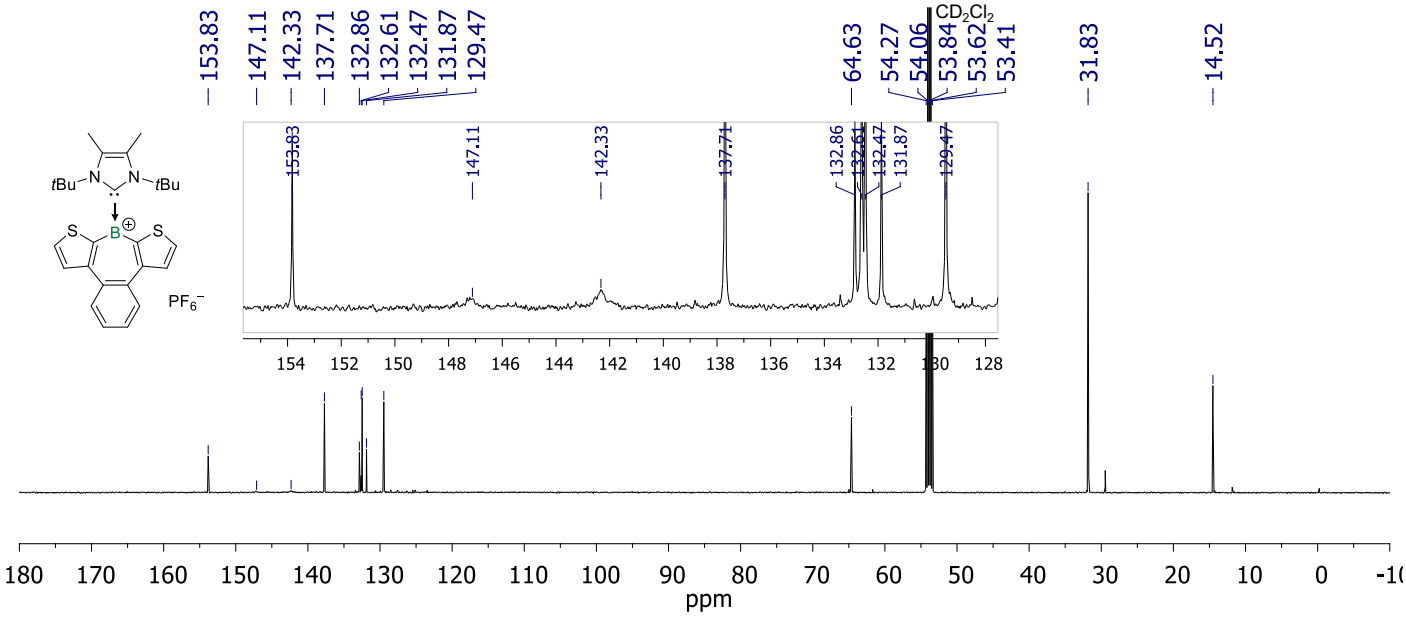



**Fig. S33** $^{13}$C NMR spectrum of **1-H** in $CD_2Cl_2$ at room temperature.

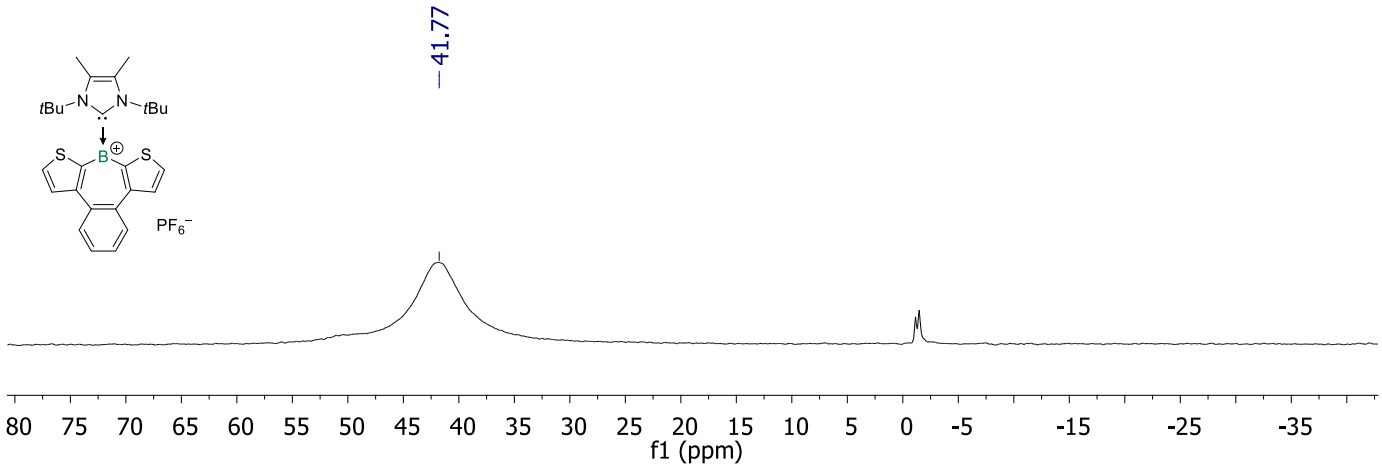



**Fig. S34** $^{11}$B NMR spectrum of **1-H** in $CD_2Cl_2$ at room temperature.

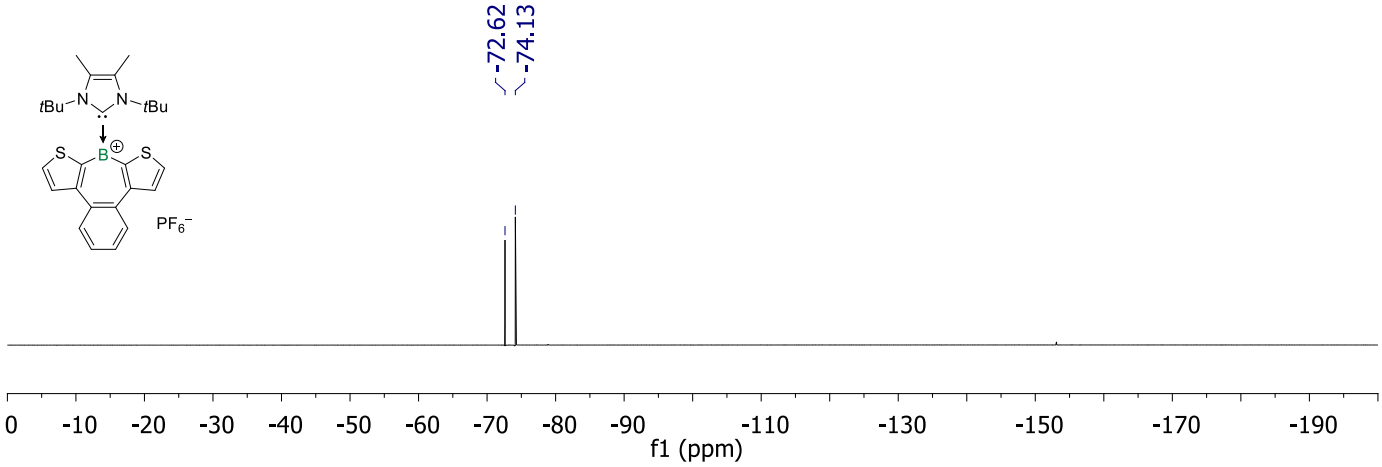



**Fig. S35** $^{19}$F NMR spectrum of **1-H** in $CD_2Cl_2$ at room temperature.

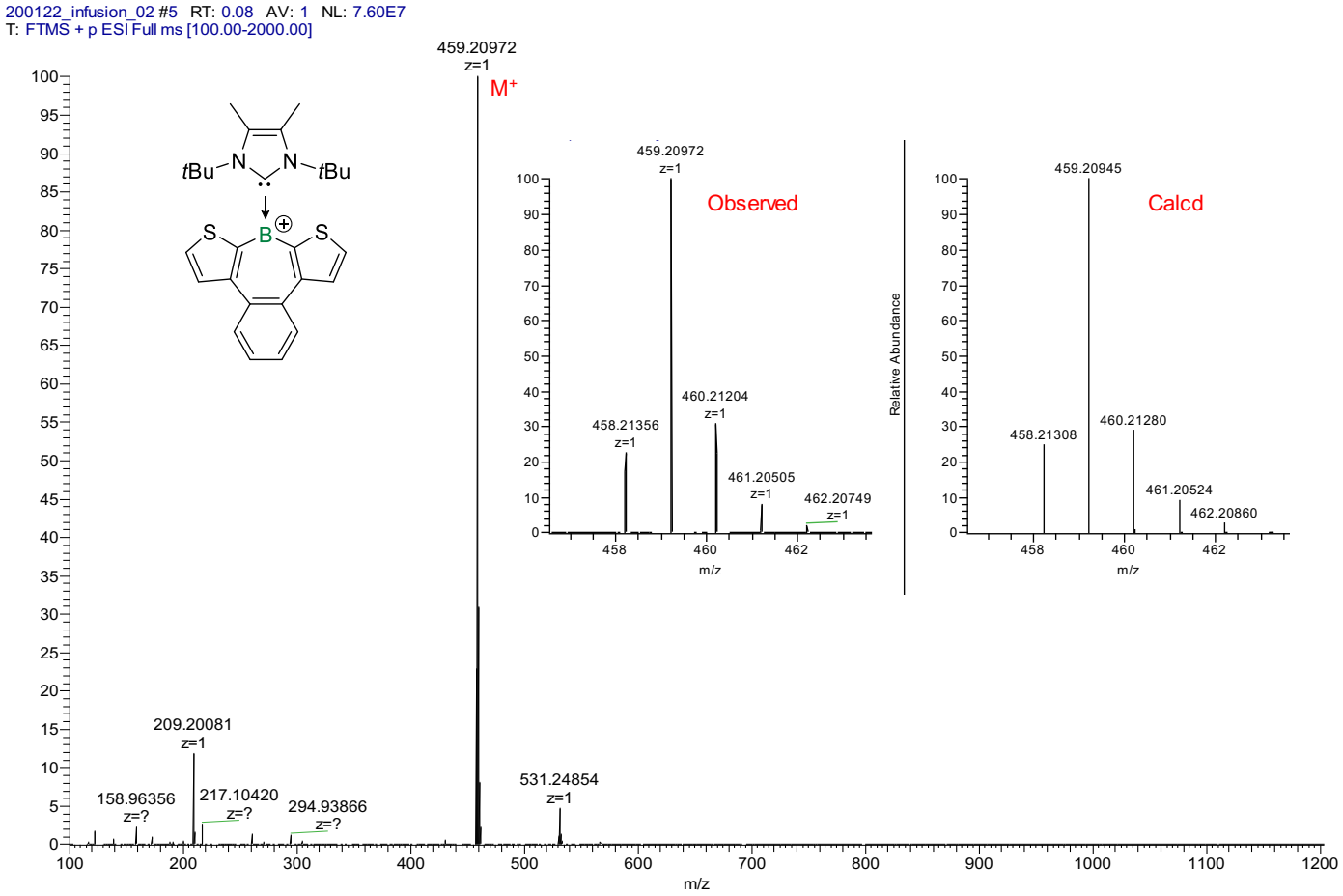



**Fig. S36** ESI mass spectrum of **1-H** (positive mode).

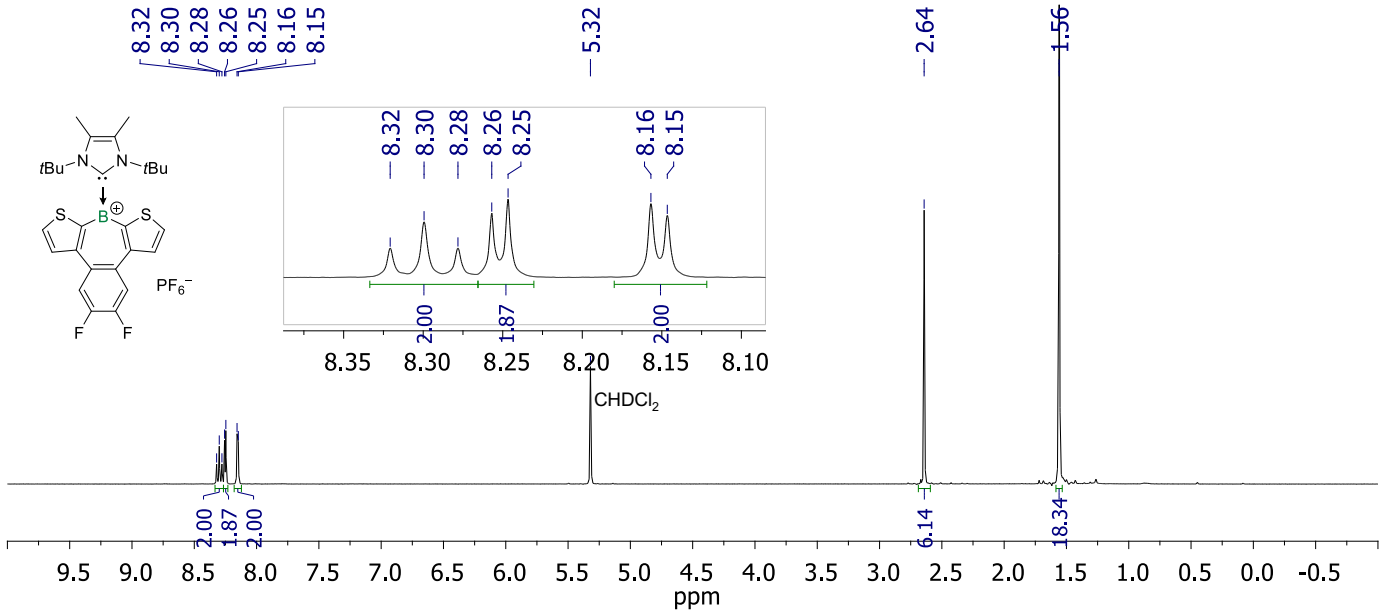



**Fig. S37** $^{1}$H NMR spectrum of **1-F** in $CD_2Cl_2$ at room temperature.

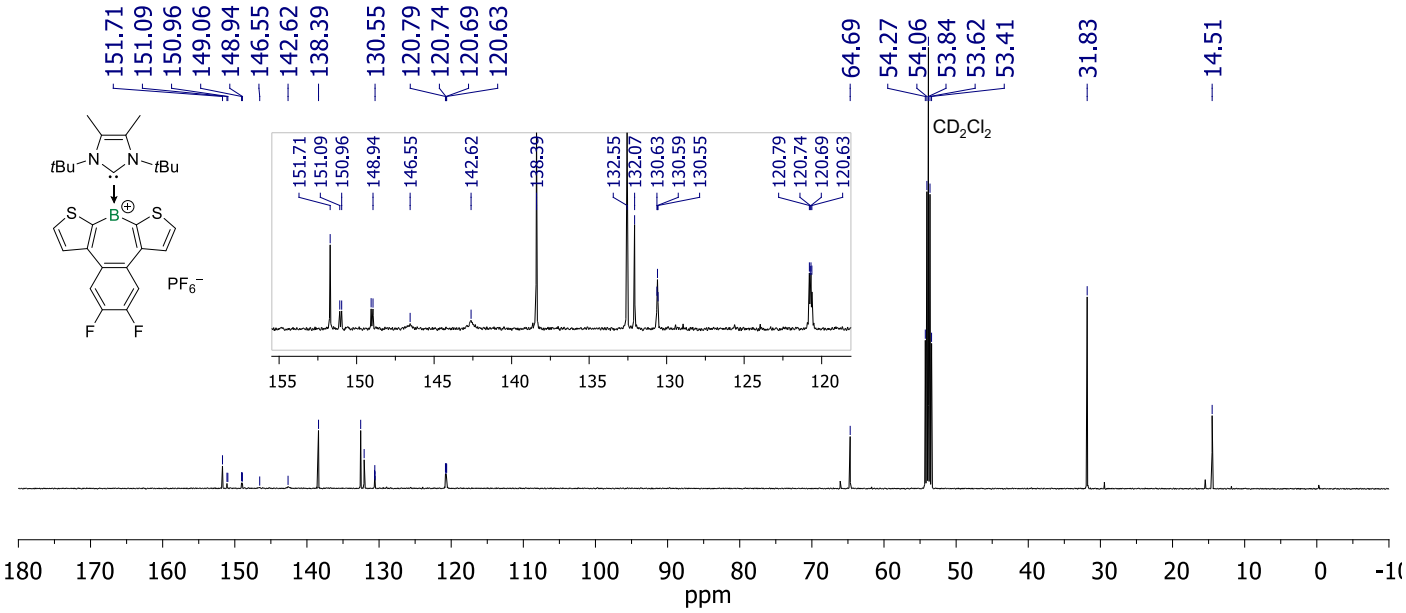



**Fig. S38** $^{13}$C NMR spectrum of **1-F** in $CD_2Cl_2$ at room temperature.

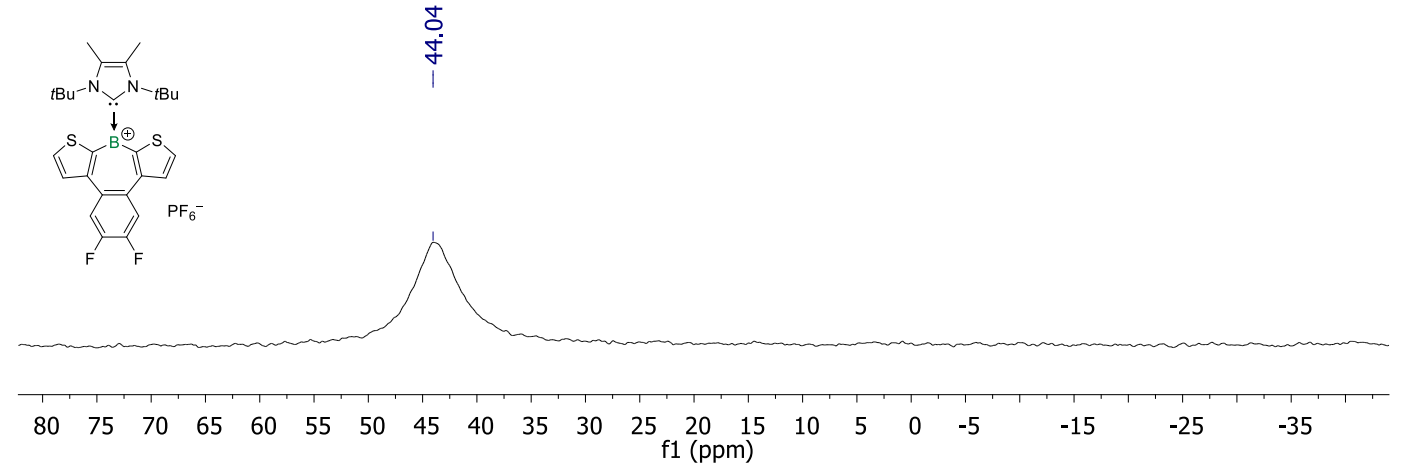



**Fig. S39** $^{11}$B NMR spectrum of **1-F** in $CD_2Cl_2$ at room temperature.

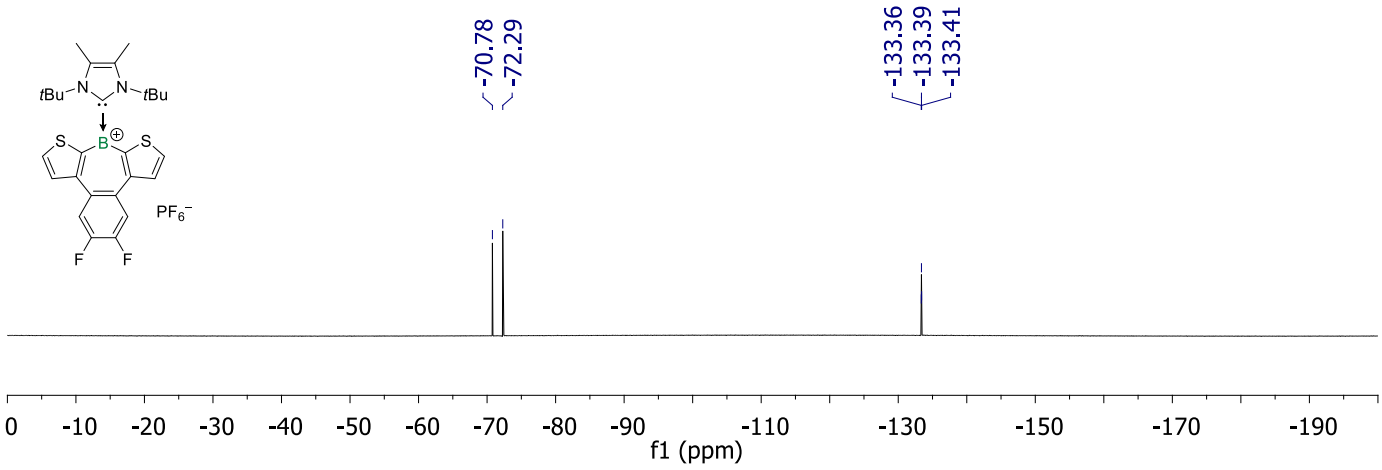



**Fig. S40** $^{19}F$ NMR spectrum of **1-F** in $CD_2Cl_2$ at room temperature.

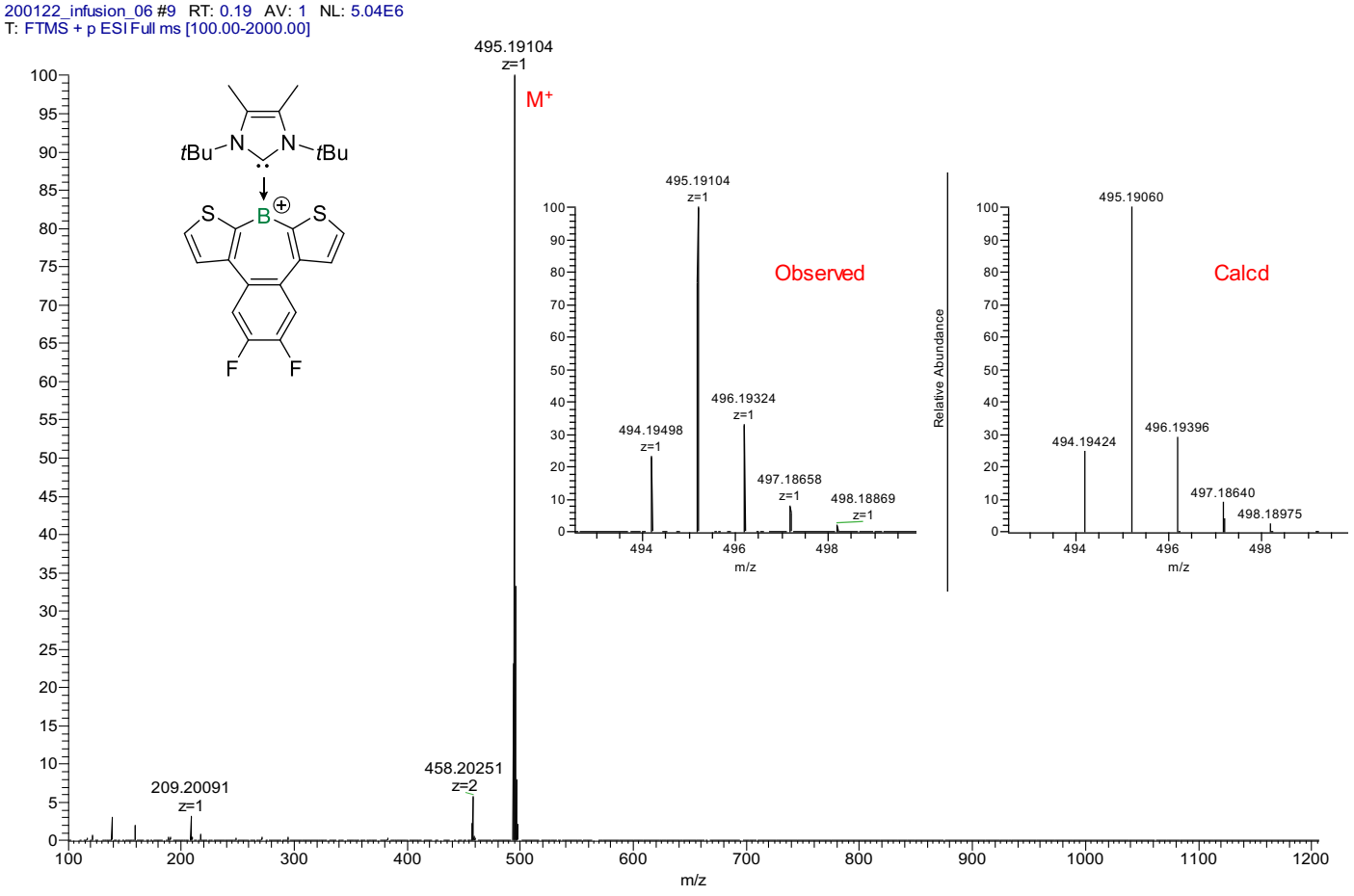



**Fig. S41** ESI mass spectrum of **1-F** (positive mode).

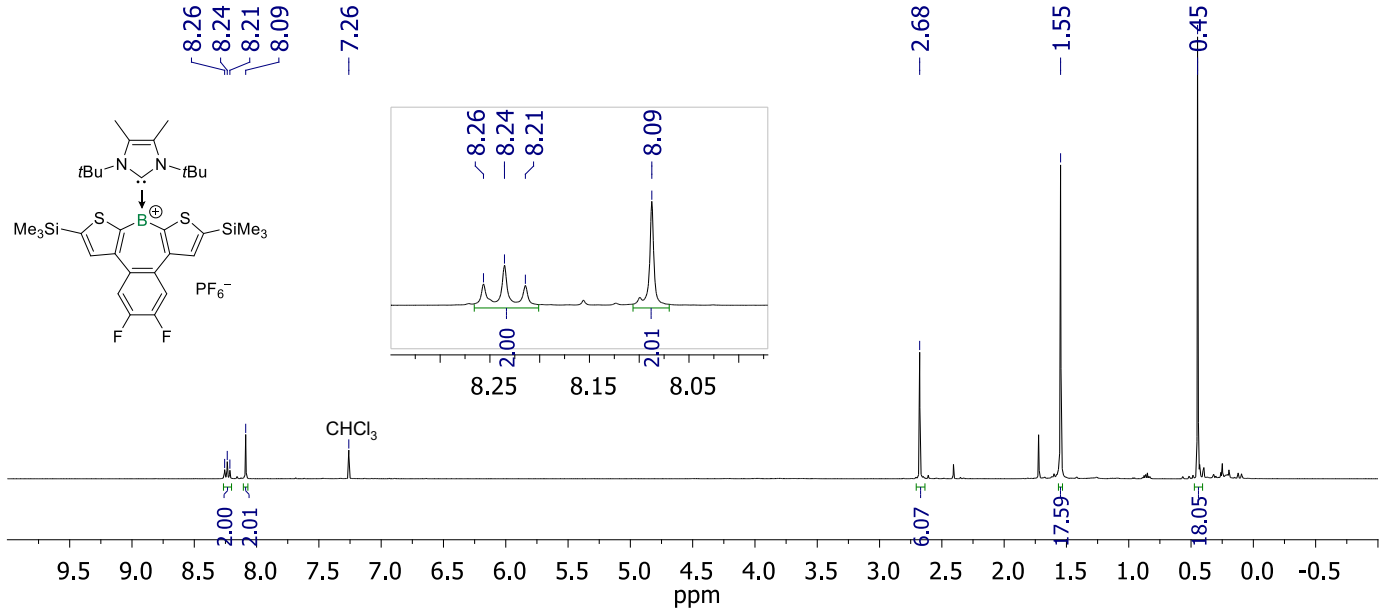



**Fig. S42** $^{1}$H NMR spectrum of **1-F-Si** in $CDCl_3$ at room temperature.

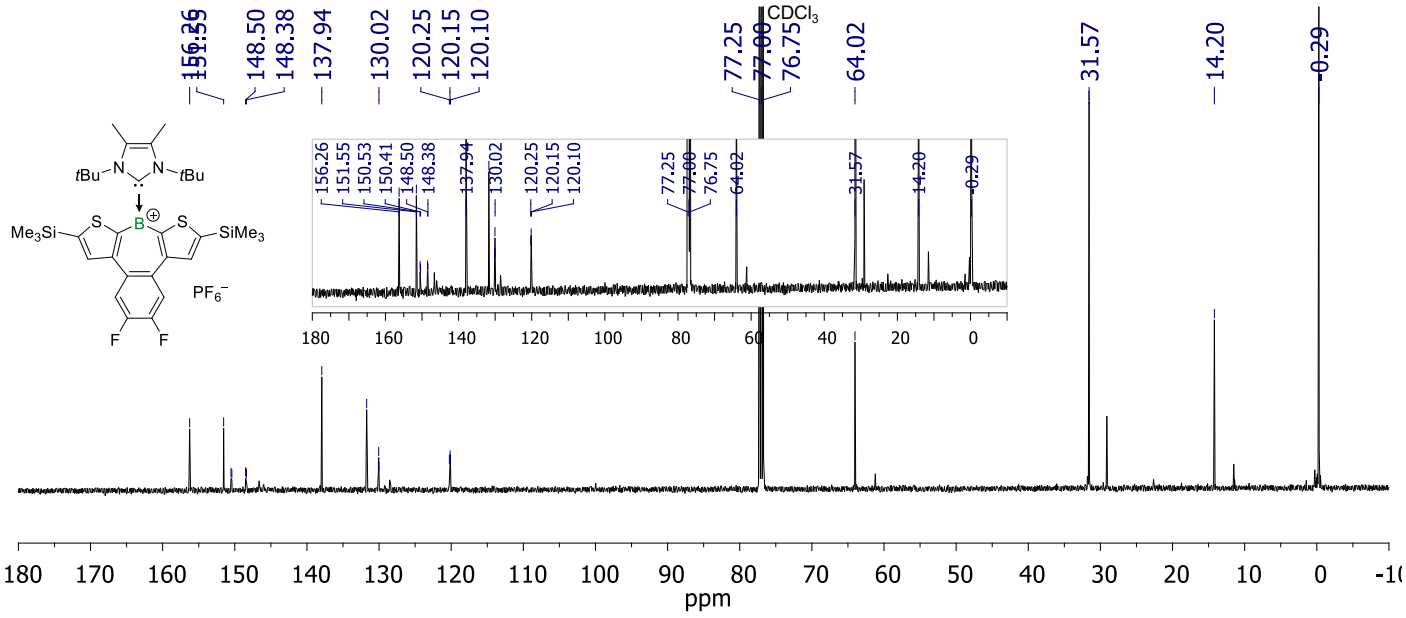



**Fig. S43** $^{13}$C NMR spectrum of **1-F-Si** in $CDCl_3$ at room temperature.

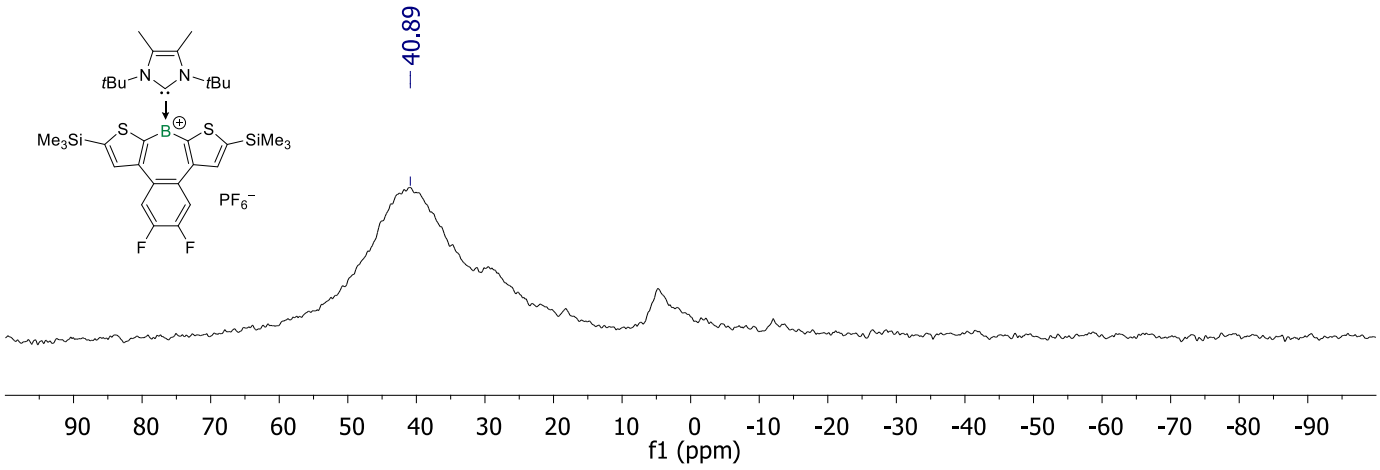



**Fig. S44** $^{11}$B NMR spectrum of **1-F-Si** in $CDCl_3$ at room temperature.

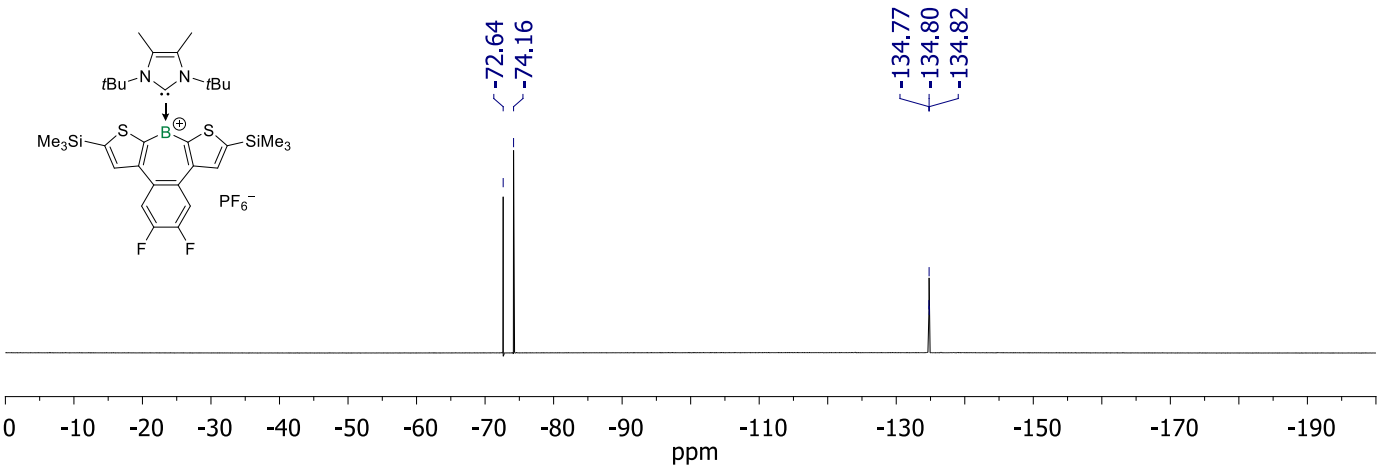



**Fig. S45** $^{19}$F NMR spectrum of **1-F-Si** in $CDCl_3$ at room temperature.

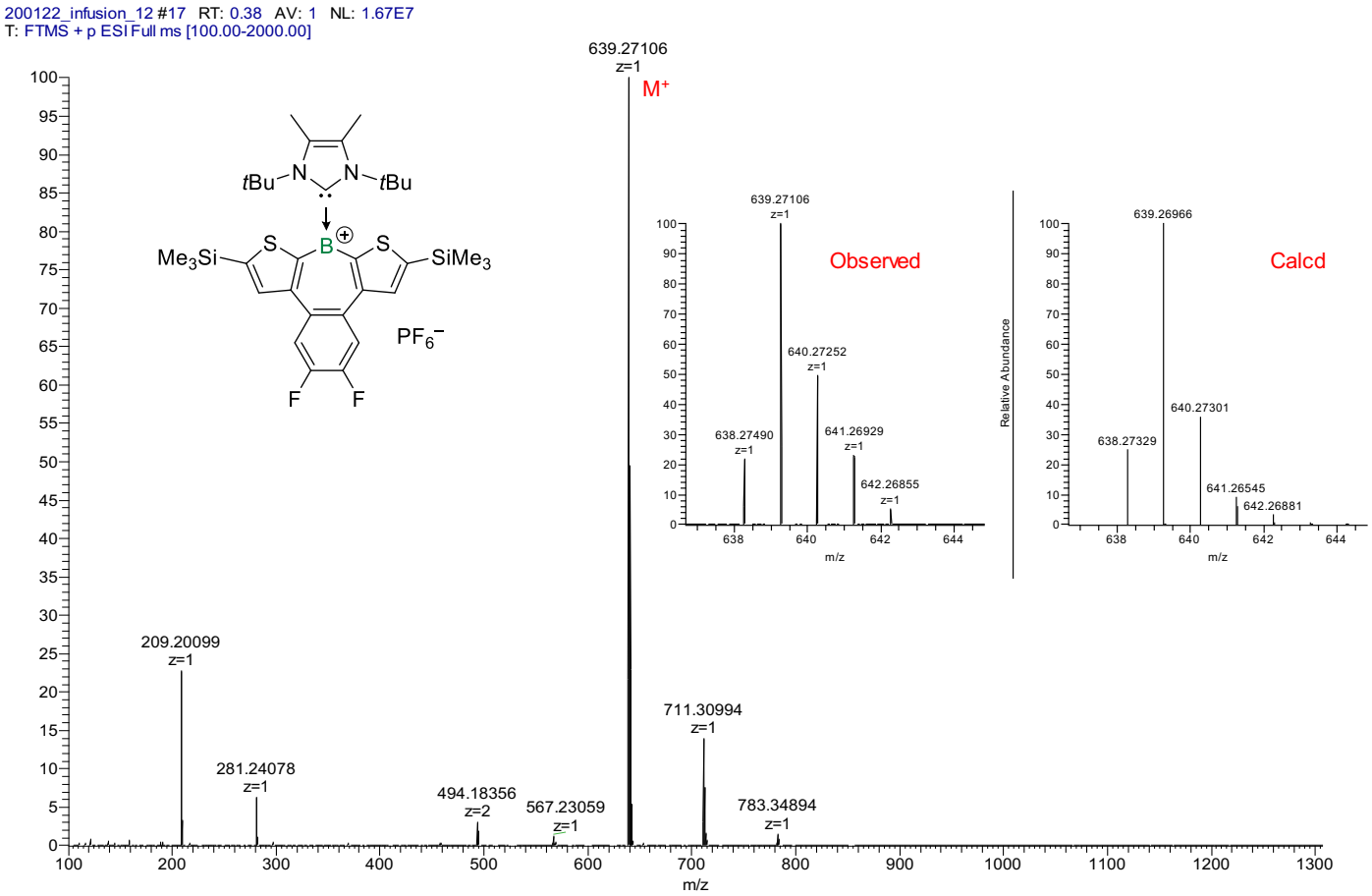



**Fig. S46** MALDI-TOF mass spectrum of **1-F-Si** (positive mode).

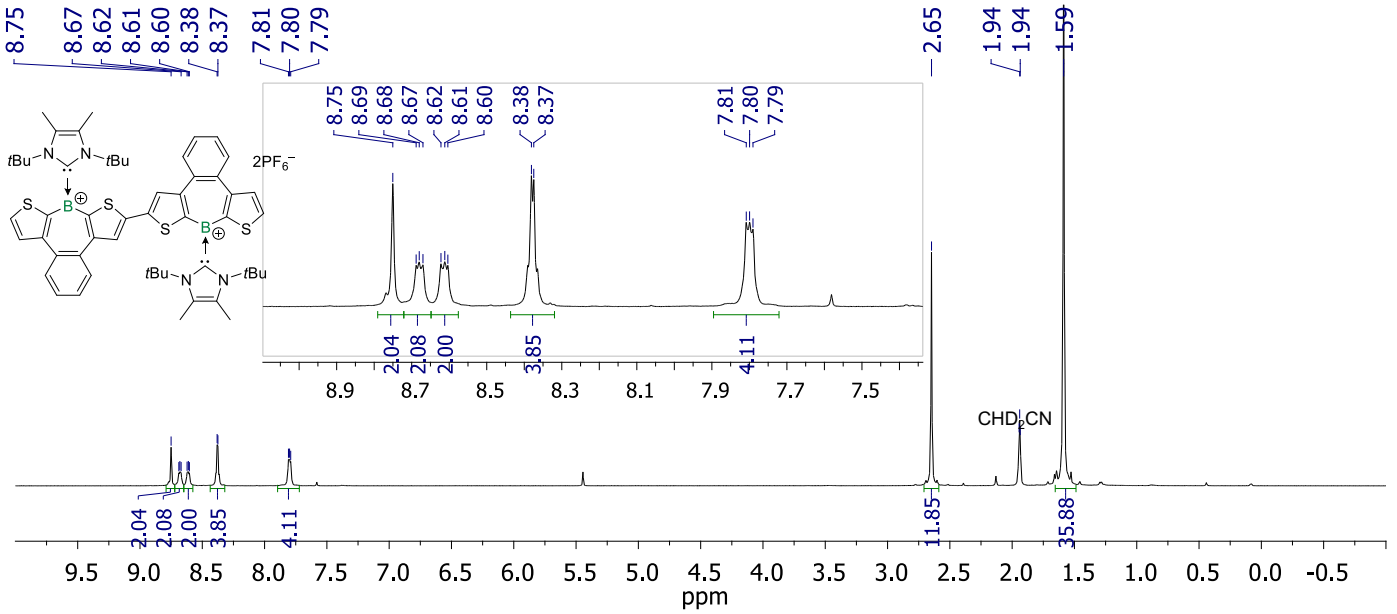



**Fig. S47** $^{1}$H NMR spectrum of **2-H** in $CD_3CN$ at room temperature.

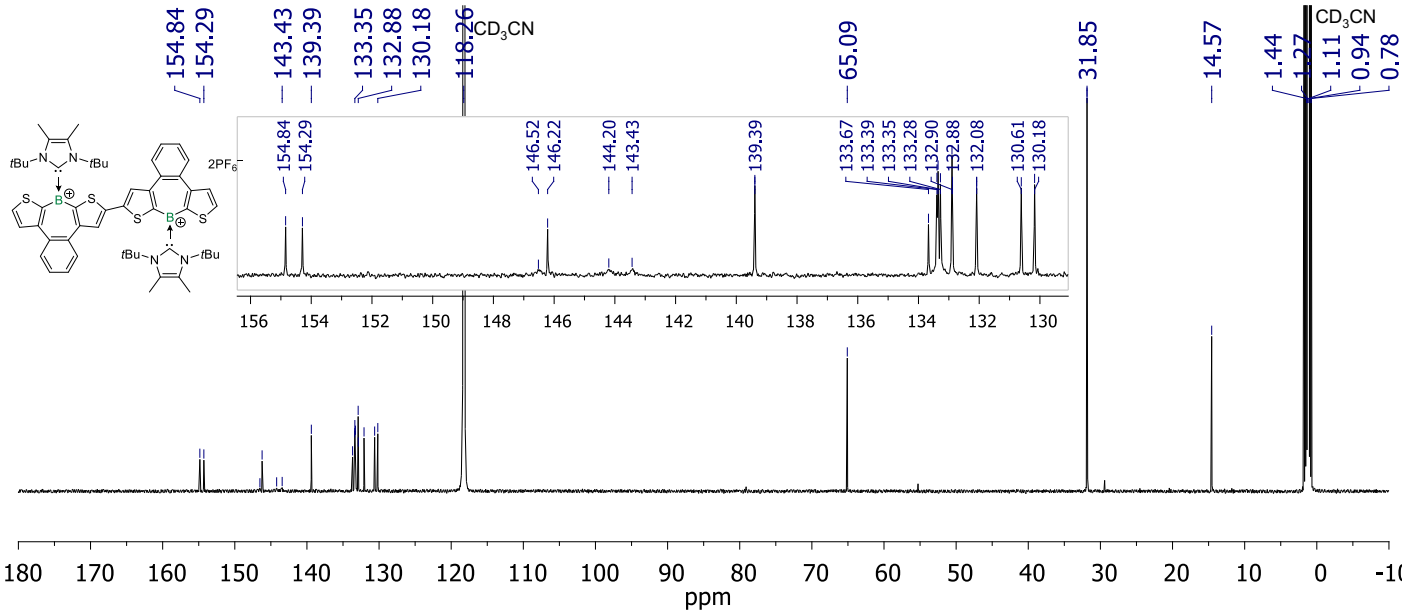



**Fig. S48** $^{13}$C NMR spectrum of **2-H** in $CD_3CN$ at room temperature.

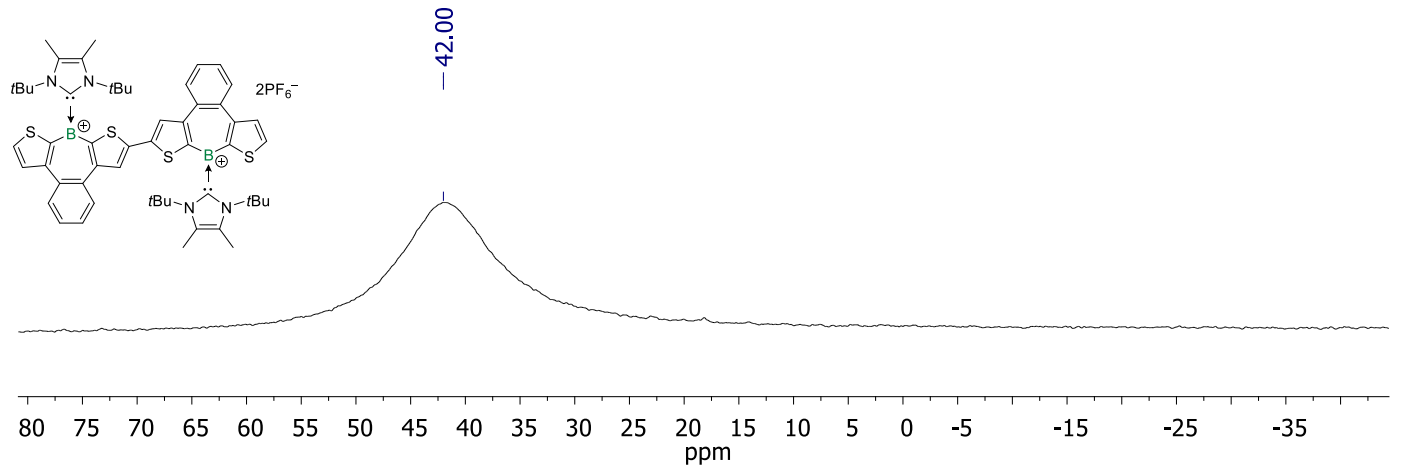



**Fig. S49** $^{11}$B NMR spectrum of **2-H** in $CD_3CN$ at room temperature.

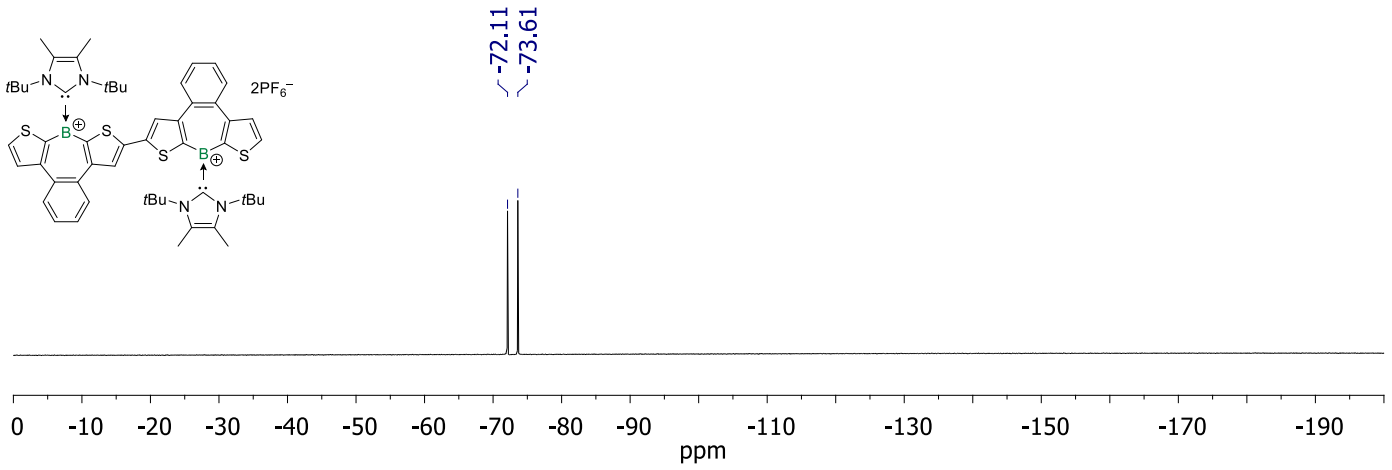



**Fig. S50** $^{19}$F NMR spectrum of **2-H** in $CD_3CN$ at room temperature.

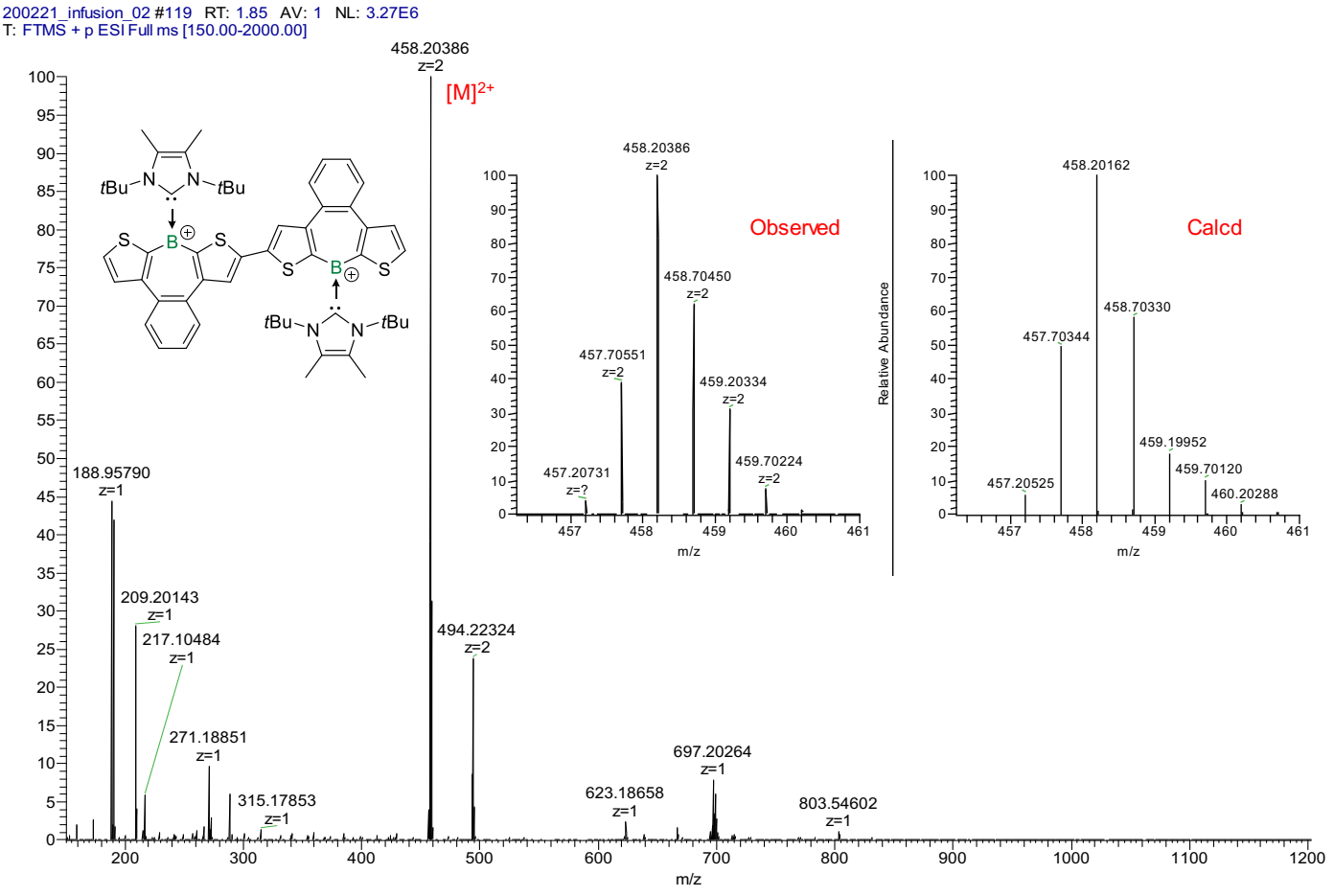



**Fig. S51** ESI mass spectrum of **2-H** (positive mode).

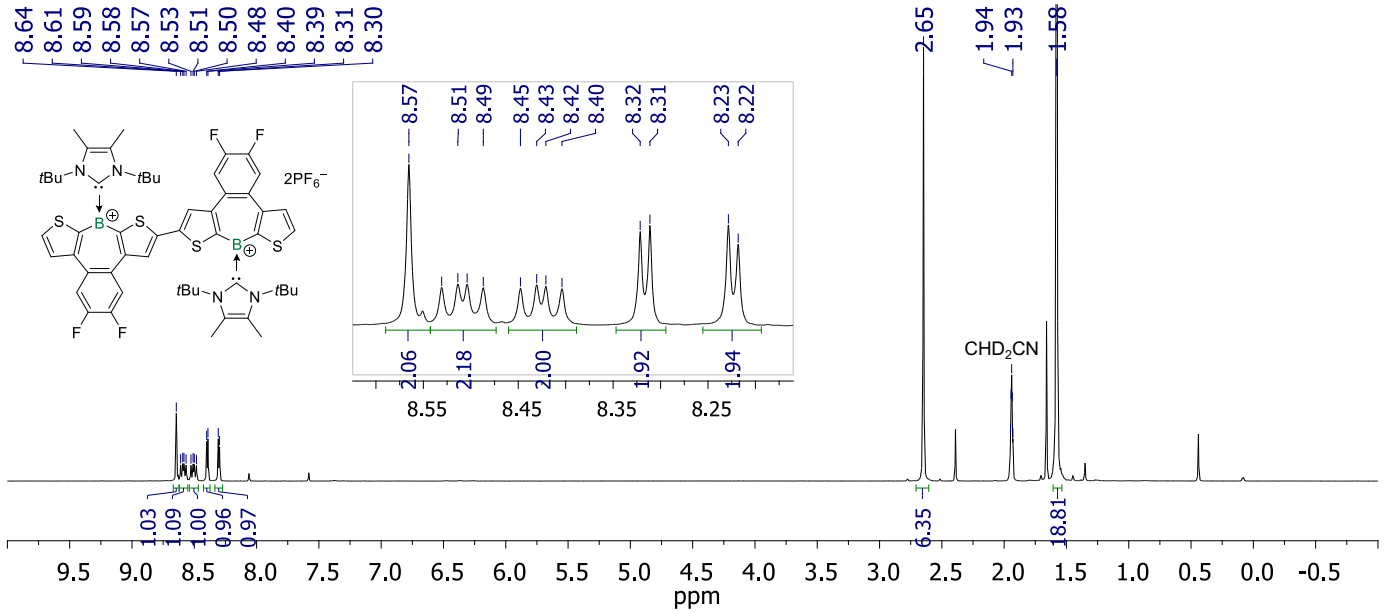



**Fig. S52** $^{1}$H NMR spectrum of **2-F** in $CD_3CN$ at room temperature.

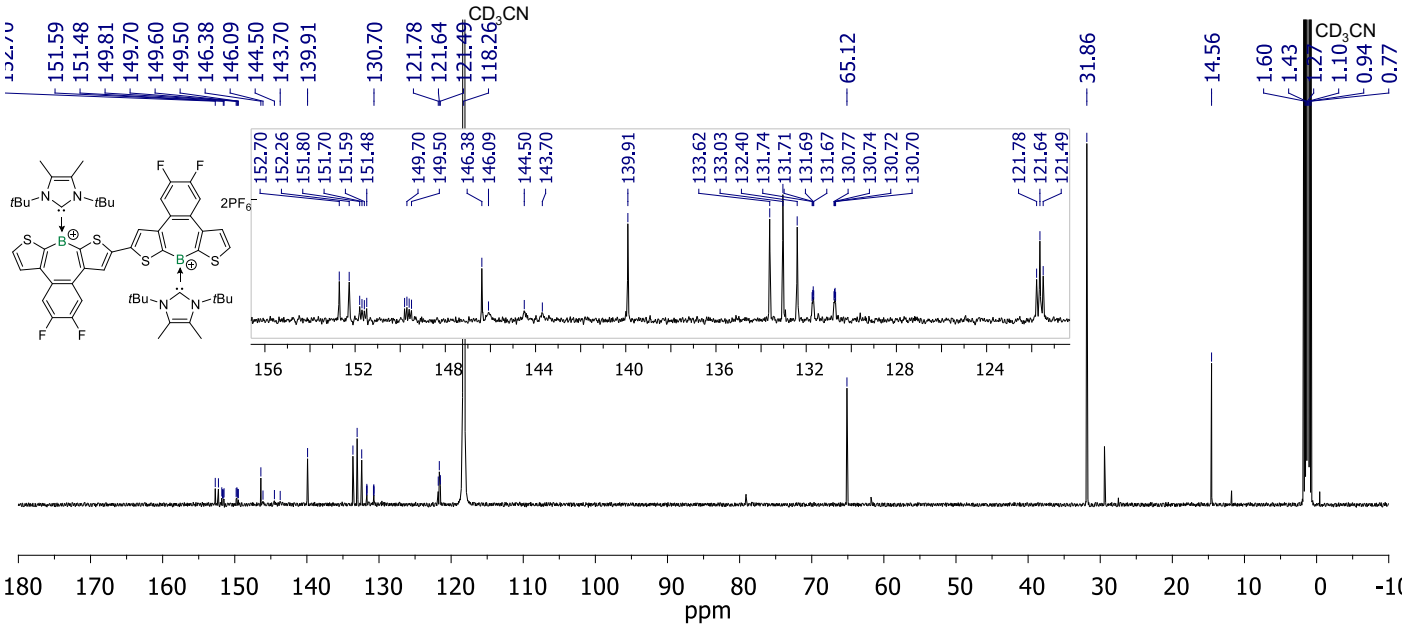



**Fig. S53** $^{13}$C NMR spectrum of **2-F** in $CD_3CN$ at room temperature.

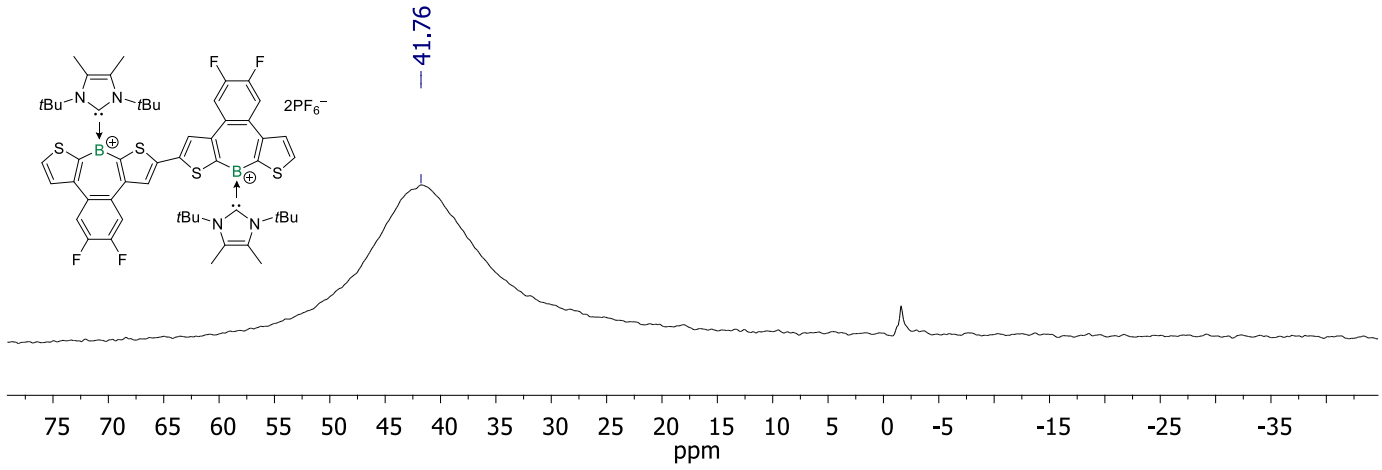



**Fig. S54** $^{11}$B NMR spectrum of **2-F** in $CD_3CN$ at room temperature.

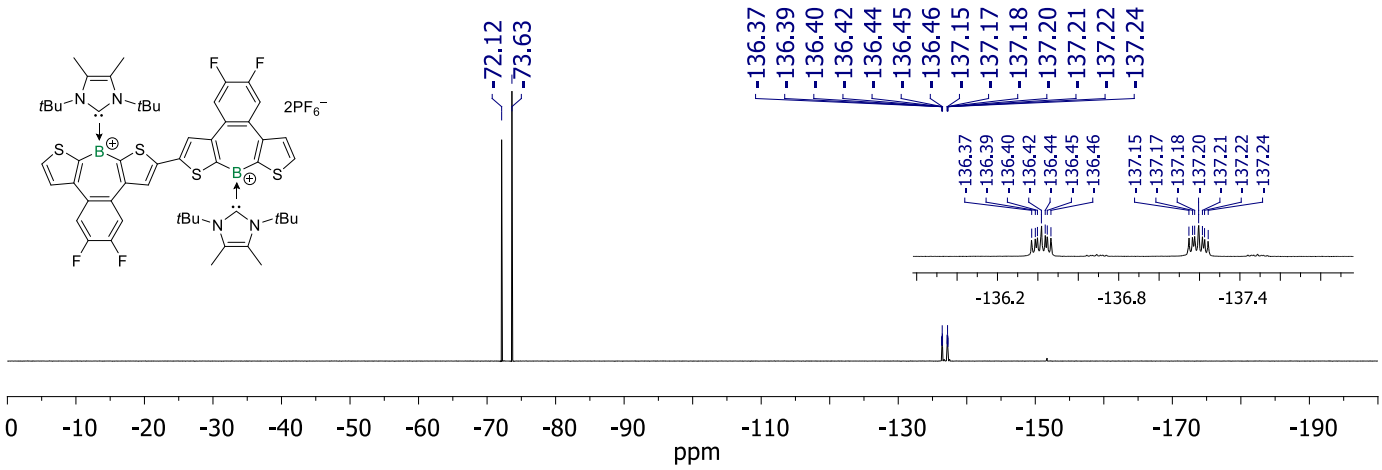



**Fig. S55** $^{19}$F NMR spectrum of **2-F** in $CD_3CN$ at room temperature.

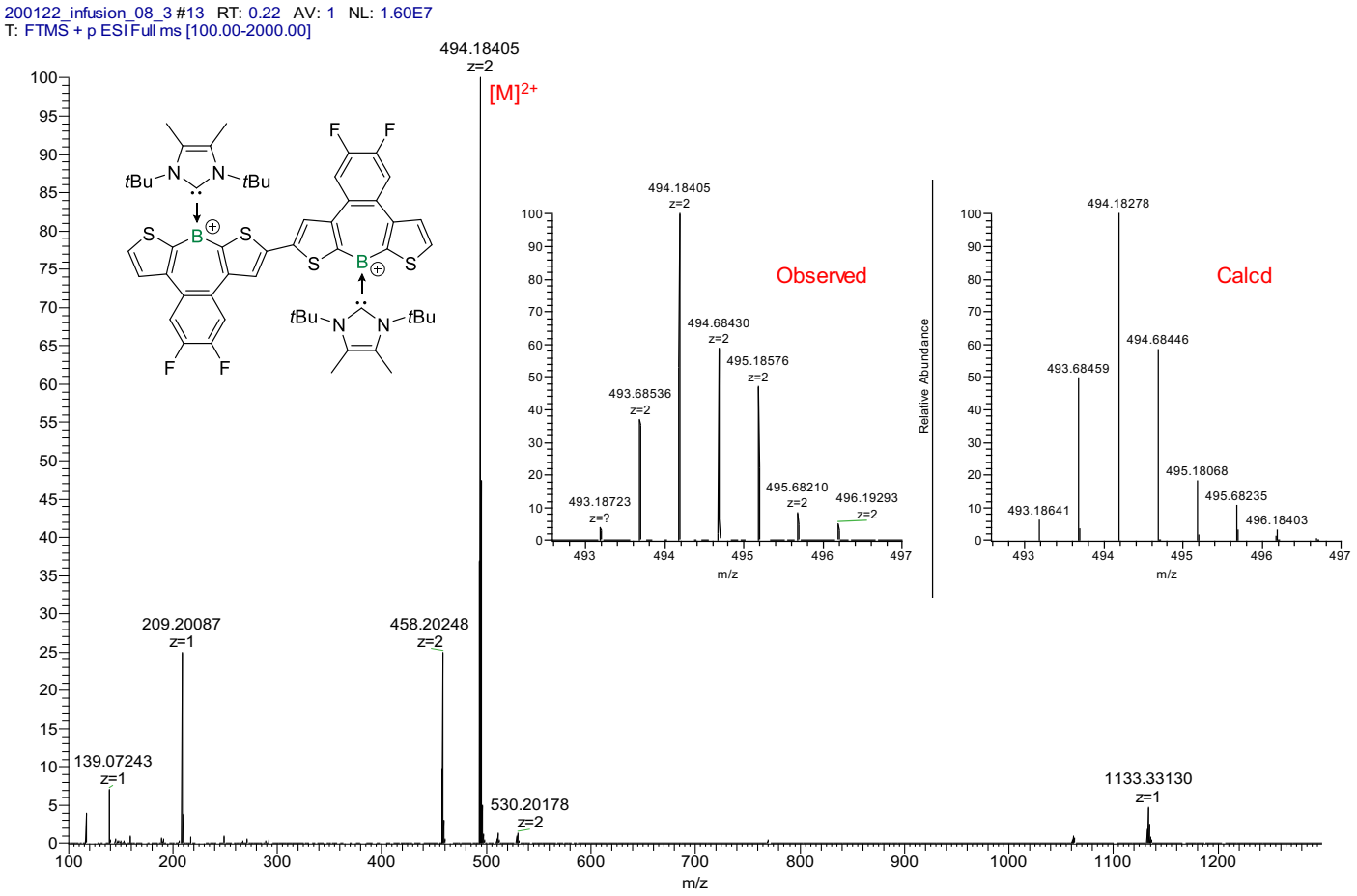



**Fig. S56** ESI mass spectrum of **2-F** (positive mode).

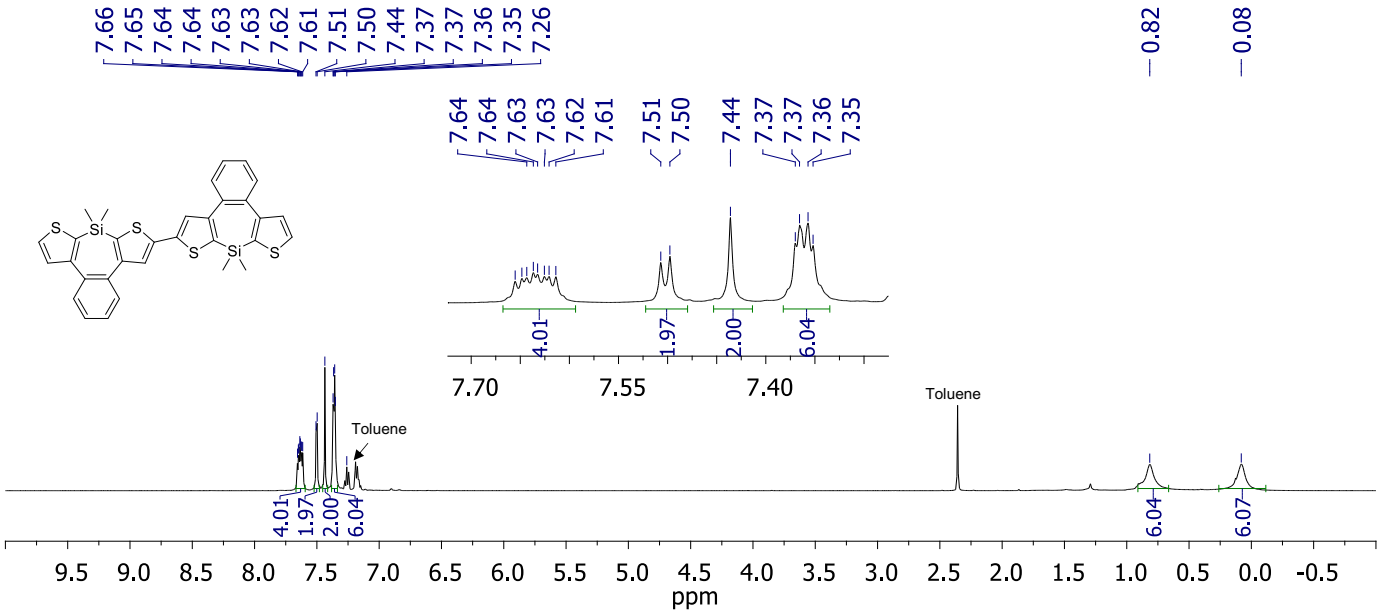



**Fig. S57** $^{1}$H NMR spectrum of **5-H** in $CDCl_3$ at room temperature.

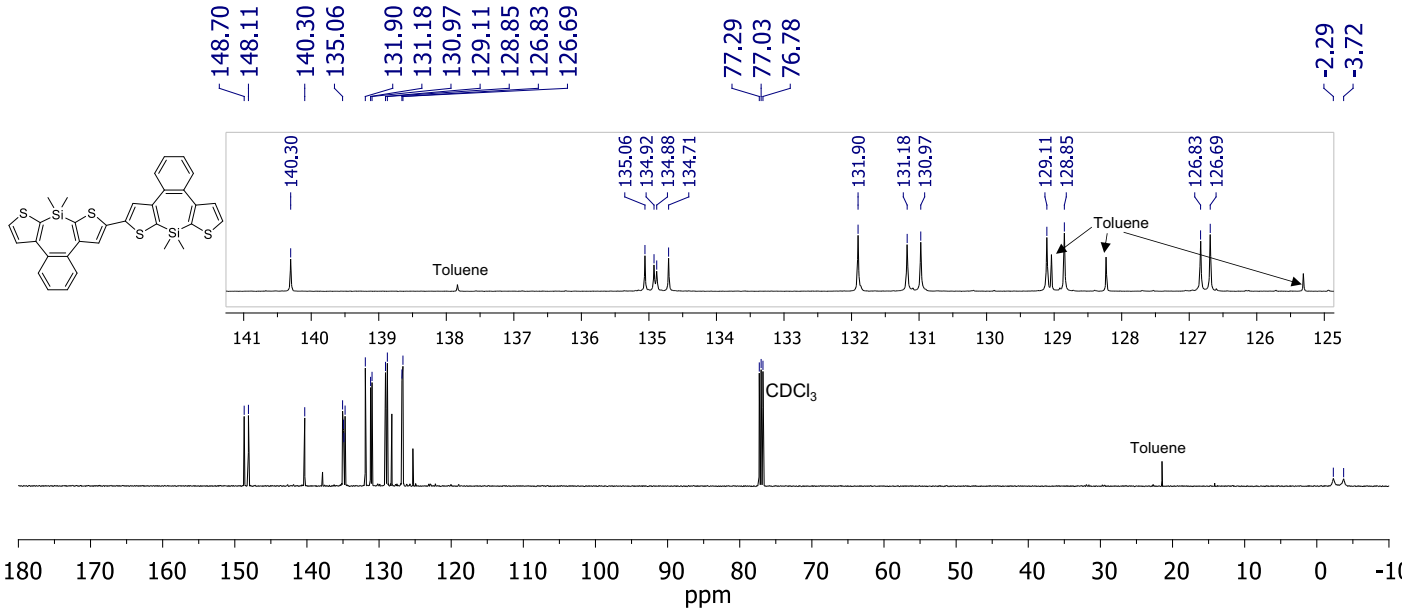



**Fig. S58** $^{13}C$ NMR spectrum of **5-H** in $CDCl_3$ at room temperature.

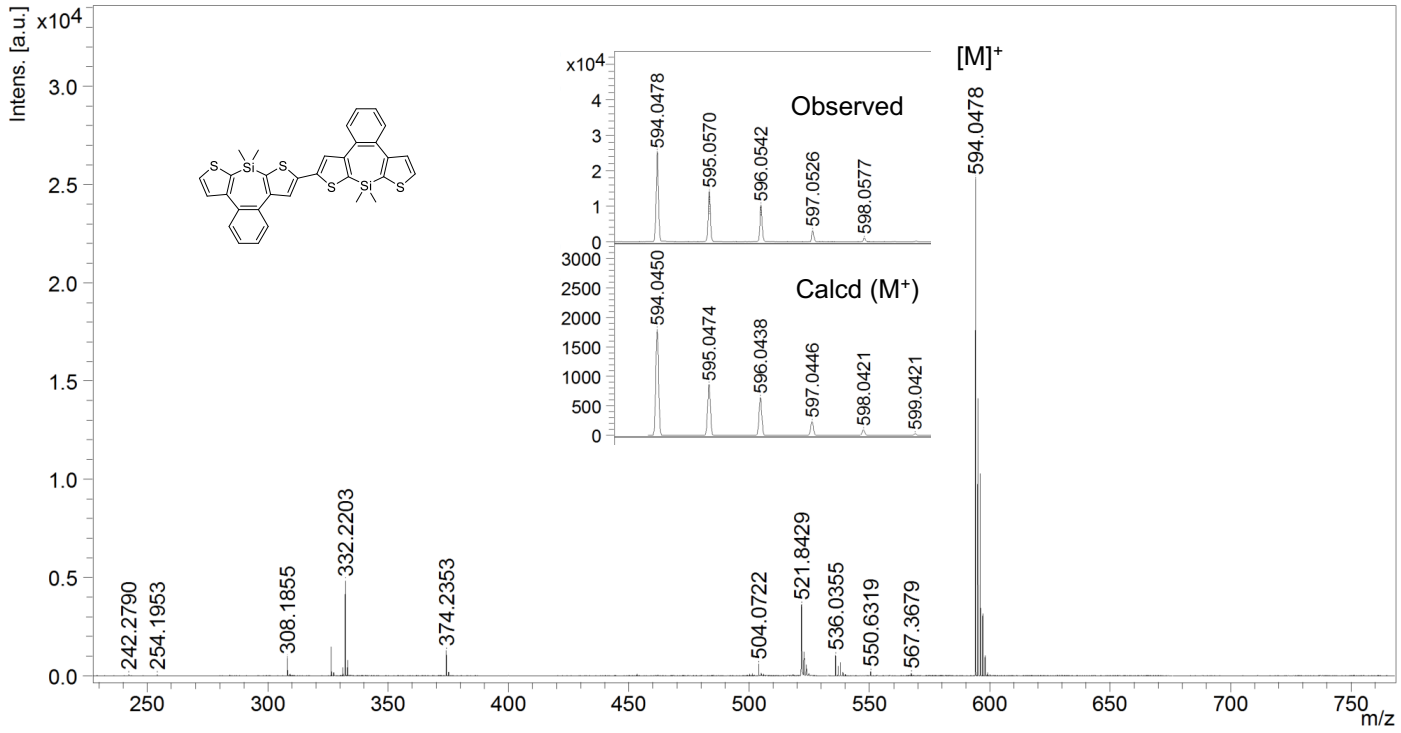



**Fig. S59** MALDI-TOF mass spectrum of **5-H** (positive mode).

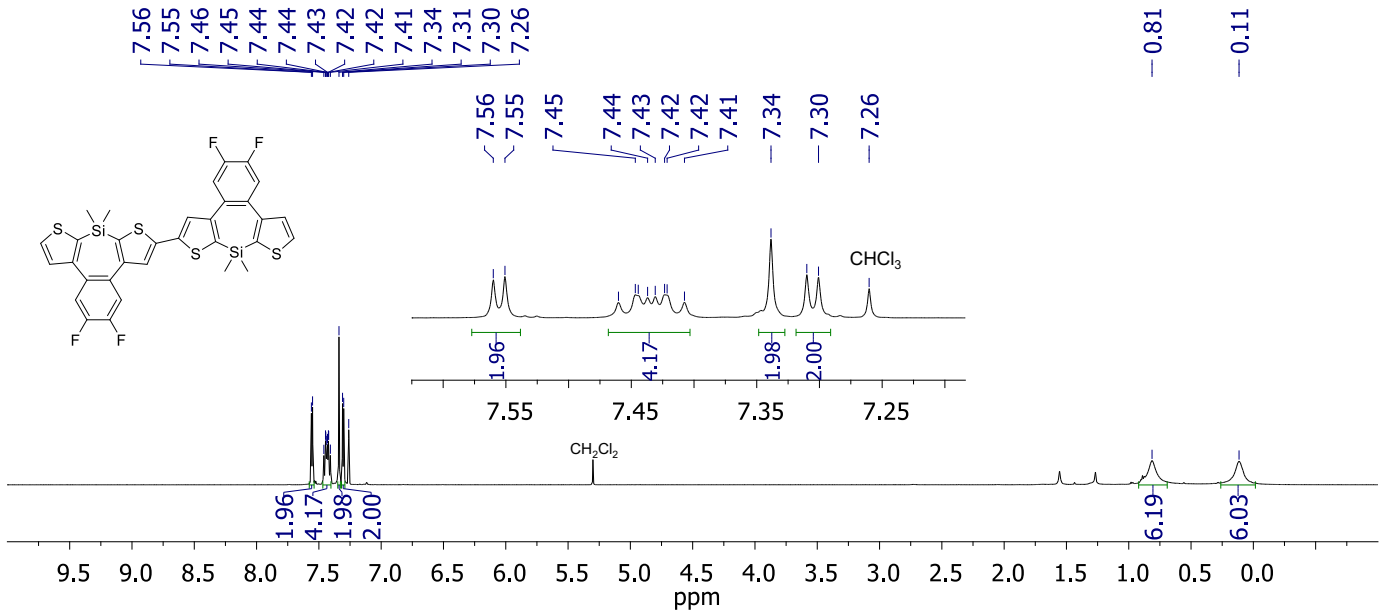



**Fig. S60** $^{1}$H NMR spectrum of **5-F** in $CDCl_3$ at room temperature.

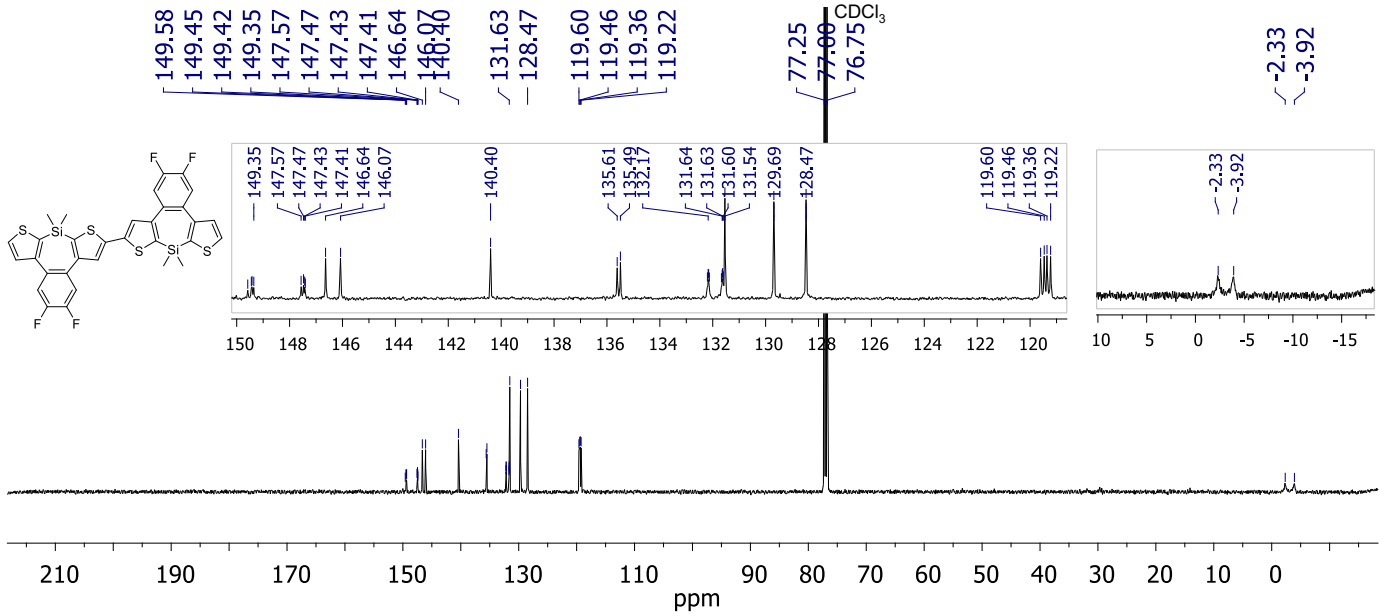



**Fig. S61** $^{13}$C NMR spectrum of **5-F** in $CDCl_3$ at room temperature.

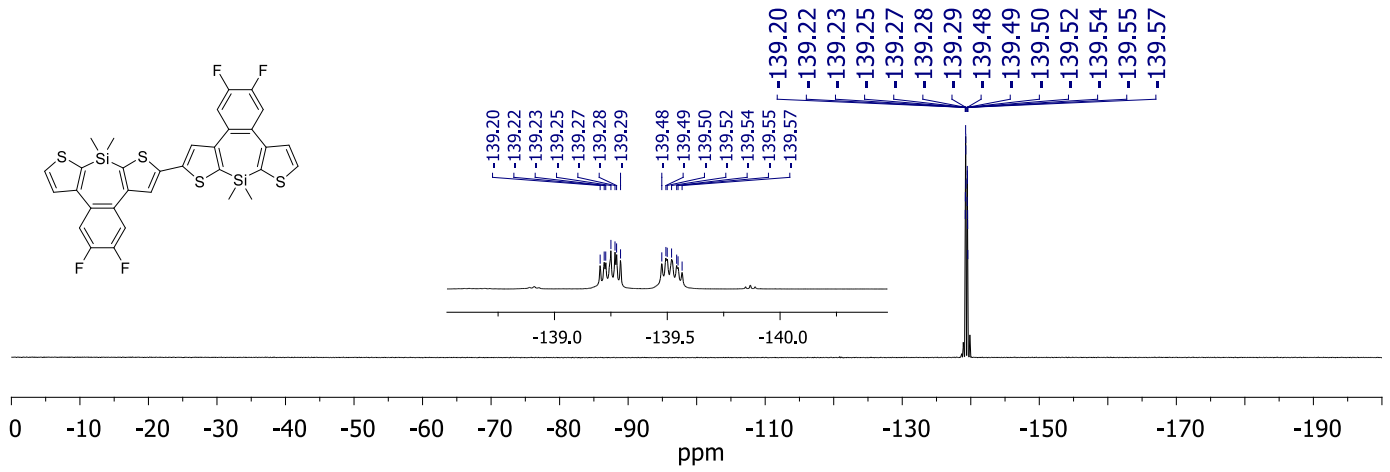



**Fig. S62** $^{19}$F NMR spectrum of **5-F** in $CDCl_3$ at room temperature.

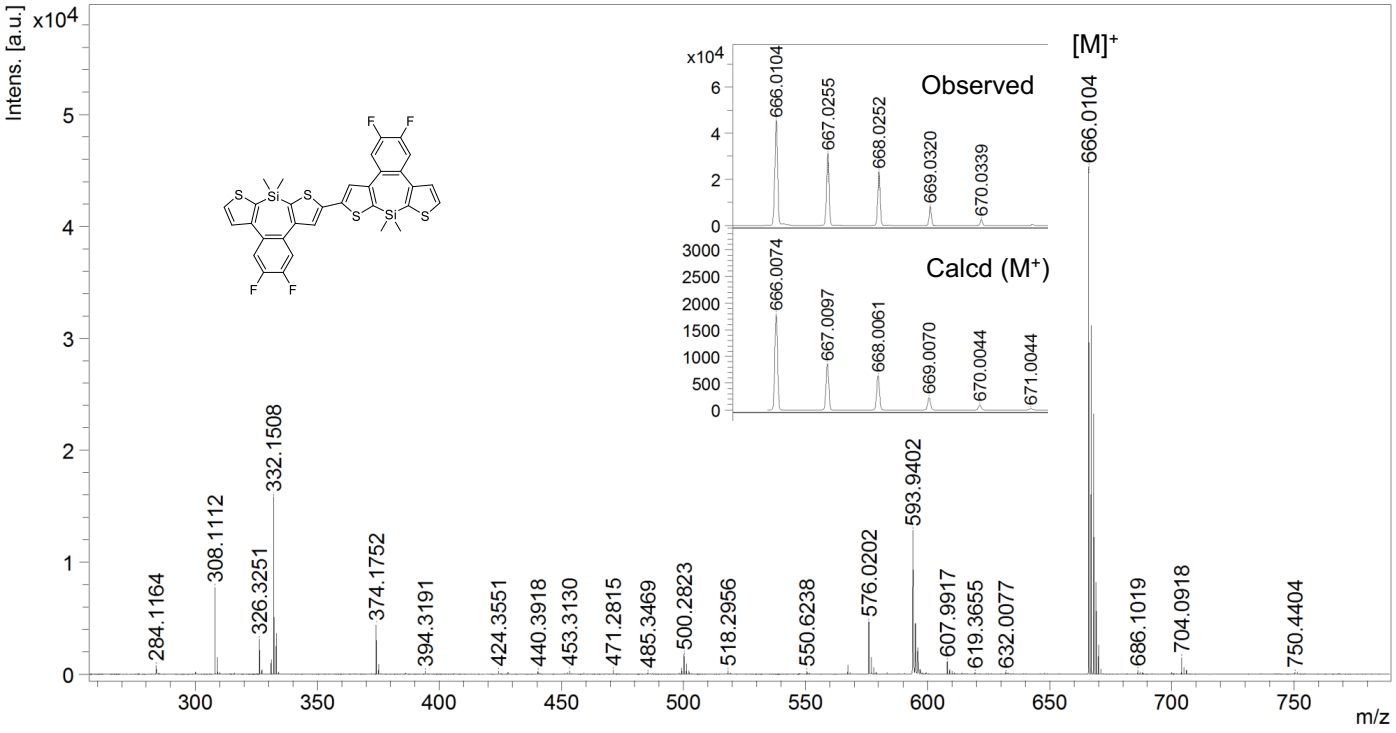



**Fig. S63** MALDI-TOF mass spectrum of **5-F** (positive mode).

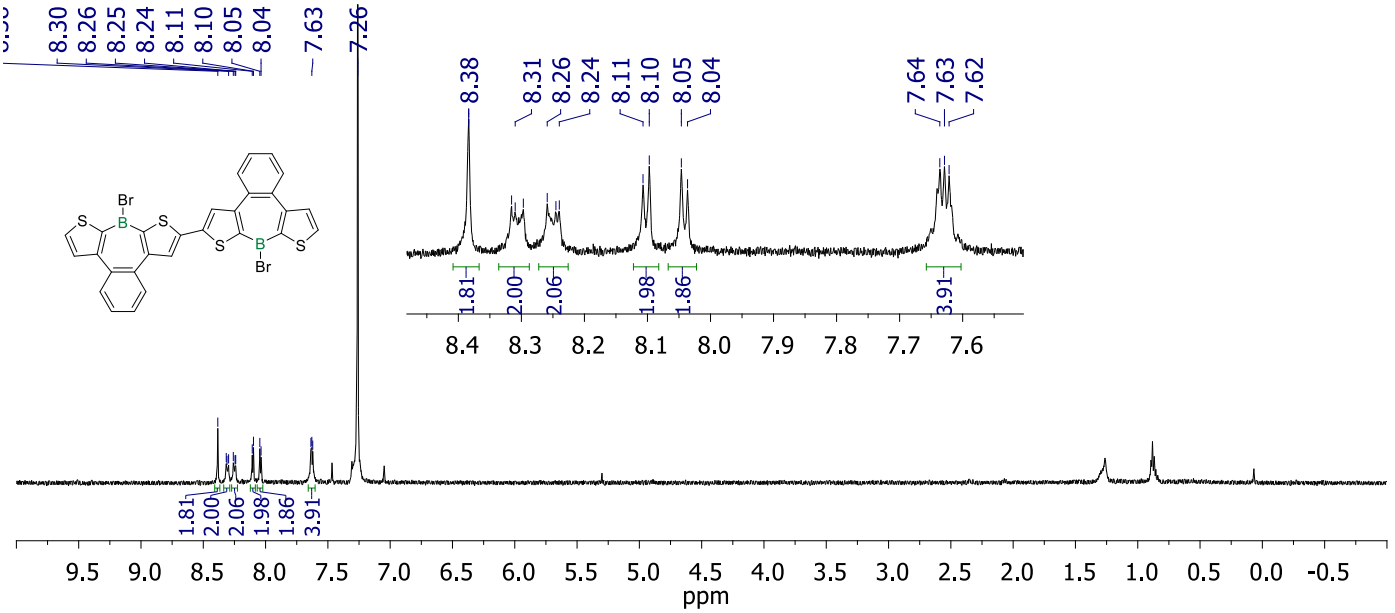



**Fig. S64** $^{1}$H NMR spectrum of **6-H** in $CDCl_3$ at room temperature.

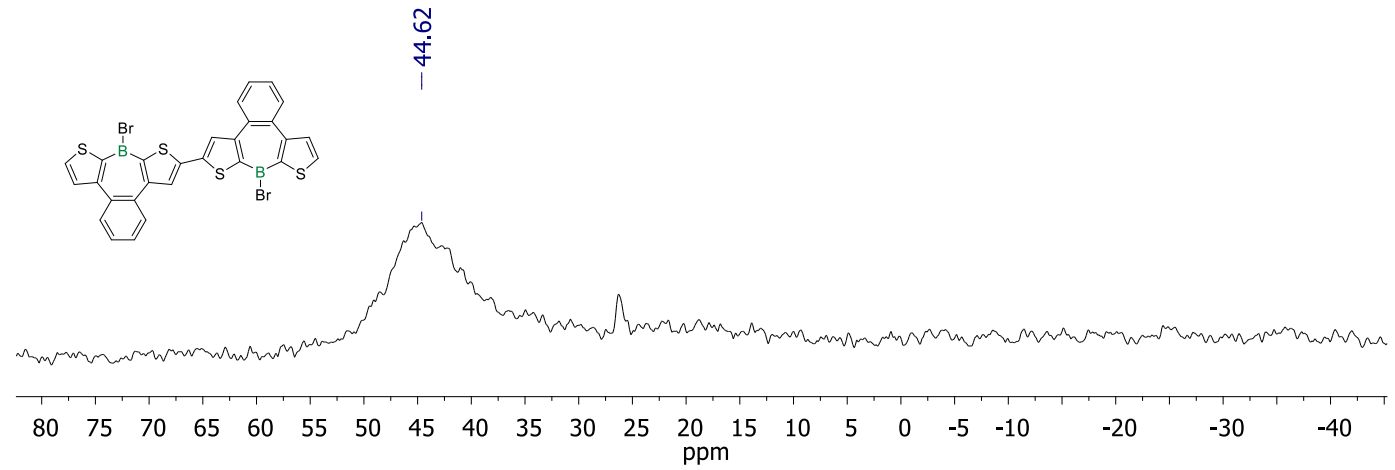



**Fig. S65** $^{11}$B NMR spectrum of **6-H** in $CDCl_3$ at room temperature.

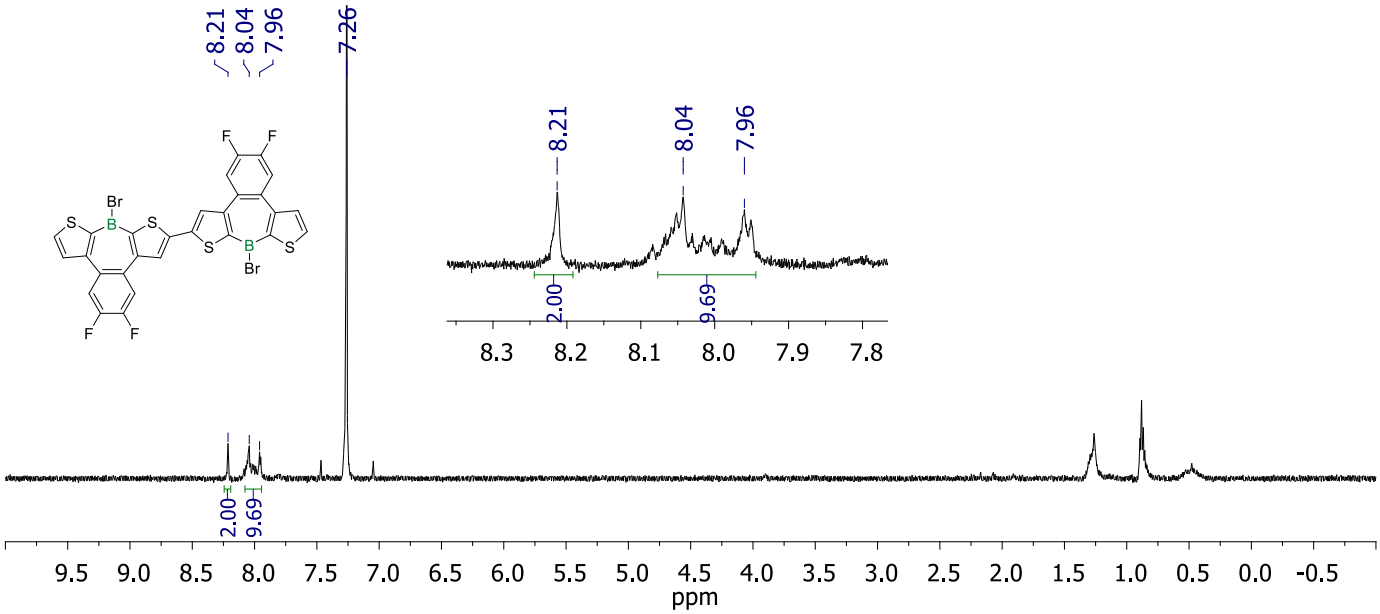



**Fig. S66** $^{1}$H NMR spectrum of a crude product of **6-F** in $CDCl_3$ at room temperature.

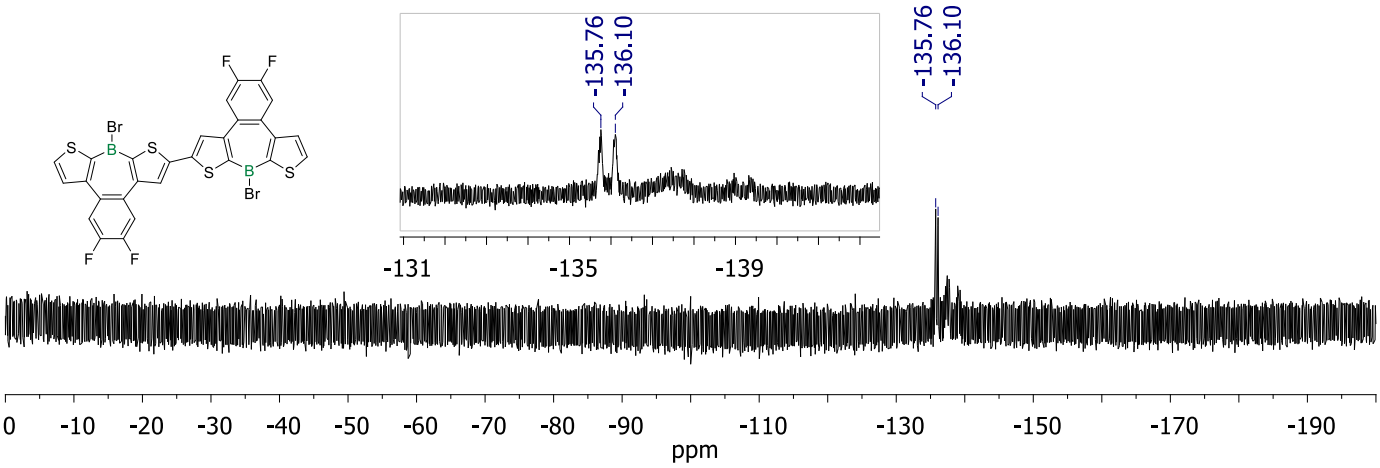



**Fig. S67** $^{19}$F NMR spectrum of a crude product of **6-F** in $CDCl_3$ at room temperature.

## ***Cartesian Coordinates for Optimized Structures***

**Table S4** Coordinates for Optimized Structure of **1-H**$^{+}$ in the ground state ($S_0$).

Total Energy: −1978.7703 Hartree

# opt b3lyp/6-31g(d,p) geom=connectivity

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 5.775411 | -0.928593 | 0.308407 |
| 2 | 6 | 0 | 5.808598 | 0.405648 | 0.716138 |
| 3 | 6 | 0 | 4.658206 | 1.166647 | 0.622683 |
| 4 | 6 | 0 | 3.431095 | 0.668736 | 0.115998 |
| 5 | 6 | 0 | 3.397184 | -0.701366 | -0.302938 |
| 6 | 6 | 0 | 4.592771 | -1.453585 | -0.178448 |
| 7 | 6 | 0 | 2.316051 | 1.633469 | 0.116620 |
| 8 | 6 | 0 | 0.941703 | 1.347751 | 0.177288 |
| 9 | 6 | 0 | 0.878390 | -1.186413 | -0.596239 |
| 10 | 6 | 0 | 2.239848 | -1.448914 | -0.828122 |
| 11 | 6 | 0 | 2.563418 | 3.050461 | 0.187414 |
| 12 | 6 | 0 | 1.440997 | 3.803557 | 0.359980 |
| 13 | 16 | 0 | 0.023003 | 2.830348 | 0.434514 |
| 14 | 16 | 0 | -0.109212 | -2.514082 | -1.209220 |
| 15 | 6 | 0 | 1.265136 | -3.335417 | -1.840014 |
| 16 | 6 | 0 | 2.422522 | -2.666998 | -1.573060 |
| 17 | 5 | 0 | 0.184473 | 0.052850 | -0.057928 |
| 18 | 6 | 0 | -1.421888 | 0.012230 | 0.138544 |
| 19 | 7 | 0 | -2.060847 | -0.376382 | 1.282385 |
| 20 | 6 | 0 | -3.439309 | -0.362532 | 1.055766 |
| 21 | 6 | 0 | -3.639003 | 0.066488 | -0.226426 |
| 22 | 7 | 0 | -2.380981 | 0.290173 | -0.796159 |
| 23 | 6 | 0 | -4.537935 | -0.747590 | 2.004135 |
| 24 | 6 | 0 | -4.992278 | 0.226155 | -0.860506 |
| 25 | 6 | 0 | -2.213222 | 0.806587 | -2.236917 |
| 26 | 6 | 0 | -2.731114 | 2.257623 | -2.290170 |
| 27 | 6 | 0 | -2.970050 | -0.143082 | -3.189302 |
| 28 | 6 | 0 | -0.754948 | 0.824493 | -2.716922 |
| 29 | 6 | 0 | -1.436810 | -0.837971 | 2.606941 |
| 30 | 6 | 0 | -2.117356 | -0.089529 | 3.772706 |
| 31 | 6 | 0 | 0.057177 | -0.506169 | 2.705206 |
| 32 | 6 | 0 | -1.600139 | -2.366525 | 2.701531 |
| 33 | 1 | 0 | 6.654580 | -1.559055 | 0.391986 |
| 34 | 1 | 0 | 6.714385 | 0.841051 | 1.125330 |
| 35 | 1 | 0 | 4.694540 | 2.179798 | 0.999278 |
| 36 | 1 | 0 | 4.576812 | -2.504660 | -0.433062 |
| 37 | 1 | 0 | 3.539939 | 3.501793 | 0.079990 |
| 38 | 1 | 0 | 1.375092 | 4.880738 | 0.433343 |
| 39 | 1 | 0 | 1.151047 | -4.262011 | -2.386403 |
| 40 | 1 | 0 | 3.379371 | -3.021072 | -1.930757 |
| 41 | 1 | 0 | -5.419726 | -1.032376 | 1.429218 |
| 42 | 1 | 0 | -4.286027 | -1.601784 | 2.629657 |
| 43 | 1 | 0 | -4.825856 | 0.079122 | 2.661475 |
| 44 | 1 | 0 | -5.039912 | 1.024985 | -1.595182 |
| 45 | 1 | 0 | -5.322452 | -0.697111 | -1.348833 |
| 46 | 1 | 0 | -5.723190 | 0.469363 | -0.088022 |
| 47 | 1 | 0 | -2.097841 | 2.909420 | -1.683818 |
| 48 | 1 | 0 | -2.686664 | 2.608812 | -3.324541 |
| 49 | 1 | 0 | -3.758491 | 2.374237 | -1.947509 |
| 50 | 1 | 0 | -4.052002 | -0.112089 | -3.088209 |
| 51 | 1 | 0 | -2.633256 | -1.173702 | -3.047363 |
| 52 | 1 | 0 | -2.736531 | 0.144687 | -4.217371 |
| 53 | 1 | 0 | -0.766246 | 1.236289 | -3.729451 |
| 54 | 1 | 0 | -0.112728 | 1.470542 | -2.122473 |
| 55 | 1 | 0 | -0.321004 | -0.172227 | -2.778662 |
| 56 | 1 | 0 | -3.140494 | -0.400123 | 3.966347 |
| 57 | 1 | 0 | -1.547939 | -0.287184 | 4.684055 |
| 58 | 1 | 0 | -2.101856 | 0.990414 | 3.599615 |
| 59 | 1 | 0 | 0.662435 | -1.015378 | 1.955592 |

| | | | | | |
|---|---|---|---|---|---|
| 60 | 1 | 0 | 0.400216 | -0.865428 | 3.678964 |
| 61 | 1 | 0 | 0.247501 | 0.566594 | 2.664039 |
| 62 | 1 | 0 | -1.194153 | -2.711253 | 3.656514 |
| 63 | 1 | 0 | -2.639265 | -2.693098 | 2.647447 |
| 64 | 1 | 0 | -1.047253 | -2.861313 | 1.898400 |

**Table S5** Coordinates for Optimized Structure of **1-F**$^{+}$ in the ground state ($S_0$).

Total Energy: −2177.2229 Hartree

# opt b3lyp/6-31g(d,p) geom=connectivity

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 5.372628 | -0.790874 | 0.065956 |
| 2 | 6 | 0 | 5.396174 | 0.567273 | 0.384302 |
| 3 | 6 | 0 | 4.234488 | 1.299380 | 0.309528 |
| 4 | 6 | 0 | 2.994985 | 0.741306 | -0.093309 |
| 5 | 6 | 0 | 2.970470 | -0.655008 | -0.419038 |
| 6 | 6 | 0 | 4.187756 | -1.374848 | -0.316490 |
| 7 | 6 | 0 | 1.864275 | 1.686446 | -0.095190 |
| 8 | 6 | 0 | 0.498436 | 1.381925 | 0.032012 |
| 9 | 6 | 0 | 0.451942 | -1.201123 | -0.563643 |
| 10 | 6 | 0 | 1.807824 | -1.463302 | -0.827855 |
| 11 | 6 | 0 | 2.088614 | 3.108785 | -0.108665 |
| 12 | 6 | 0 | 0.958990 | 3.851471 | 0.061976 |
| 13 | 16 | 0 | -0.437271 | 2.860887 | 0.236654 |
| 14 | 16 | 0 | -0.535411 | -2.586690 | -1.027877 |
| 15 | 6 | 0 | 0.826946 | -3.440830 | -1.638869 |
| 16 | 6 | 0 | 1.982674 | -2.737517 | -1.474117 |
| 17 | 5 | 0 | -0.244860 | 0.064010 | -0.093325 |
| 18 | 6 | 0 | -1.843950 | 0.013844 | 0.154927 |
| 19 | 7 | 0 | -2.443743 | -0.308006 | 1.339949 |
| 20 | 6 | 0 | -3.827984 | -0.330059 | 1.153292 |
| 21 | 6 | 0 | -4.071062 | 0.010554 | -0.148111 |
| 22 | 7 | 0 | -2.833605 | 0.213938 | -0.767902 |
| 23 | 6 | 0 | -4.891781 | -0.669732 | 2.157061 |
| 24 | 6 | 0 | -5.443298 | 0.109931 | -0.752454 |
| 25 | 6 | 0 | -2.714335 | 0.638986 | -2.243343 |
| 26 | 6 | 0 | -3.247833 | 2.079250 | -2.372862 |
| 27 | 6 | 0 | -3.491058 | -0.373289 | -3.111534 |
| 28 | 6 | 0 | -1.271063 | 0.635363 | -2.766701 |
| 29 | 6 | 0 | -1.776012 | -0.670401 | 2.674675 |
| 30 | 6 | 0 | -2.441465 | 0.139570 | 3.807958 |
| 31 | 6 | 0 | -0.286888 | -0.304861 | 2.709453 |
| 32 | 6 | 0 | -1.905140 | -2.191859 | 2.874522 |
| 33 | 1 | 0 | 4.301994 | 2.331419 | 0.622573 |
| 34 | 1 | 0 | 4.218670 | -2.440231 | -0.494835 |
| 35 | 1 | 0 | 3.051415 | 3.572135 | -0.273983 |
| 36 | 1 | 0 | 0.876811 | 4.929874 | 0.080338 |
| 37 | 1 | 0 | 0.708256 | -4.412028 | -2.100208 |
| 38 | 1 | 0 | 2.929680 | -3.110510 | -1.838921 |
| 39 | 1 | 0 | -5.785511 | -1.002603 | 1.628359 |
| 40 | 1 | 0 | -4.607840 | -1.479470 | 2.826534 |
| 41 | 1 | 0 | -5.173376 | 0.192358 | 2.770126 |
| 42 | 1 | 0 | -5.527894 | 0.872923 | -1.521492 |
| 43 | 1 | 0 | -5.765099 | -0.841913 | -1.188363 |
| 44 | 1 | 0 | -6.159070 | 0.373450 | 0.027296 |

| | | | | | |
|---|---|---|---|---|---|
| 45 | 1 | 0 | -2.606350 | 2.773508 | -1.825222 |
| 46 | 1 | 0 | -3.234015 | 2.365673 | -3.427874 |
| 47 | 1 | 0 | -4.267453 | 2.207388 | -2.011291 |
| 48 | 1 | 0 | -4.570502 | -0.333599 | -2.989373 |
| 49 | 1 | 0 | -3.151078 | -1.392513 | -2.908153 |
| 50 | 1 | 0 | -3.280543 | -0.155916 | -4.161608 |
| 51 | 1 | 0 | -1.315781 | 0.975918 | -3.804400 |
| 52 | 1 | 0 | -0.617874 | 1.326186 | -2.238018 |
| 53 | 1 | 0 | -0.829126 | -0.359972 | -2.772679 |
| 54 | 1 | 0 | -3.445766 | -0.189757 | 4.060608 |
| 55 | 1 | 0 | -1.834984 | 0.027045 | 4.709743 |
| 56 | 1 | 0 | -2.470047 | 1.204065 | 3.558156 |
| 57 | 1 | 0 | 0.307586 | -0.850213 | 1.976753 |
| 58 | 1 | 0 | 0.089223 | -0.595787 | 3.693722 |
| 59 | 1 | 0 | -0.119175 | 0.766583 | 2.595766 |
| 60 | 1 | 0 | -1.477756 | -2.461980 | 3.844090 |
| 61 | 1 | 0 | -2.937868 | -2.541604 | 2.859376 |
| 62 | 1 | 0 | -1.353706 | -2.729495 | 2.098513 |
| 63 | 9 | 0 | 6.489865 | -1.514740 | 0.167585 |
| 64 | 9 | 0 | 6.535672 | 1.133413 | 0.788577 |

**Table S6** Coordinates for Optimized Structure of **2-H$^{2+}$** in the ground state ($S_0$).

Total Energy: −3956.3016 Hartree

# opt b3lyp/6-31g(d,p) geom=connectivity

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.417803 | -6.053759 | 0.279646 |
| 2 | 6 | 0 | -2.145254 | -5.580250 | 0.602136 |
| 3 | 6 | 0 | -1.874889 | -4.230804 | 0.467071 |
| 4 | 6 | 0 | -2.825127 | -3.288118 | 0.000784 |
| 5 | 6 | 0 | -4.133261 | -3.772535 | -0.322571 |
| 6 | 6 | 0 | -4.376217 | -5.159801 | -0.160959 |
| 7 | 6 | 0 | -2.346399 | -1.894070 | -0.067632 |
| 8 | 6 | 0 | -3.111030 | -0.720750 | 0.036787 |
| 9 | 6 | 0 | -5.539946 | -1.619393 | -0.522410 |
| 10 | 6 | 0 | -5.291606 | -2.981611 | -0.774840 |
| 11 | 6 | 0 | -0.943696 | -1.605574 | -0.130237 |
| 12 | 6 | 0 | -0.613486 | -0.276928 | -0.008222 |
| 13 | 16 | 0 | -2.057358 | 0.684044 | 0.179147 |
| 14 | 16 | 0 | -7.184198 | -1.205612 | -1.011735 |
| 15 | 6 | 0 | -7.473706 | -2.785691 | -1.624462 |
| 16 | 6 | 0 | -6.402041 | -3.608642 | -1.437814 |
| 17 | 5 | 0 | -4.617612 | -0.504977 | -0.062200 |
| 18 | 6 | 0 | -5.270690 | 0.954835 | 0.186741 |
| 19 | 7 | 0 | -5.811663 | 1.372790 | 1.370582 |
| 20 | 6 | 0 | -6.417733 | 2.615868 | 1.175973 |
| 21 | 6 | 0 | -6.212817 | 2.971689 | -0.128536 |
| 22 | 7 | 0 | -5.507024 | 1.931383 | -0.742267 |
| 23 | 6 | 0 | -7.185381 | 3.434986 | 2.172817 |
| 24 | 6 | 0 | -6.706846 | 4.252256 | -0.740957 |
| 25 | 6 | 0 | -5.073344 | 1.992237 | -2.218374 |
| 26 | 6 | 0 | -3.989901 | 3.081293 | -2.349960 |
| 27 | 6 | 0 | -6.314468 | 2.267329 | -3.092369 |
| 28 | 6 | 0 | -4.467124 | 0.678972 | -2.732941 |
| 29 | 6 | 0 | -5.857764 | 0.618797 | 2.708079 |

| | | | | | |
|---|---|---|---|---|---|
| 30 | 6 | 0 | -5.433459 | 1.574304 | 3.844447 |
| 31 | 6 | 0 | -4.872196 | -0.555229 | 2.750769 |
| 32 | 6 | 0 | -7.283188 | 0.069500 | 2.897715 |
| 33 | 1 | 0 | -0.900745 | -3.878827 | 0.780147 |
| 34 | 1 | 0 | -5.371705 | -5.540037 | -0.345680 |
| 35 | 1 | 0 | -0.189981 | -2.362242 | -0.302664 |
| 36 | 1 | 0 | -8.414316 | -3.027822 | -2.101045 |
| 37 | 1 | 0 | -6.399209 | -4.629081 | -1.795275 |
| 38 | 1 | 0 | -7.854634 | 4.109292 | 1.637783 |
| 39 | 1 | 0 | -7.811672 | 2.831589 | 2.827408 |
| 40 | 1 | 0 | -6.531367 | 4.048527 | 2.800078 |
| 41 | 1 | 0 | -6.057205 | 4.646604 | -1.517524 |
| 42 | 1 | 0 | -7.707846 | 4.136130 | -1.169809 |
| 43 | 1 | 0 | -6.768264 | 5.018549 | 0.032853 |
| 44 | 1 | 0 | -3.089797 | 2.787979 | -1.803561 |
| 45 | 1 | 0 | -3.725875 | 3.190149 | -3.405326 |
| 46 | 1 | 0 | -4.301977 | 4.059697 | -1.986602 |
| 47 | 1 | 0 | -6.740023 | 3.259452 | -2.967424 |
| 48 | 1 | 0 | -7.092365 | 1.523792 | -2.899311 |
| 49 | 1 | 0 | -6.020996 | 2.176163 | -4.141080 |
| 50 | 1 | 0 | -4.175415 | 0.856582 | -3.771345 |
| 51 | 1 | 0 | -3.565936 | 0.383193 | -2.200707 |
| 52 | 1 | 0 | -5.181698 | -0.142631 | -2.735418 |
| 53 | 1 | 0 | -6.175021 | 2.328839 | 4.091324 |
| 54 | 1 | 0 | -5.275309 | 0.980328 | 4.747662 |
| 55 | 1 | 0 | -4.488929 | 2.070911 | 3.603714 |
| 56 | 1 | 0 | -5.103197 | -1.339330 | 2.029606 |
| 57 | 1 | 0 | -4.959724 | -1.011239 | 3.740229 |
| 58 | 1 | 0 | -3.837556 | -0.232271 | 2.626472 |
| 59 | 1 | 0 | -7.345179 | -0.439091 | 3.863636 |
| 60 | 1 | 0 | -8.047587 | 0.847425 | 2.885146 |
| 61 | 1 | 0 | -7.523919 | -0.654868 | 2.115202 |
| 62 | 6 | 0 | 0.706096 | 0.322121 | -0.039258 |
| 63 | 16 | 0 | 2.150751 | -0.646077 | -0.165765 |
| 64 | 6 | 0 | 1.035083 | 1.654887 | 0.035202 |
| 65 | 6 | 0 | 3.204026 | 0.764464 | -0.070658 |
| 66 | 6 | 0 | 2.438082 | 1.941782 | -0.022948 |
| 67 | 1 | 0 | 0.278326 | 2.417158 | 0.163228 |
| 68 | 5 | 0 | 4.707656 | 0.550242 | 0.065460 |
| 69 | 6 | 0 | 2.918442 | 3.332010 | -0.142040 |
| 70 | 6 | 0 | 5.629199 | 1.683852 | 0.473038 |
| 71 | 6 | 0 | 5.307657 | -0.944149 | -0.099793 |
| 72 | 6 | 0 | 4.226457 | 3.828345 | 0.166109 |
| 73 | 6 | 0 | 1.969808 | 4.256036 | -0.648121 |
| 74 | 6 | 0 | 5.384980 | 3.057816 | 0.652992 |
| 75 | 16 | 0 | 7.273307 | 1.290885 | 0.973225 |
| 76 | 7 | 0 | 5.746068 | -1.486297 | -1.275635 |
| 77 | 7 | 0 | 5.445889 | -1.898407 | 0.871615 |
| 78 | 6 | 0 | 4.468991 | 5.208194 | -0.051375 |
| 79 | 6 | 0 | 2.240146 | 5.598993 | -0.835768 |
| 80 | 1 | 0 | 0.996653 | 3.892625 | -0.950619 |
| 81 | 6 | 0 | 6.502197 | 3.715438 | 1.275764 |
| 82 | 6 | 0 | 7.572950 | 2.900969 | 1.498215 |
| 83 | 6 | 0 | 6.147126 | -2.803935 | -1.043075 |
| 84 | 6 | 0 | 5.756551 | -0.846819 | -2.672275 |
| 85 | 6 | 0 | 5.977294 | -3.054689 | 0.290536 |
| 86 | 6 | 0 | 5.147694 | -1.800453 | 2.379103 |
| 87 | 6 | 0 | 3.512099 | 6.084236 | -0.529355 |
| 88 | 1 | 0 | 5.463650 | 5.596406 | 0.119133 |
| 89 | 1 | 0 | 6.506008 | 4.753111 | 1.579177 |

| | | | | | |
|---|---|---|---|---|---|
| 90 | 1 | 0 | 8.517762 | 3.165095 | 1.954244 |
| 91 | 6 | 0 | 6.667720 | -3.801753 | -2.037137 |
| 92 | 6 | 0 | 7.141028 | -1.064711 | -3.318956 |
| 93 | 6 | 0 | 5.541460 | 0.671520 | -2.630654 |
| 94 | 6 | 0 | 4.610995 | -1.475062 | -3.487254 |
| 95 | 6 | 0 | 6.303182 | -4.365573 | 0.950081 |
| 96 | 6 | 0 | 6.487694 | -1.824254 | 3.140791 |
| 97 | 6 | 0 | 4.211597 | -2.964020 | 2.767582 |
| 98 | 6 | 0 | 4.417225 | -0.510292 | 2.775798 |
| 99 | 1 | 0 | 6.508741 | -4.807352 | -1.646914 |
| 100 | 1 | 0 | 6.159135 | -3.757476 | -2.998462 |
| 101 | 1 | 0 | 7.740878 | -3.684474 | -2.217126 |
| 102 | 1 | 0 | 7.325976 | -2.085337 | -3.642383 |
| 103 | 1 | 0 | 7.205779 | -0.433923 | -4.208557 |
| 104 | 1 | 0 | 7.939563 | -0.758729 | -2.637173 |
| 105 | 1 | 0 | 4.570329 | 0.960086 | -2.227945 |
| 106 | 1 | 0 | 5.565859 | 1.024418 | -3.664887 |
| 107 | 1 | 0 | 6.332647 | 1.189431 | -2.087838 |
| 108 | 1 | 0 | 4.623759 | -1.062172 | -4.499621 |
| 109 | 1 | 0 | 4.687644 | -2.559575 | -3.572582 |
| 110 | 1 | 0 | 3.644164 | -1.237292 | -3.034691 |
| 111 | 1 | 0 | 6.643492 | -4.267372 | 1.977104 |
| 112 | 1 | 0 | 5.445876 | -5.047410 | 0.945726 |
| 113 | 1 | 0 | 7.111050 | -4.851047 | 0.401051 |
| 114 | 1 | 0 | 7.067862 | -0.926076 | 2.917522 |
| 115 | 1 | 0 | 6.282287 | -1.836218 | 4.214597 |
| 116 | 1 | 0 | 7.108915 | -2.689892 | 2.916167 |
| 117 | 1 | 0 | 4.671776 | -3.947167 | 2.711375 |
| 118 | 1 | 0 | 3.316194 | -2.958748 | 2.139270 |
| 119 | 1 | 0 | 3.894389 | -2.817984 | 3.803111 |
| 120 | 1 | 0 | 4.288750 | -0.546239 | 3.860697 |
| 121 | 1 | 0 | 4.983637 | 0.392241 | 2.557664 |
| 122 | 1 | 0 | 3.423554 | -0.439492 | 2.335379 |
| 123 | 1 | 0 | -3.668211 | -7.103005 | 0.395985 |
| 124 | 1 | 0 | -1.381179 | -6.252355 | 0.978891 |
| 125 | 1 | 0 | 1.477005 | 6.255528 | -1.240750 |
| 126 | 1 | 0 | 3.763607 | 7.127836 | -0.686905 |

**Table S7** Coordinates for Optimized Structure of **2-F**$^{2+}$ in the ground state ($S_0$).

Total Energy: −4353.2056 Hartree

# opt b3lyp/6-31g(d,p) geom=connectivity

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.861397 | 5.784653 | -0.354918 |
| 2 | 6 | 0 | 2.551329 | 5.438809 | -0.021081 |
| 3 | 6 | 0 | 2.182860 | 4.113825 | -0.010741 |
| 4 | 6 | 0 | 3.075605 | 3.063495 | -0.339379 |
| 5 | 6 | 0 | 4.422957 | 3.416591 | -0.674177 |
| 6 | 6 | 0 | 4.763794 | 4.792574 | -0.662622 |
| 7 | 6 | 0 | 2.492723 | 1.711098 | -0.269044 |
| 8 | 6 | 0 | 3.166510 | 0.500507 | -0.040657 |
| 9 | 6 | 0 | 5.669137 | 1.158331 | -0.613118 |
| 10 | 6 | 0 | 5.533805 | 2.505277 | -1.000289 |
| 11 | 6 | 0 | 1.072279 | 1.523968 | -0.320807 |
| 12 | 6 | 0 | 0.643531 | 0.241118 | -0.078070 |

| | | | | | |
|---|---|---|---|---|---|
| 13 | 16 | 0 | 2.009440 | -0.801388 | 0.219080 |
| 14 | 16 | 0 | 7.291162 | 0.581961 | -0.995613 |
| 15 | 6 | 0 | 7.722532 | 2.072059 | -1.735918 |
| 16 | 6 | 0 | 6.711215 | 2.985040 | -1.670034 |
| 17 | 5 | 0 | 4.653885 | 0.163475 | -0.080536 |
| 18 | 6 | 0 | 5.173964 | -1.313725 | 0.327993 |
| 19 | 7 | 0 | 5.633944 | -1.663337 | 1.567035 |
| 20 | 6 | 0 | 6.110167 | -2.975156 | 1.517978 |
| 21 | 6 | 0 | 5.908338 | -3.437088 | 0.246366 |
| 22 | 7 | 0 | 5.334816 | -2.397147 | -0.492509 |
| 23 | 6 | 0 | 6.749206 | -3.769015 | 2.620804 |
| 24 | 6 | 0 | 6.283081 | -4.816656 | -0.218163 |
| 25 | 6 | 0 | 4.945506 | -2.559650 | -1.973022 |
| 26 | 6 | 0 | 3.762984 | -3.545899 | -2.049849 |
| 27 | 6 | 0 | 6.183530 | -3.038014 | -2.759731 |
| 28 | 6 | 0 | 4.494771 | -1.250011 | -2.634119 |
| 29 | 6 | 0 | 5.726244 | -0.788713 | 2.826005 |
| 30 | 6 | 0 | 5.156403 | -1.570769 | 4.028629 |
| 31 | 6 | 0 | 4.885836 | 0.489966 | 2.715729 |
| 32 | 6 | 0 | 7.199660 | -0.387132 | 3.020337 |
| 33 | 1 | 0 | 1.173311 | 3.903149 | 0.312919 |
| 34 | 1 | 0 | 5.777776 | 5.113841 | -0.854170 |
| 35 | 1 | 0 | 0.376728 | 2.310508 | -0.581637 |
| 36 | 1 | 0 | 8.695148 | 2.199795 | -2.192239 |
| 37 | 1 | 0 | 6.801004 | 3.964383 | -2.119530 |
| 38 | 1 | 0 | 7.355825 | -4.561244 | 2.181414 |
| 39 | 1 | 0 | 7.417352 | -3.177411 | 3.244057 |
| 40 | 1 | 0 | 6.009732 | -4.244319 | 3.272819 |
| 41 | 1 | 0 | 5.623657 | -5.217673 | -0.982842 |
| 42 | 1 | 0 | 7.305794 | -4.847954 | -0.608782 |
| 43 | 1 | 0 | 6.233379 | -5.504218 | 0.627123 |
| 44 | 1 | 0 | 2.880805 | -3.118953 | -1.565698 |
| 45 | 1 | 0 | 3.520418 | -3.724068 | -3.100849 |
| 46 | 1 | 0 | 3.964154 | -4.512981 | -1.591109 |
| 47 | 1 | 0 | 6.504478 | -4.048032 | -2.519243 |
| 48 | 1 | 0 | 7.023260 | -2.355750 | -2.602121 |
| 49 | 1 | 0 | 5.939752 | -3.025312 | -3.824937 |
| 50 | 1 | 0 | 4.216903 | -1.498920 | -3.661532 |
| 51 | 1 | 0 | 3.614048 | -0.811667 | -2.169209 |
| 52 | 1 | 0 | 5.291685 | -0.509965 | -2.687086 |
| 53 | 1 | 0 | 5.798894 | -2.371365 | 4.384444 |
| 54 | 1 | 0 | 5.031067 | -0.874105 | 4.860735 |
| 55 | 1 | 0 | 4.172326 | -1.985374 | 3.791251 |
| 56 | 1 | 0 | 5.225151 | 1.163582 | 1.928812 |
| 57 | 1 | 0 | 5.004040 | 1.031872 | 3.657511 |
| 58 | 1 | 0 | 3.823198 | 0.278084 | 2.588782 |
| 59 | 1 | 0 | 7.292720 | 0.200502 | 3.937669 |
| 60 | 1 | 0 | 7.869780 | -1.242908 | 3.107797 |
| 61 | 1 | 0 | 7.543753 | 0.228695 | 2.185121 |
| 62 | 6 | 0 | -0.717001 | -0.260335 | -0.073558 |
| 63 | 16 | 0 | -2.092475 | 0.808347 | -0.140971 |
| 64 | 6 | 0 | -1.136168 | -1.567618 | -0.007281 |
| 65 | 6 | 0 | -3.239391 | -0.526151 | -0.044217 |
| 66 | 6 | 0 | -2.556743 | -1.754505 | -0.030623 |
| 67 | 1 | 0 | -0.428524 | -2.380866 | 0.081365 |
| 68 | 5 | 0 | -4.721710 | -0.207225 | 0.122834 |
| 69 | 6 | 0 | -3.135718 | -3.105541 | -0.151611 |
| 70 | 6 | 0 | -5.717521 | -1.281789 | 0.516667 |
| 71 | 6 | 0 | -5.214227 | 1.329280 | 0.000112 |
| 72 | 6 | 0 | -4.473455 | -3.514584 | 0.160395 |

| | | | | | |
|---|---|---|---|---|---|
| 73 | 6 | 0 | -2.251145 | -4.087420 | -0.663955 |
| 74 | 6 | 0 | -5.576044 | -2.674640 | 0.660188 |
| 75 | 16 | 0 | -7.326112 | -0.781972 | 1.033240 |
| 76 | 7 | 0 | -5.631124 | 1.929553 | -1.155409 |
| 77 | 7 | 0 | -5.271430 | 2.266379 | 0.996144 |
| 78 | 6 | 0 | -4.811785 | -4.873533 | -0.060000 |
| 79 | 6 | 0 | -2.616557 | -5.399764 | -0.851482 |
| 80 | 1 | 0 | -1.251453 | -3.824722 | -0.979364 |
| 81 | 6 | 0 | -6.740132 | -3.264906 | 1.263532 |
| 82 | 6 | 0 | -7.747053 | -2.379077 | 1.510198 |
| 83 | 6 | 0 | -5.936144 | 3.265140 | -0.884795 |
| 84 | 6 | 0 | -5.706156 | 1.327306 | -2.566116 |
| 85 | 6 | 0 | -5.729601 | 3.470366 | 0.451588 |
| 86 | 6 | 0 | -4.956408 | 2.112414 | 2.495676 |
| 87 | 6 | 0 | -3.917043 | -5.800301 | -0.542987 |
| 88 | 1 | 0 | -5.819315 | -5.227845 | 0.104636 |
| 89 | 1 | 0 | -6.824311 | -4.307275 | 1.538000 |
| 90 | 1 | 0 | -8.709581 | -2.585246 | 1.959039 |
| 91 | 6 | 0 | -6.400346 | 4.321632 | -1.845218 |
| 92 | 6 | 0 | -7.081827 | 1.654457 | -3.186007 |
| 93 | 6 | 0 | -5.596536 | -0.203067 | -2.563381 |
| 94 | 6 | 0 | -4.532347 | 1.895098 | -3.385223 |
| 95 | 6 | 0 | -5.954571 | 4.784461 | 1.145654 |
| 96 | 6 | 0 | -6.279093 | 2.212327 | 3.281052 |
| 97 | 6 | 0 | -3.931606 | 3.195516 | 2.892477 |
| 98 | 6 | 0 | -4.317343 | 0.762974 | 2.850847 |
| 99 | 1 | 0 | -6.163186 | 5.303343 | -1.434347 |
| 100 | 1 | 0 | -5.912519 | 4.264932 | -2.816457 |
| 101 | 1 | 0 | -7.482064 | 4.285743 | -2.007518 |
| 102 | 1 | 0 | -7.201496 | 2.692530 | -3.483998 |
| 103 | 1 | 0 | -7.201521 | 1.050624 | -4.088455 |
| 104 | 1 | 0 | -7.889702 | 1.387112 | -2.498994 |
| 105 | 1 | 0 | -4.644636 | -0.569330 | -2.178063 |
| 106 | 1 | 0 | -5.654634 | -0.527786 | -3.605500 |
| 107 | 1 | 0 | -6.417569 | -0.677915 | -2.025383 |
| 108 | 1 | 0 | -4.591693 | 1.512915 | -4.407909 |
| 109 | 1 | 0 | -4.532538 | 2.984204 | -3.439898 |
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| 112 | 1 | 0 | -5.056072 | 5.410814 | 1.129135 |
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| 114 | 1 | 0 | -6.924905 | 1.363496 | 3.044982 |
| 115 | 1 | 0 | -6.056341 | 2.180980 | 4.350943 |
| 116 | 1 | 0 | -6.841513 | 3.124993 | 3.089982 |
| 117 | 1 | 0 | -4.317703 | 4.211036 | 2.861672 |
| 118 | 1 | 0 | -3.047370 | 3.136910 | 2.251194 |
| 119 | 1 | 0 | -3.612509 | 3.006258 | 3.920394 |
| 120 | 1 | 0 | -4.167097 | 0.764780 | 3.933531 |
| 121 | 1 | 0 | -4.955289 | -0.088916 | 2.625934 |
| 122 | 1 | 0 | -3.339361 | 0.626069 | 2.391044 |
| 123 | 9 | 0 | -4.286623 | -7.063929 | -0.750612 |
| 124 | 9 | 0 | -1.750201 | -6.282372 | -1.355591 |
| 125 | 9 | 0 | 1.677399 | 6.390910 | 0.315840 |
| 126 | 9 | 0 | 4.231612 | 7.065007 | -0.338196 |

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