CHEMISTRY
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Supporting Information

Transition-Metal-Free Cleavage of CO

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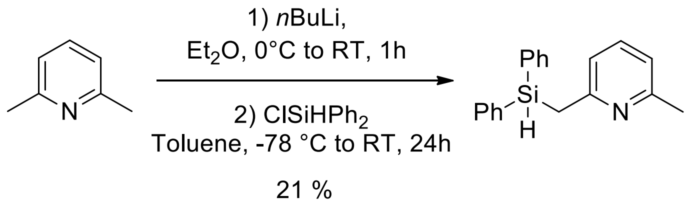
Supporting Information

Procedures and spectroscopic data

General comments: All reactions and manipulations were carried out under an atmosphere of dry dinitrogen using standard Schlenk techniques or in a glove-box. All solvents were purged with dinitrogen and dried using an MBRAUN Solvent Purification System (SPS). ^{1}H, ^{13}C, ^{29}Si, ^{11}B and ^{19}F NMR spectra were recorded on Bruker AV 300, Bruker DRX 300 or Bruker AV 400 spectrometers. Chemical shifts were expressed in positive sign, in parts per million, calibrated to residual ^{1}H (5.32 ppm), ^{13}C (53.84 ppm), external tetramethylsilane (0 ppm) solvent signals and external $BF_3.Et_2O$ respectively. Mass spectra were recorded on an AccuTOF LC, JMS-T100LP or an AccuTOF GC v 4g, JMS-T100GCV Mass spectrometer. Triphenylcarbenium tetrakis(pentafluorophenyl)borate[S1] and lithium *tris*[2-(dimethylamino)ethyl]amine hydridotris(pentafluorophenyl)borate[S2] were prepared from reported procedures. Tris(pentafluorophenyl)borane was purchased from Sigma Aldrich and was sublimed prior to use. Microanalysis was performed by Kolbe Mikroanalytisches Laboratorium in Muehlheim a/d Ruhr, Germany.

Synthesis of 1^H



n-BuLi in hexanes (17.0 mmol, 2.5 M, 6.79 mL, 1.01 eq) was added dropwise at 0 °C to a solution of lutidine (16.8 mmol, 1.95 mL, 1.80 g) in diethylether (20 mL) and the resulting mixture was stirred for an additional hour at room temperature giving a dark red solution. Chlorodiphenylsilane (16.8 mmol, 3.29 mL, 1.0 eq) in solution in toluene (10 mL) was then added dropwise to the solution at -78 °C under stirring. The reaction mixture was then allowed to warm up slowly to room temperature (in the cold bath) over 1 day under stirring giving a colorless solution and a white precipitate. After removal of the volatiles under vacuum, the residue was extracted with pentane (3 times 10 mL) and filtered over filter frit. The obtained colorless solution was concentrated until saturation and cooled down to -30 °C leading to the precipitation of a colorless oil. After elimination of the mother liquor via syringe, the oil was washed at the same temperature with pentane (20 mL) and dried under reduced pressure (yield: 21%).

^1H NMR (300 MHz, CD_2Cl_2, δ): 2.42 (s, 3H, CH_3), 2.91 (d, 2H, $^3J_{HH}$ = 3.7 Hz, Si-CH_2), 5.01 (m, 1H, $^1J_{HSi}$ = 199.9 Hz, Si-H), 6.77 (d, 1H, $^3J_{HH}$ = 7.8 Hz, $H_{m\text{-}Py}$), 6.85 (d, 1H, $^3J_{HH}$ = 7.7 Hz, $H_{m\text{-}Py}$), 7.30-7.46 (m, 7H, $H_{arom.}$), 7.51-7.62 (m, 4H, $H_{arom.}$).

$^{13}C\{^1H\}$ NMR (76 MHz, CD_2Cl_2, δ): 24.5 (s, 1C, CH_3), 25.8 (s, 1C, CH_2), 119.5 (s, 1C, $CH_{m\text{-}Py}$), 120.1 (s, 1C, $CH_{m\text{-}Py}$), 128.3 (s, 4C, CH_{Ph}), 130.1 (s, 2C, $CH_{p\text{-}Ph}$), 134.2 (s, 2C, Si-$C_{quat.}$), 135.7 (s, 4C, CH_{Ph}), 136.5 (s, 1C, $CH_{p\text{-}Py}$), 158.1 (s, 1C, $C_{o\text{-}Py}$), 159.1 (s, 1C, $C_{o\text{-}Py}$).

$^{29}Si\{^1H\}$ NMR (60 MHz, CD_2Cl_2, δ): -14.6 (s).

Anal. Calcd. For $C_{19}H_{19}NSi$; C, 78.84; H, 6.62; N, 4.84. Found: C, 78.78; H, 6.88; N, 4.74.

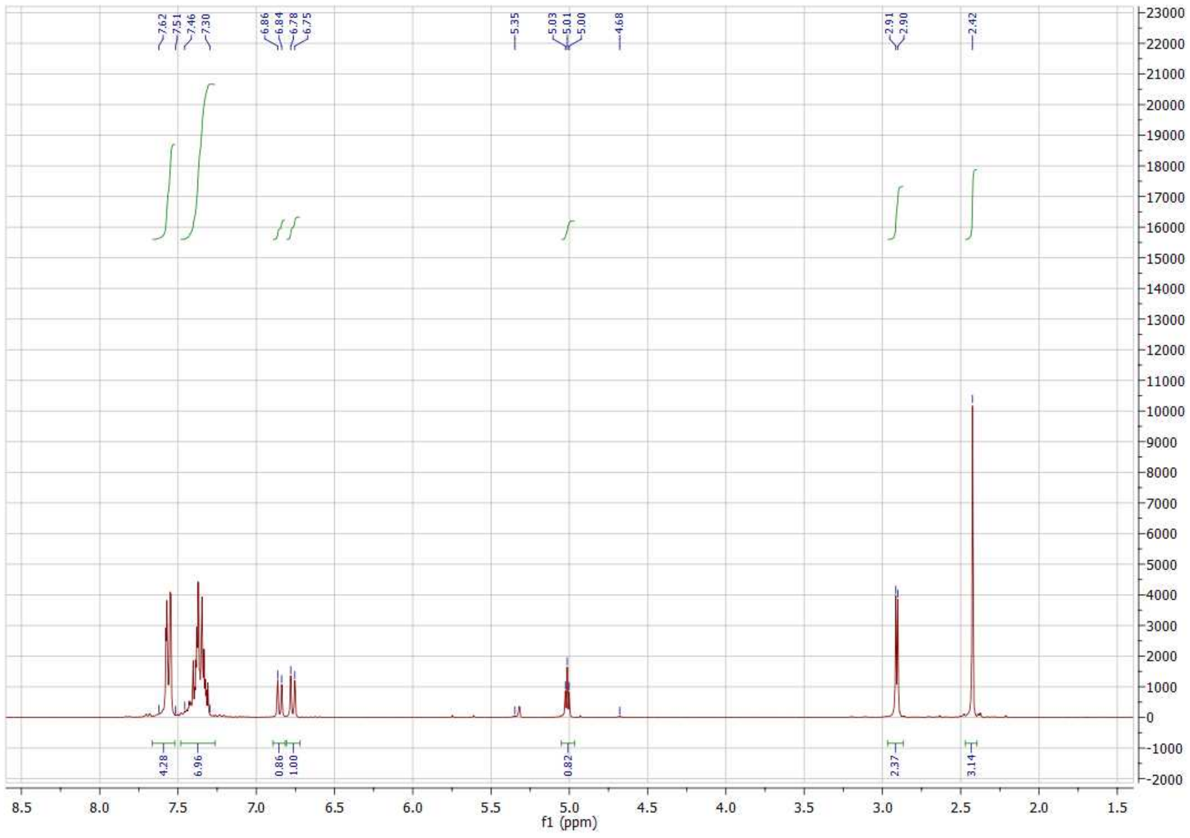


Figure S1. ^{1}H NMR spectrum of $\mathbf{1^{H}}$ (300 MHz, 20 °C) in CD_2Cl_2

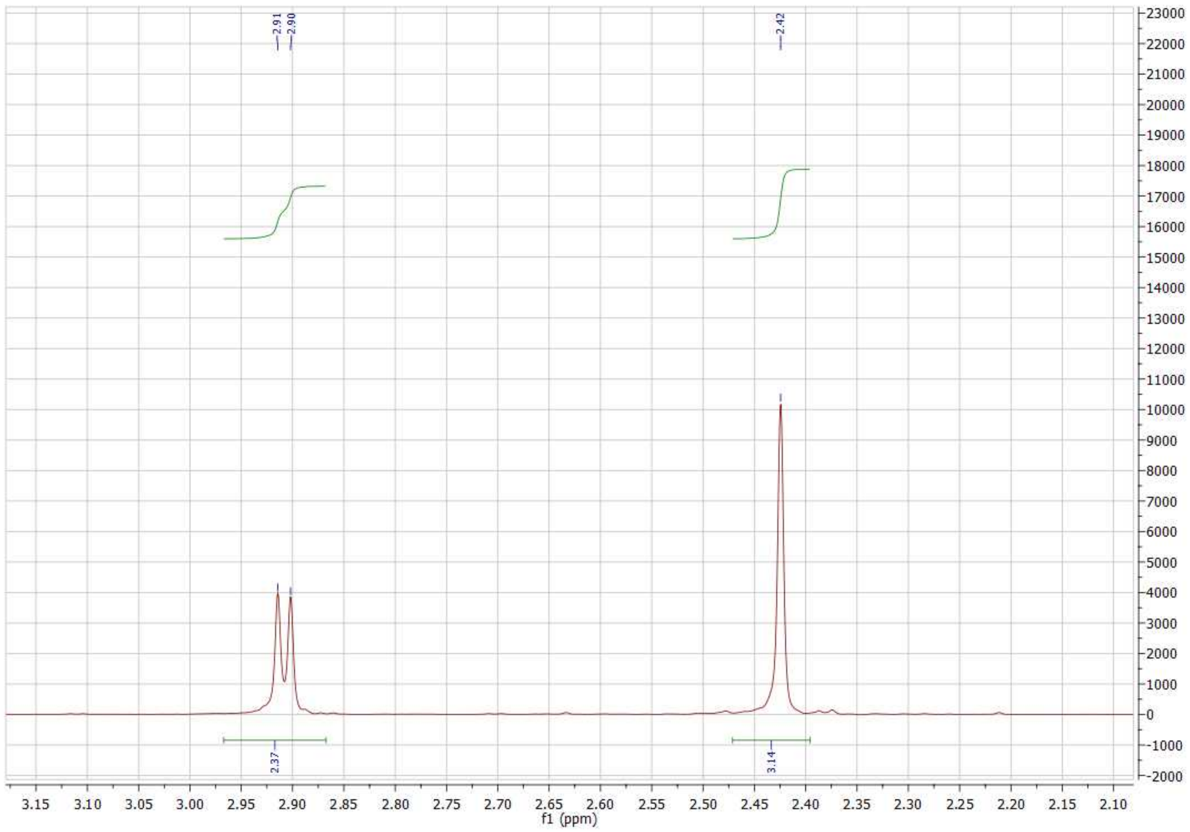


Figure S2. ^{1}H NMR spectrum of $\mathbf{1^{H}}$ (300 MHz, 20 °C) in CD_2Cl_2: aliphatic region

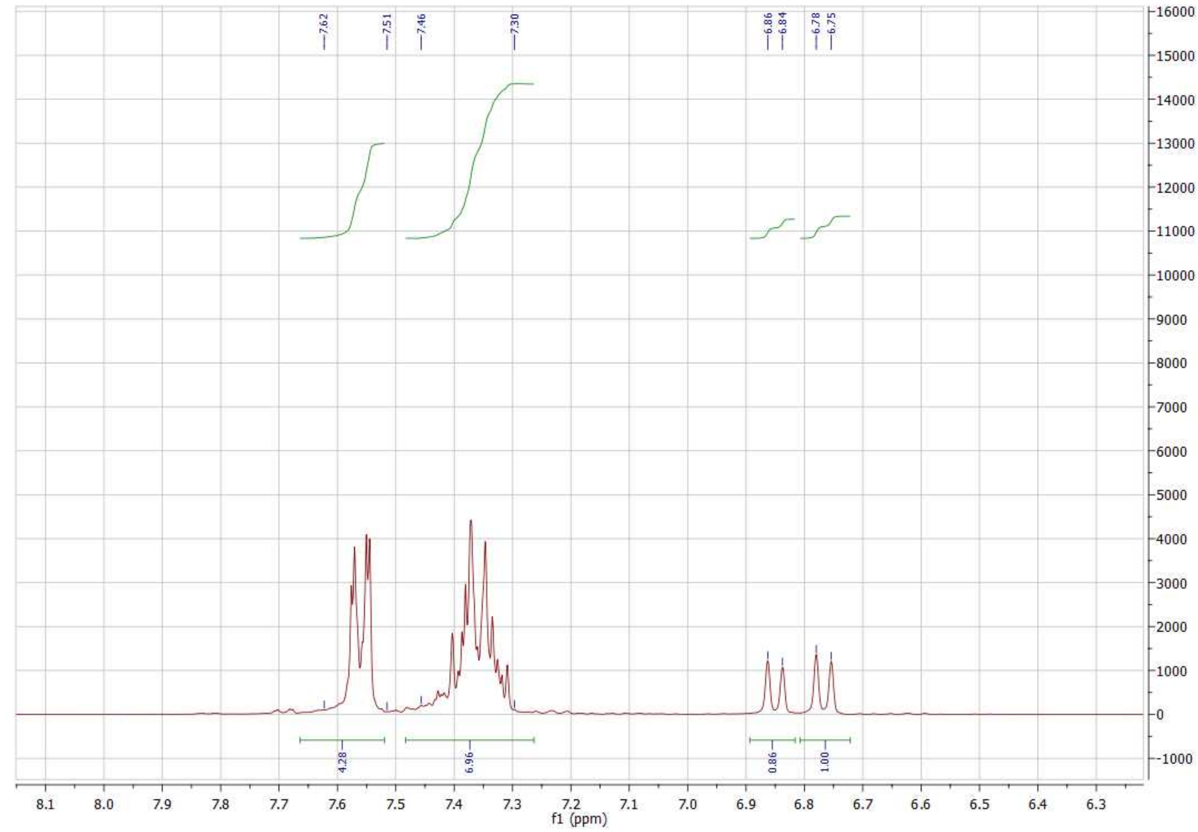


Figure S3. ^{1}H NMR spectrum of $\mathbf{1^{H}}$ (300 MHz, 20 °C) in CD_2Cl_2: aromatic region

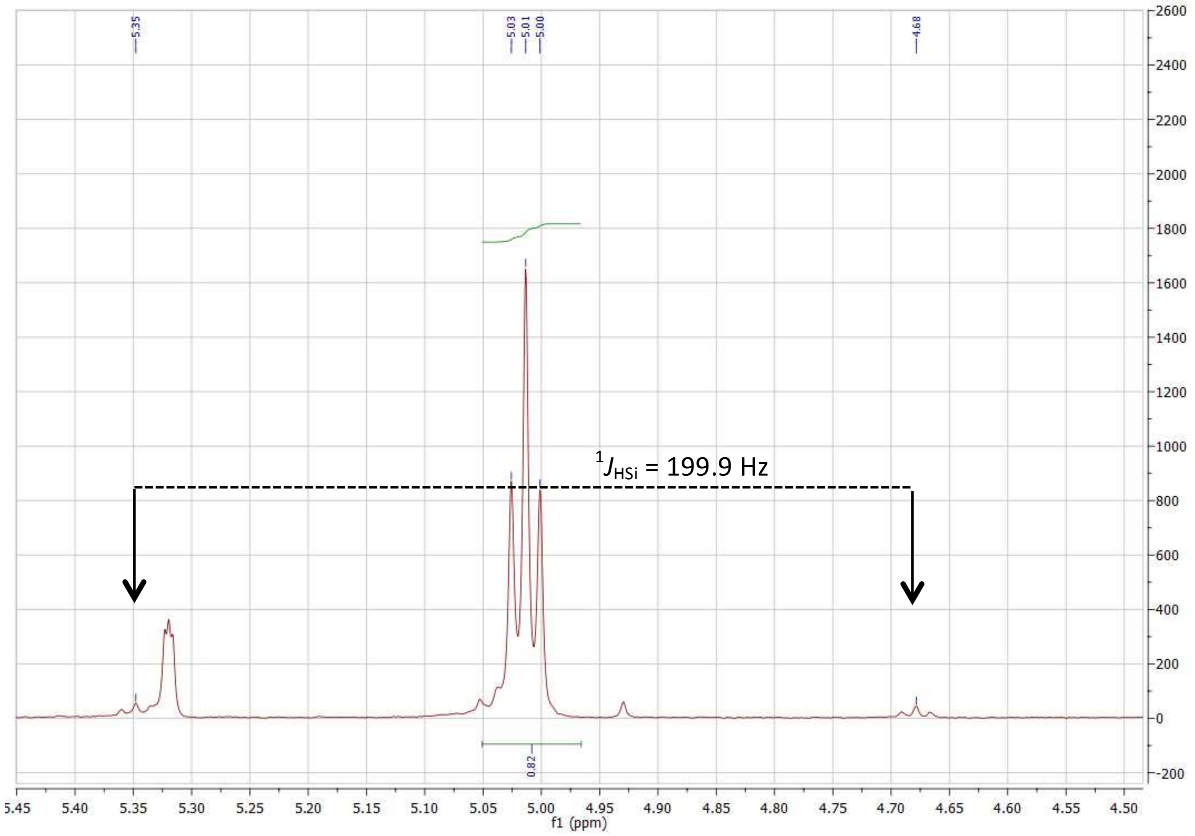


Figure S4. ^{1}H NMR spectrum of $\mathbf{1^{H}}$ (300 MHz, 20 °C) in CD_2Cl_2: silyl hydride

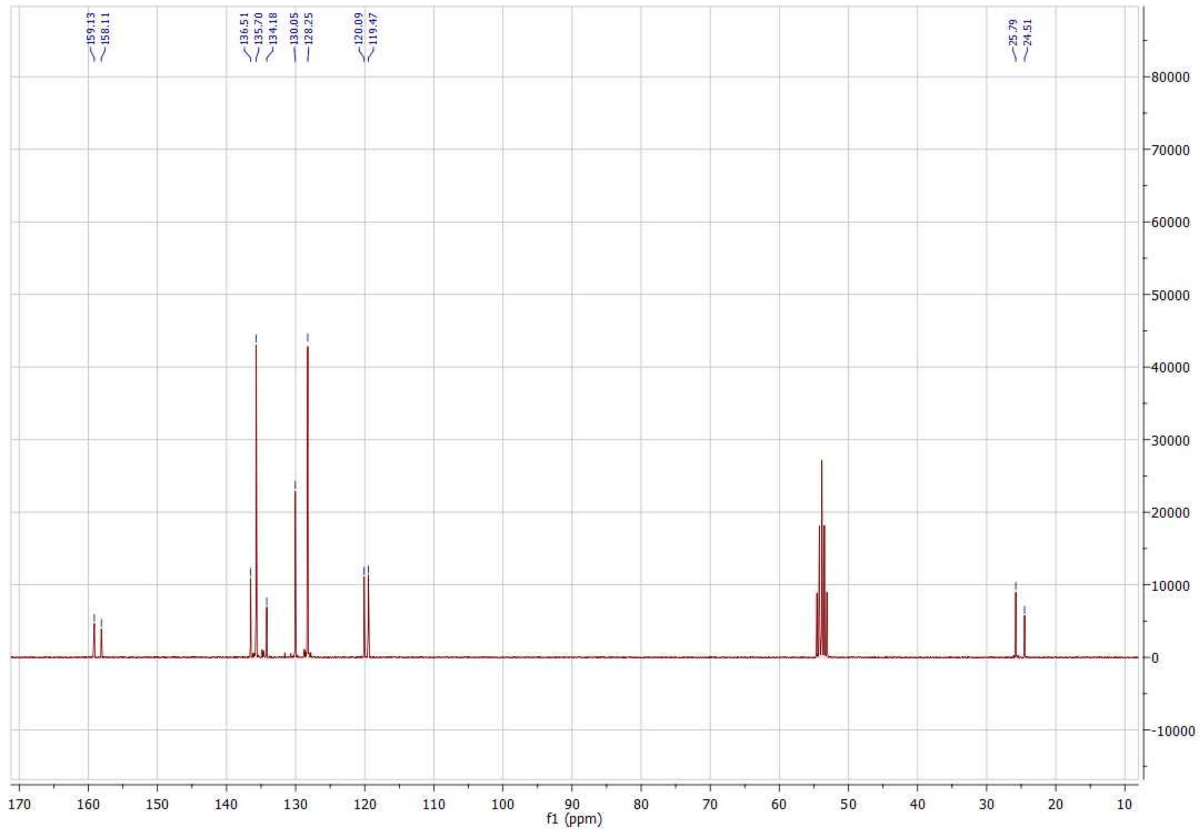


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of **1^H^** (76 MHz, 20 °C) in CD_2Cl_2

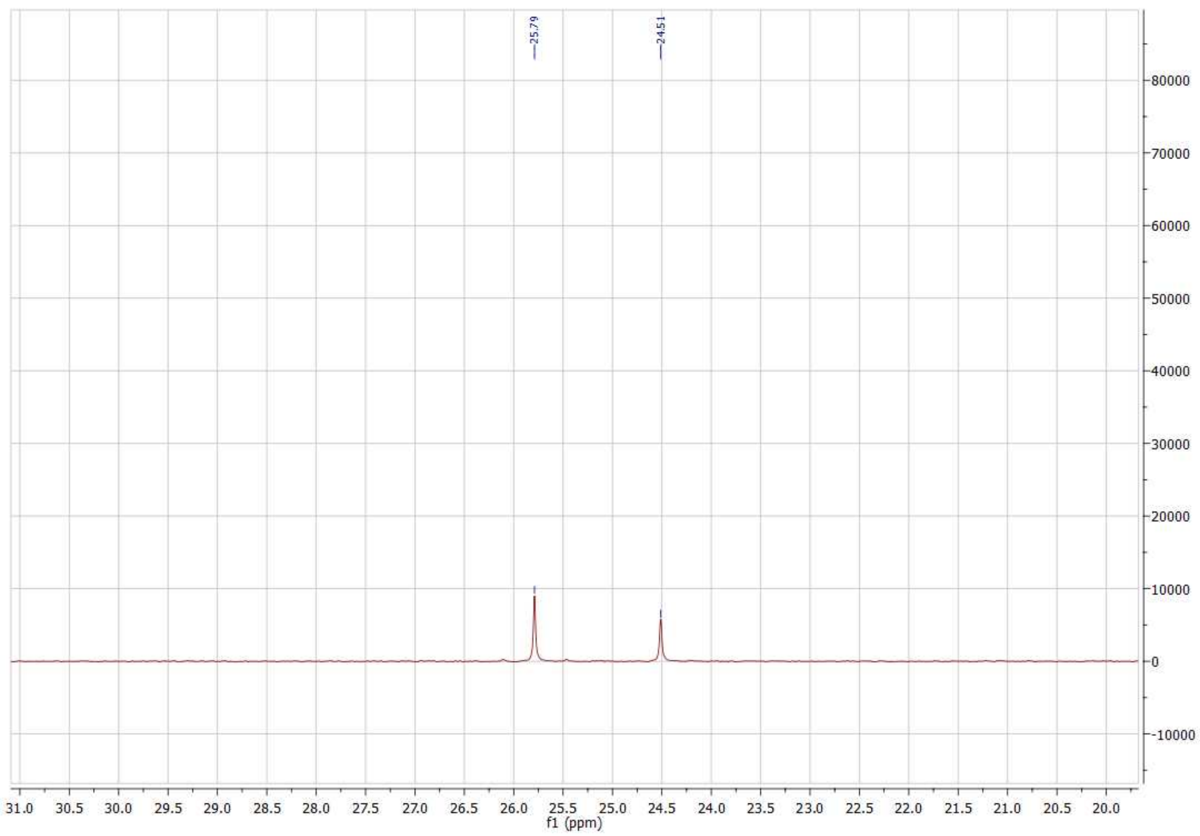


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of **1^H^** (76 MHz, 20 °C) in CD_2Cl_2: aliphatic region

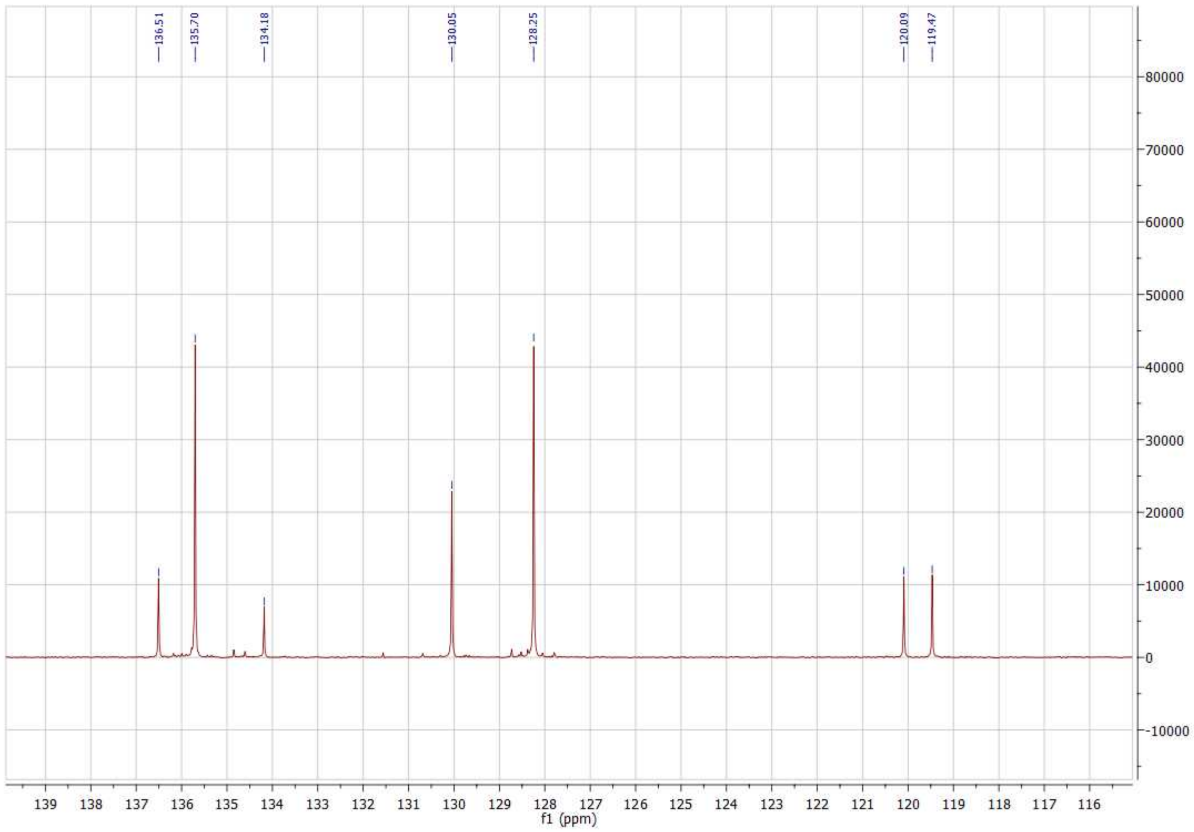


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of $\mathbf{1^{H}}$ (76 MHz, 20 °C) in CD_2Cl_2: aromatic region

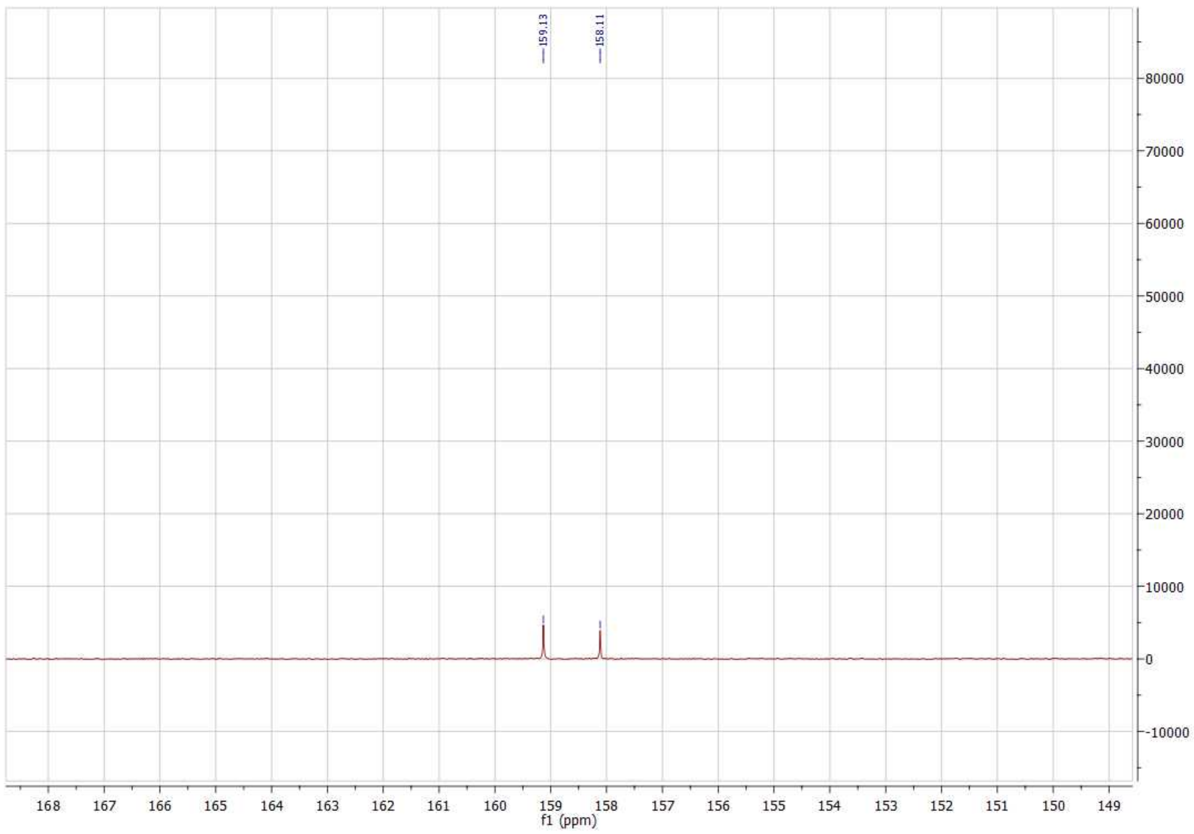


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of $\mathbf{1^{H}}$ (76 MHz, 20 °C) in CD_2Cl_2: aromatic region 2

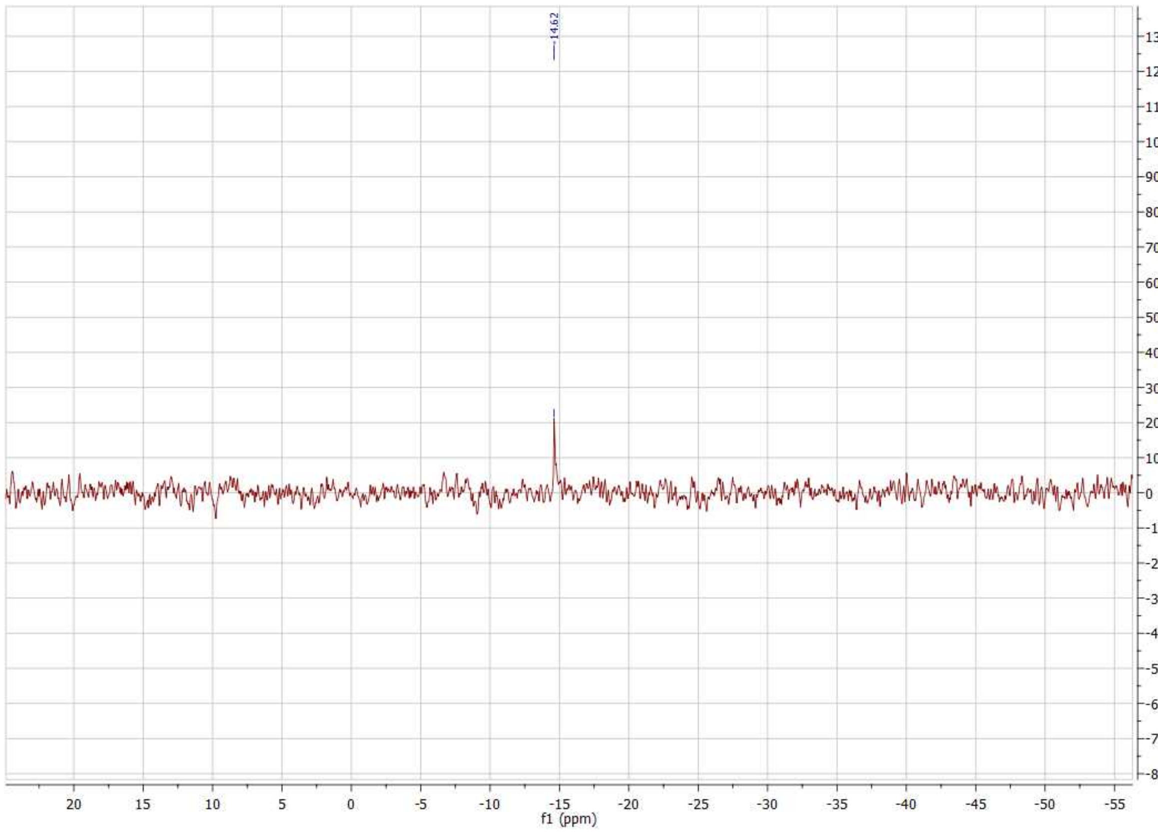
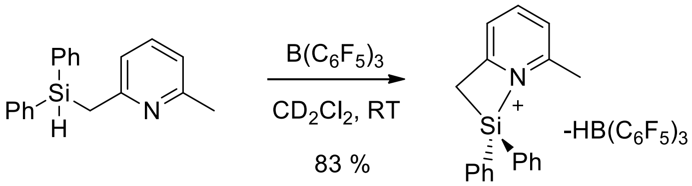


Figure S9. $^{29}Si\{^{1}H\}$ DEPT NMR spectrum of $\mathbf{1^{H}}$ (60 MHz, 20 °C) in CD_2Cl_2

Synthesis of 1^+-HBCF



In an NMR tube, CD_2Cl_2 (0.5 mL) was added to a neat mixture of $\mathbf{1^H}$ (8.7 mg, 30.1 μmol) and tris(pentafluorophenyl)borane (15.1 mg, 29.5 μmol, 0.98 eq.) at room temperature, leading to the instantaneous formation of the expected salt in 83% conversion (relative to the borane reagent). The yield was determined by relative integration of the –CH_2 resonance of the product against the –CH_2 resonance of dichloroethane (internal standard) in the $^1H\{^{11}B\}$ NMR spectrum (D1 = 10 s).

HRMS (CSI, -40 °C): exact mass (monoisotopic) calcd for $[C_{19}H_{18}NSi]^+$, 288.1209; found 288.1198 and $[C_{18}H_1B_1F_{15}]^-$, 512.9935; found 512.9951.

^{1}H NMR (300 MHz, CD_2Cl_2, δ): 2.50 (s, 3H, CH_3), 3.43 (s, 2H, Si-CH_2), 3.57 (br., 1H, B-H), 7.54-7.67 (m, 5H, $4H_{Ph}$ and $1H_{m\text{-py}}$), 7.71-7.82 (m, 7H, $6H_{Ph}$ and $1H_{m\text{-py}}$), 8.34 (t, 1H, $CH_{p\text{-Py}}$).

The resonance signals of the two $H_{m\text{-py}}$ (overlapping with the resonance signals of the H_{Ph}) have been detected at δ 7.62 and δ 7.78 by means of [^{1}H, ^{1}H] COSY NMR spectroscopy.

$^{13}C\{^1H\}$ NMR (76 MHz, CD_2Cl_2, δ): 20.4 (s, CH_3), 20.6 (s, Si-CH_2), 123.3 (s, Si-$C_{quat.}$), 124.6 (s, $CH_{m\text{-Py}}$), 127.0 (s, $CH_{m\text{-Py}}$), 130.1 (s, CH_{Ph}), 134.7 (s, $CH_{p\text{-Ph}}$), 135.9 (s, CH_{Ph}), 137.0 (d br., $^1J_{CF}$ = 246.2 Hz, C-$F_{o\text{-C6F5}}$ or C-$F_{m\text{-C6F5}}$), 139.2 (d br., $^1J_{CF}$ = 245.2 Hz, C-$F_{p\text{-C6F5}}$), 148.1 (s, $CH_{p\text{-Py}}$), 148.6 (br., $^1J_{CF}$ = 238.3 Hz, C-$F_{o\text{-C6F5}}$ or C-$F_{m\text{-C6F5}}$), 156.2 (s, $C_{o\text{-Py}}$), 162.0 (s, $C_{o\text{-Py}}$), the quaternary carbons B-$C_{ipso\text{-C6F5}}$ were not observed.

$^{29}Si\{^1H\}$ NMR (60 MHz, CD_2Cl_2, δ): 23.2 (s).

$^{11}B\{^1H\}$ NMR (96 MHz, CD_2Cl_2, δ): -25.3 (br.).

$^{19}F\{^1H\}$ NMR (282 MHz, CD_2Cl_2, δ): -167.1 (br., 6F, $F_{m\text{-C6F5}}$), -164.5 (br., 3F, $F_{p\text{-C6F5}}$), -133.4 (d, 6F, $^3J_{FF}$ = 21.1 Hz, $F_{o\text{-C6F5}}$).

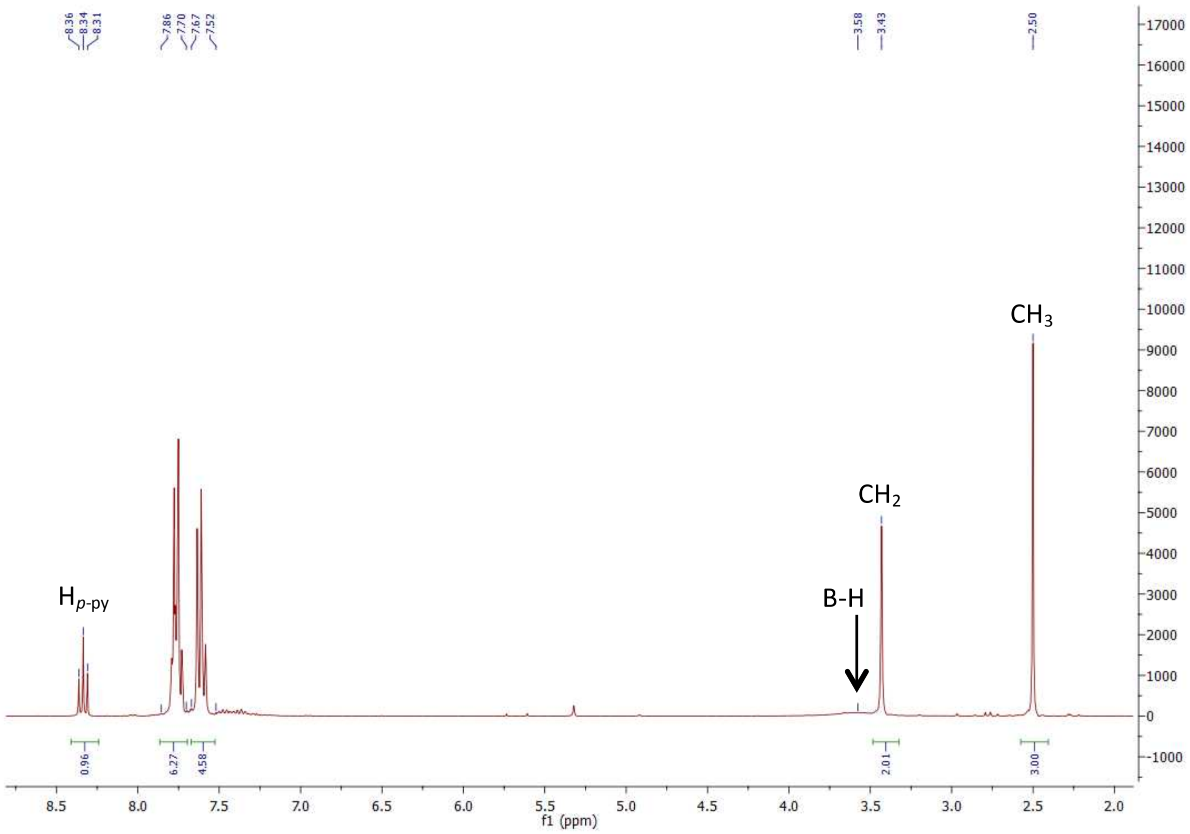


Figure S10. ^{1}H NMR spectrum of **1$^+$-HBCF** (300 MHz, 20 °C) in CD_2Cl_2

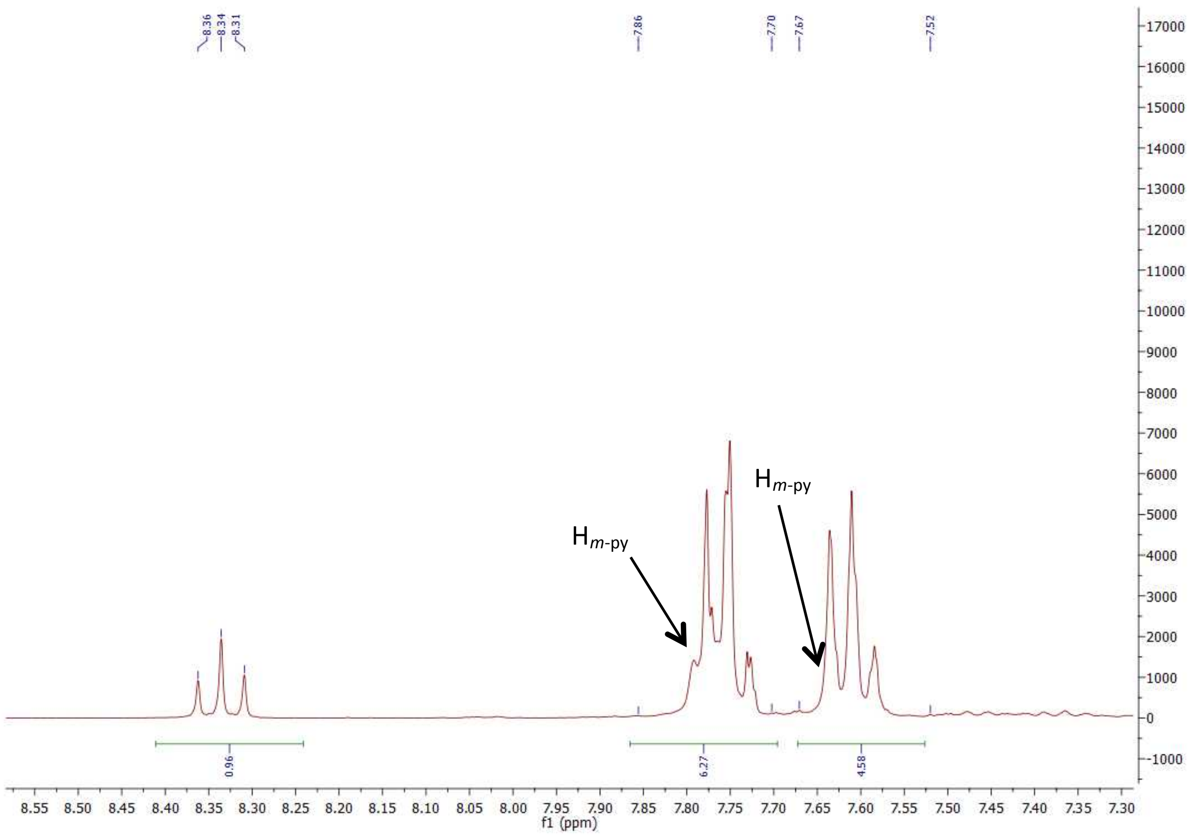


Figure S11. ^{1}H NMR spectrum of **1$^+$-HBCF** (300 MHz, 20 °C) in CD_2Cl_2: aromatic region

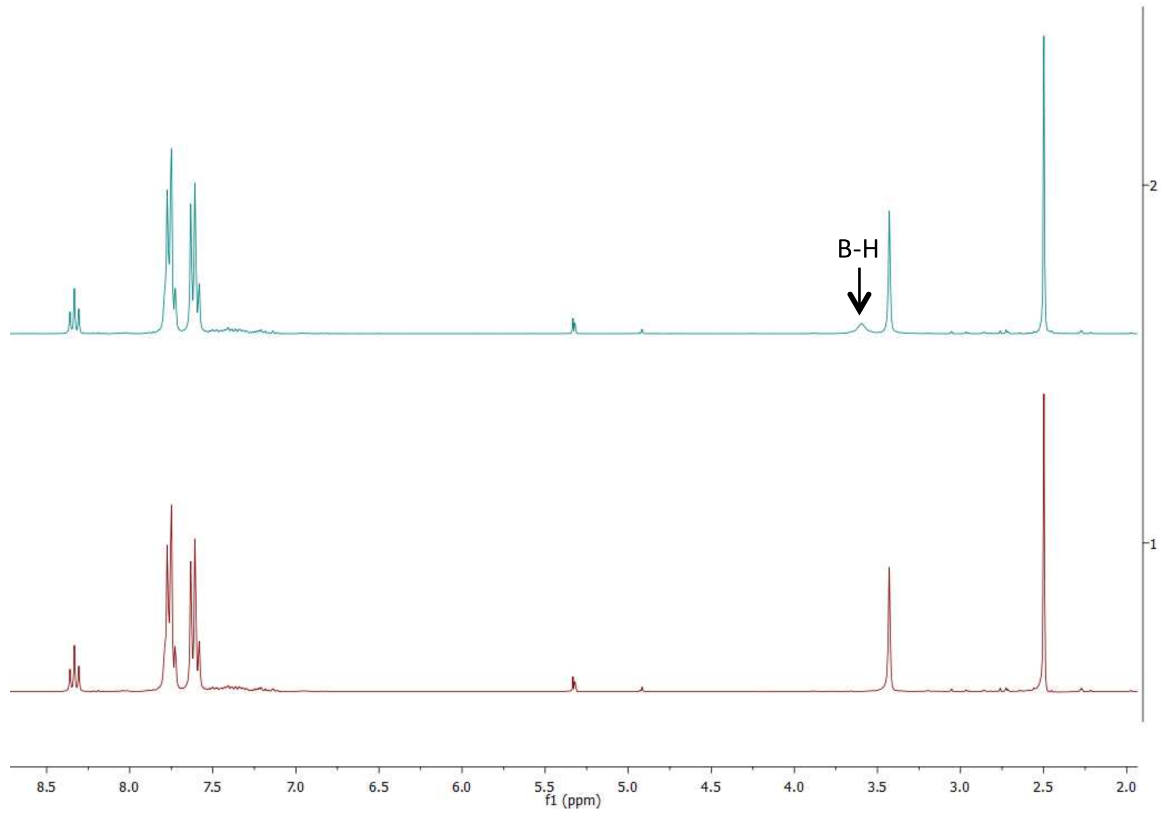


Figure S12. Stacked ^{1}H (bottom) and $^{1}H\{^{11}B\}$ (top) NMR spectra of **1^{+}-HBCF** (300 MHz, 20 °C) in CD_2Cl_2

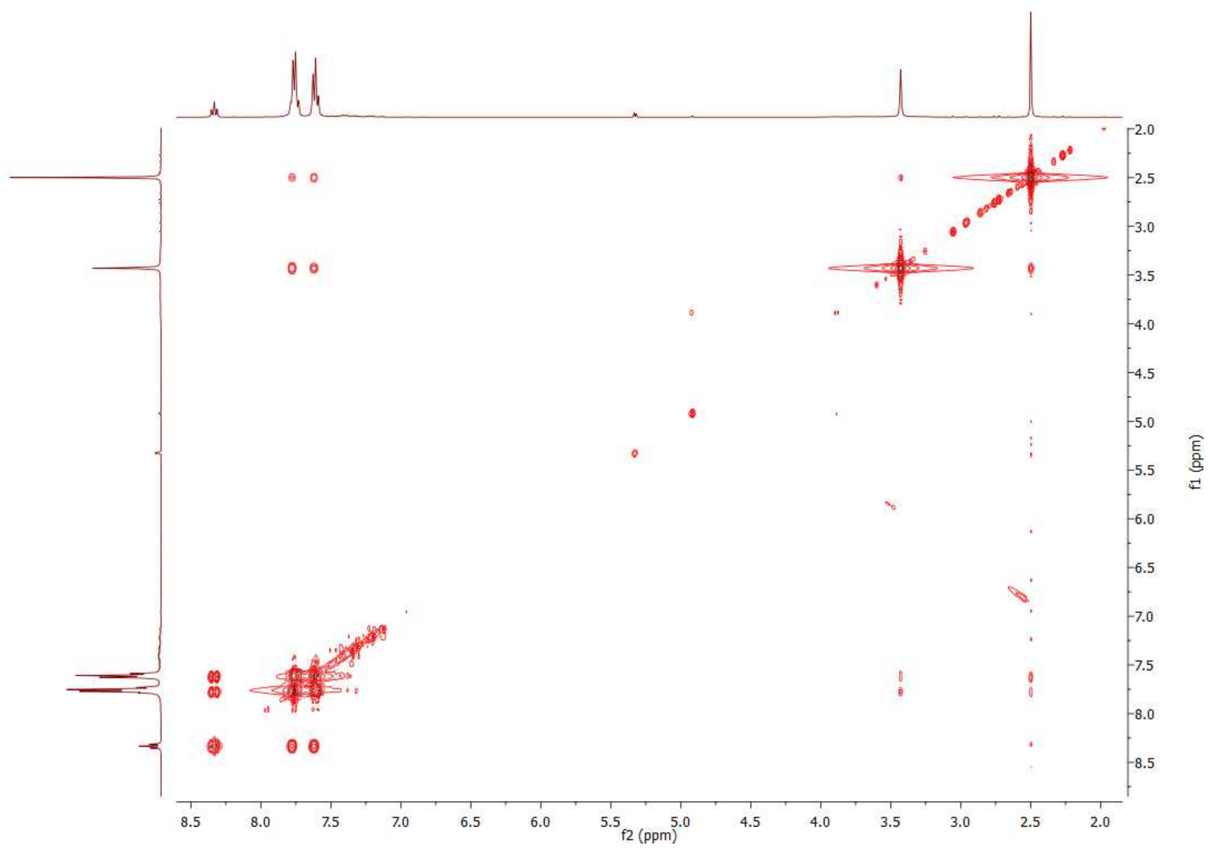


Figure S13. COSY [^{1}H,^{1}H] of **1^{+}-HBCF** (400 MHz, 20 °C) in CD_2Cl_2

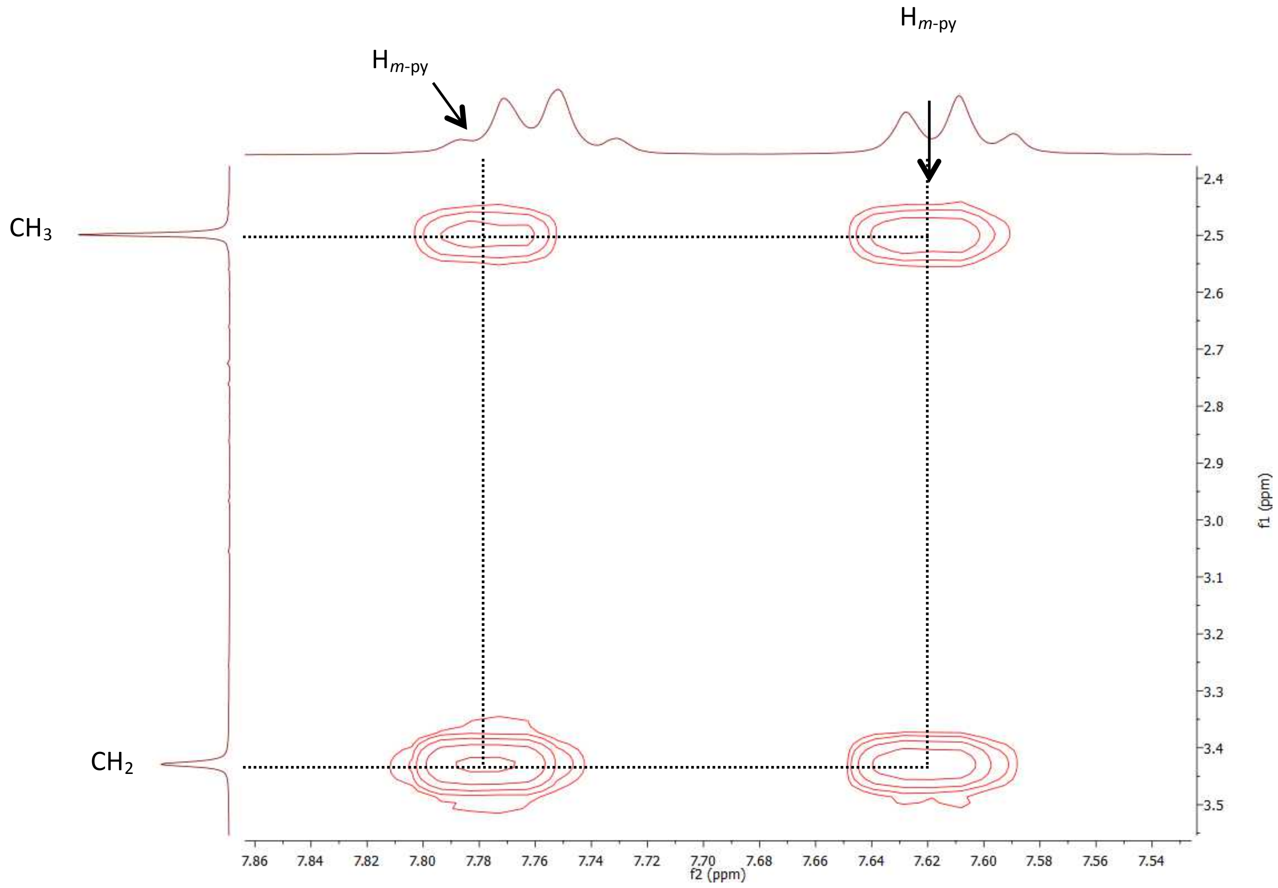


Figure S14. COSY [^{1}H,^{1}H] of **1$^+$-HBCF** (400 MHz, 20 °C) in CD_2Cl_2: zoom 1

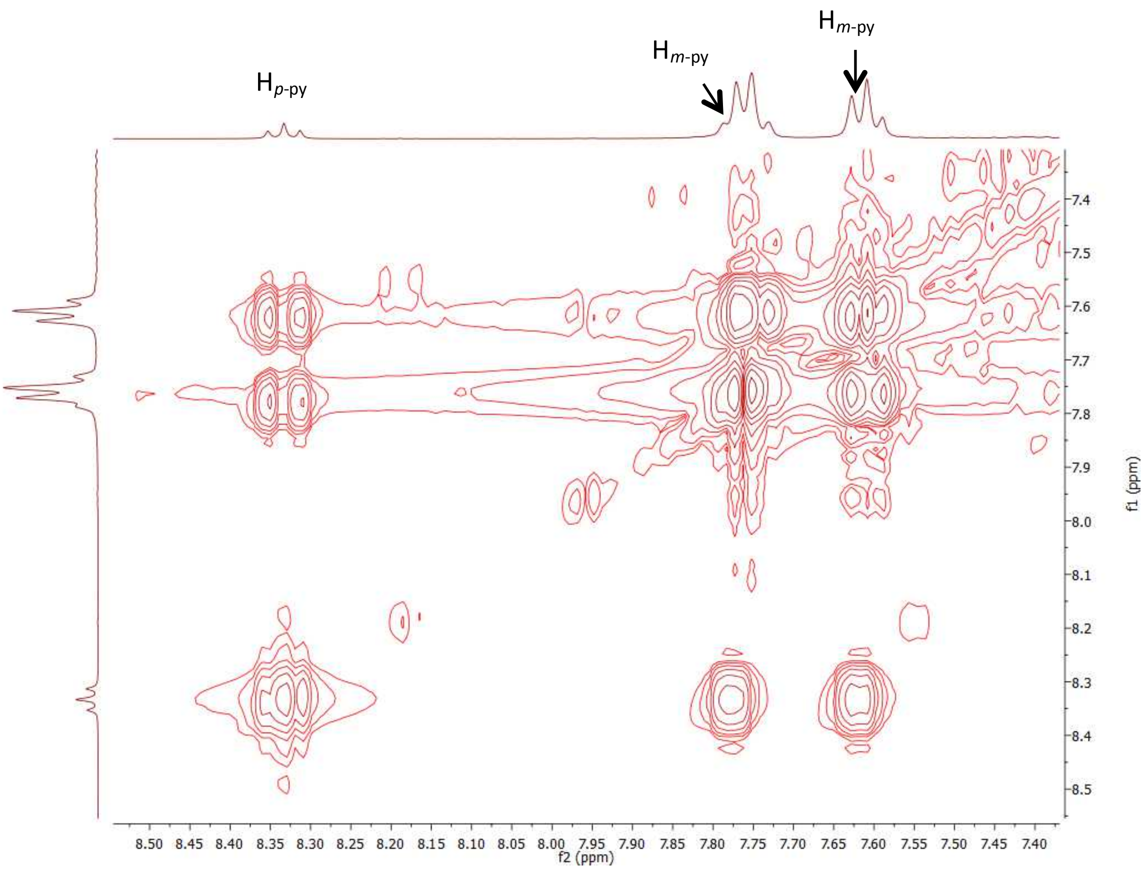


Figure S15. COSY [^{1}H,^{1}H] of **1$^+$-HBCF** (400 MHz, 20 °C) in CD_2Cl_2: zoom 2

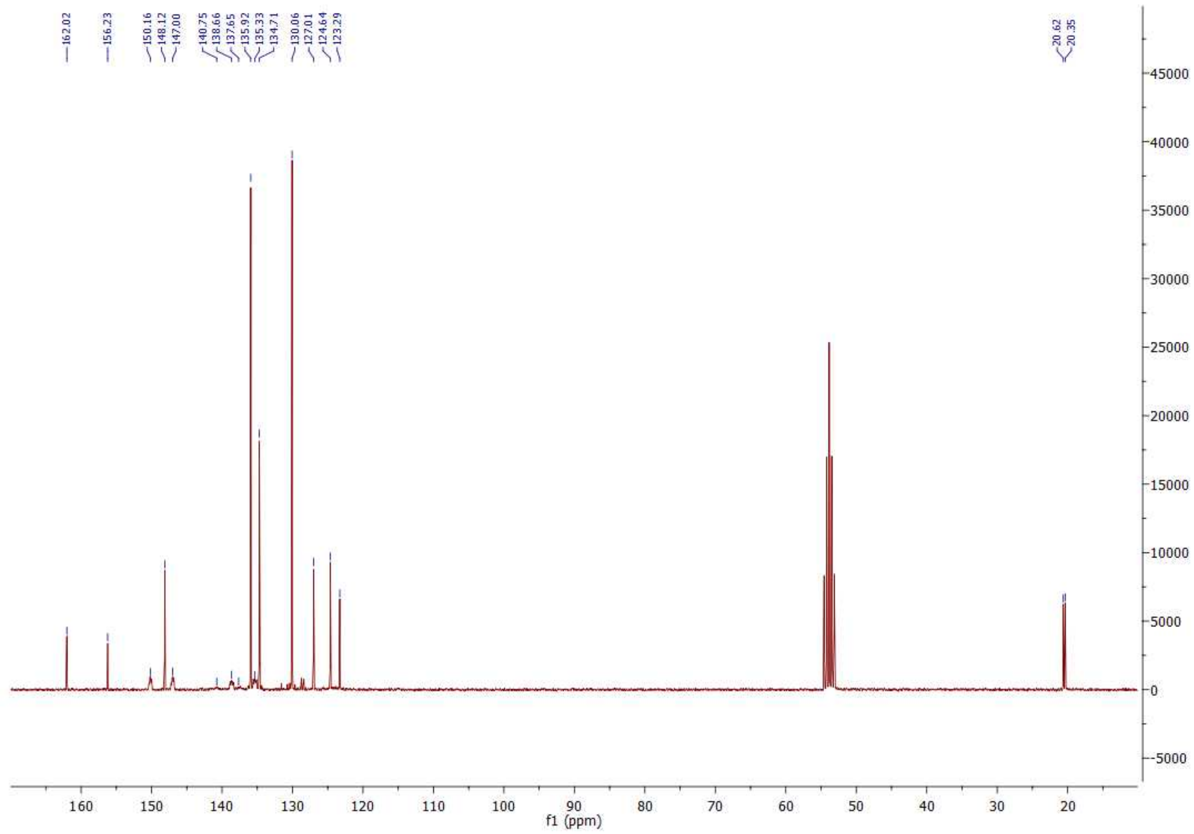


Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of **1^{+}-HBCF** (76 MHz, 20 °C) in CD_2Cl_2

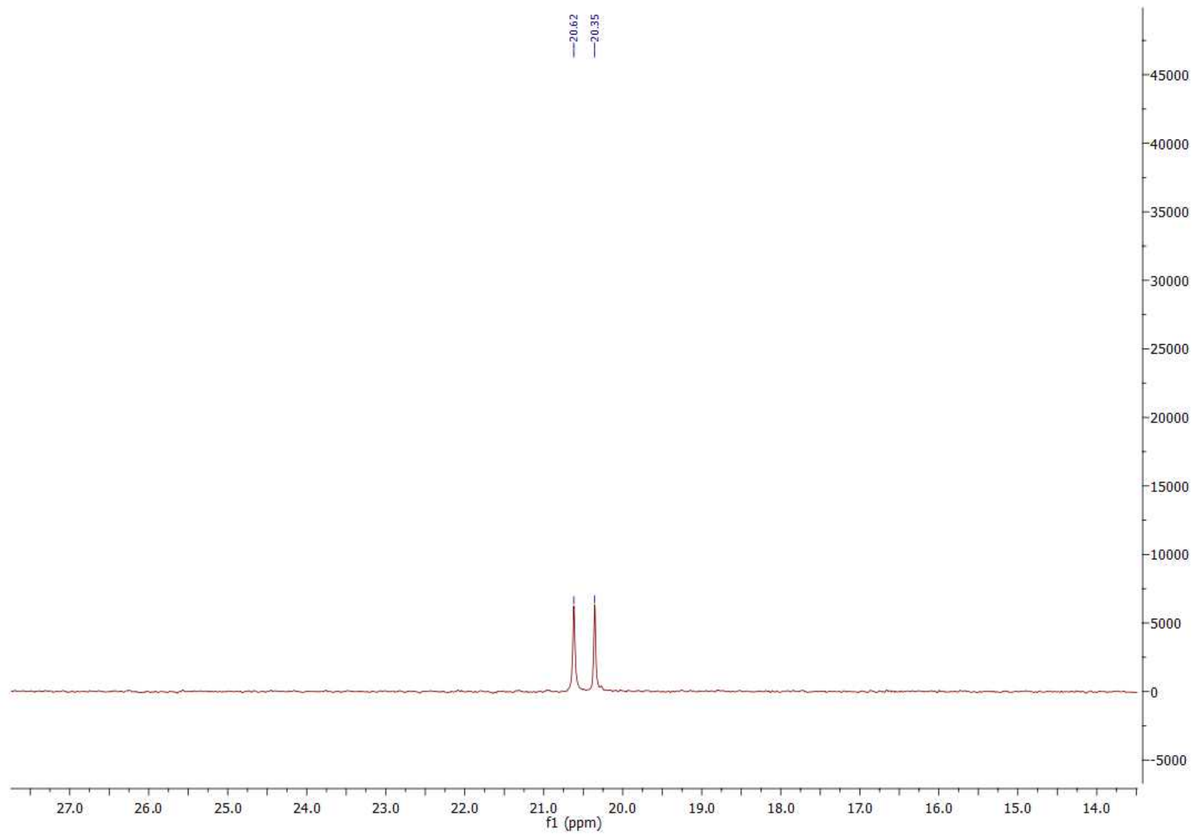


Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum of **1^{+}-HBCF** (76 MHz, 20 °C) in CD_2Cl_2: aliphatic region

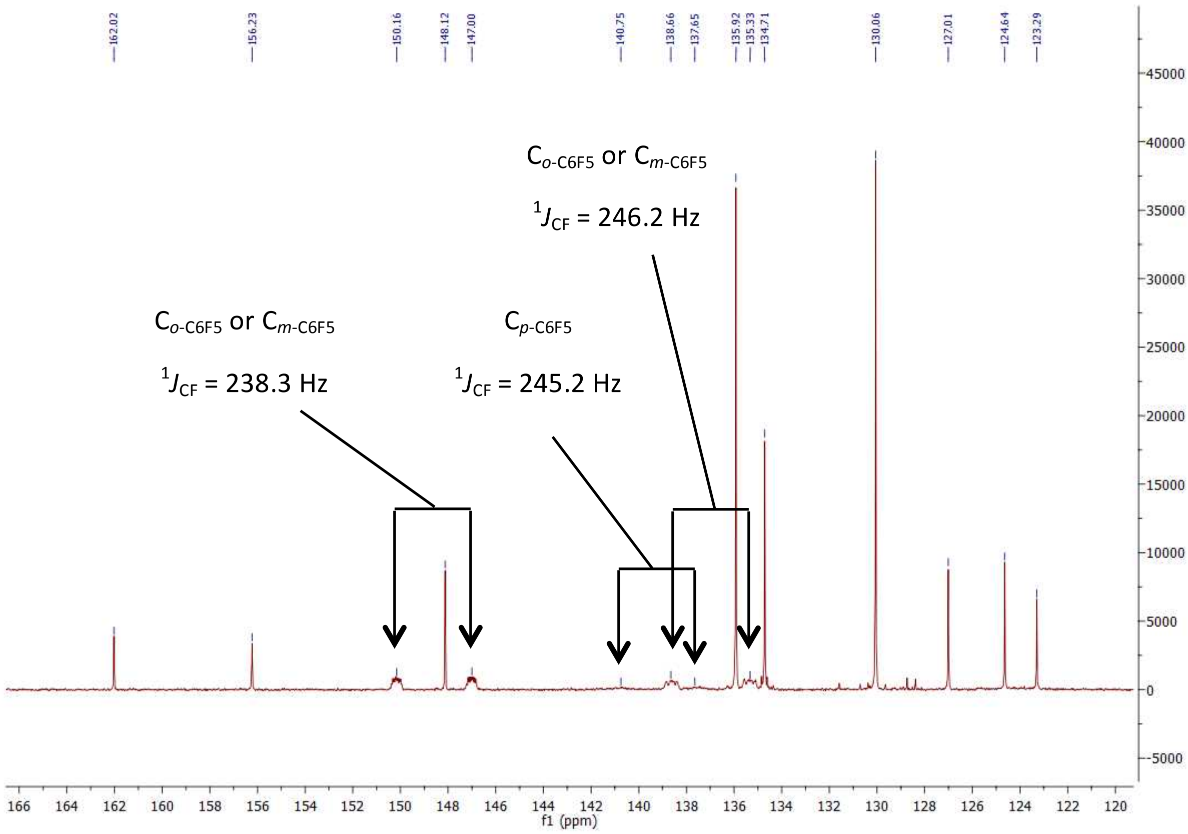


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of **1⁺-HBCF** (76 MHz, 20 °C) in CD_2Cl_2: aromatic region

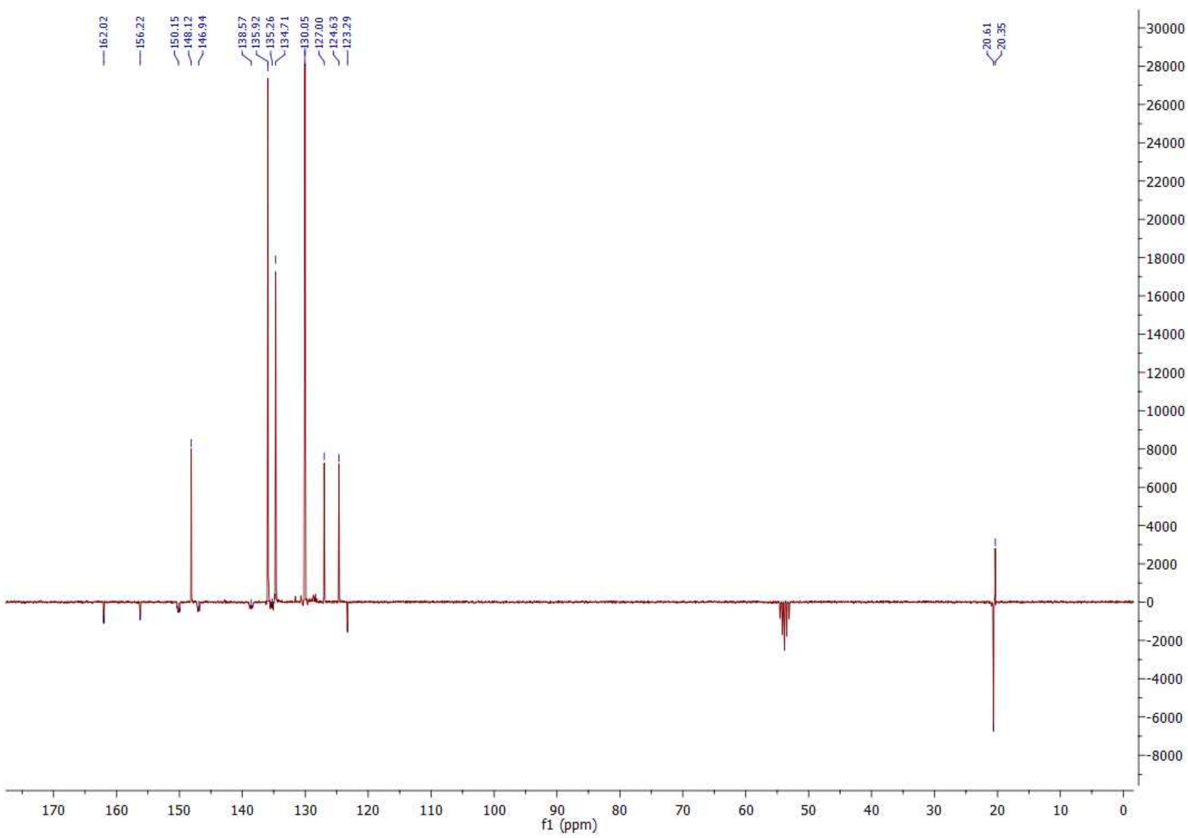


Figure S19. $^{13}C\{^{1}H\}$ jmod NMR spectrum of **1^+-HBCF** (76 MHz, 20 °C) in CD_2Cl_2

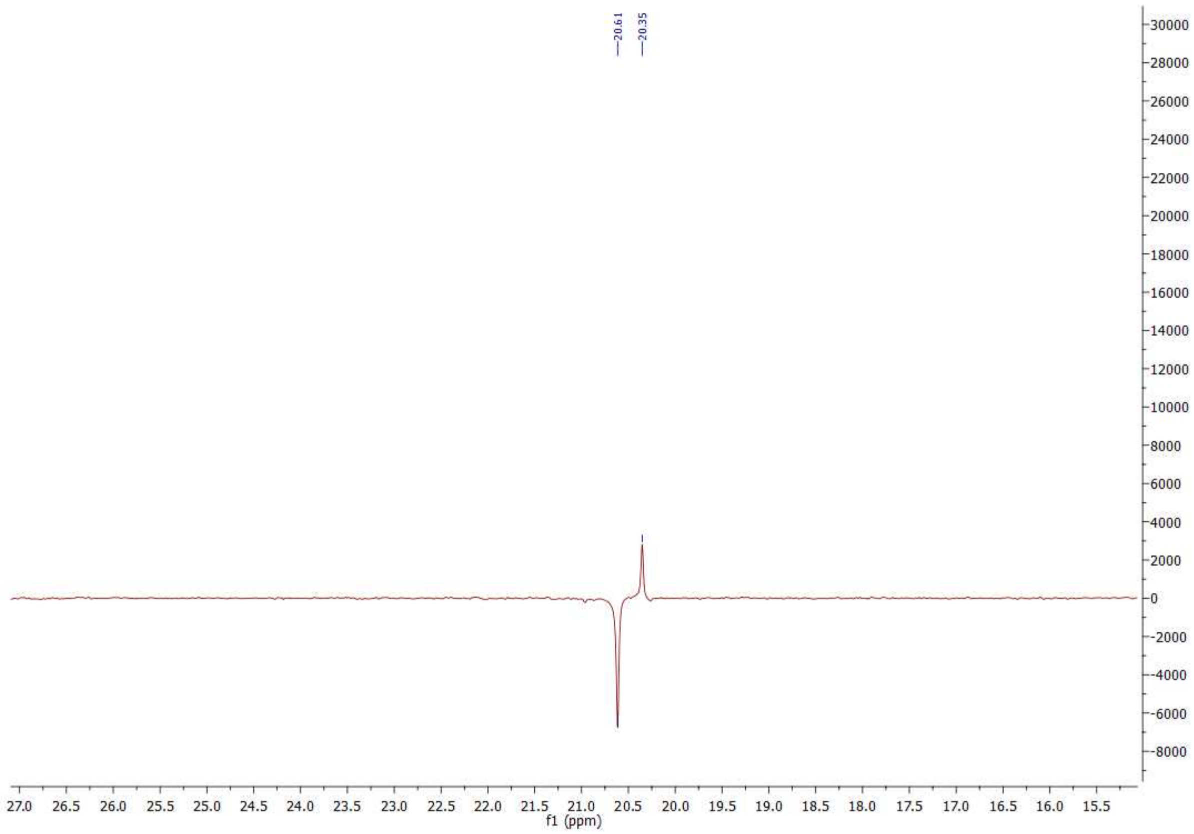


Figure S20. $^{13}C\{^{1}H\}$ jmod NMR spectrum of **1⁺-HBCF** (76 MHz, 20 °C) in CD_2Cl_2: aliphatic region

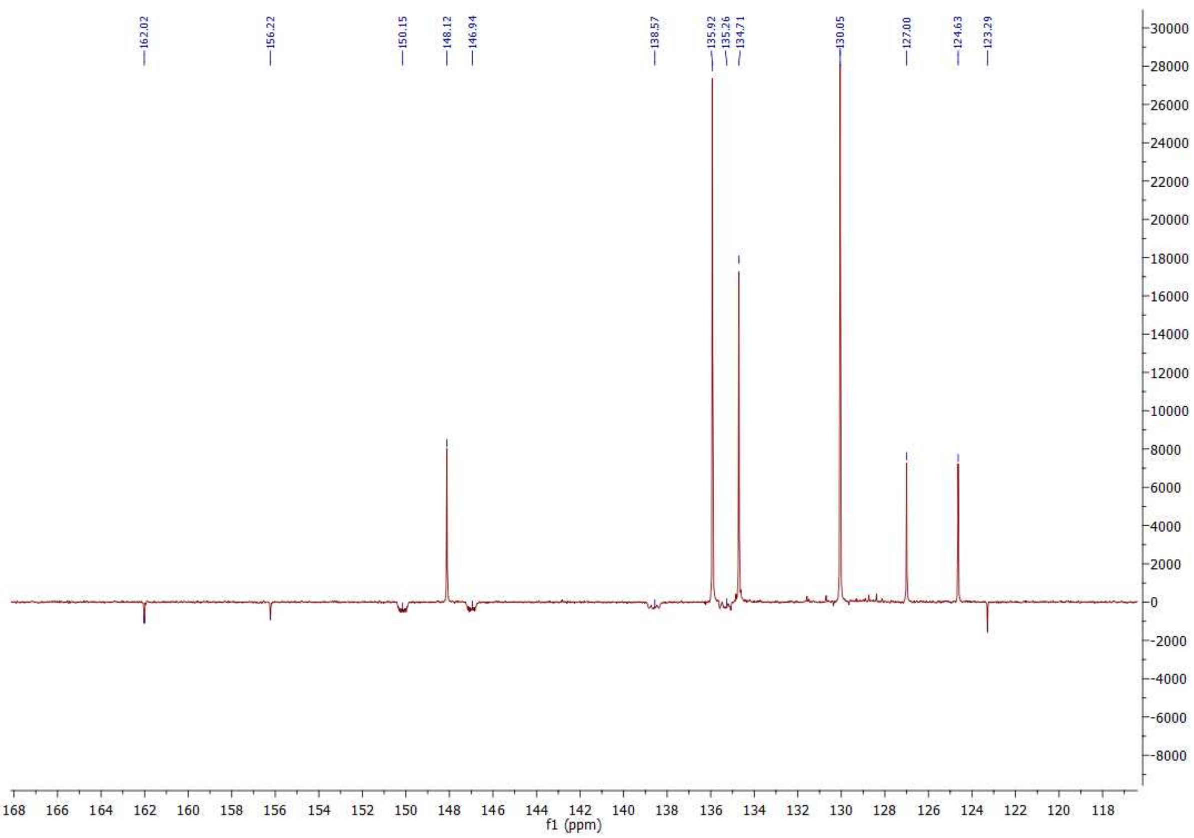


Figure S21. $^{13}C\{^{1}H\}$ jmod NMR spectrum of **1⁺-HBCF** (76 MHz, 20 °C) in CD_2Cl_2: aromatic region

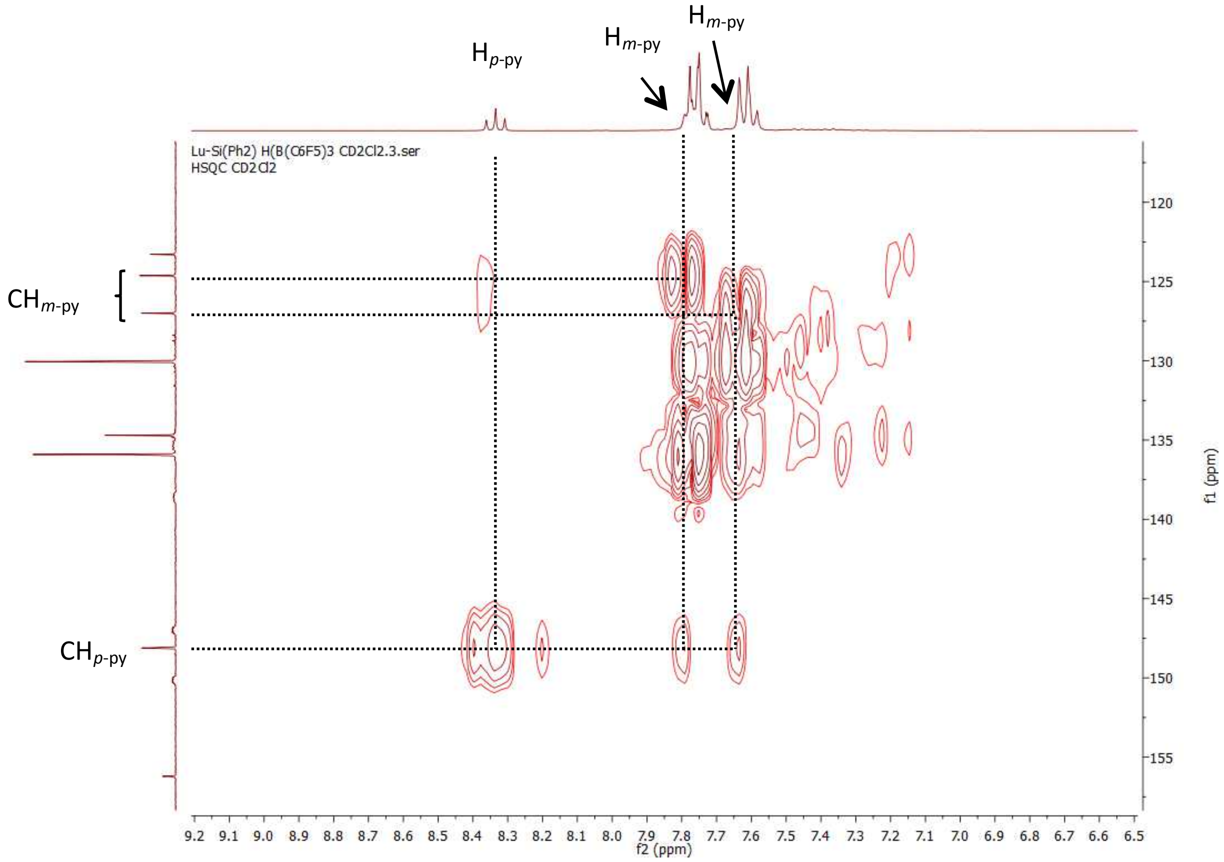


Figure S22. HSQC [^{13}C,^{1}H] NMR spectrum of **1$^+$-HBCF** (76 MHz, 20 °C) in CD_2Cl_2

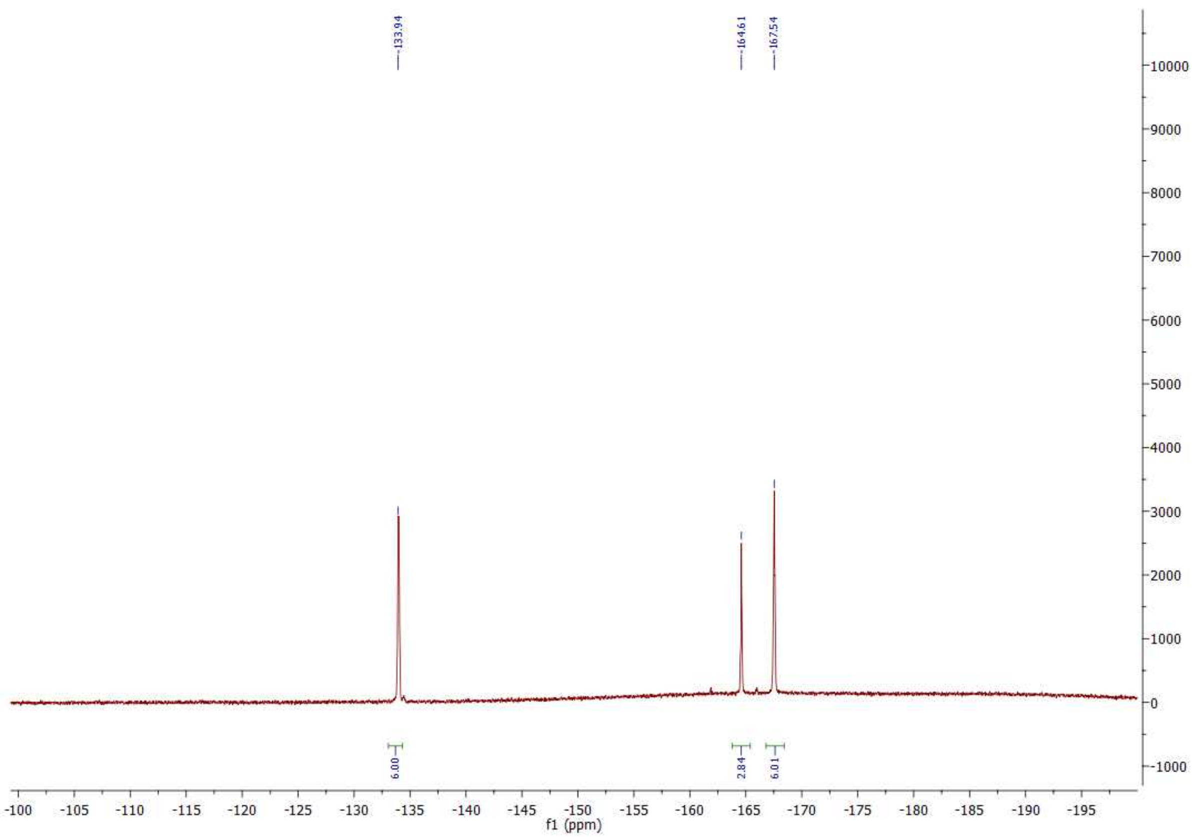


Figure S23. ^{19}F{^{1}H} NMR spectrum of **1$^+$-HBCF** (282 MHz, 20 °C) in CD_2Cl_2

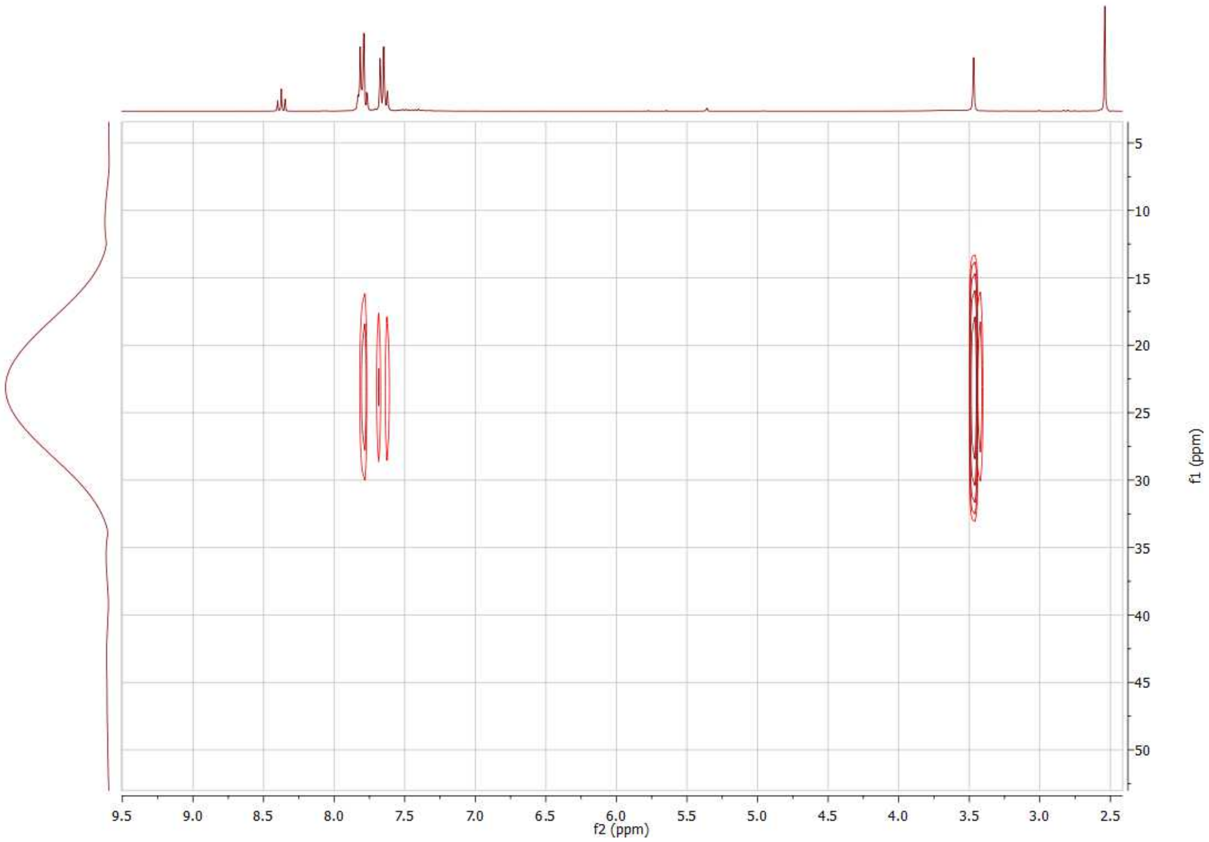
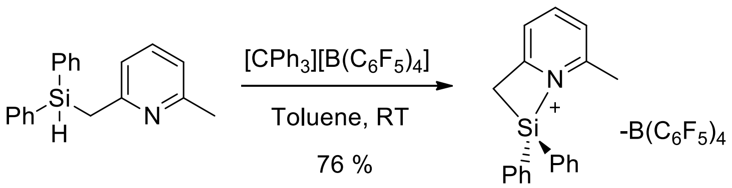


Figure S24. HSQC [^{29}Si,^{1}H] NMR spectrum of **1^{+}-HBCF** (60 MHz, 20 °C) in CD_2Cl_2

Synthesis of 1^{+}-BAr$^{F}_{4}$



Neat triphenylcarbenium tetrakis(pentafluorophenyl)borate (117 mg, 0.127 mmol, 0.95 eq.) was added at room temperature to a solution of **1^{H}** (37.5 mg, 0.129 mmol) in toluene (2 mL) in a Schlenk protected from light under stirring. After 10 minutes of stirring at room temperature, the cloudy yellowish reaction mixture was left to stand, leading to the formation of a yellowish oil and a colorless mother liquor. The mother liquor was removed via siringe and the precipitate was washed again with toluene (2.5 mL). The resulting oil was dried under reduced pressure for 2 hours (0.023 mbar) and **1^{+}-BAr$^{F}_{4}$** was obtained as a yellowish oil in a yield of 76%. The compound still contains toluene (**1^{+}-BAr$^{F}_{4}$** / toluene = 1 / 1.39); attempts to dry the sample for a prolonged period of time led to hydrolysis. HRMS (CSI, -43 °C): exact mass (monoisotopic) calcd for $[C_{19}H_{18}NSi]^{+}$, 288.1209; found 288.1218 and HRMS (ESI): exact mass (monoisotopic) calcd for $[C_{24}B_{1}F_{20}]^{-}$, 678.9778; found 678.9792.

^{1}H NMR (300 MHz, CD_2Cl_2, δ): 2.49 (s, 3H, CH_3), 3.41 (s, 2H, Si-CH_2), 3.57 (br., 1H, B-H), 7.57-7.67 (m, 5H, $4H_{Ph}$ and $1H_{m\text{-py}}$), 7.71-7.81 (m, 7H, $6H_{Ph}$ and $1H_{m\text{-py}}$), 8.33 (t, 1H, $CH_{p\text{-Py}}$).

^{13}C{^{1}H} NMR (76 MHz, CD_2Cl_2, δ): 20.4 (s, CH_3), 20.6 (s, Si-CH_2), 123.2 (s, Si-$C_{quat.}$), 124.6 (s, $CH_{m\text{-Py}}$), 127.0 (s, $CH_{m\text{-Py}}$), 130.1 (s, CH_{Ph}), 134.8 (s, $CH_{p\text{-Ph}}$), 135.9 (s, CH_{Ph}), 136.7 (d br., $^{1}J_{CF}$ = 249.7 Hz, C-$F_{o\text{-C6F5}}$ or C-$F_{m\text{-C6F5}}$), 138.6 (d br., $^{1}J_{CF}$ = 245.2 Hz, C-$F_{p\text{-C6F5}}$), 148.1 (s, $CH_{p\text{-Py}}$), 148.5 (br., $^{1}J_{CF}$ = 240.7 Hz, C-$F_{o\text{-C6F5}}$ or C-$F_{m\text{-C6F5}}$), 156.3 (s, $C_{o\text{-Py}}$), 162.0 (s, $C_{o\text{-Py}}$).

^{29}Si{^{1}H} NMR (60 MHz, CD_2Cl_2, δ): 23.2 (s).

^{11}B{^{1}H} NMR (96 MHz, CD_2Cl_2, δ): -16.7 (s).

^{19}F{^{1}H} NMR (282 MHz, CD_2Cl_2, δ): -167.4 (br., 8F, $F_{m\text{-C6F5}}$), -163.5 (t, 4F, $^{3}J_{FF}$ = 20.1 Hz, $F_{p\text{-C6F5}}$), -133.1 (br., 8F, $F_{o\text{-C6F5}}$).

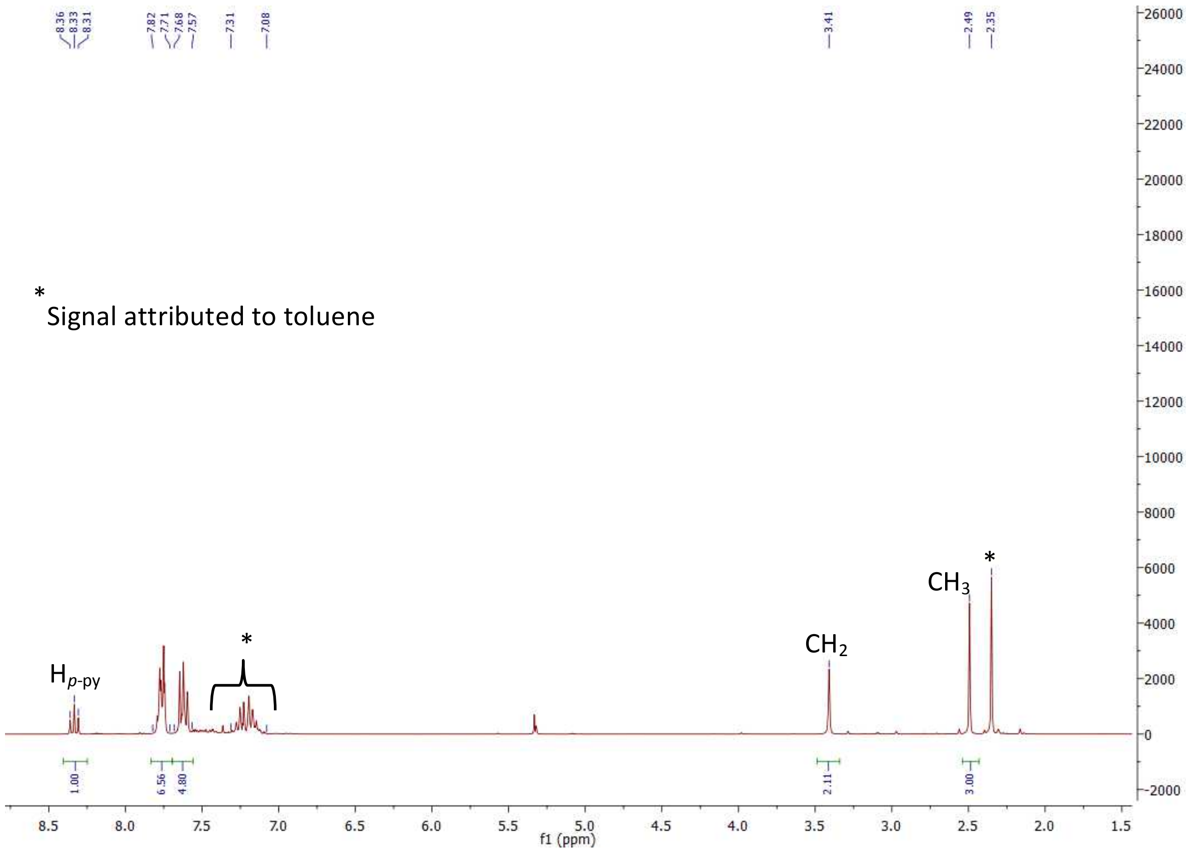


Figure S25. ^{1}H NMR spectrum of **1^{+}-BAr$^{F}_{4}$** (300 MHz, 20 °C) in CD_2Cl_2

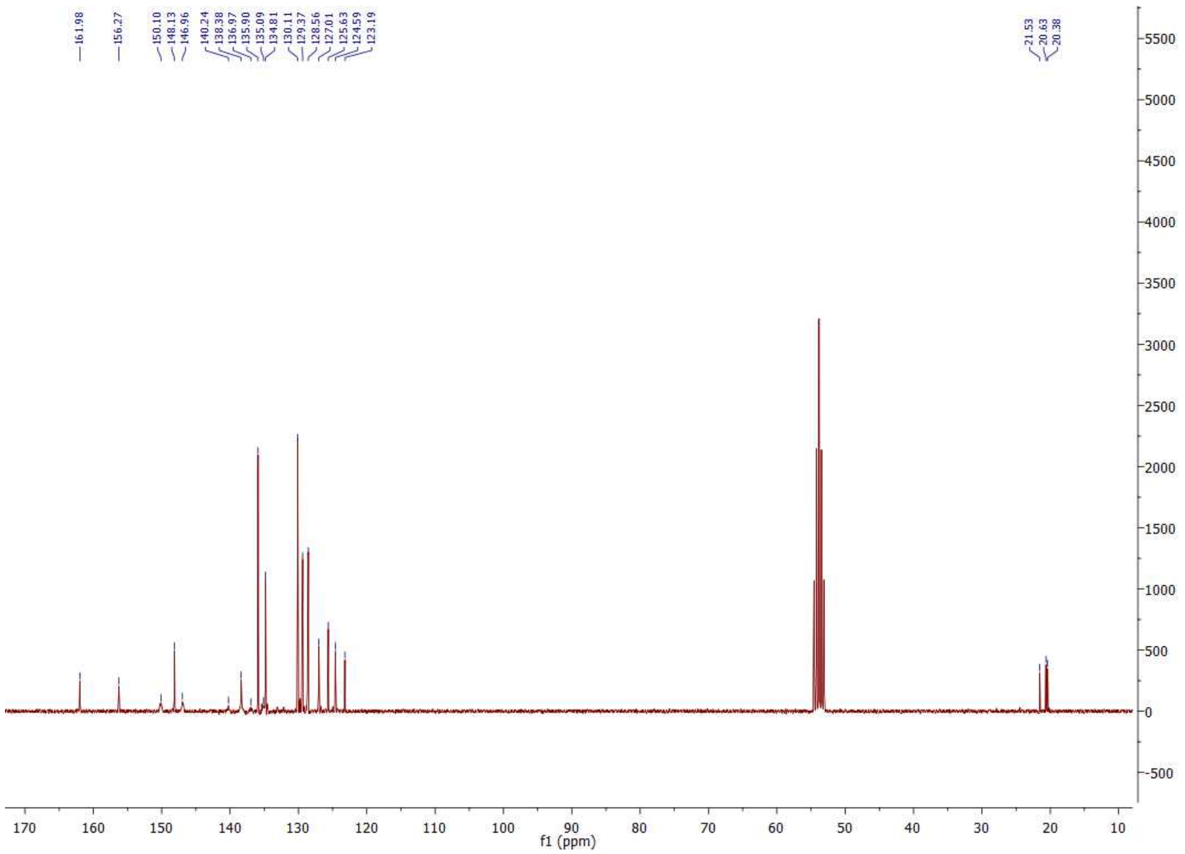


Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of **1^{+}-BAr$^{F}_{4}$** (76 MHz, 20 °C) in CD_2Cl_2

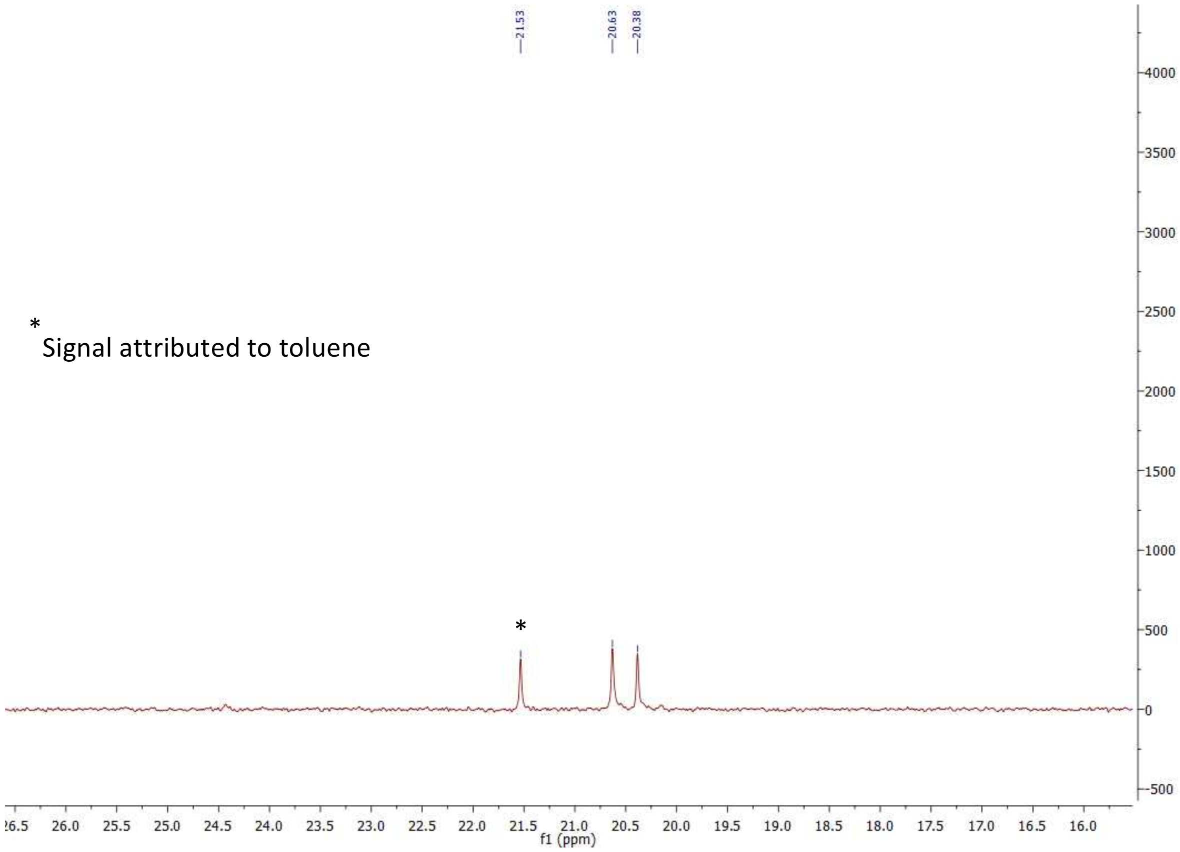


Figure S27. $^{13}C\{^{1}H\}$ NMR spectrum of **1^{+}-BAr$^{F}_{4}$** (76 MHz, 20 °C) in CD_2Cl_2: aliphatic region

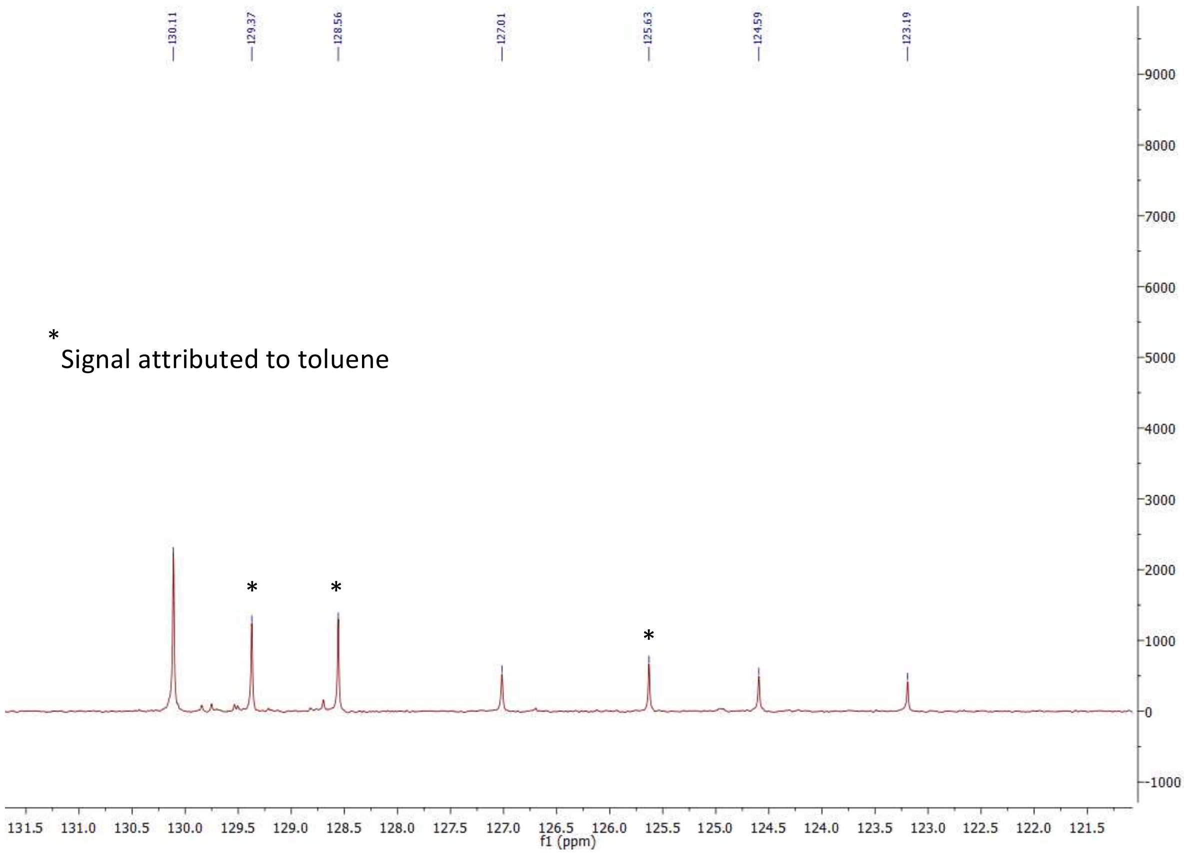


Figure S28. $^{13}C\{^{1}H\}$ NMR spectrum of **1^{+}-BAr$^{F}_{4}$** (76 MHz, 20 °C) in CD_2Cl_2: aromatic region 1

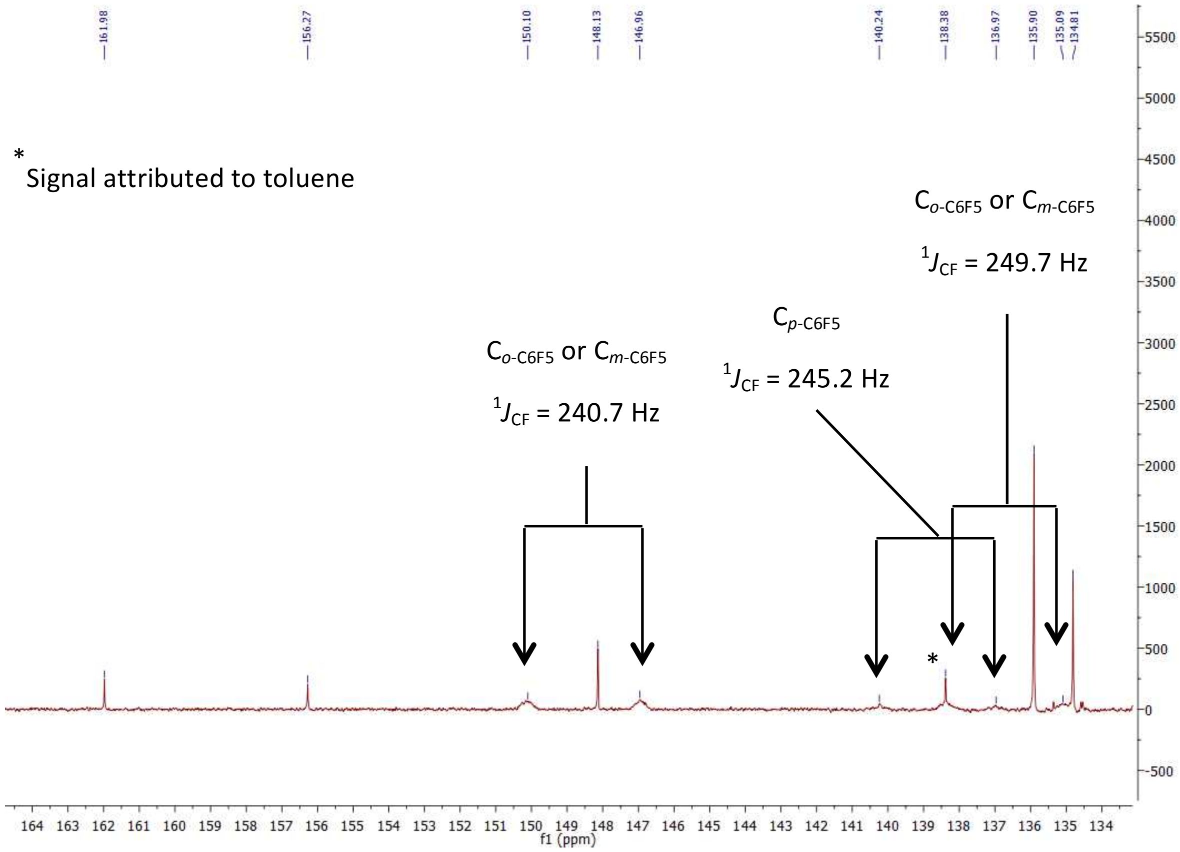


Figure S29. $^{13}C\{^{1}H\}$ NMR spectrum of $\mathbf{1^{+}\text{-}BAr^{F}_{4}}$ (76 MHz, 20 °C) in CD_2Cl_2: aromatic region 2

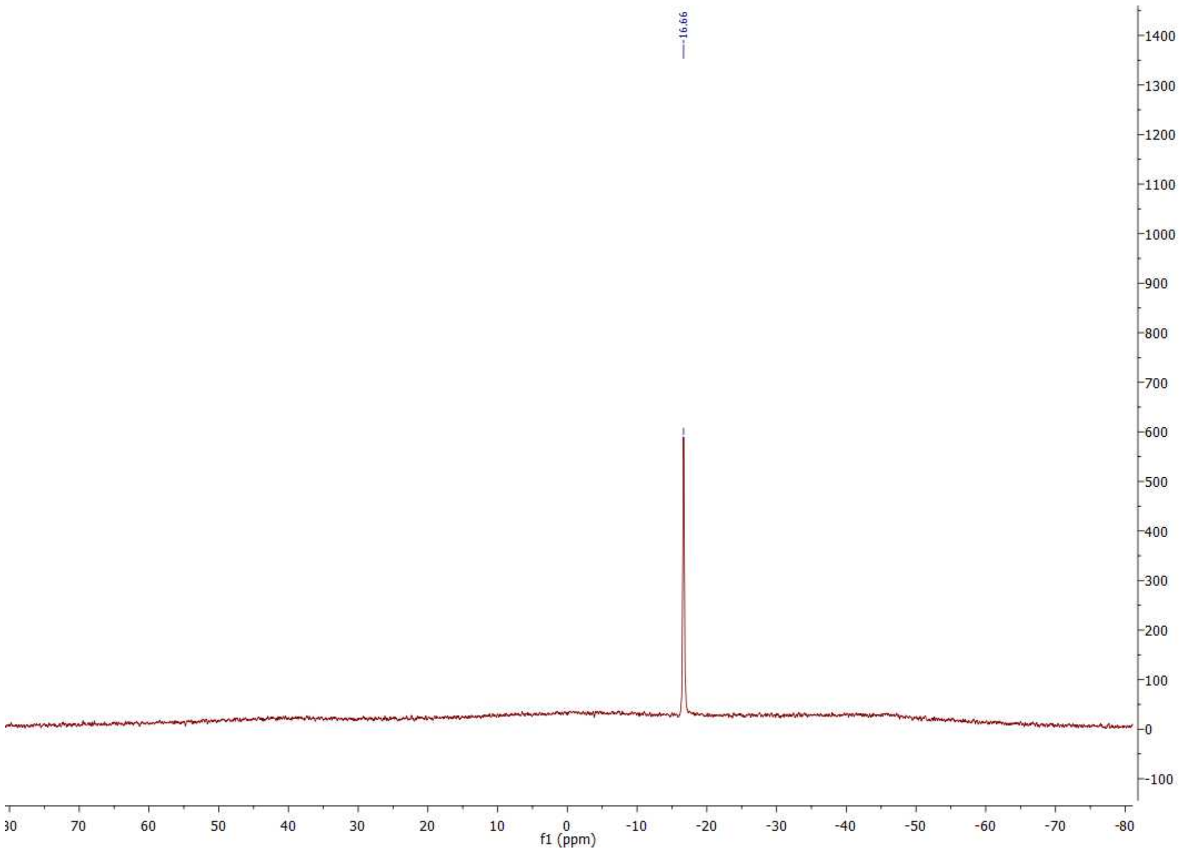


Figure S30. $^{11}B\{^{1}H\}$ NMR spectrum of $\mathbf{1^{+}\text{-}BAr^{F}_{4}}$ (96 MHz, 20 °C) in CD_2Cl_2: aromatic region 2

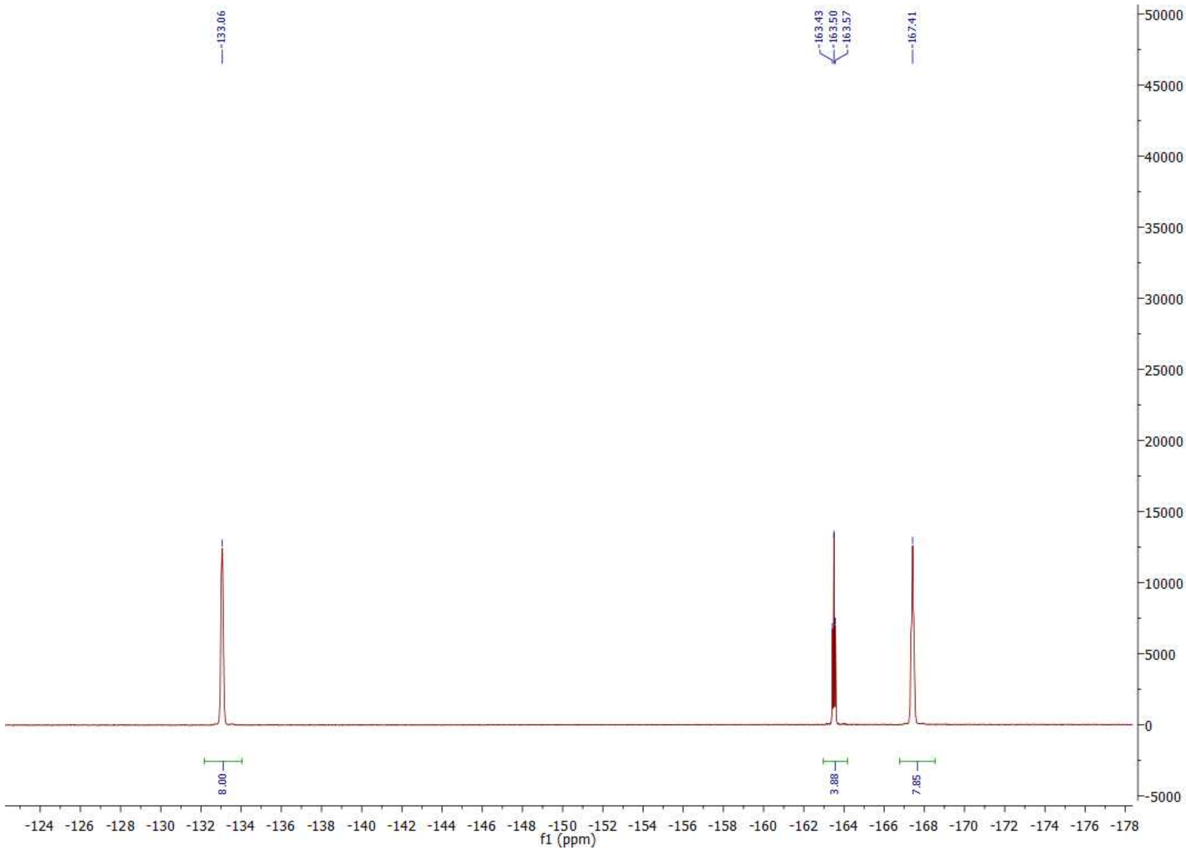


Figure S31. $^{19}F\{^{1}H\}$ NMR spectrum of **1^{+}-BAr$^{F}_{4}$** (282 MHz, 20 °C) in CD_2Cl_2

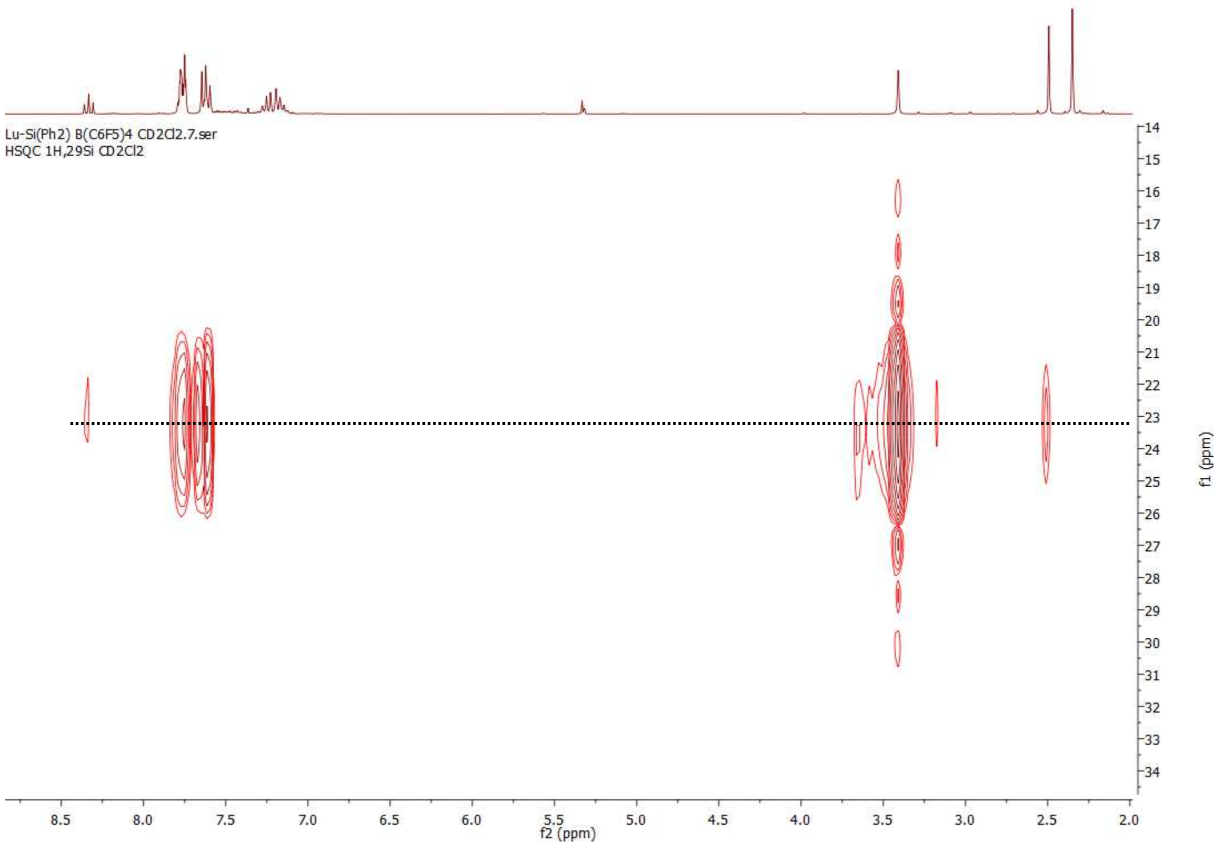
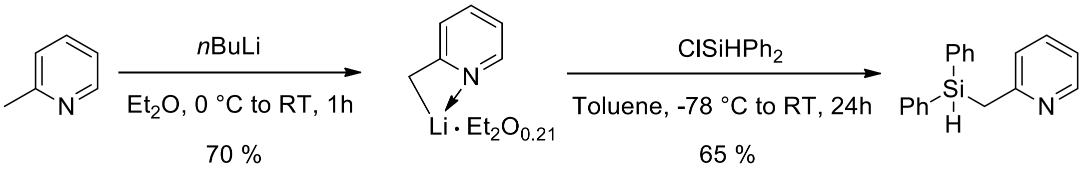


Figure S32. HSQC [^{29}Si,^{1}H] NMR spectrum of **1^{+}-BAr$^{F}_{4}$** (60 MHz, 20 °C) in CD_2Cl_2

Synthesis of 2^H



n-Butyl lithium in solution in hexanes (2.83 mL, 2.5 M, 1 eq.) was added dropwise to an ice-cold solution of 2-picoline (7.09 mmol, 0.70 mL) in diethylether (30 mL). The resulting solution was then allowed to warm up to room temperature and was further stirred for 1 hour at room temperature leading to an orange solution. The solution was then cooled down to -60 °C, leading to the precipitation of the lithiated species as an orange powder. The mother liquor was eliminated via syringe at -60 °C and the resulting solid was dried under vacuum at room temperature during 30 minutes. The analysis of the solid by ^{1}H NMR in THF-d_8 showed the presence of 0.21 molecule of diethylether per lithiated species (570 mg; 70%).

Chlorodiphenylsilane (0.98 mL, 5.03 mmol, 1.01 eq) in solution in toluene (10 mL) was then added dropwise to a stirred suspension of this lithiated species (570 mg, 4.98 mmol) in toluene (20 mL) cooled down to -78 °C. The reaction mixture was allowed to warm up slowly to room temperature overnight and was stirred for an additional 10 hours leading to a colorless solution and a white precipitate. After elimination of volatiles under vacuum, the residue was extracted with pentane (15 mL) and filtered. The pentane solution was concentrated to saturation and then cooled down slowly to -30 °C leading to the crystallization of the expected compound in 65% yield. The crystals liquefy slowly at room temperature giving a colorless oil.

^{1}H NMR (300 MHz, CD_2Cl_2, δ): 2.95 (d, 2H, $^3J_{HH}$ = 3.8 Hz, Si-CH$_2$), 5.02 (m, 1H, $^1J_{HSi}$ = 201.3 Hz, Si-H), 6.93-7.03 (m, 2H, $H_{m\text{-Py}}$), 7.29-7.99 (m, 11H, $H_{arom.}$), 8.37-8.45 (m, 1H, $H_{arom.}$).

^{13}C{^{1}H} NMR (76 MHz, CD_2Cl_2, δ): 25.9 (s, 1C, CH$_2$), 120.2 (s, 1C, $CH_{m\text{-Py}}$), 123.3 (s, 1C, $CH_{m\text{-Py}}$), 128.3 (s, 4C, CH_{Ph}), 130.1 (s, 2C, $CH_{p\text{-Ph}}$), 134.0 (s, 2C, Si-$C_{quat.}$), 135.6 (s, 4C, CH_{Ph}), 136.3 (s, 1C, $CH_{p\text{-Py}}$), 145.9 (s, 1C, $CH_{o\text{-Py}}$), 160.1 (s, 1C, $C_{o\text{-Py}}$).

^{29}Si{^{1}H} NMR (60 MHz, CD_2Cl_2, δ): -14.5 (s).

HRMS (CSI, -40 °C): exact mass (monoisotopic) calcd for $[C_{18}H_{16}NSi+H]^+$, 276.1209; found 276.1206.

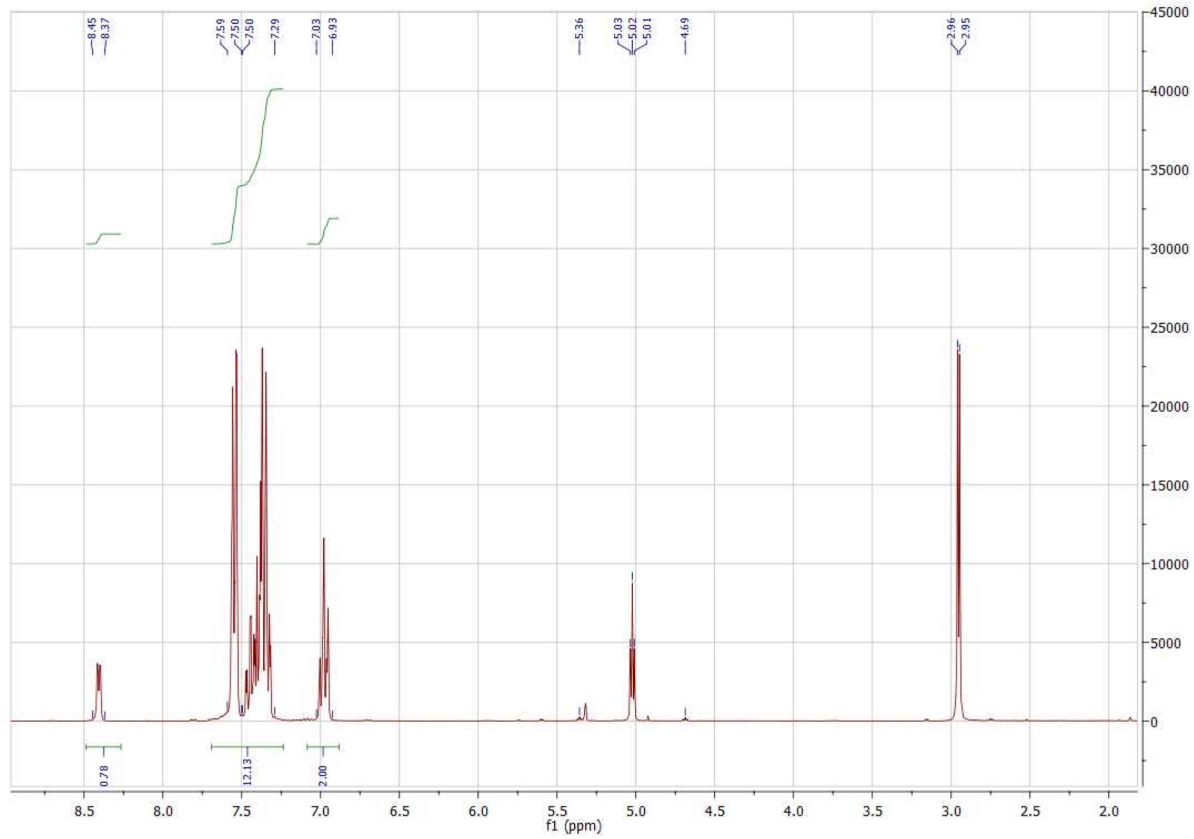


Figure S33. ^{1}H NMR spectrum of $\mathbf{2^{H}}$ (300 MHz, 20 °C) in CD_2Cl_2

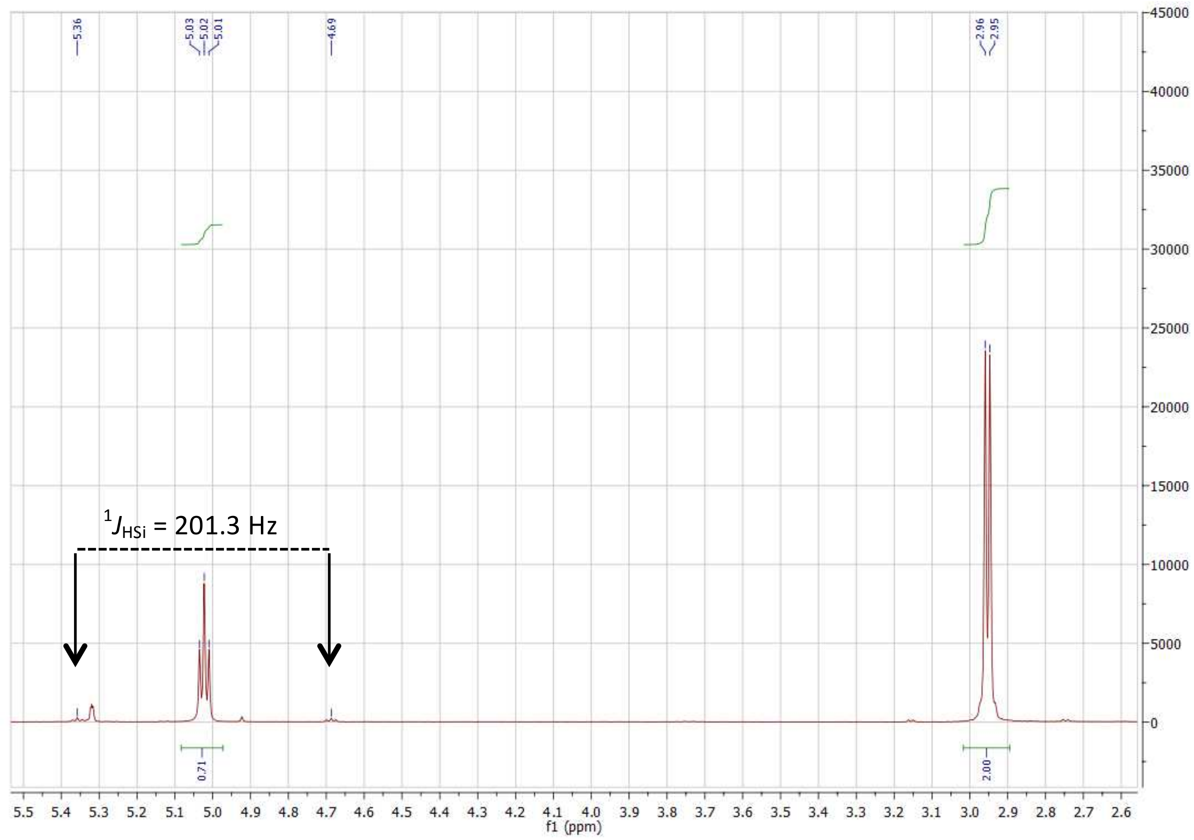


Figure S34. ^{1}H NMR spectrum of $\mathbf{2^{H}}$ (300 MHz, 20 °C) in CD_2Cl_2: aliphatic region

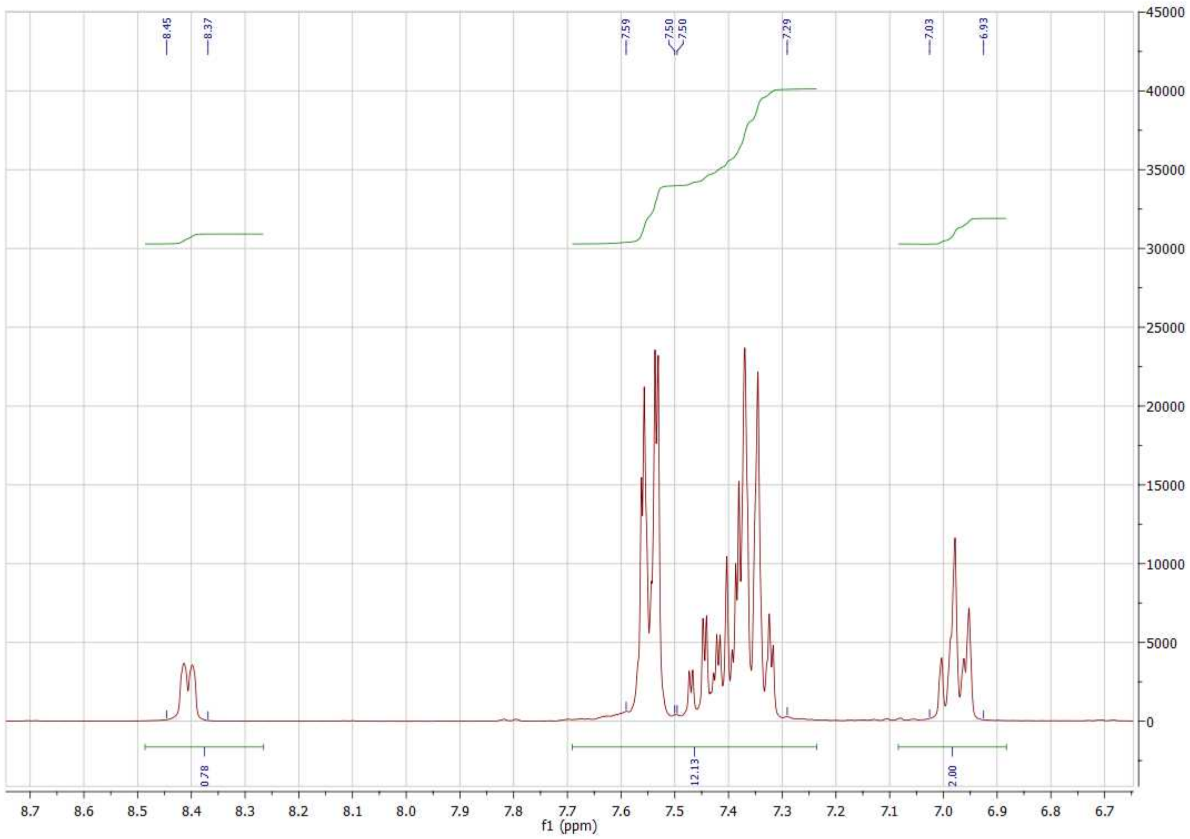


Figure S35. ^{1}H NMR spectrum of **2^{H}** (300 MHz, 20 °C) in CD_2Cl_2: aromatic region

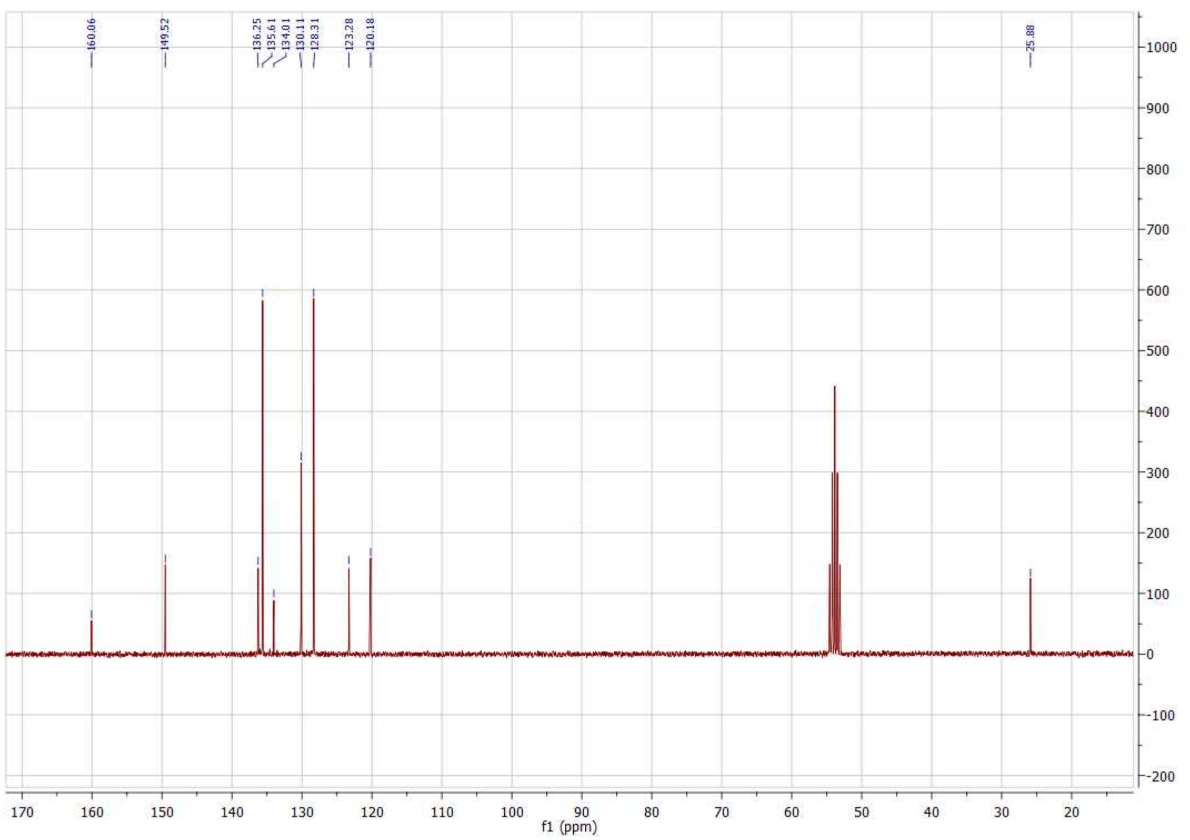


Figure S36. $^{13}C\{^{1}H\}$ NMR spectrum of **2^{H}** (76 MHz, 20 °C) in CD_2Cl_2

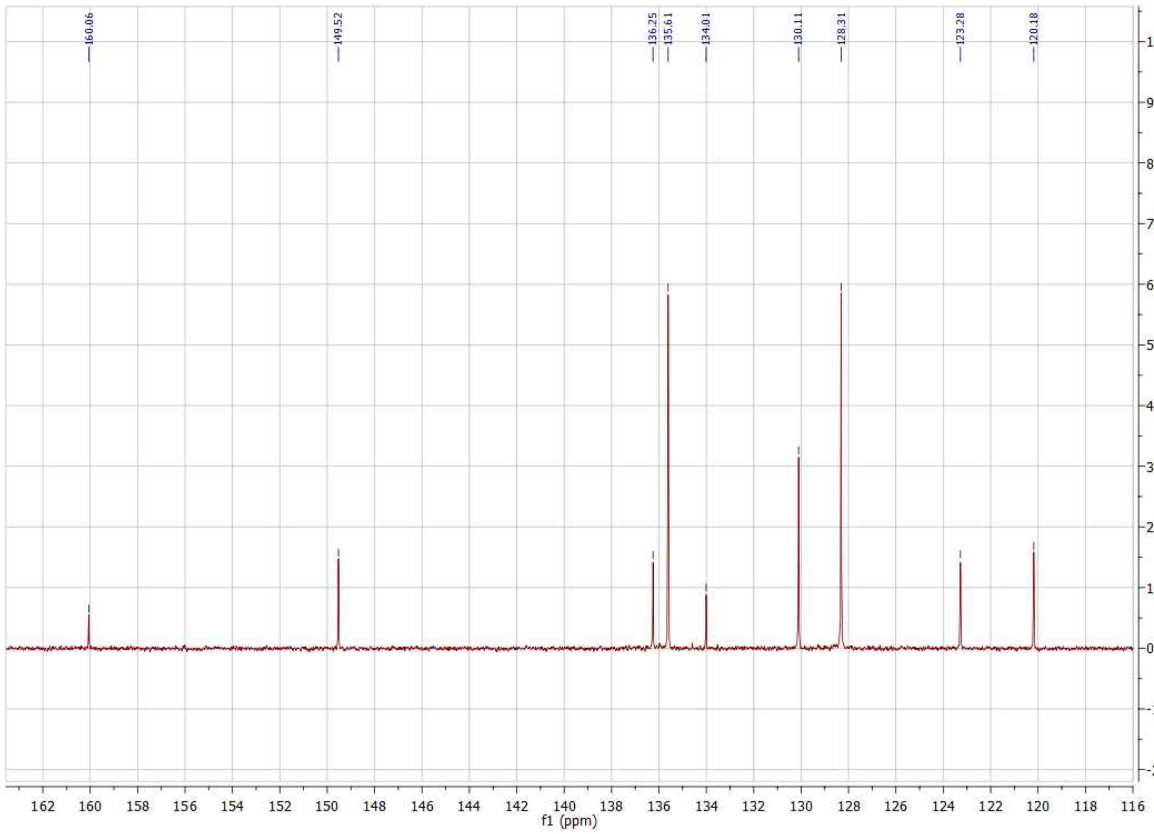


Figure S37. $^{13}C\{^{1}H\}$ NMR spectrum of $\mathbf{2^H}$ (76 MHz, 20 °C) in CD_2Cl_2: aromatic region

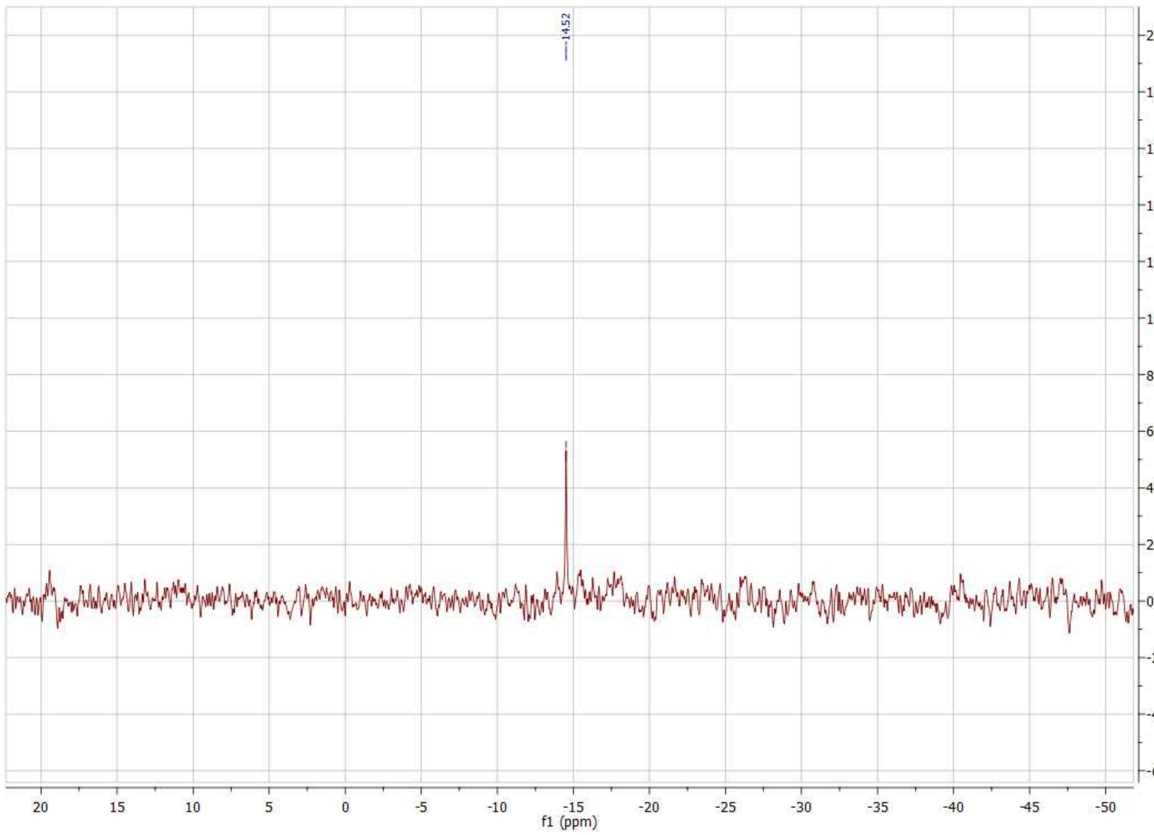
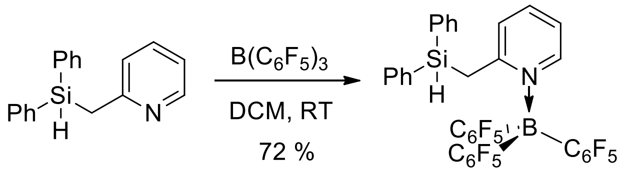


Figure S38. $^{29}Si\{^{1}H\}$ DEPT NMR spectrum of $\mathbf{2^H}$ (60 MHz, 20 °C) in CD_2Cl_2

Synthesis of 2^H-BCF



Tris(pentafluorophenyl)borane (356.9 mg, 0.70 mmol, 1 eq.) in solution in dichloromethane (1 mL) was added at room temperature to a solution of $\mathbf{2^H}$ (192 mg, 0.70 mmol) in dichloromethane (3 mL). After 5 minutes of stirring, the solvent was removed under reduced pressure and the residue was solubilized in toluene (2 mL). Slow concentration of this solution at room temperature led to the formation of a crystalline precipitate. After elimination of the mother liquor, the crystalline solid was solubilized in a mixture of DCM / pentane (3 mL / 11 mL) and the resulting colorless solution was concentrated under reduced pressure leading to the formation of colorless crystals at room temperature in 72% yield. Crystals suitable for X-ray diffraction analysis were obtained from a saturated toluene solution at room temperature.

^{1}H NMR (300 MHz, CD_2Cl_2, δ): 3.30 (s, 2H, Si-CH_2), 3.95 (s, 1H, $^1J_{HSi}$ = 205.4 Hz, Si-H), 7.08 (d, 1H, $^3J_{HH}$ = 8.0 Hz, $H_{arom.}$), 7.23-7.51 (m, 11H, $H_{arom.}$), 7.83 (pseudo-t,* 1H, $^3J_{HH}$ = 7.5 Hz, $H_{arom.}$), 8.66 (m, 1H, $H_{arom.}$).

$^{13}C\{^1H\}$ NMR (76 MHz, CD_2Cl_2, δ): 23.6 (s br., 1C, CH_2), 121.7 (s, 1C, CH_{Py}), 128.3 (s, 1C, CH_{Py}), 128.8 (s, 2C, CH_{Ph}), 128.8 (s, 2C, CH_{Ph}), 130.9 (s, 1C, CH_{Ph}), 131.1 (s, 1C, CH_{Ph}), 131.7 (s, 1C, Si-$C_{quat.}$), 131.8 (s, 1C, Si-$C_{quat.}$), 134.7 (s, 2C, CH_{Ph}), 135.5 (s, 2C, CH_{Ph}), 141.8 (s, 1C, CH_{Py}), 148.2 (m, 1C, CH_{Py}), 162.3 (d, 1C, $^5J_{CF}$ = 4.3 Hz, $C_{o\text{-}Py}$), no signals were observed for the C-F carbons.

$^{11}B\{^1H\}$ NMR (96 MHz, CD_2Cl_2, δ): -3.5.

$^{29}Si\{^1H\}$ NMR (60 MHz, CD_2Cl_2, δ): -15.9 (s).

$^{19}F\{^1H\}$ NMR (282 MHz, CD_2Cl_2, δ): -125.8 (m, 1F), -128.7 (m, 1F), -132.2 (m, 1F), -132.7 (m, 1F), -133.4 (m, 1F), -136.3 (m, 1F), -156.6 (pseudo-t, 1F, $^3J_{FF}$ = 21.7 Hz), -156.8 (pseudo-t, 1F, $^3J_{FF}$ = 20.9 Hz), -158.7 (pseudo-t, 1F, $^3J_{FF}$ = 20.2 Hz), -162.8 (m, 1F), -163.3 (m, 1F), -163.7 (m, 1F), -164.4 (m, 1F), -164.7 (m, 2F).

Anal. Calcd. For $C_{36}H_{17}BF_{15}NSi$; C, 54.91; H, 2.18; N, 1.78. Found: C, 55.17; H, 2.13; N, 1.77.

* we have opted to describe this signal as a 'pseudo-triplet', although 'apparent triplet' is an alternative assignment, to distinguish the situation of chemical equivalency and chemical inequivalency in the coupling and brings accuracy in the relationship between structure and NMR pattern

For references, see:

K. Gholivand, Z. Shariatinia, Z. Ahmadian Tabasi, A. Tadjarodi, *Heteroatom Chem.* **2006***, 17*, 337

T. R. Hoye, P. R. Hanson, J. R. Vyvyan, *J. Org. Chem.* **1994**, *59*, 4096

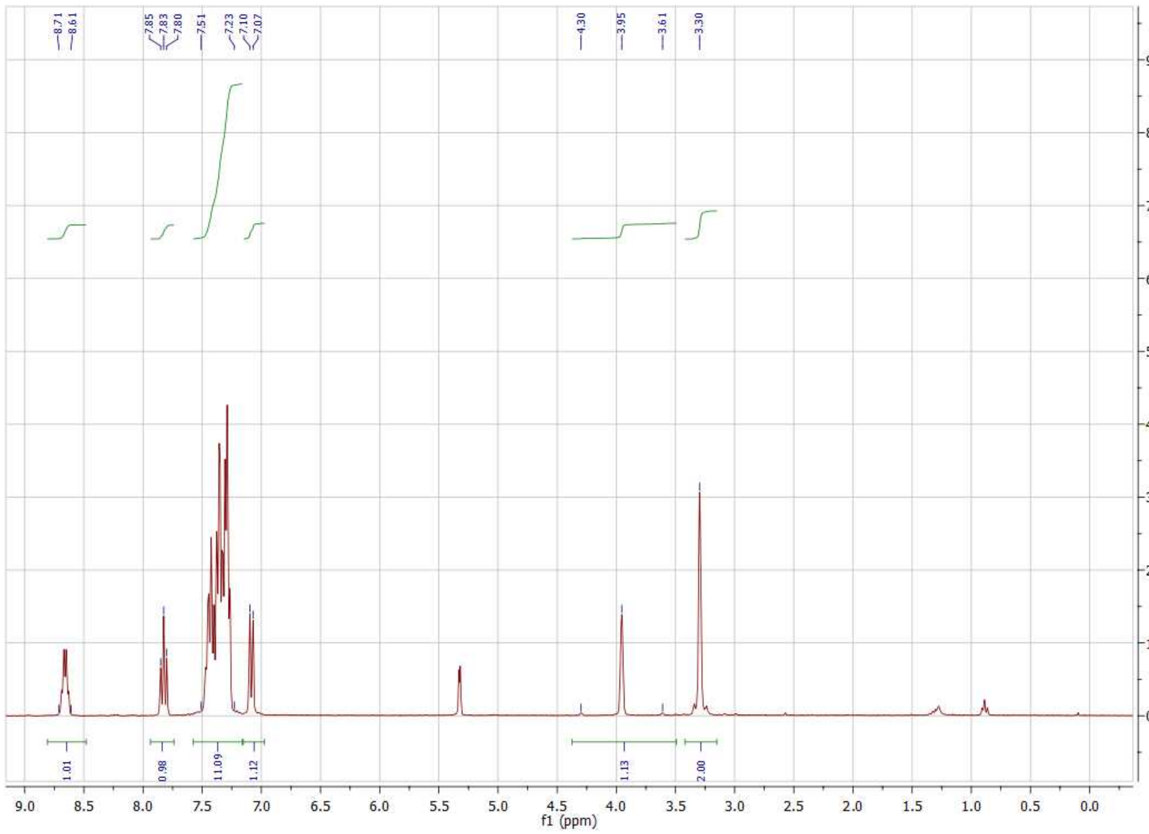


Figure S39. ^{1}H NMR spectrum of **2^{H}-BCF** (300 MHz, 20 °C) in CD_2Cl_2

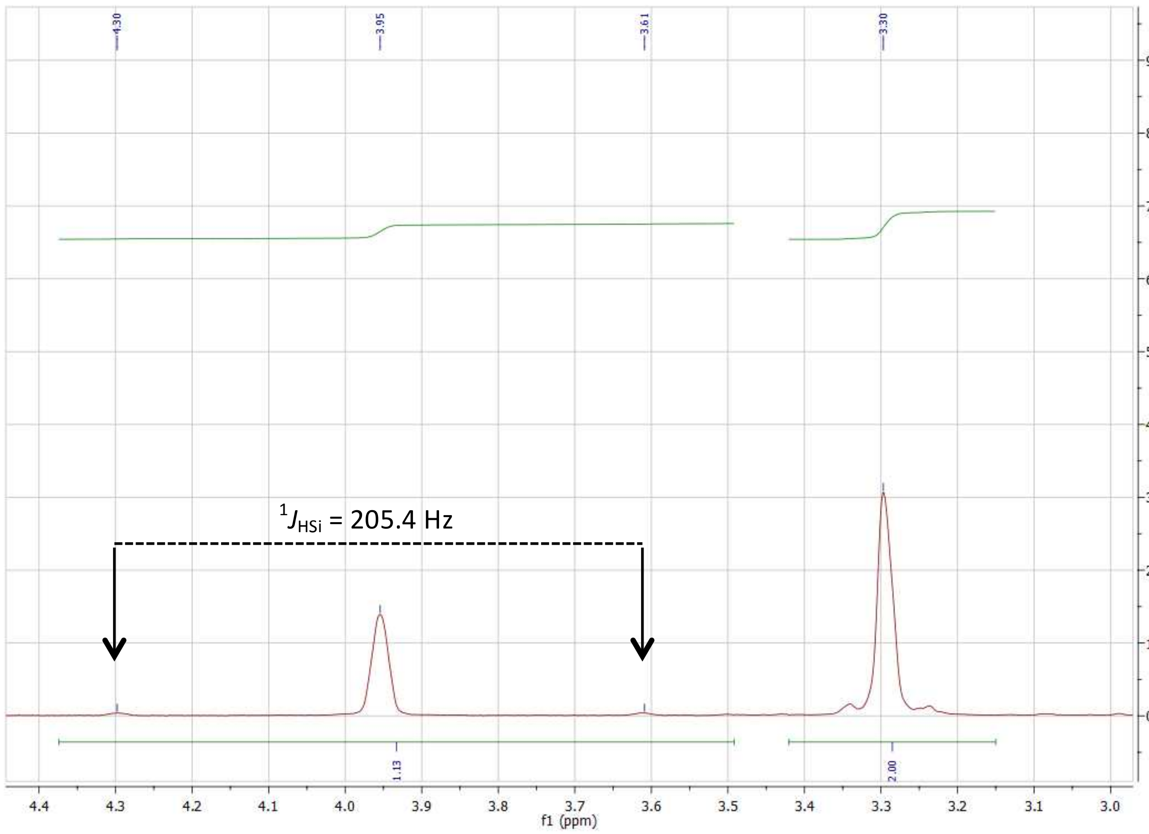


Figure S40. ^{1}H NMR spectrum of **2^{H}-BCF** (300 MHz, 20 °C) in CD_2Cl_2: aliphatic region

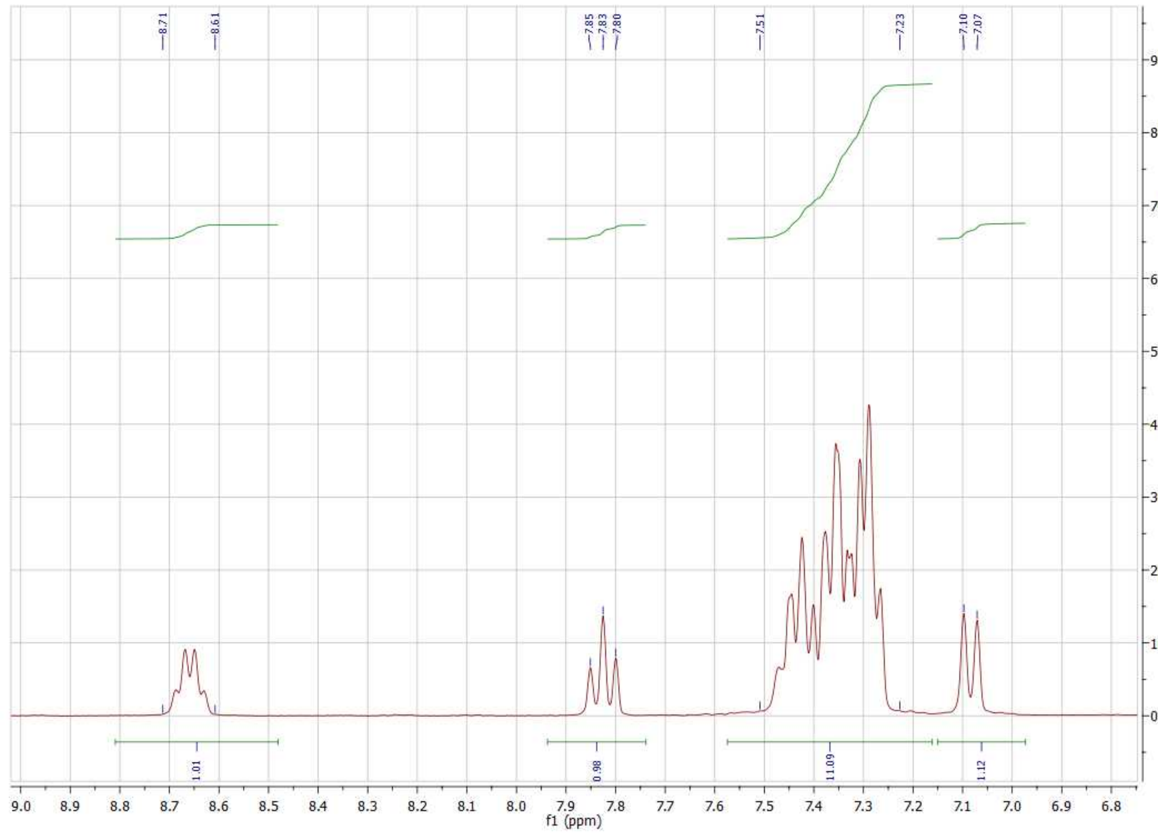


Figure S41. ^{1}H NMR spectrum of **2^H-BCF** (300 MHz, 20 °C) in CD_2Cl_2: aromatic region

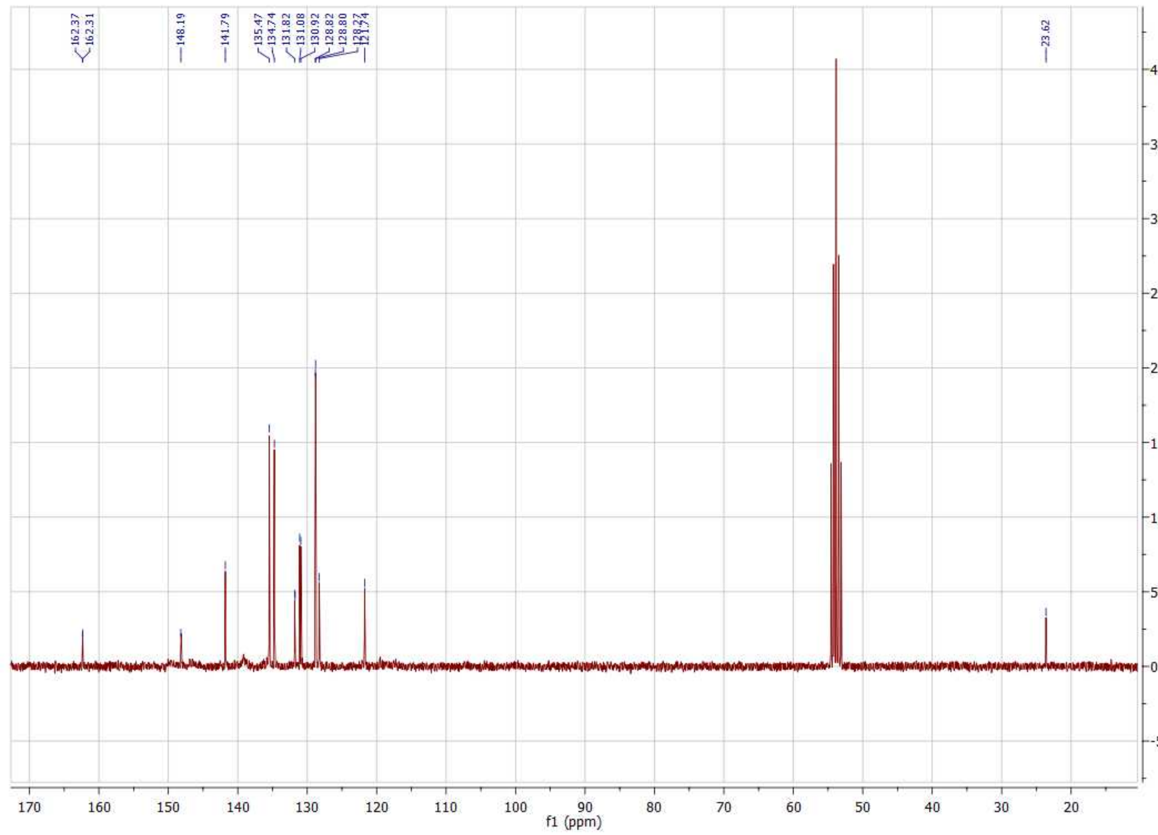


Figure S42. $^{13}C\{^{1}H\}$ NMR spectrum of **2^H-BCF** (76 MHz, 20 °C) in CD_2Cl_2

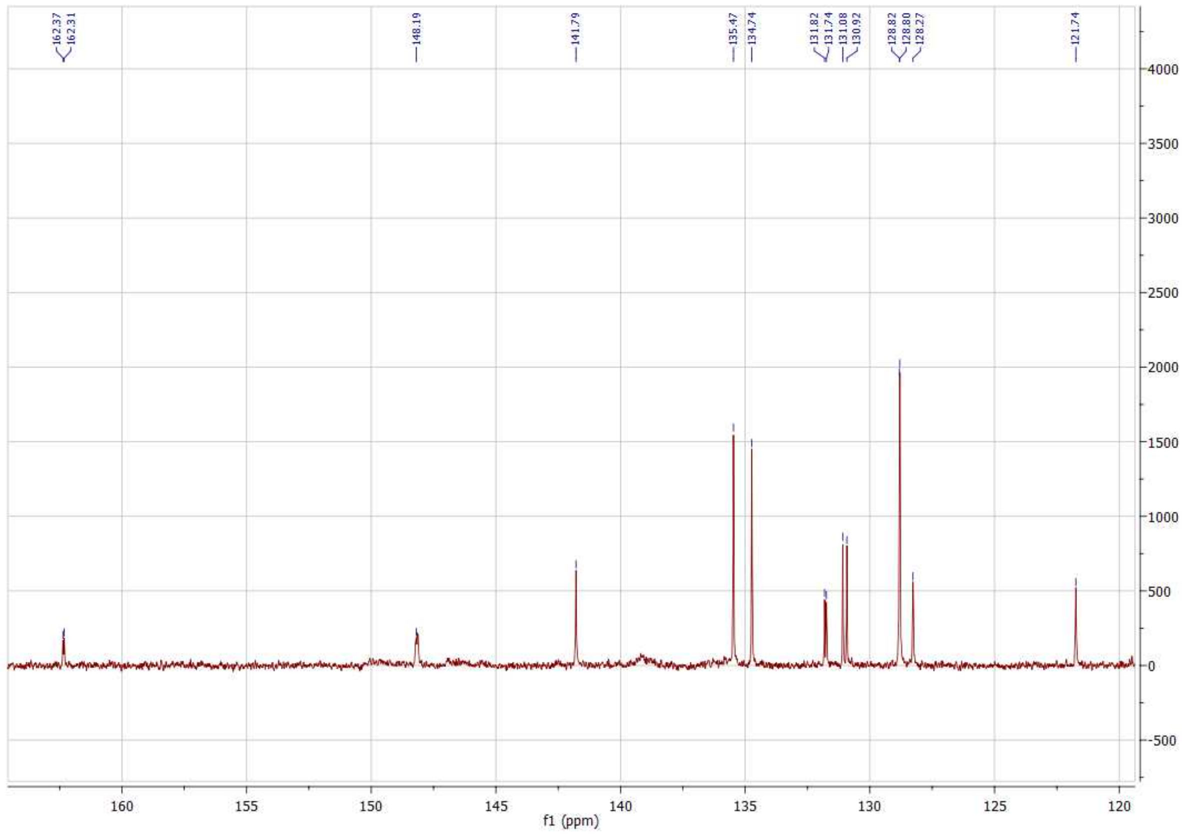


Figure S43. $^{13}C\{^1H\}$ NMR spectrum of **2^H-BCF** (76 MHz, 20 °C) in CD_2Cl_2: aromatic region

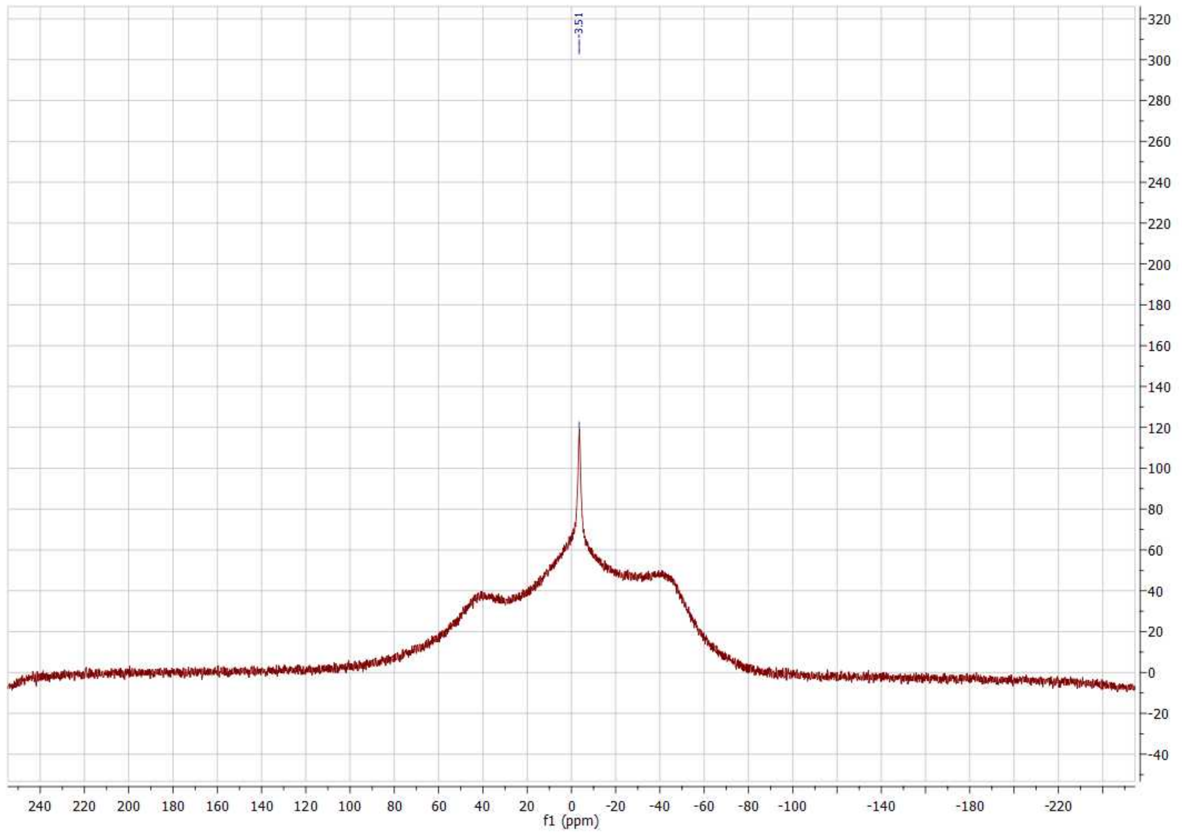


Figure S44. $^{11}B\{^1H\}$ NMR spectrum of **2^H-BCF** (96 MHz, 20 °C) in CD_2Cl_2

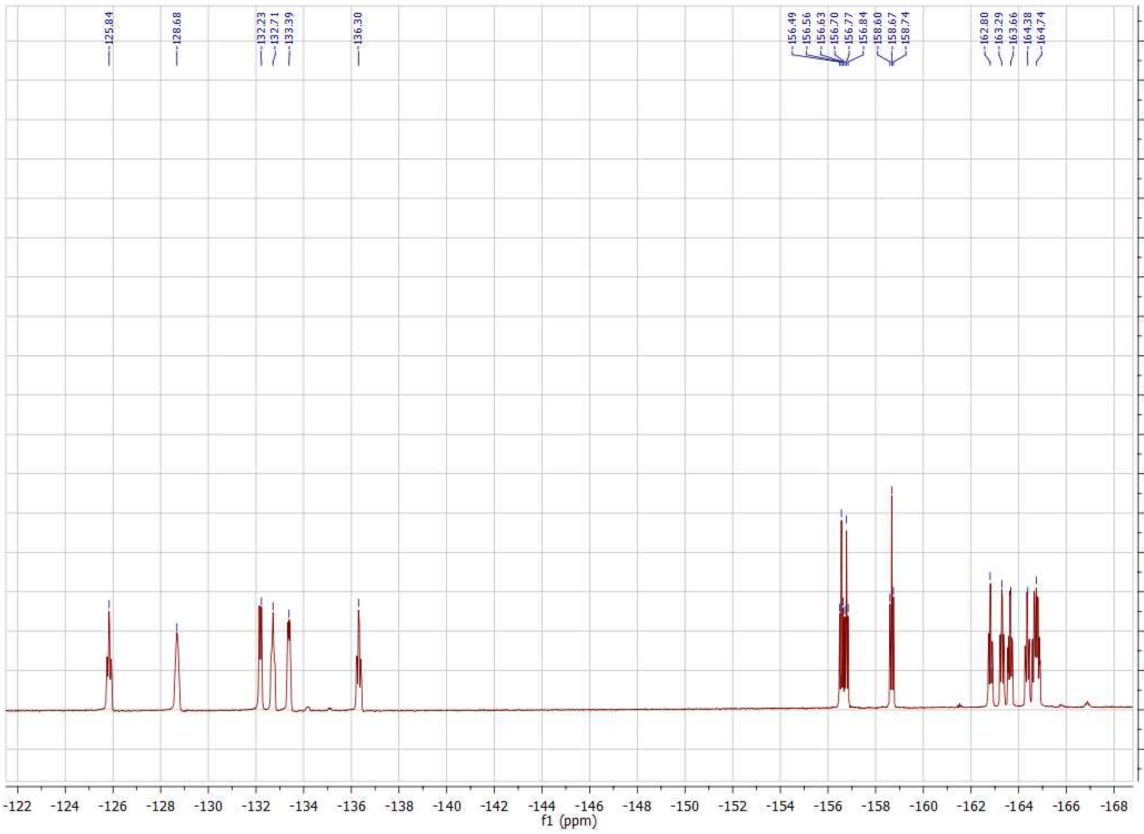


Figure S45. $^{19}F\{^{1}H\}$ NMR spectrum of **2^H-BCF** (282 MHz, 20 °C) in CD_2Cl_2

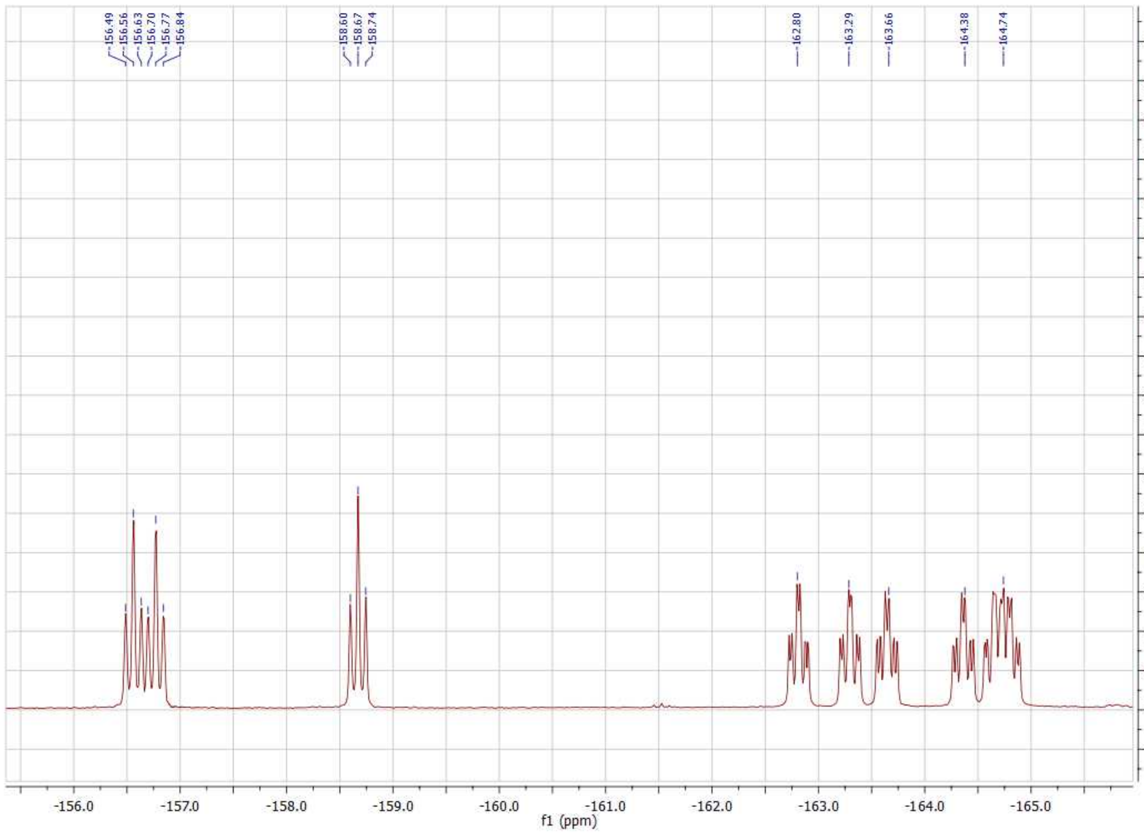


Figure S46. $^{19}F\{^{1}H\}$ NMR spectrum of **2^H-BCF** (282 MHz, 20 °C) in CD_2Cl_2: zoom

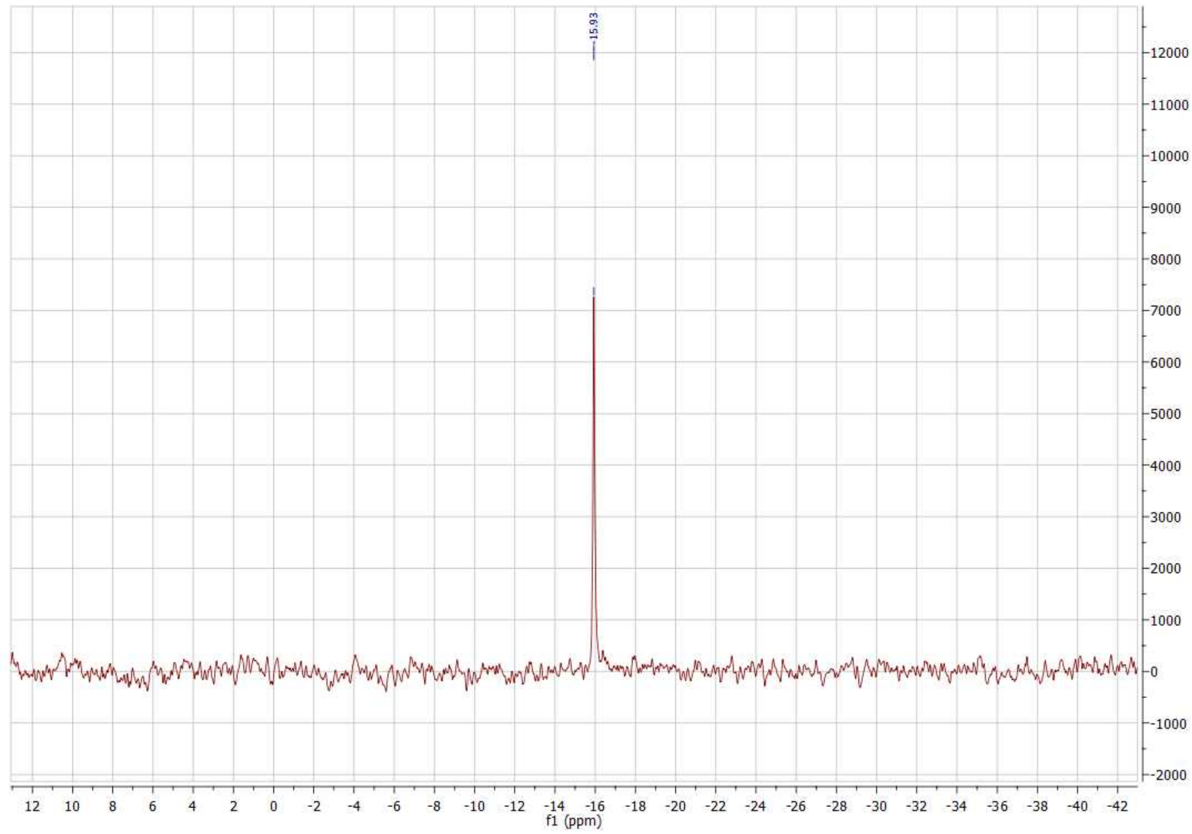
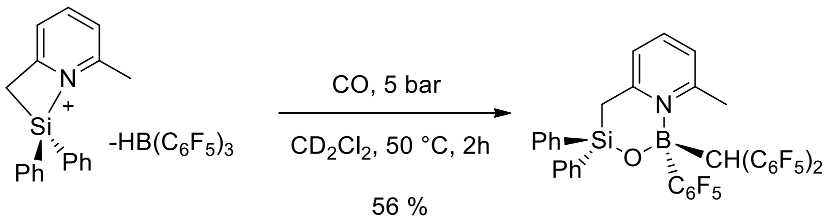
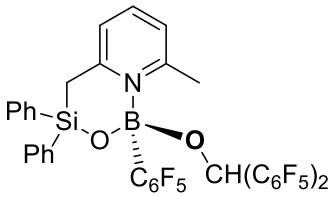


Figure S47. $^{29}Si\{^1H\}$ DEPT NMR spectrum of **2^H-BCF** (60 MHz, 20 °C) in CD_2Cl_2

Synthesis of 3



An NMR tube suited for experiments under pressure containing a solution of **1⁺-HBCF** (19.6 mg, $2.45.10^{-2}$ mmol) in CD_2Cl_2 (0.5 mL) was pressurized with 5 bar of carbon monoxide and heated for two hours at 50 °C affording compound **3** in 56% yield. The yield was determined by integration of the methylene proton resonance signal of the product relative to the methylene proton resonance signal of dichloroethane (internal standard) in the $^{1}H\{^{11}B\}$ NMR spectrum (D1 = 10 s). Crystals of the oxidized compound **3O** (depicted below) were obtained from a saturated pentane solution at -20 °C.



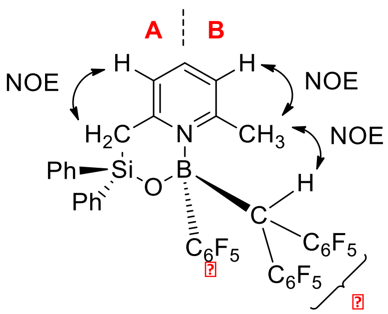
HRMS

Both protonated and not-protonated compound have been detected in HRMS using cold-spray ionization. Due to its high sensitivity, the compound could be detected only in flow-injection in absence of acetonitrile.

Non-labeled compound HRMS (CSI, -40 °C): exact mass (monoisotopic) calcd for $[C_{38}H_{19}N_1Si_1B_1F_{15}O_1]^+$, 829.1096; found 829.2196 and $[C_{38}H_{29}N_1SiB_1F_{15}O_1+H]^+$, 830.1175; found 830.2028.

^{13}C-labeled compound HRMS (CSI, -40 °C): exact mass (monoisotopic) calcd for $[C_{37}{}^{13}C_1H_{19}N_1Si_1B_1F_{15}O_1]^+$, 830.1130; found 830.1925 and $[C_{37}{}^{13}C_1H_{20}N_1Si_1B_1F_{15}O_1+H]^+$, 831.1208; found 830.1084.

NMR characterization



Non-labeled compound

^{1}H NMR (300 MHz, CD_2Cl_2, δ): 2.41 (s, 3H, CH_3), 2.91 (s, 2H, Si-CH_2), 4.75 (s, 1H, $\underline{H}C(C_6F_5)_2$), 6.68 (d, 1H, $^{3}J_{HH}$ = 7.6 Hz, $H_{m\text{-pyA}}$), 6.86 (d, 1H, $^{3}J_{HH}$ = 7.6 Hz, $H_{m\text{-pyB}}$), 7.10-7.48 (m, 11H, H_{Ph} and $H_{p\text{-py}}$).

$^{13}C\{^{1}H\}$ NMR (76 MHz, CD_2Cl_2, δ): 24.2 (s, 1C, CH_3), 25.9 (br., 1C, B-CH), 27.3 (s, 1C, CH_2), 113.1 (br., 2C, $C_{ipso\text{-C6F5}}(\beta)$), 120.0 (s, 1C, $CH_{m\text{-py}}$(A)), 120.7 (s, 1C, $CH_{m\text{-py}}$(B)), 128.1 (s, 4C, $CH_{o\text{-Ph}}$ or $CH_{m\text{-Ph}}$), 130.8 (s, 2C, $CH_{p\text{-Ph}}$), 133.5 (s, 2C, Si-C_{Ph}), 134.9 (s, 4C, $CH_{o\text{-Ph}}$ or $CH_{m\text{-Ph}}$), 136.8 (s, 1C, $CH_{p\text{-py}}$), 137.4 ($C_{m\text{-C6F5}}$ (α) or $C_{m\text{-C6F5}}(\beta)$), 137.9 ($C_{m\text{-C6F5}}$ (α) or $C_{m\text{-C6F5}}(\beta)$), 140.6 (2C, $C_{p\text{-C6F5}}$ (β)), 142.7 (1C, $C_{p\text{-C6F5}}$ (α)), 145.6 (d br., 4C, $^{1}J_{CF}$ = 246.2 Hz, $C_{o\text{-C6F5}}$ (β)), 147.6 (2C, $C_{o\text{-C6F5}}$ (α)), 157.5 (s, 1C, $C_{o\text{-py}}$(A)), 158.2 (s, 1C, $C_{o\text{-py}}$(B)).

$C_{o\text{-C6F5}}$ (β) or $C_{m\text{-C6F5}}(\beta)$, $C_{p\text{-C6F5}}$ (β), $C_{ipso\text{-C6F5}}$ (b), $C_{o\text{-C6F5}}$ (α), $C_{m\text{-C6F5}}(\alpha)$ and $C_{p\text{-C6F5}}(\alpha)$ have been detected based on 2D $\{^{13}C,^{19}F\}$ HSQC experiment. The B-$\underline{C}_{ipso\text{-C6F5}}$ couldn't be detected.

$^{29}Si\{^{1}H\}$ NMR (60 MHz, CD_2Cl_2, δ): -8.6 (s).

$^{11}B\{^{1}H\}$ NMR (96 MHz, CD_2Cl_2, δ): 2.3 (br.).

$^{19}F\{^{1}H\}$ NMR (282 MHz, CD_2Cl_2, δ): -162.5 (m, 4F, $F_{m\text{-C6F5}}(\beta)$), -161.6 (m, 2F, $F_{m\text{-C6F5}}(\alpha)$), -156.1 (t, 2F, $^{3}J_{FF}$ = 20.7 Hz, $F_{p\text{-C6F5}}(\beta)$), -150.8 (t, 1F, $^{3}J_{FF}$ = 20.0 Hz, $F_{p\text{-C6F5}}(\alpha)$),-139.7 (d br., 4F, $^{3}J_{FF}$ = 14.6 Hz, $F_{o\text{-C6F5}}(\beta)$), -131.3 (d br., 2F, $^{3}J_{FF}$ = 20.5 Hz, $F_{o\text{-C6F5}}(\alpha)$).

Labeled compound

^{1}H NMR (300 MHz, CD_2Cl_2, δ): 2.41 (s, 3H, CH_3), 2.90 (s, 2H, Si-CH_2), 4.75 (d, 1H, $^{1}J_{HC}$ = 116.8 Hz, $\underline{H}^{13}C(C_6F_5)_2$), 6.68 (d, 1H, $^{3}J_{HH}$ = 7.7 Hz, $H_{m\text{-pyA}}$), 6.86 (d, 1H, $^{3}J_{HH}$ = 7.6 Hz, $H_{m\text{-pyB}}$), 7.10-7.48 (m, 11H, H_{Ph} and $H_{p\text{-py}}$).

$^{13}C\{^{1}H\}$ NMR (76 MHz, CD_2Cl_2, δ): 24.2 (s, 1C, CH_3), 25.9 (br., B-^{13}CH), 27.3 (s, 1C, CH_2), 113.1 (br., 2C, $C_{ipso\text{-C6F5}}(\beta)$), 120.0 (s, 1C, $CH_{m\text{-py}}$(A)), 120.7 (s, 1C, $CH_{m\text{-py}}$(B)), 128.1 (s, 4C, $CH_{o\text{-Ph}}$ or $CH_{m\text{-Ph}}$), 130.8 (s, 2C, $CH_{p\text{-Ph}}$), 133.5 (s, 2C, Si-C_{Ph}), 134.9 (s, 4C, $CH_{o\text{-Ph}}$ or $CH_{m\text{-Ph}}$), 136.8 (s, 1C, $CH_{p\text{-py}}$), 137.4 ($C_{m\text{-C6F5}}$ (α) or $C_{m\text{-C6F5}}(\beta)$), 137.9 ($C_{m\text{-C6F5}}$ (α) or $C_{m\text{-C6F5}}(\beta)$), 140.6 (2C, $C_{p\text{-C6F5}}$ (β)), 142.7 (1C, $C_{p\text{-C6F5}}$ (α)), 145.6 (d br., 4C, $^{1}J_{CF}$ = 248.3 Hz, $C_{o\text{-C6F5}}$ (β)), 147.6 (2C, $C_{o\text{-C6F5}}$ (α)), 157.4 (s, 1C, $C_{o\text{-py}}$(A)), 158.2 (s, 1C, $C_{o\text{-py}}$(B)).

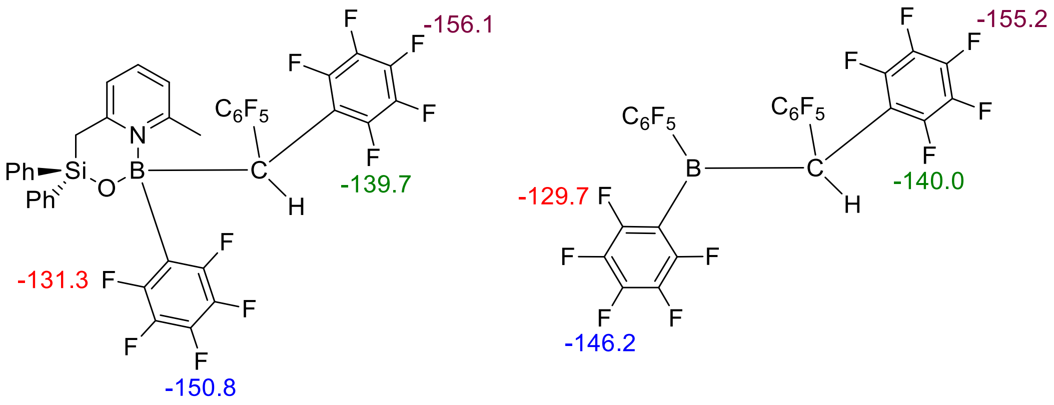
$C_{o\text{-C6F5}}$ (β) or $C_{m\text{-C6F5}}(\beta)$, $C_{p\text{-C6F5}}$ (β), $C_{ipso\text{-C6F5}}$ (β), $C_{o\text{-C6F5}}$ (α), $C_{m\text{-C6F5}}(\alpha)$ and $C_{p\text{-C6F5}}(\alpha)$ have been detected based on 2D $\{^{13}C,^{19}F\}$ HSQC experiment. The B-$\underline{C}_{ipso\text{-C6F5}}$ couldn't be detected.

$C_{ipso\text{-C6F5}}$ (α) and $C_{ipso\text{-C6F5}}$ (β) were not observed.

$^{29}Si\{^{1}H\}$ NMR (60 MHz, CD_2Cl_2, δ): -8.6 (s).

$^{11}B\{^{1}H\}$ NMR (96 MHz, CD_2Cl_2, δ): 2.3 (br.).

$^{19}F\{^{1}H\}$ NMR (282 MHz, CD_2Cl_2, δ): -162.5 (m, 4F, $F_{m\text{-C6F5}}(\beta)$), -161.6 (m, 2F, $F_{m\text{-C6F5}}(\alpha)$), -156.1 (t, 2F, $^{3}J_{FF}$ = 20.7 Hz, $F_{p\text{-C6F5}}(\beta)$), -150.8 (t, 1F, $^{3}J_{FF}$ = 20.0 Hz, $F_{p\text{-C6F5}}(\alpha)$),-139.7 (d br., 4F, $^{3}J_{FF}$ = 14.6 Hz, $F_{o\text{-C6F5}}(\beta)$), -139.3 (d br., 2F, $^{3}J_{FF}$ = 20.5 Hz, $F_{o\text{-C6F5}}(\alpha)$).



Comparison of the ^{19}F NMR chemical shift (ppm) of **3** with that reported for a structurally related reported compound[S3] (right).

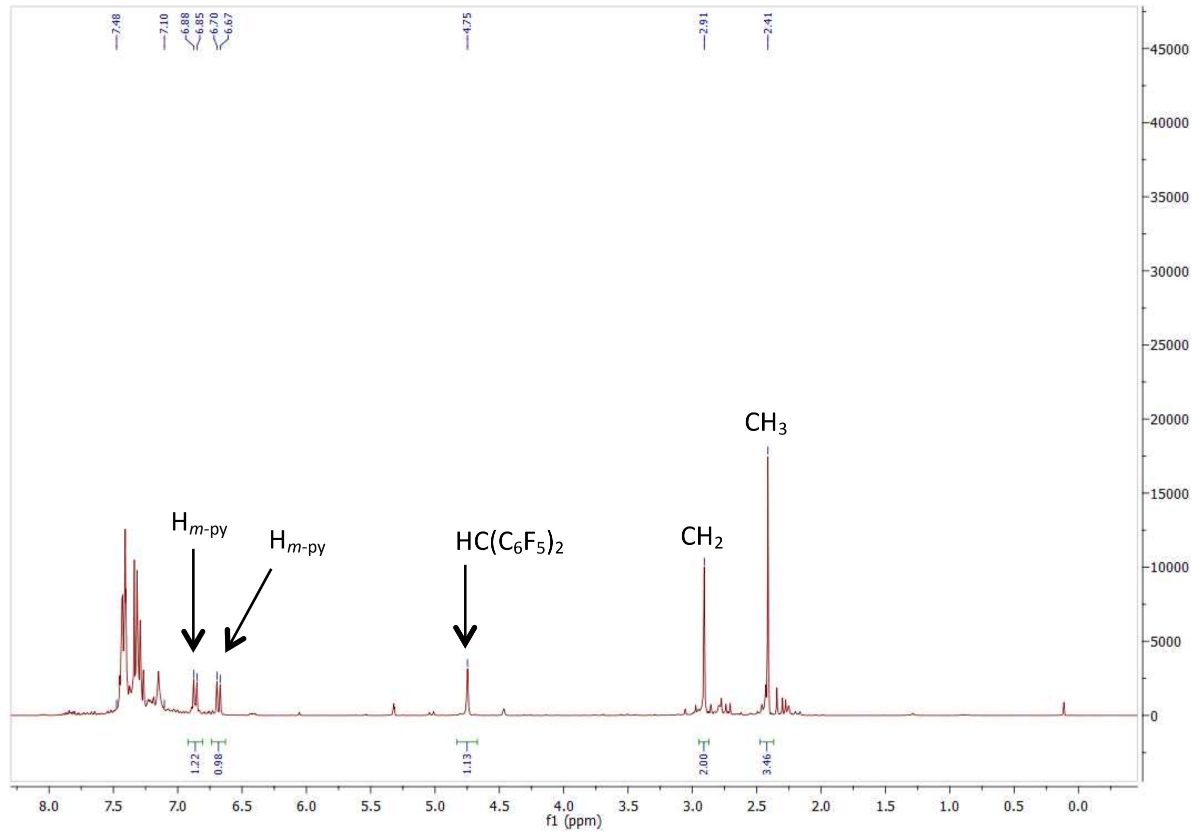


Figure S48. ^{1}H NMR spectrum of **3** (300 MHz, 20 °C) in CD_2Cl_2

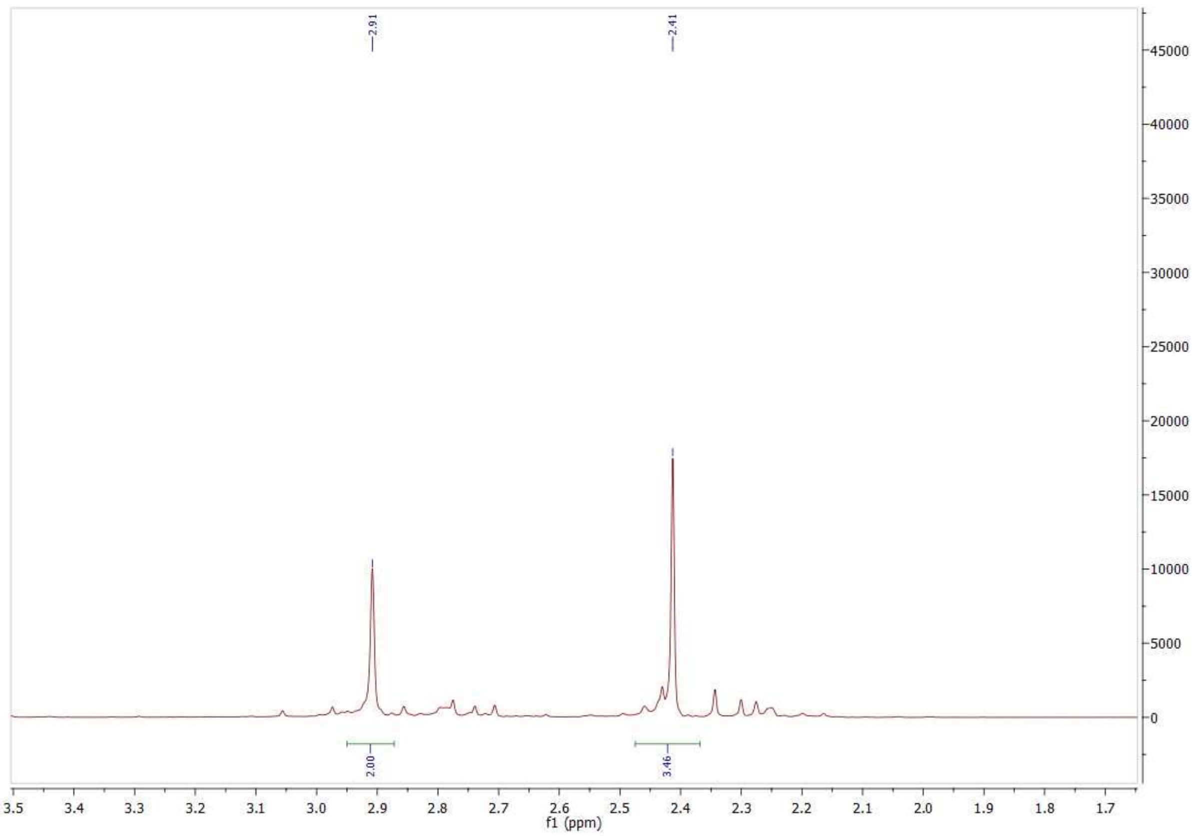


Figure S49. ^{1}H NMR spectrum of **3** (300 MHz, 20 °C) in CD_2Cl_2: aliphatic region

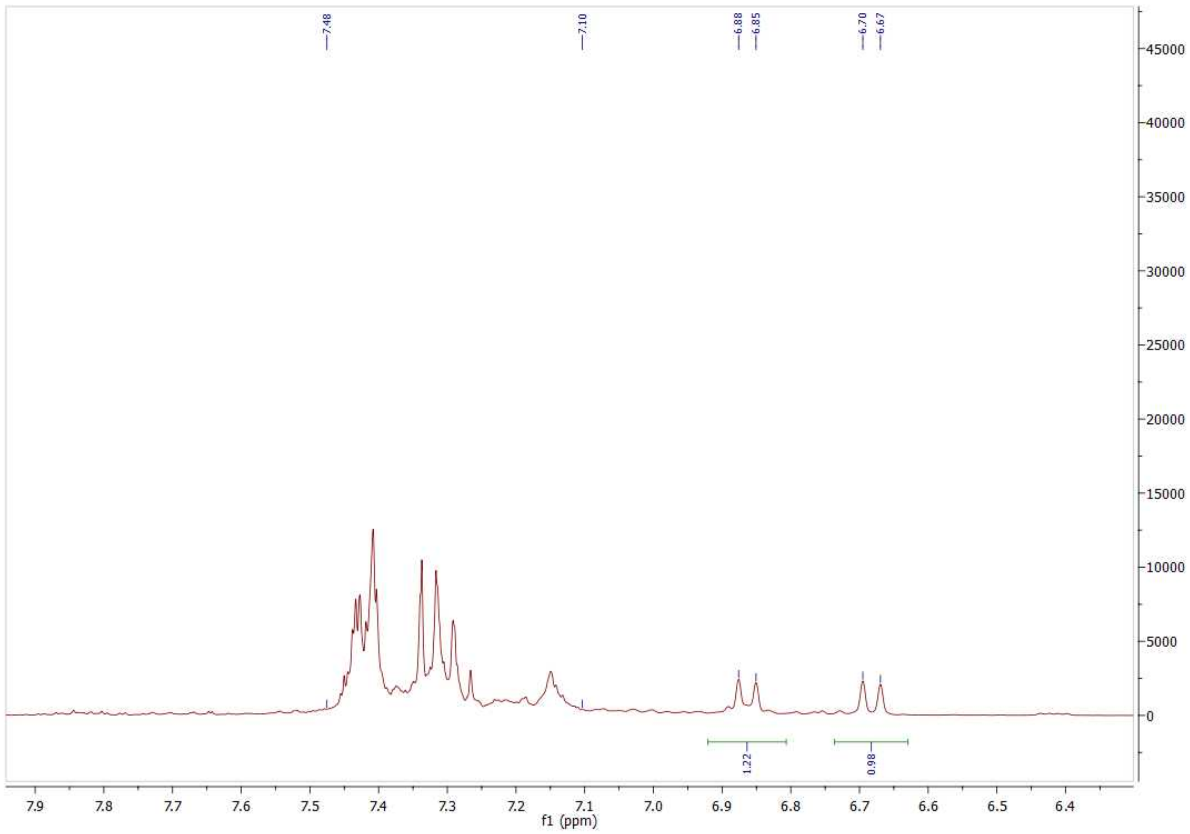


Figure S50. [1]H NMR spectrum of **3** (300 MHz, 20 °C) in CD_2Cl_2: aromatic region

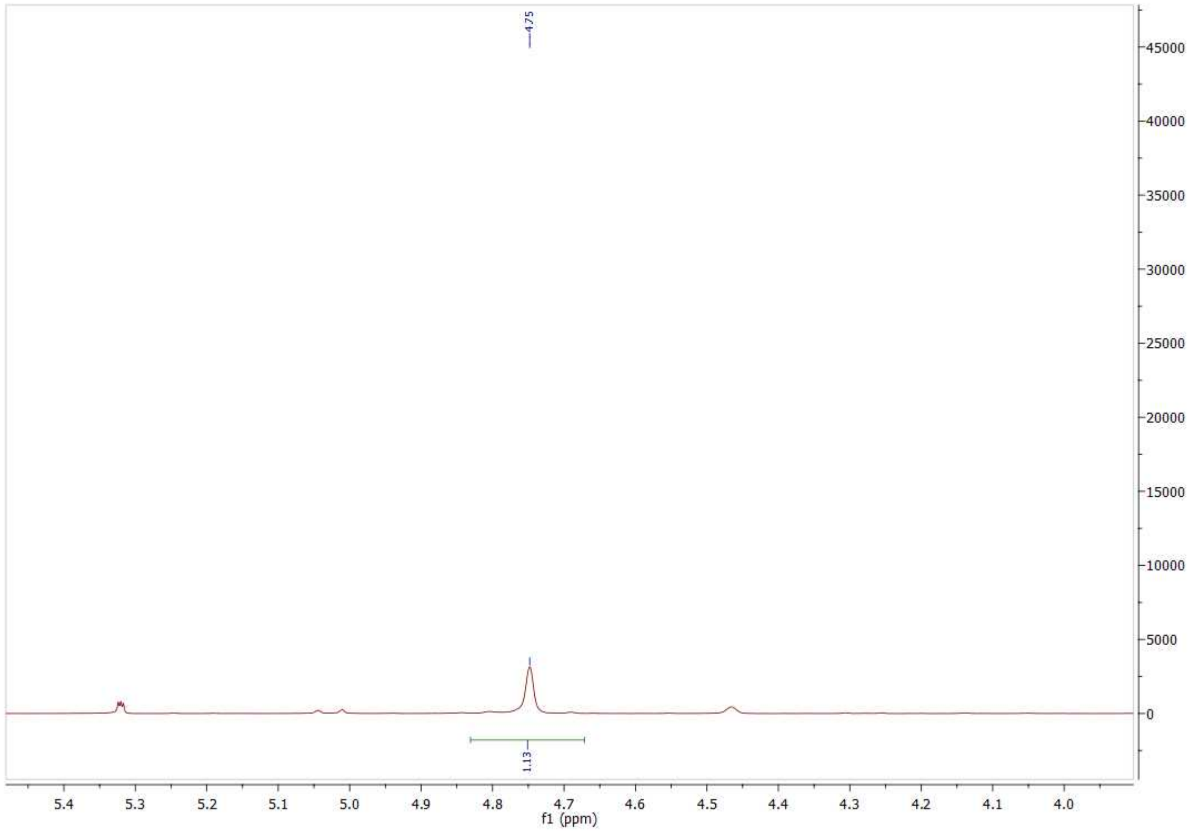


Figure S51. [1]H NMR spectrum of **3** (300 MHz, 20 °C) in CD_2Cl_2: H-C$(C_6F_5)_2$

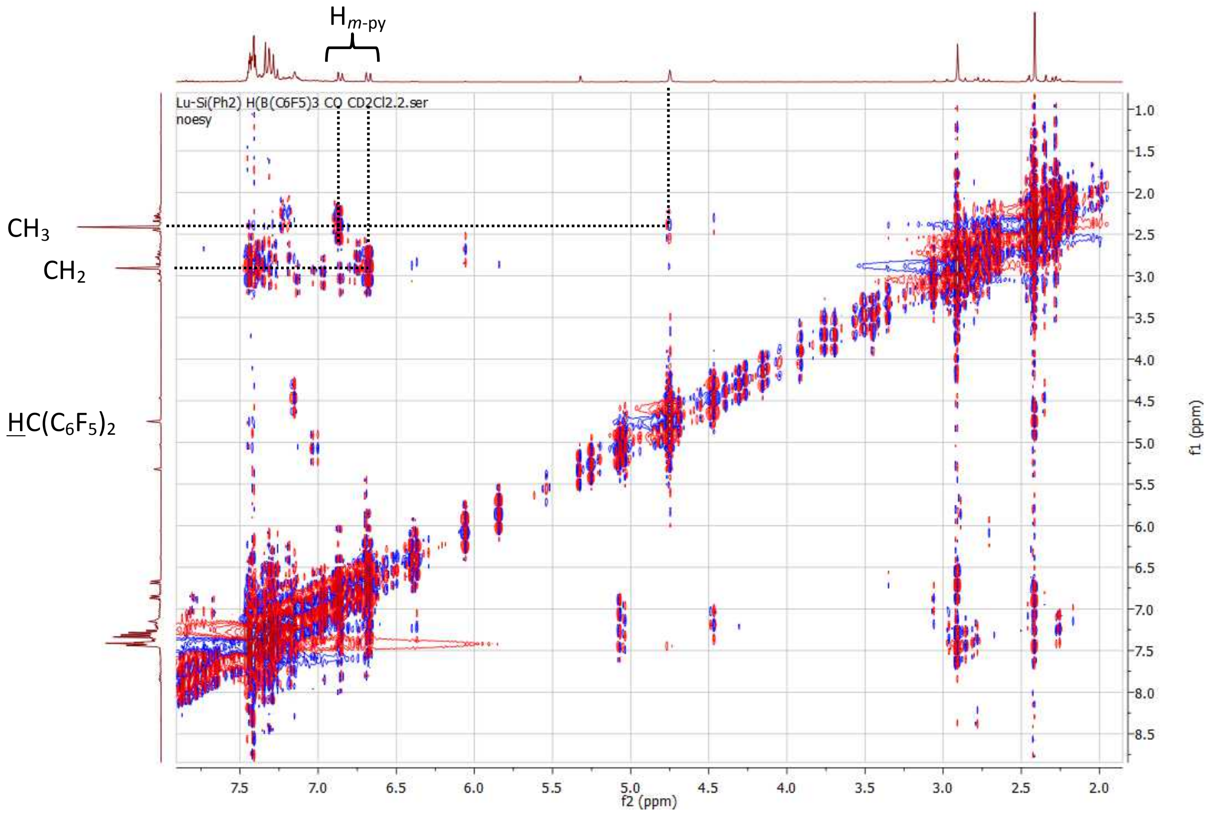


Figure S52. NOESY [^{1}H, ^{1}H] NMR spectrum of **3** (300 MHz, 20 °C) in CD_2Cl_2

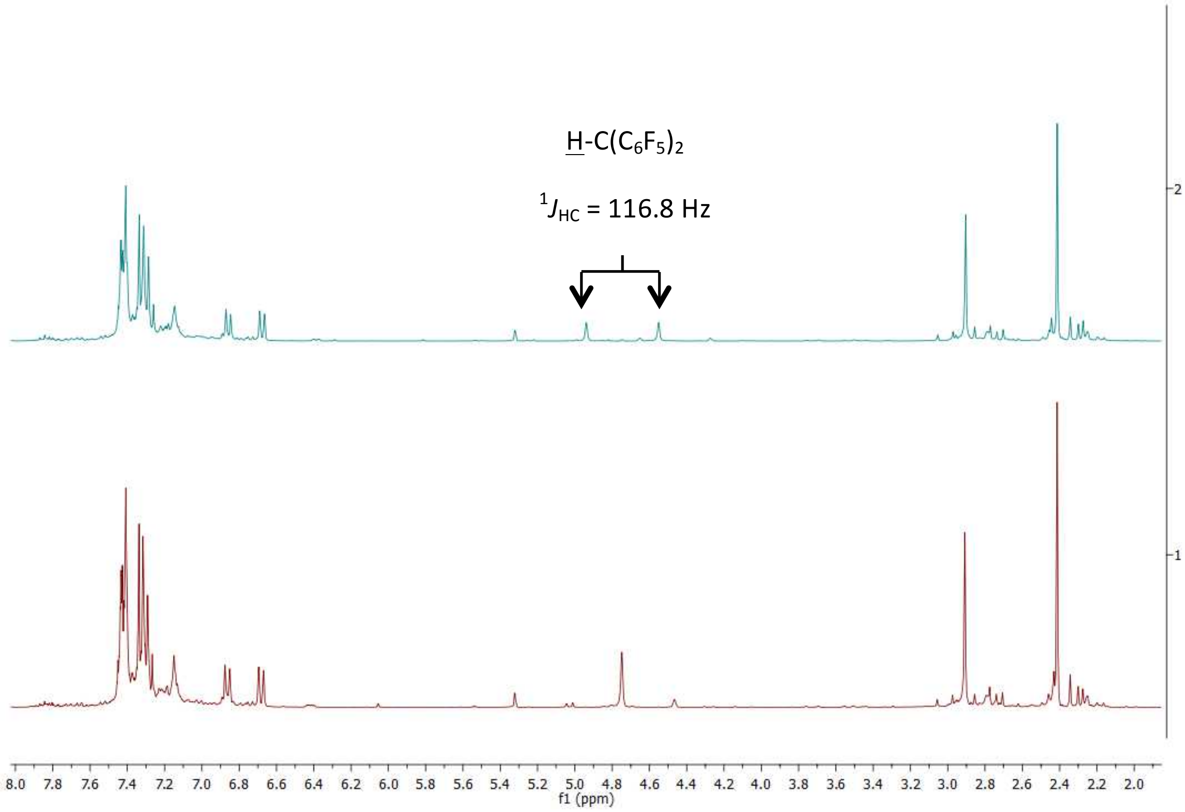


Figure S53. Stacked ^{1}H of **3** (bottom) and ^{1}H of ^{13}C-labeled **3** (top) NMR spectra (300 MHz, 20 °C) in CD_2Cl_2

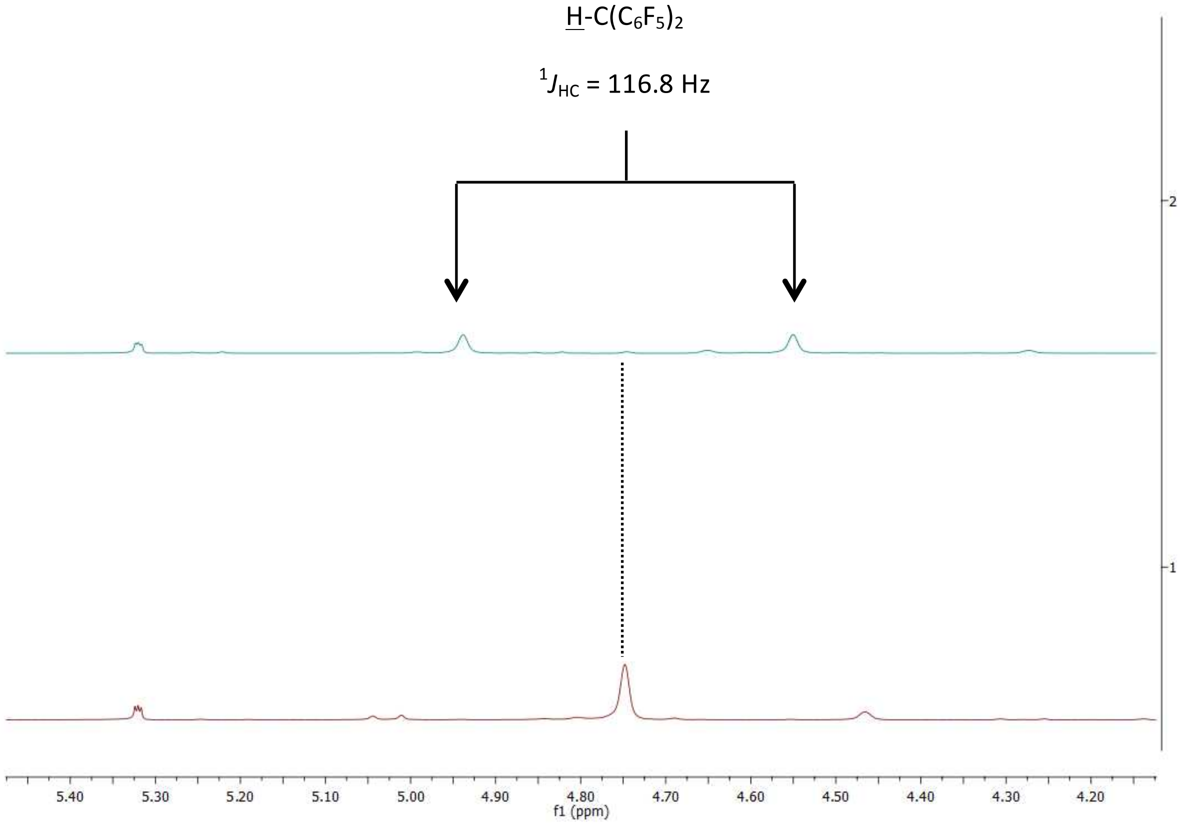


Figure S54. Stacked [1]H of **3** (bottom) and [1]H of [13]C-labeled **3** (top) NMR spectra (300 MHz, 20 °C) in CD_2Cl_2: zoom on H-C(C_6F_5)$_2$

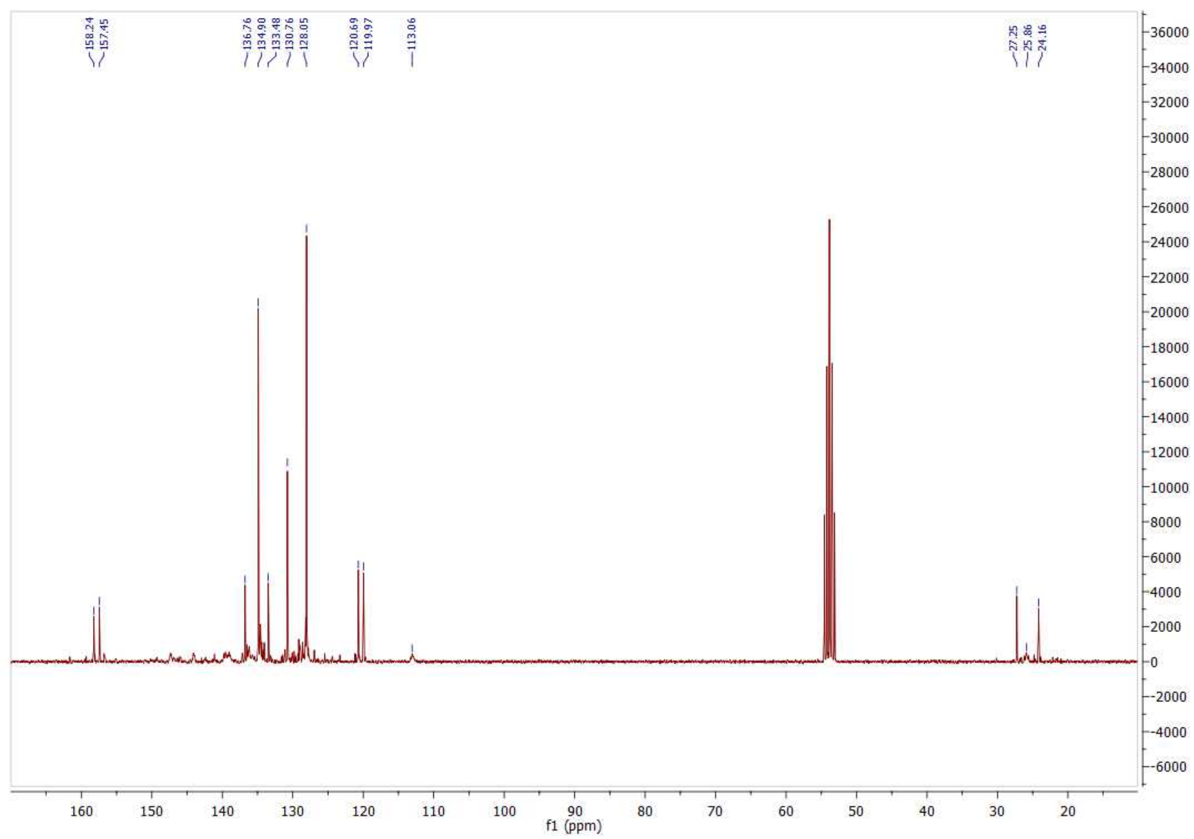


Figure S55. $^{13}C\{^{1}H\}$ NMR spectrum of **3** (76 MHz, 20 °C) in CD_2Cl_2

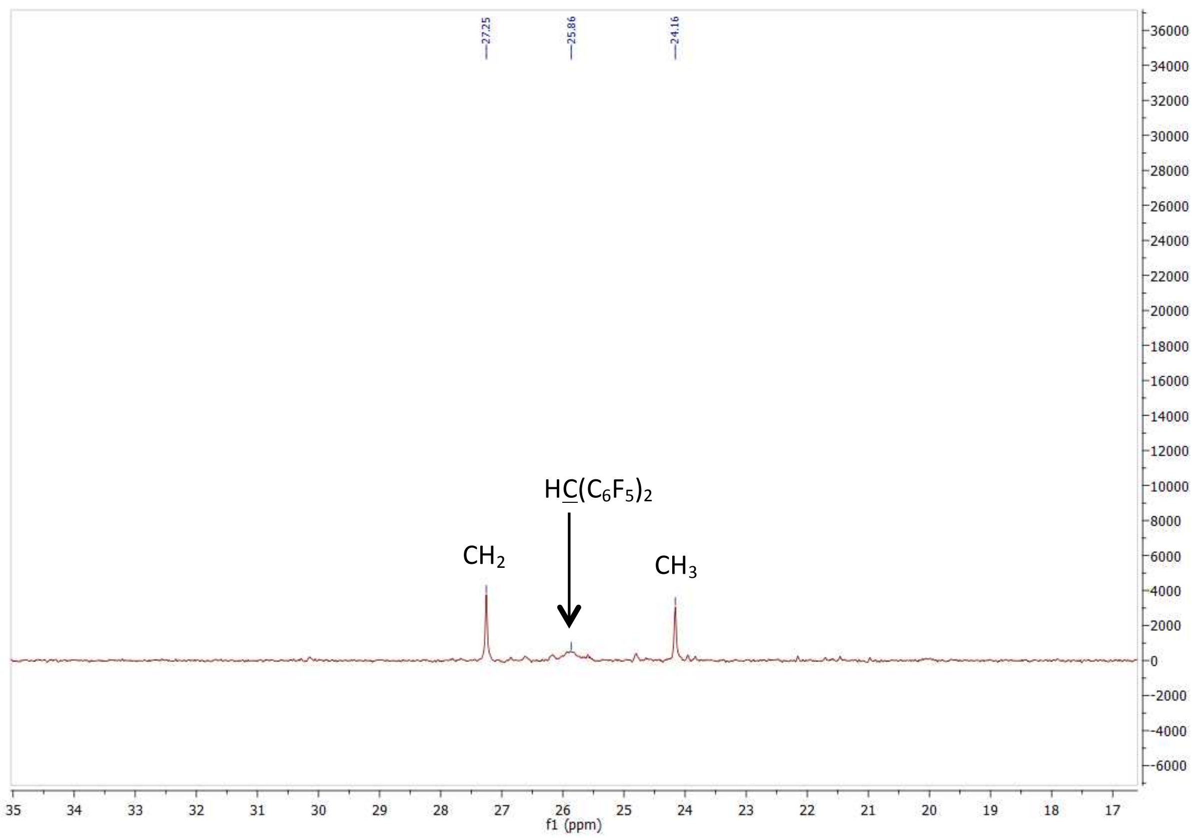


Figure S56. $^{13}C\{^{1}H\}$ NMR spectrum of **3** (76 MHz, 20 °C) in CD_2Cl_2: aliphatic region

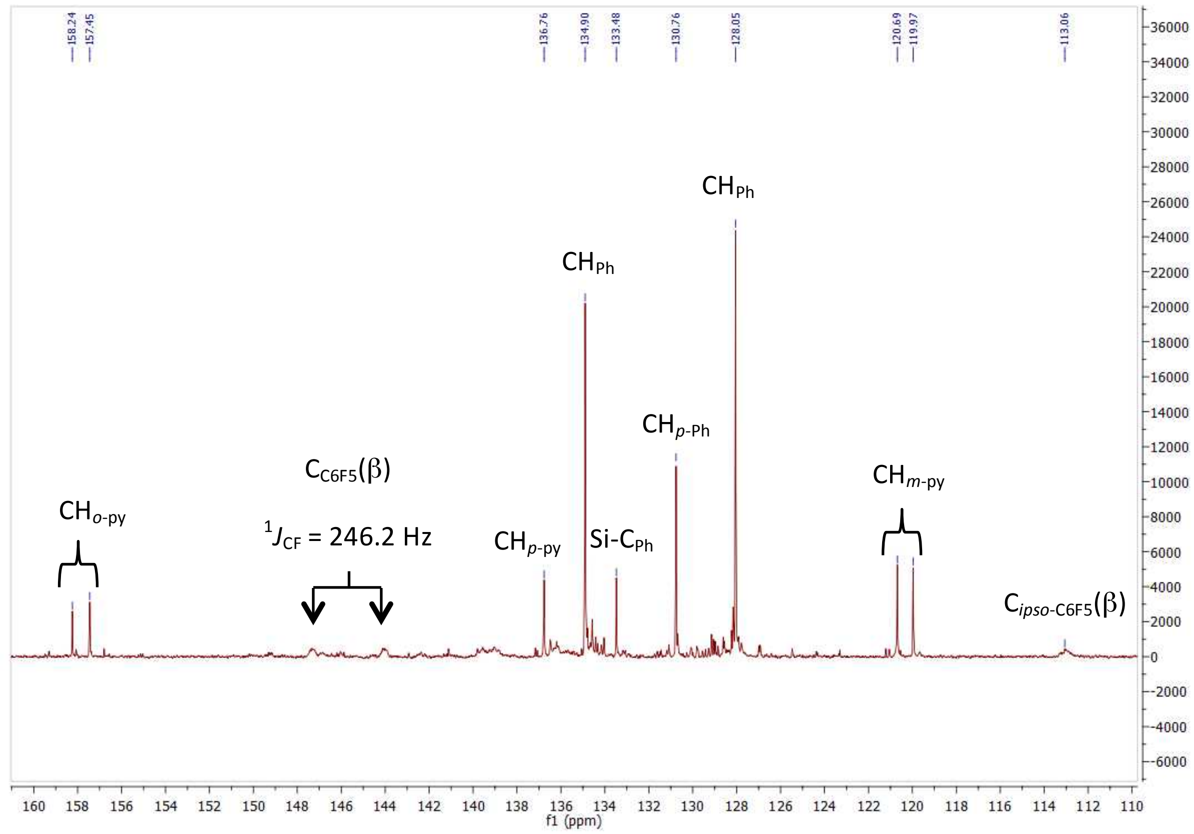


Figure S57. $^{13}C\{^{1}H\}$ NMR spectrum of **3** (76 MHz, 20 °C) in CD_2Cl_2: aromatic region

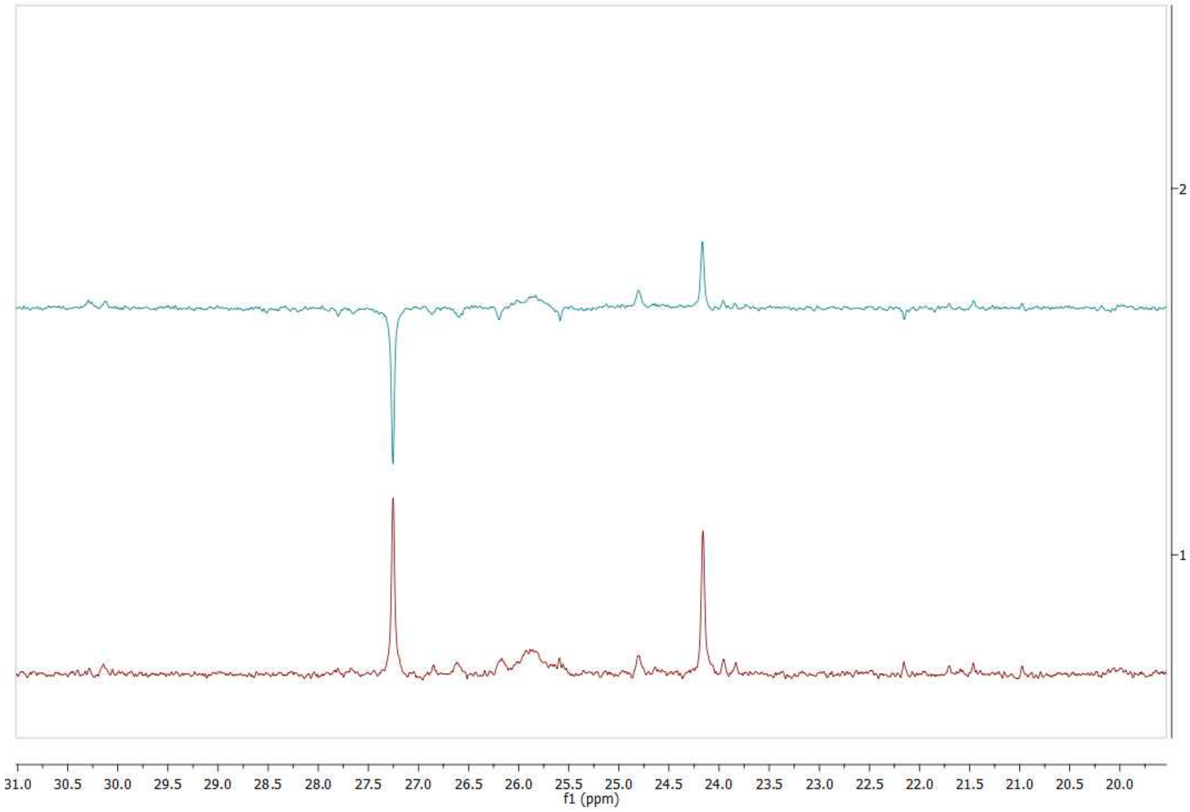


Figure S58. Stacked $^{13}C\{^1H\}$ (bottom) and $^{13}C\{^1H\}$ jmod (top) NMR spectra of **3** (76 MHz, 20 °C) in CD_2Cl_2: aliphatic region

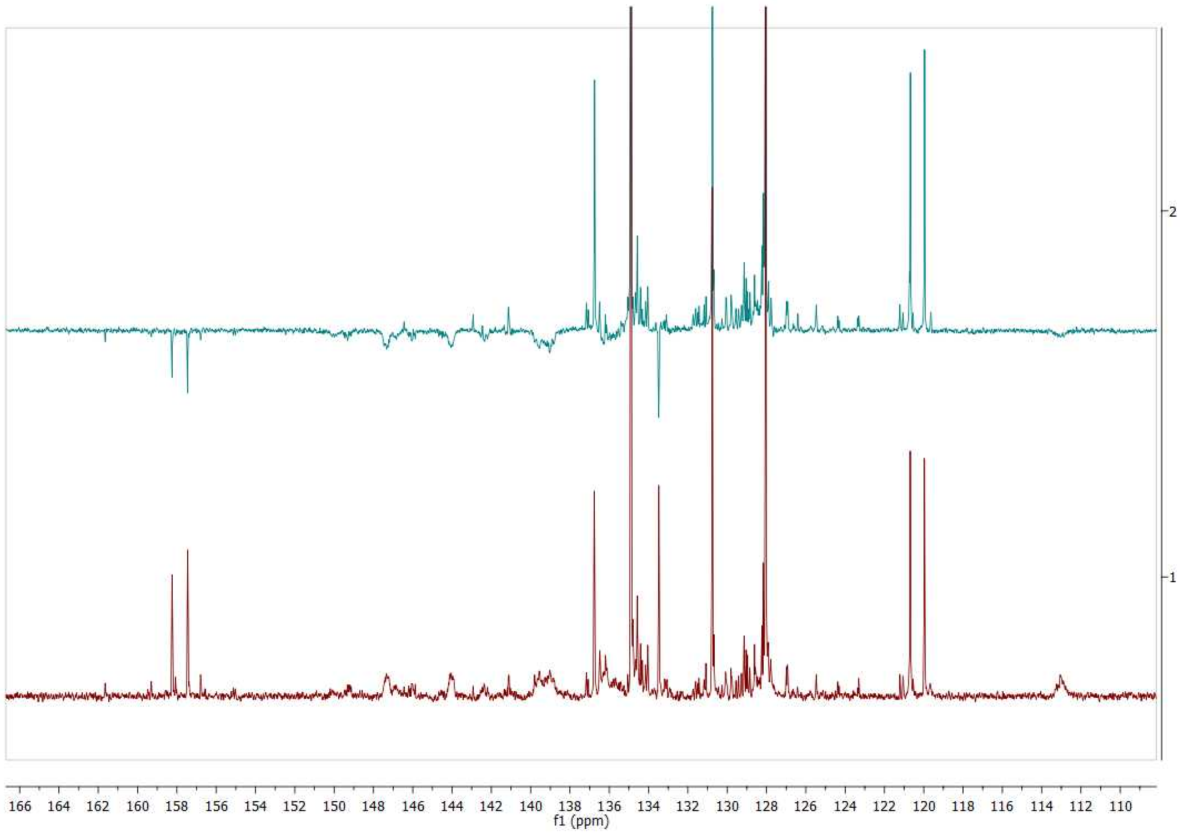


Figure S59. Stacked $^{13}C\{^{1}H\}$ (bottom) and $^{13}C\{^{1}H\}$ jmod (top) NMR spectra of **3** (76 MHz, 20 °C) in CD_2Cl_2: aromatic region

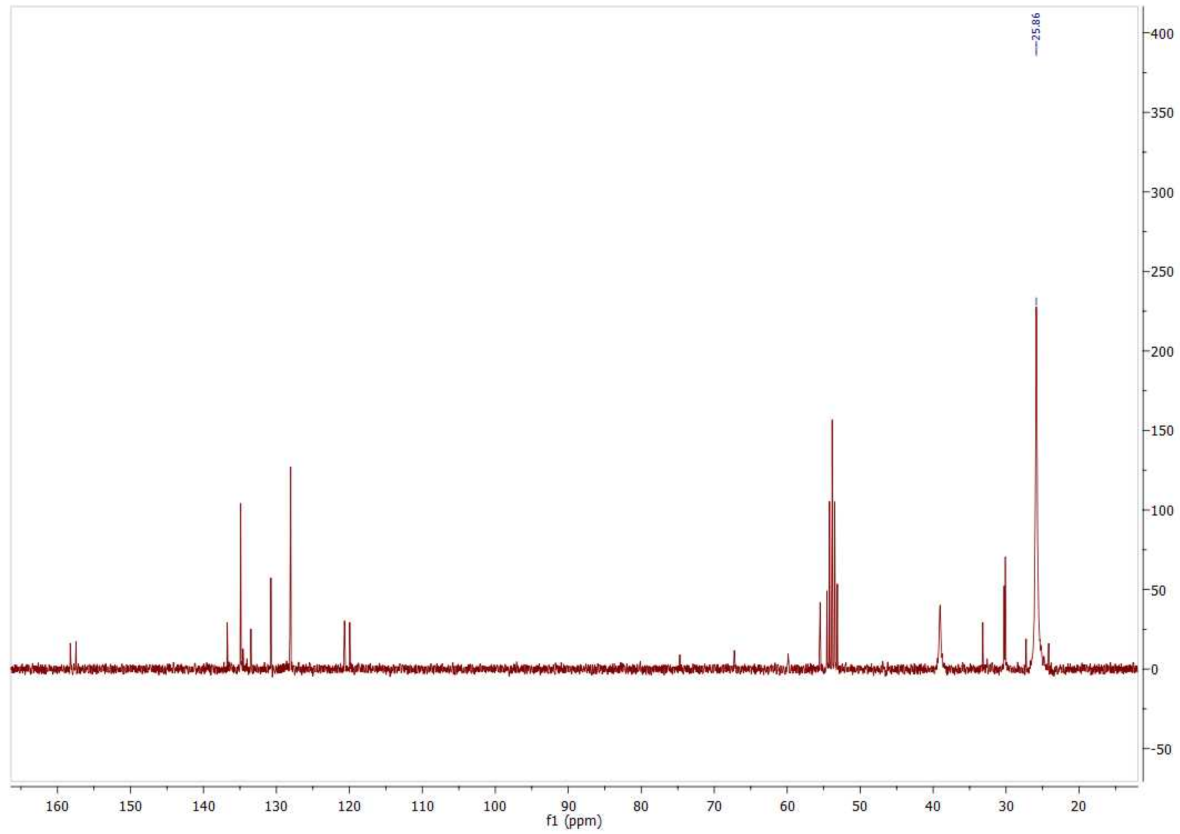


Figure S60. $^{13}C\{^{1}H\}$ NMR spectrum of ^{13}C-labeled **3** (76 MHz, 20 °C) in CD_2Cl_2

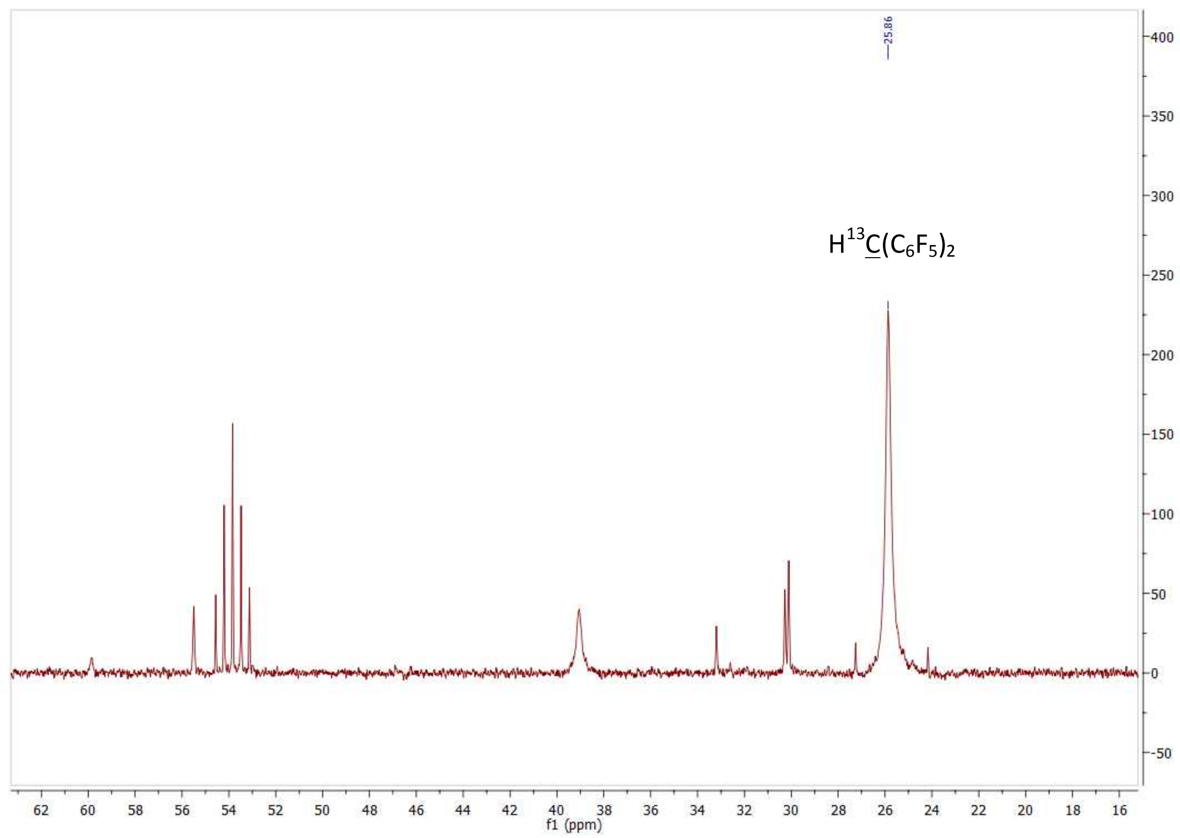


Figure S61. $^{13}C\{^{1}H\}$ NMR spectrum of ^{13}C-labeled **3** (76 MHz, 20 °C) in CD_2Cl_2: aliphatic region

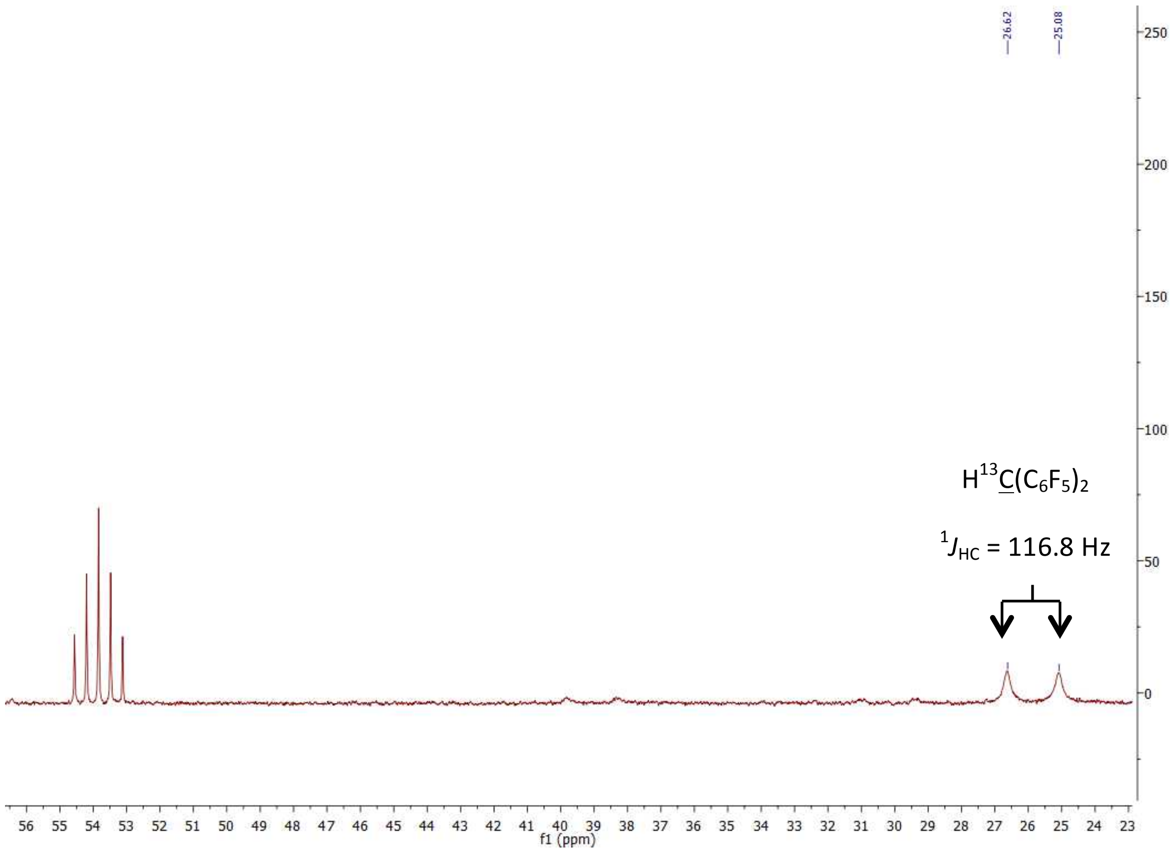


Figure S62. ^{13}C NMR spectrum of ^{13}C-labeled **3** (76 MHz, 20 °C) in CD_2Cl_2: aliphatic region

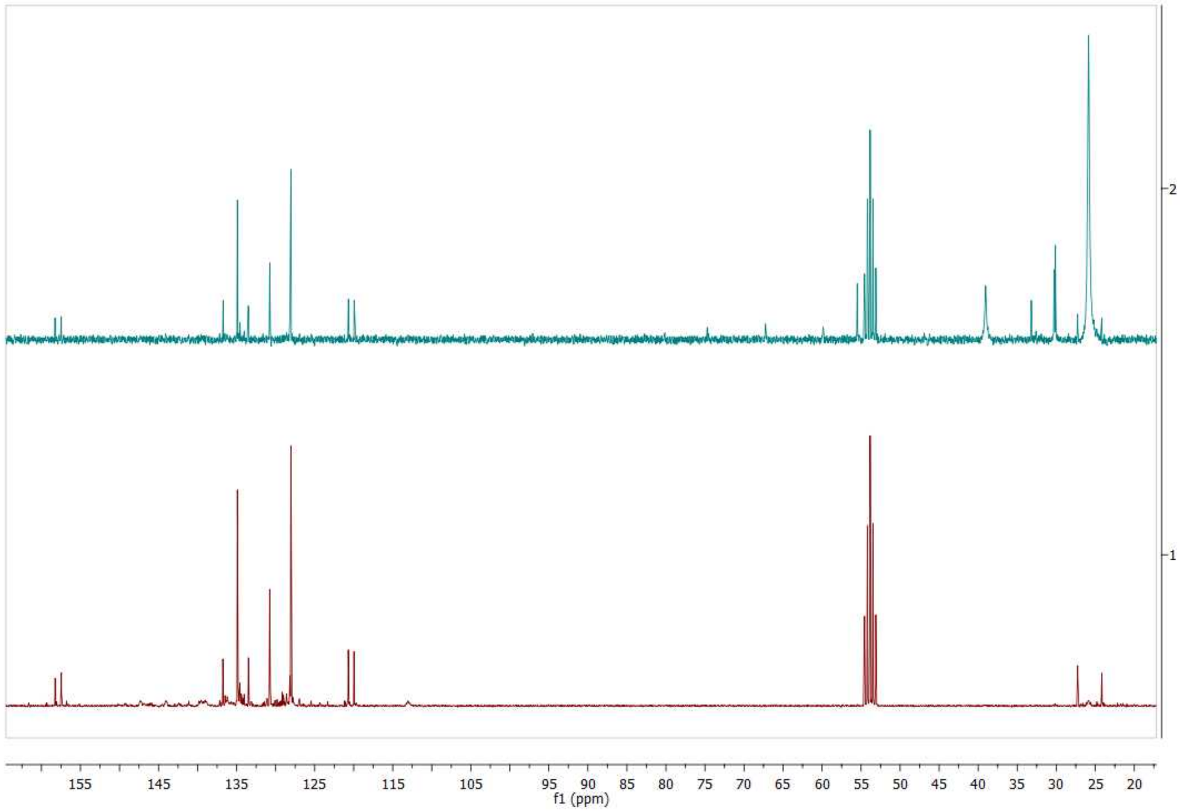


Figure S63. Stacked $^{13}C\{^{1}H\}$ of **3** (bottom) and $^{13}C\{^{1}H\}$ of ^{13}C-labeled **3** (top) NMR spectra (76 MHz, 20 °C) in CD_2Cl_2

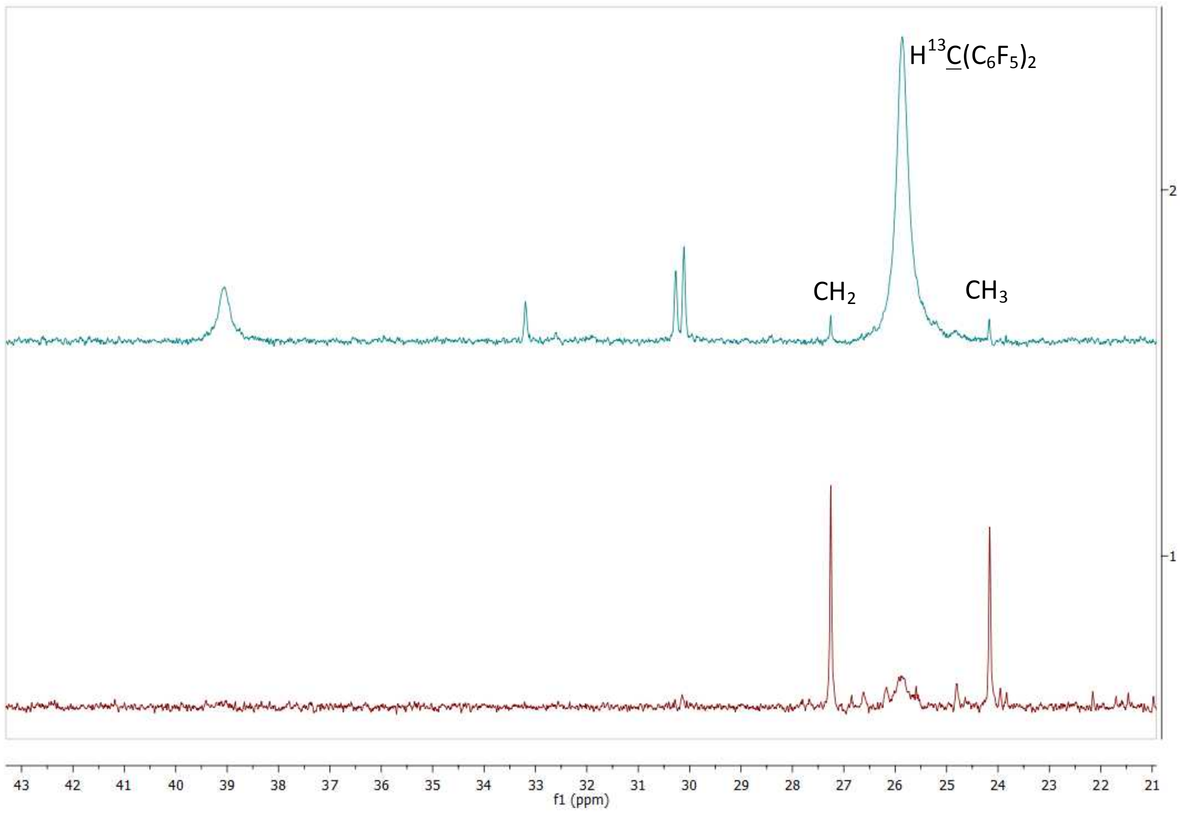


Figure S64. Stacked $^{13}C\{^{1}H\}$ of **3** (bottom) and $^{13}C\{^{1}H\}$ of ^{13}C-labeled **3** (top) NMR spectra (76 MHz, 20 °C) in CD_2Cl_2: aliphatic region

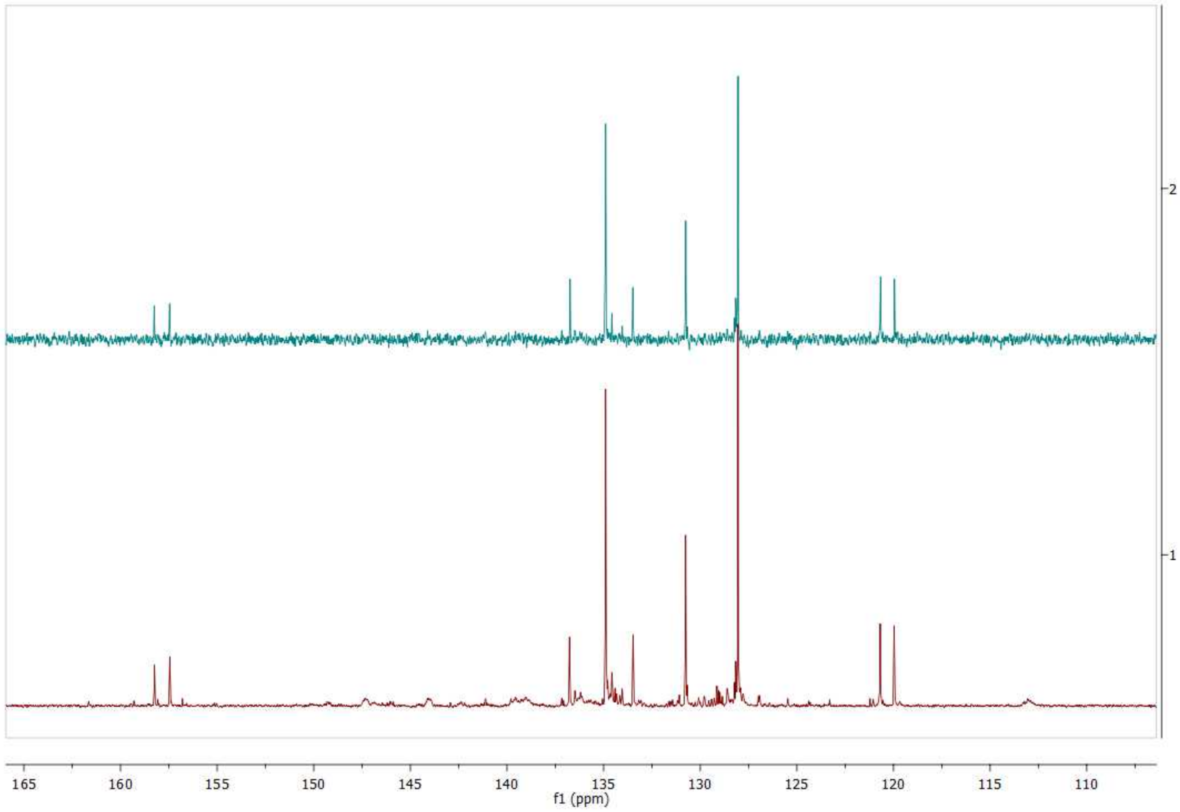


Figure S65. Stacked $^{13}C\{^{1}H\}$ of **3** (bottom) and $^{13}C\{^{1}H\}$ of ^{13}C-labeled **3** (top) NMR spectra (76 MHz, 20 °C) in CD_2Cl_2: aromatic region

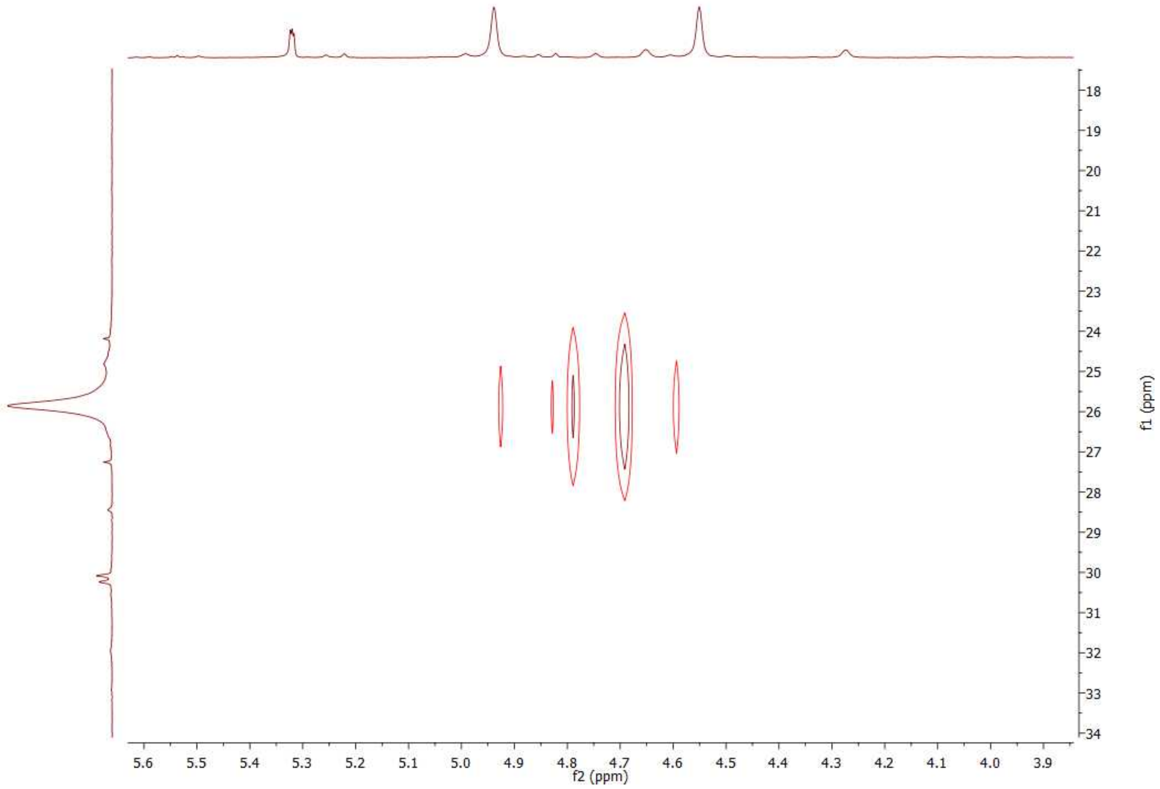


Figure S66. HSQC [^{13}C,^{1}H] NMR spectrum of ^{13}C-labeled **3** (76 MHz, 20 °C) in CD_2Cl_2

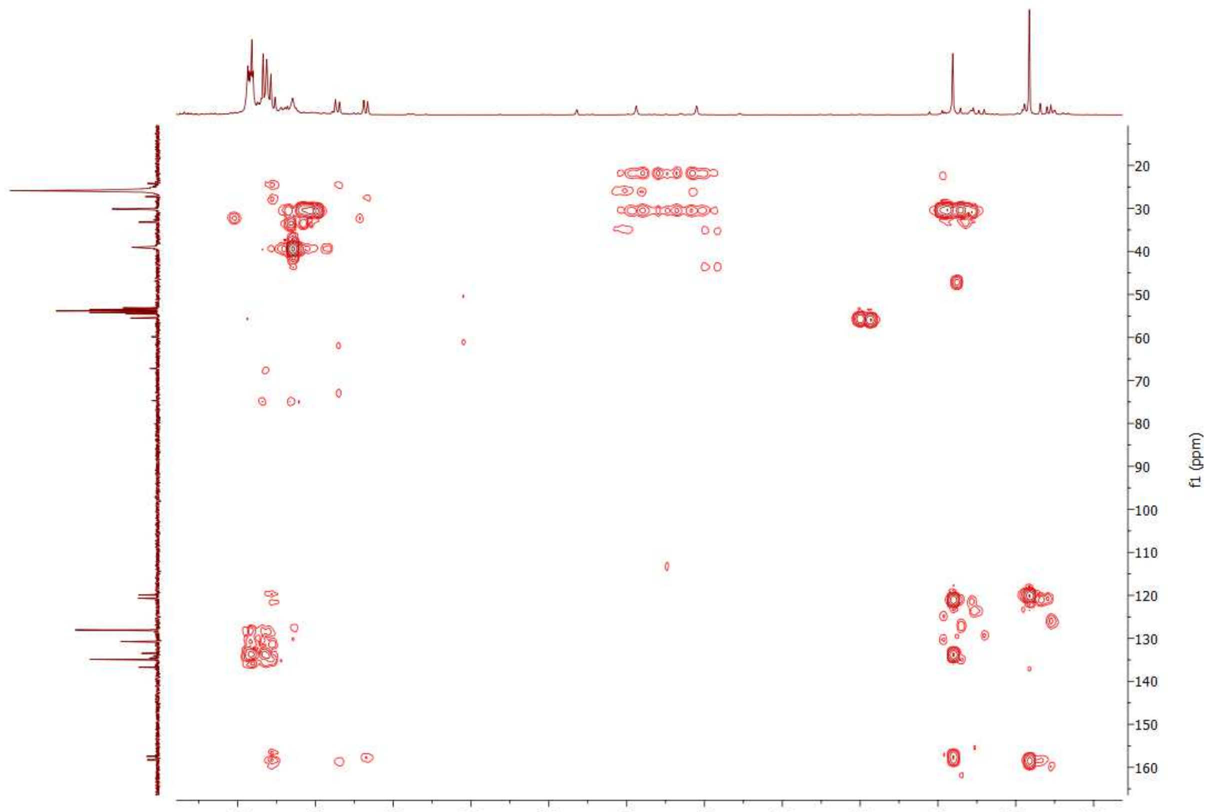


Figure S67. HMQC [^{13}C,^{1}H] NMR spectrum of ^{13}C-labeled **3** (76 MHz, 20 °C) in CD_2Cl_2

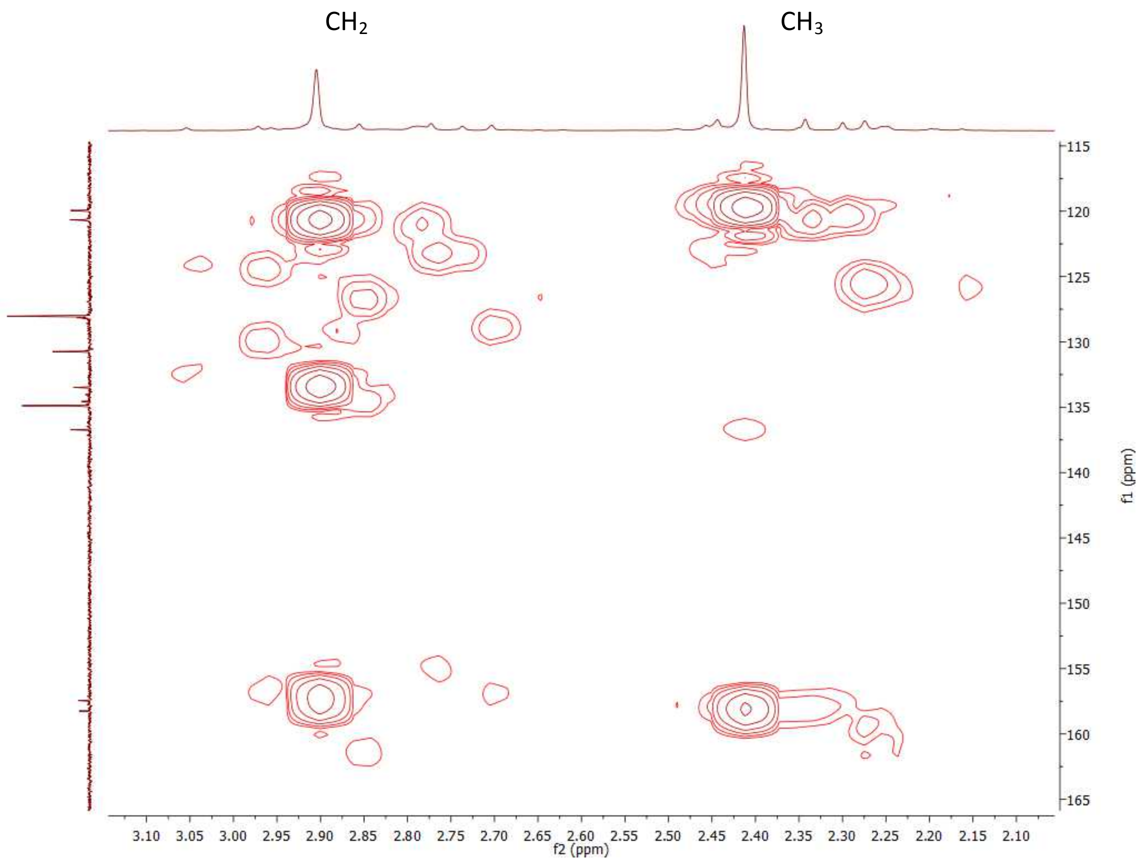


Figure S68. HMBC [$^{13}C,^{1}H$] NMR spectrum of ^{13}C-labeled **3** (76 MHz, 20 °C) in CD_2Cl_2: zoom 1

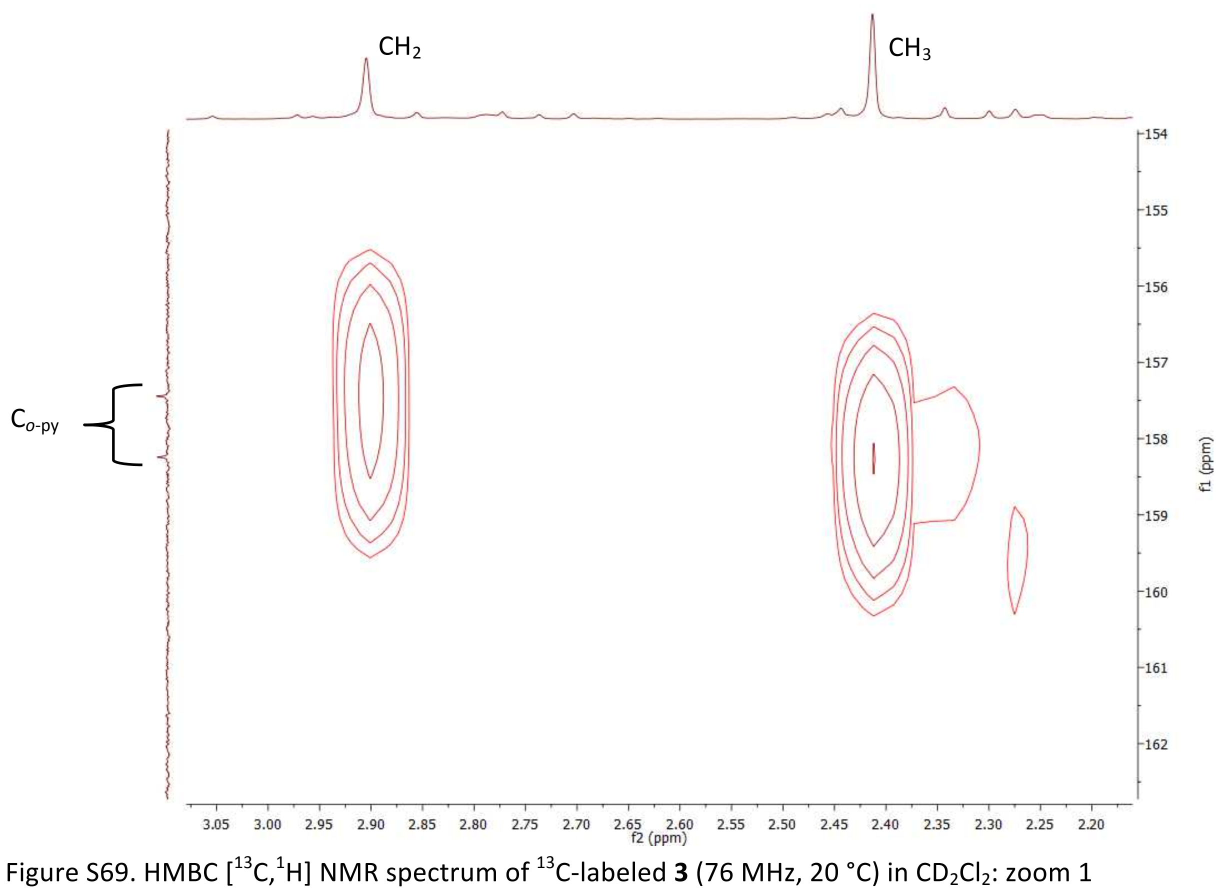


Figure S69. HMBC [$^{13}C,^{1}H$] NMR spectrum of ^{13}C-labeled **3** (76 MHz, 20 °C) in CD_2Cl_2: zoom 1

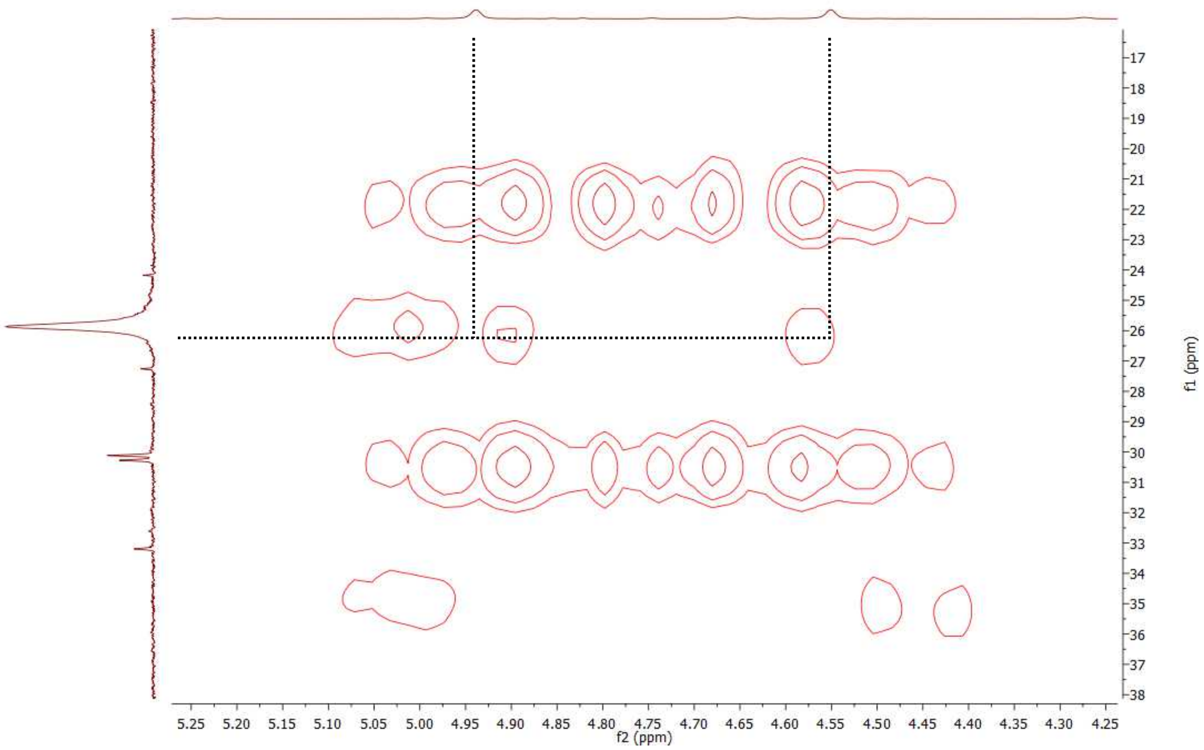


Figure S70. HMBC [^{13}C,^{1}H] NMR spectrum of ^{13}C-labeled **3** (76 MHz, 20 °C) in CD_2Cl_2: zoom 2

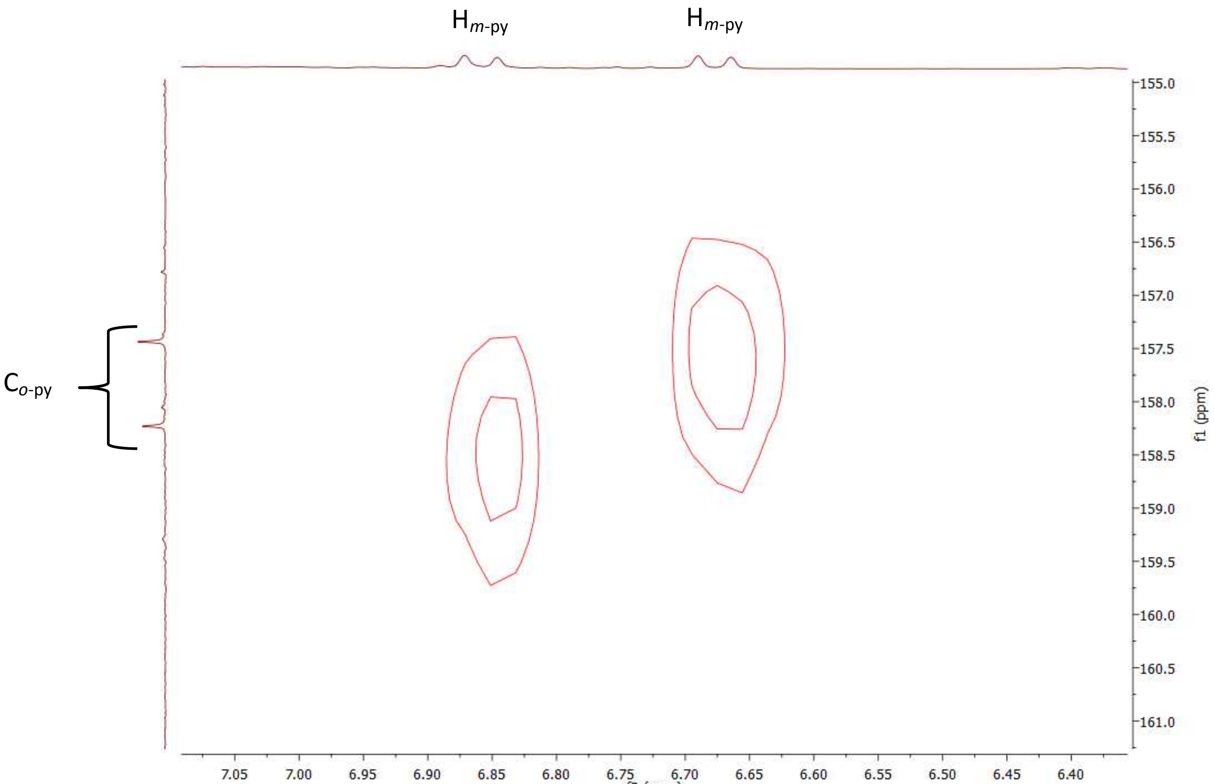


Figure S71. HMBC [^{13}C,^{1}H] NMR spectrum of ^{13}C-labeled **3** (76 MHz, 20 °C) in CD_2Cl_2: zoom 5

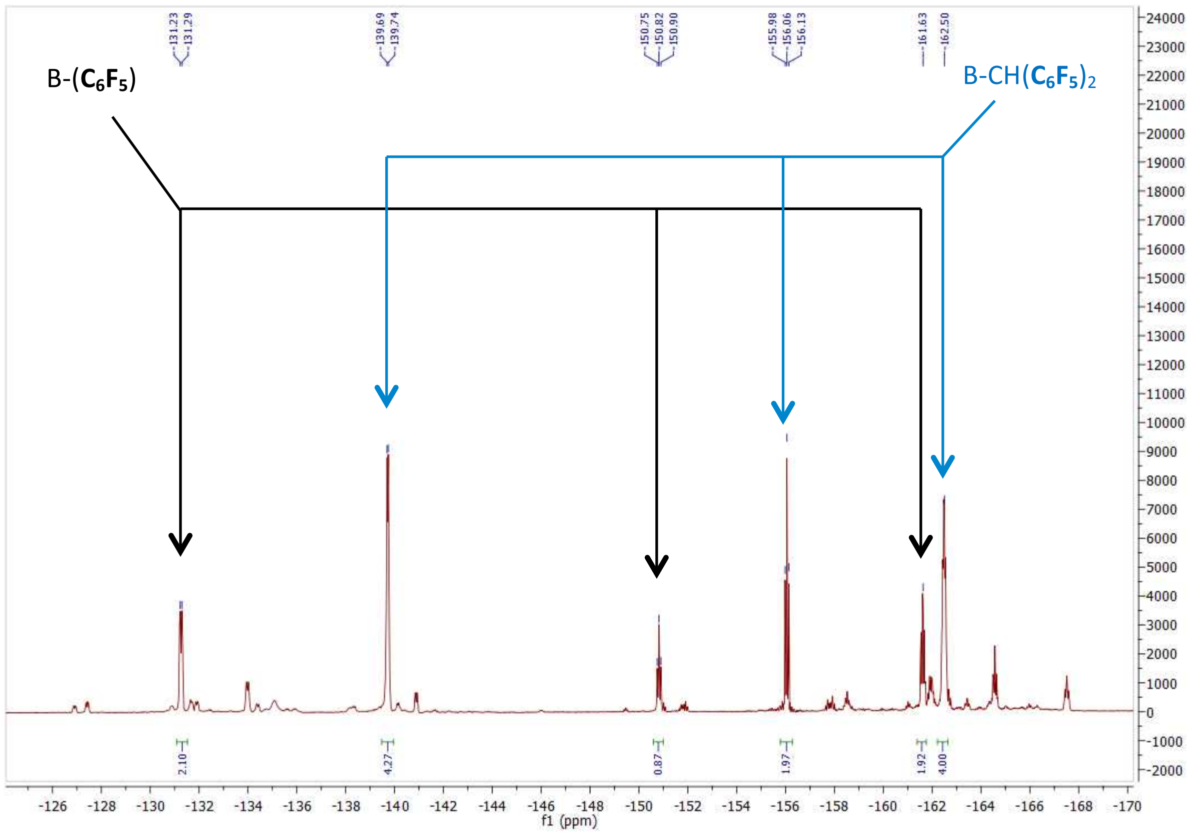


Figure S72. $^{19}F\{^{1}H\}$ NMR spectrum of **3** (282 MHz, 20 °C) in CD_2Cl_2

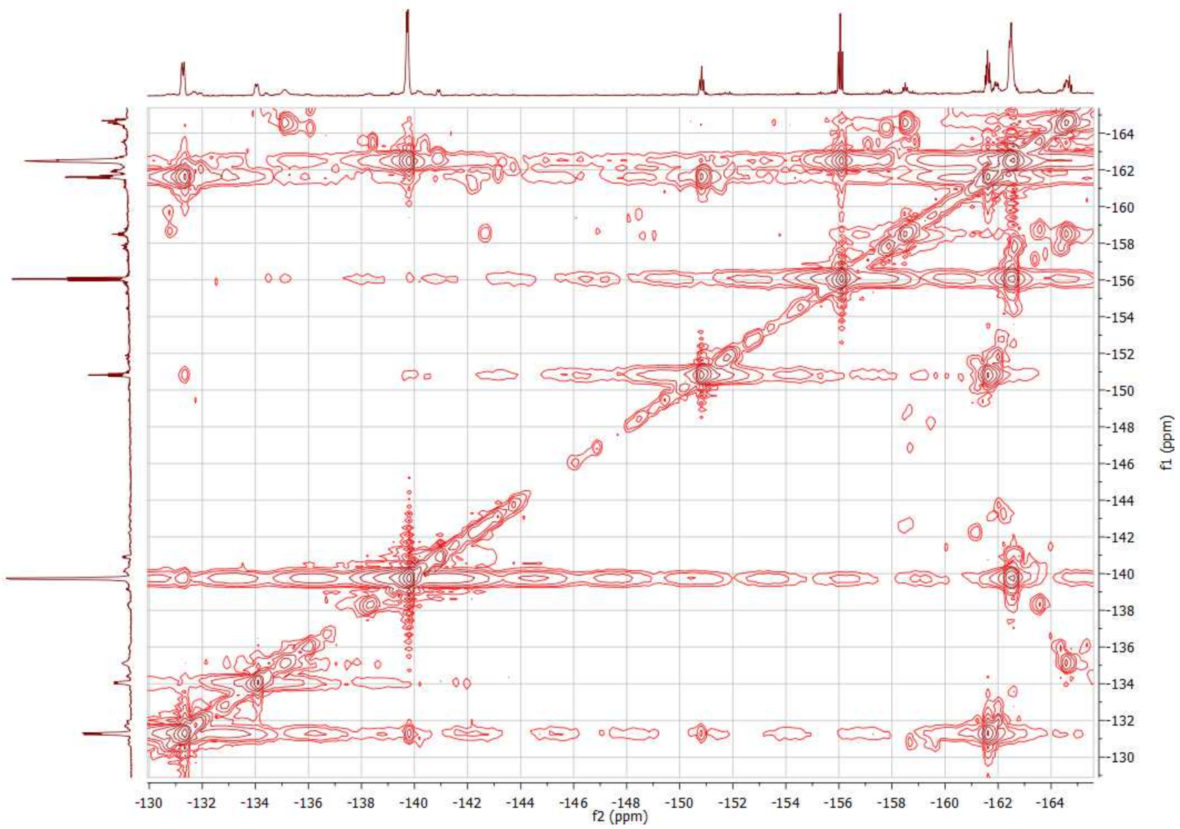


Figure S73. COSY [^{19}F, ^{19}F] NMR spectrum of **3** (282 MHz, 20 °C) in CD_2Cl_2

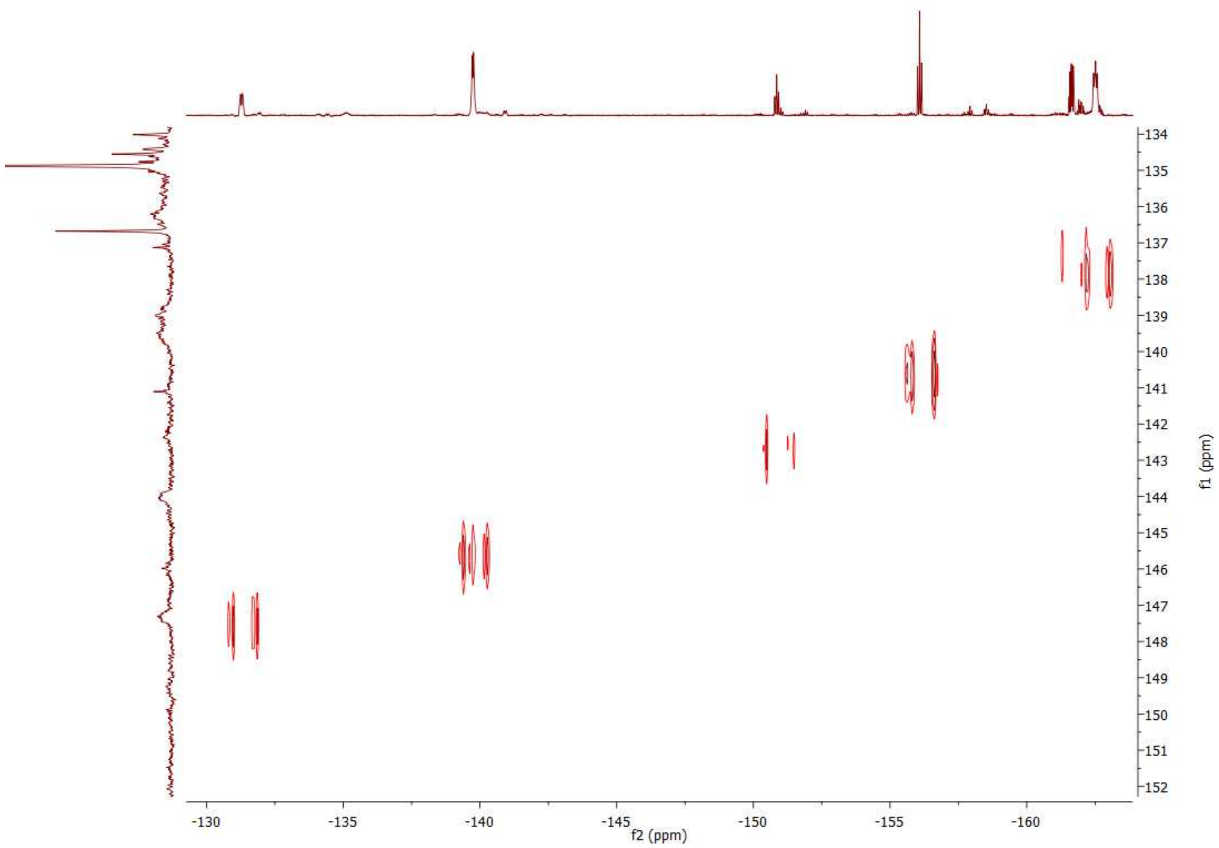


Figure S74. HSQC [^{19}F,^{13}C] NMR spectrum of **3** (282 MHz, 20 °C) in CD_2Cl_2

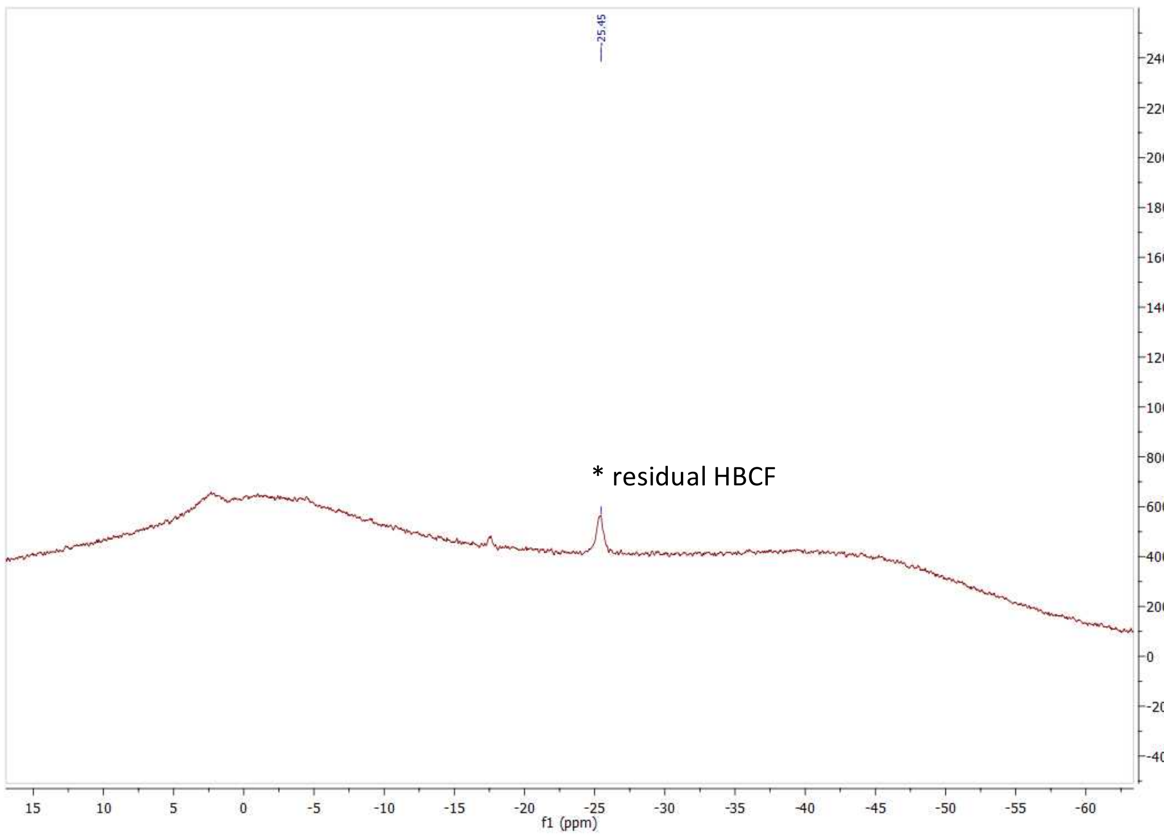


Figure S75. $^{11}B\{^1H\}$ NMR spectrum of **3** (96 MHz, 20 °C) in CD_2Cl_2

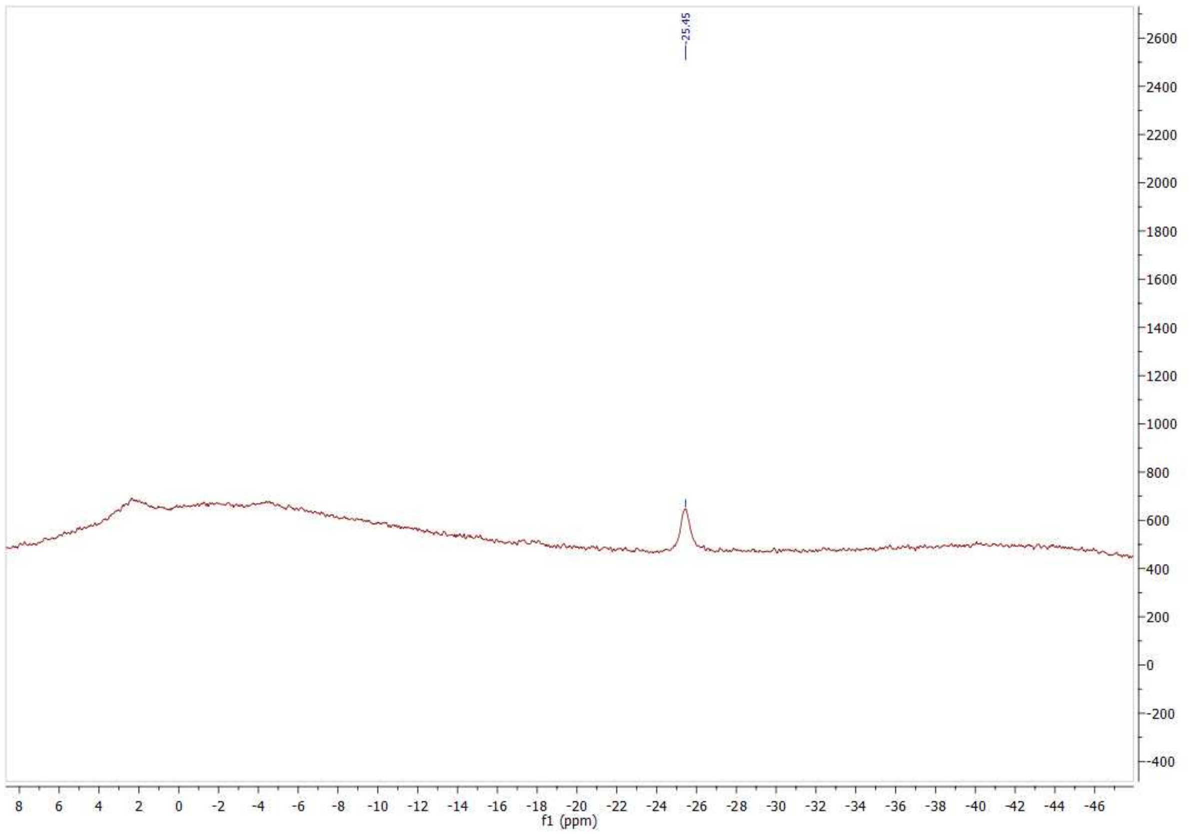


Figure S76. $^{11}B\{^{1}H\}$ NMR spectrum of ^{13}C-labeled **3** (96 MHz, 20 °C) in CD_2Cl_2

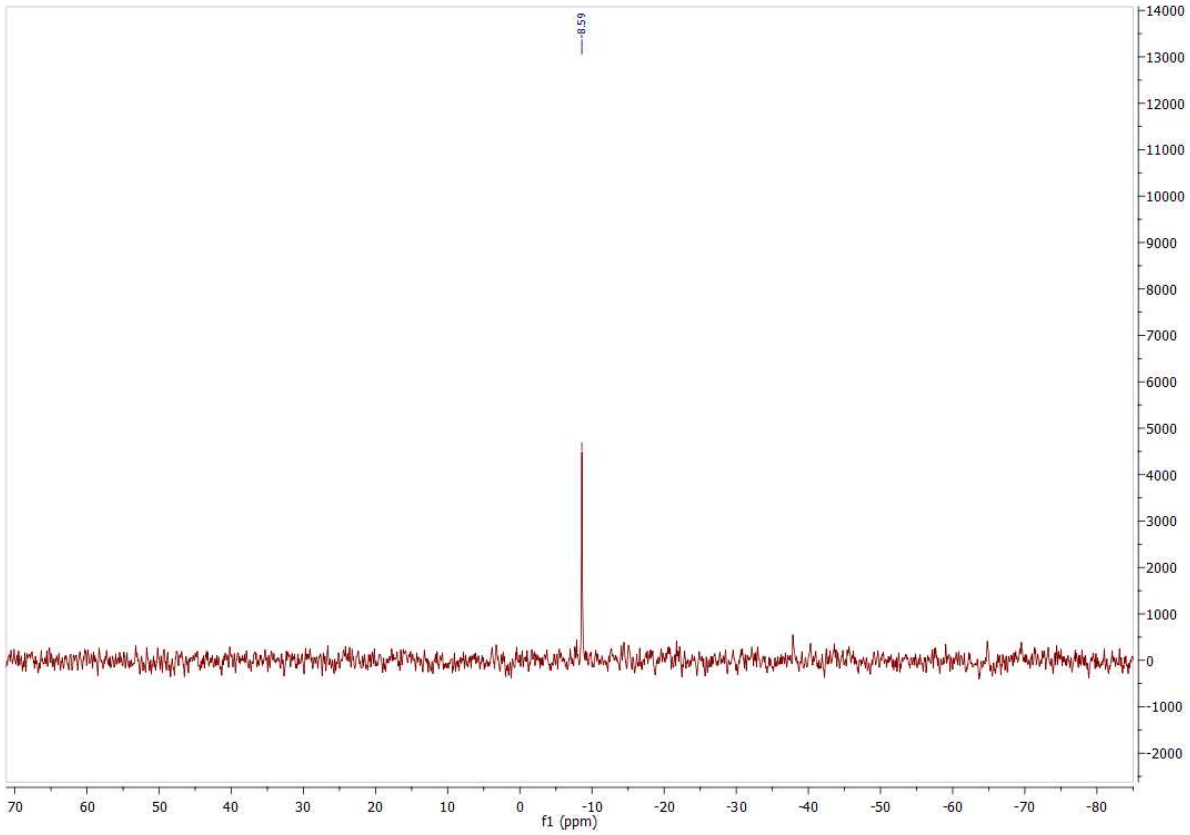


Figure S77. $^{29}Si\{^{1}H\}$ NMR spectrum of **3** (60 MHz, 20 °C) in CD_2Cl_2

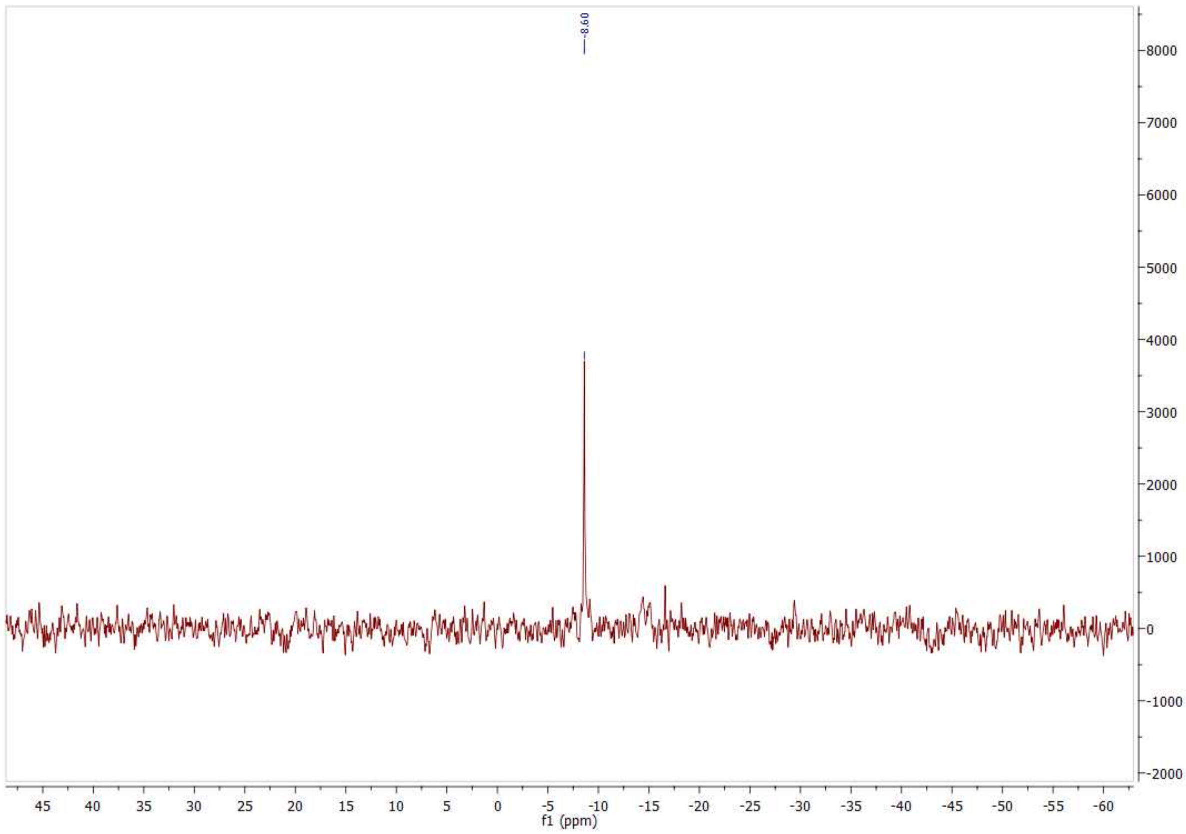


Figure S78. $^{29}Si\{^1H\}$ NMR spectrum of ^{13}C-labeled **3** (60 MHz, 20 °C) in CD_2Cl_2

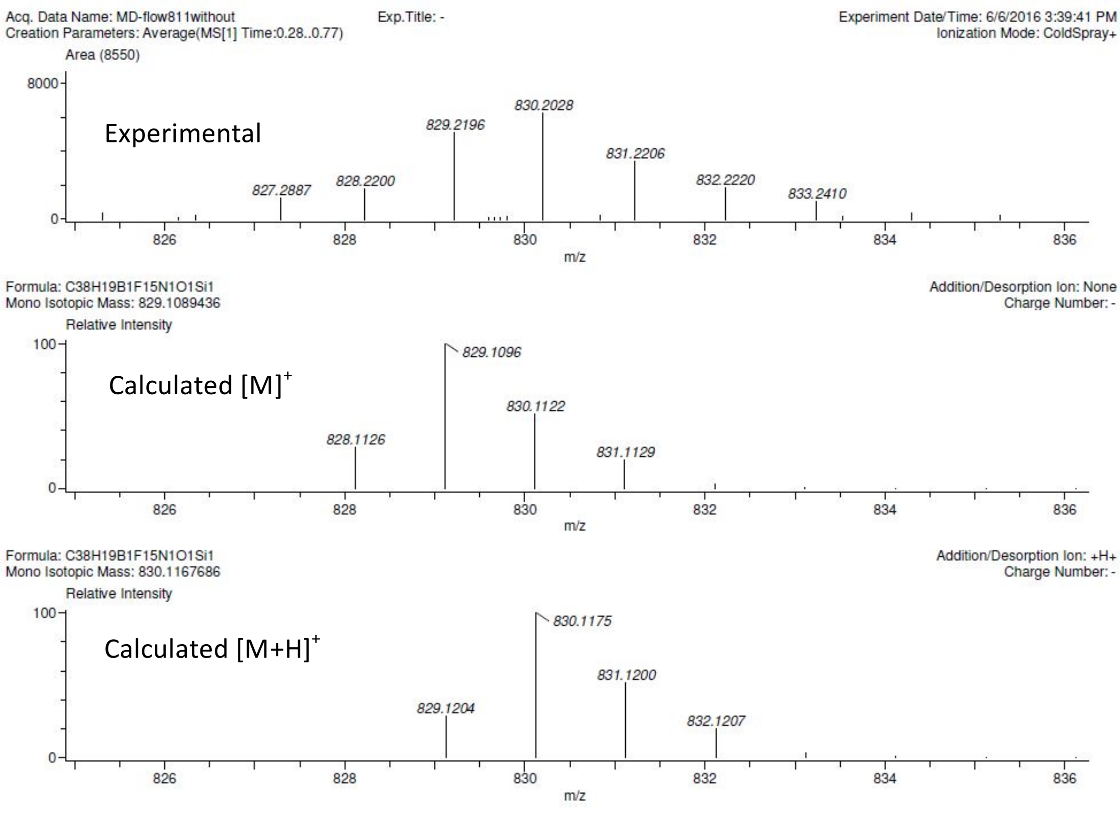


Figure S79. High-resolution mass spectrum of **3**, coldspray ionization, flow injection

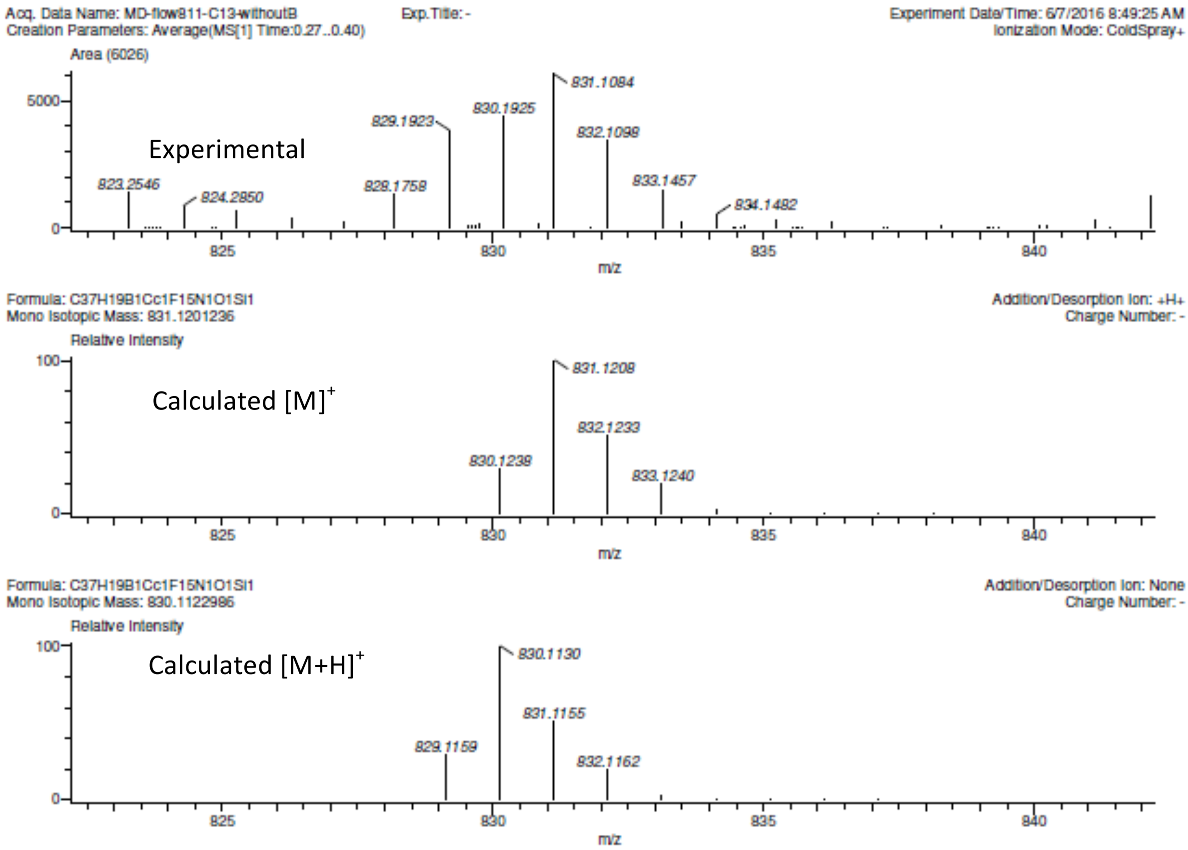
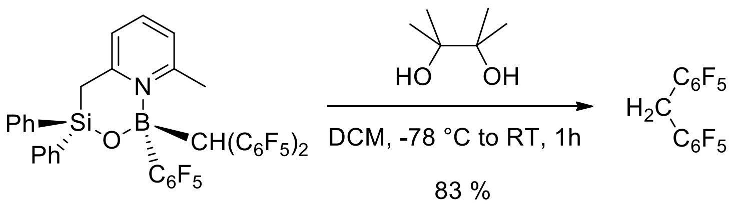


Figure S80. High-resolution mass spectrum of ^{13}C-labeled **3**, coldspray ionization, flow injection

Synthesis of 4



To a in situ prepared solution of **3** (165.8 mg, 0.200 mmol) in dichloromethane (7.3 mL) at -78 °C was dropwise added a solution of pinacol (23.9 mg, 0.201 mmol, 1.01 eq.) in dichloromethane (3.2 mL) under stirring. After completion of the addition, the reaction mixture was allowed to warm up to room temperature and further stirred at this temperature for an additional 30 minutes. The compound was purified by flash chromatography on silica gel and then sublimed under slight vacuum at 45 °C. After work-up, compound **4** was obtained in 83% yield. Crystals suitable for X-ray diffraction were obtained by slow evaporation of a pentane solution at room temperature.

Flash chromatography on silica gel:

-dimension of the column: 22.5 cm X 3 cm
-Rf = 0.45
-mass of silica: 80 g
-eluent: pentane
-volume of eluent before the compound goes out: 200 mL
-volume of solvent for the elution of the compound: 70 mL

Non-labeled bis(pentafluorophenyl)methane

HRMS (GC-EI): exact mass (monoisotopic) calcd for $[C_{13}H_2F10]^+$, 347.9997; found 347.9999.

^{1}H NMR (300 MHz, CD_2Cl_2, δ): 4.10 (s, 2H, CH_2).

$^{13}C\{^1H\}$ NMR (76 MHz, CD_2Cl_2, δ): 15.8 (s, 1C, CH_2), 111.2 (br, 2C, $C_{ipso\text{-}C6F5}$), 138.1 (d br., 4C, $^1J_{CF}$ = 248.5 Hz, $C_{o\text{-}C6F5}$ or $C_{m\text{-}C6F5}$), 141.1 (d br., 2C, $^1J_{CF}$ = 253.5 Hz, $C_{p\text{-}C6F5}$), 145.7 (d br., 4C, $^1J_{CF}$ = 249.3 Hz, $C_{o\text{-}C6F5}$ or $C_{m\text{-}C6F5}$).

$^{19}F\{^1H\}$ NMR (282 MHz, CD_2Cl_2, δ): -163.0 (m, 4F, $F_{m\text{-}C6F5}$), -156.3 (t, 2F, $^3J_{FF}$ = 20.8 Hz, $F_{p\text{-}C6F5}$), -143.0 (m, 4F, $F_{o\text{-}C6F5}$).

Labeled bis(pentafluorophenyl)methane

HRMS (GC-EI): exact mass (monoisotopic) calcd for $[^{13}C_1{}^{12}C_{12}H_2F10]^+$, 349.0030; found 349.0030.

^{1}H NMR (400 MHz, CD_2Cl_2, δ): 4.10 (d, $^1J_{HC}$ = 136.1 Hz, $^{13}CH_2$).

$^{13}C\{^1H\}$ NMR (101 MHz, CD_2Cl_2, δ): 15.8 (s, $^{13}CH_2$), 111.2 (d br., 2C, $^1J_{CC}$ = 46.3 Hz, $C_{ipso\text{-}C6F5}$), 138.1 (d br., 4C, $^1J_{CF}$ = 253.4 Hz, $C_{o\text{-}C6F5}$ or $C_{m\text{-}C6F5}$), 141.0 (d br., 2C, $^1J_{CF}$ = 253.4 Hz, $C_{p\text{-}C6F5}$), 145.7 (d br., 4C, $^1J_{CF}$ = 250.2 Hz, $C_{o\text{-}C6F5}$ or $C_{m\text{-}C6F5}$).

$^{19}F\{^1H\}$ NMR (282 MHz, CD_2Cl_2, δ): -163.0 (m, 4F, $F_{m\text{-}C6F5}$), -156.3 (t, 2F, $^3J_{FF}$ = 20.9 Hz, $F_{p\text{-}C6F5}$), -143.0 (m, 4F, $F_{o\text{-}C6F5}$).

Anal. Calcd. For $C_{13}H_2F_{10}$; C, 44.85; H, 0.58. Found: C, 44.79; H, 0.60.

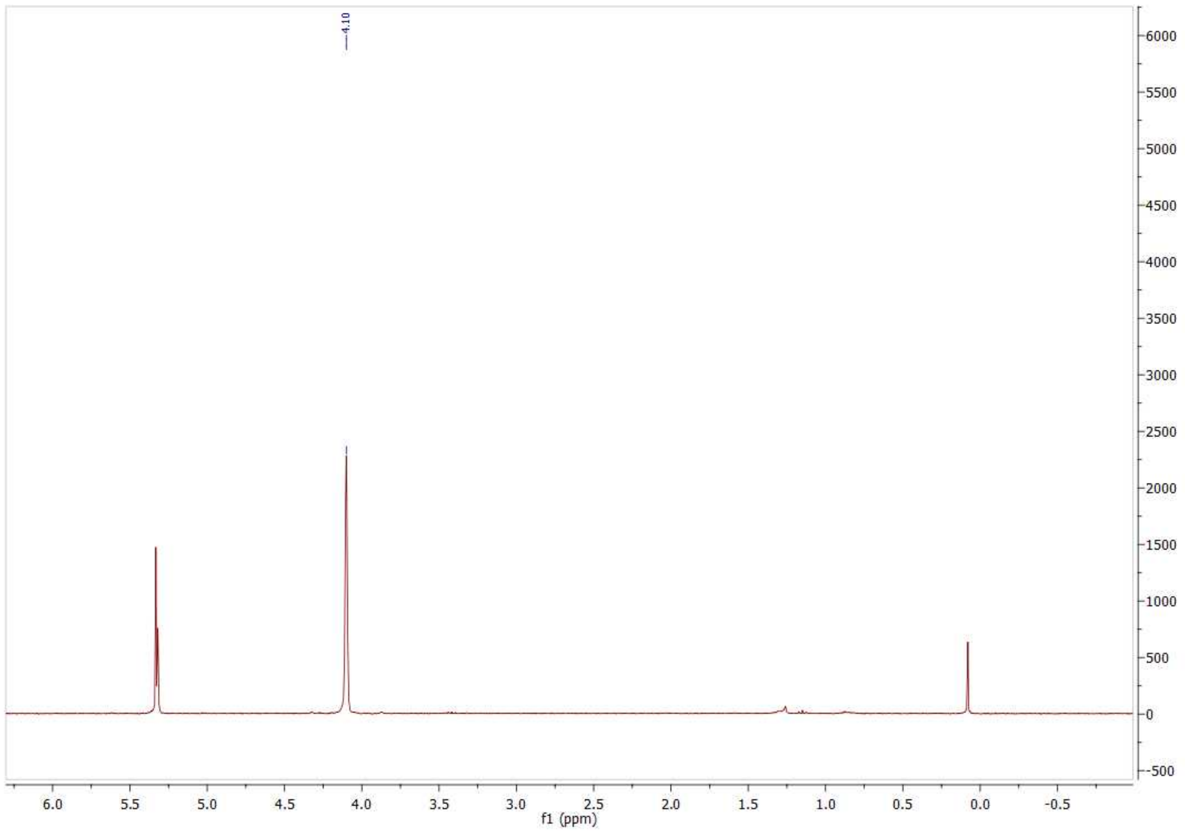


Figure S81. ^{1}H NMR spectrum of **4** (300 MHz, 20 °C) in CD_2Cl_2

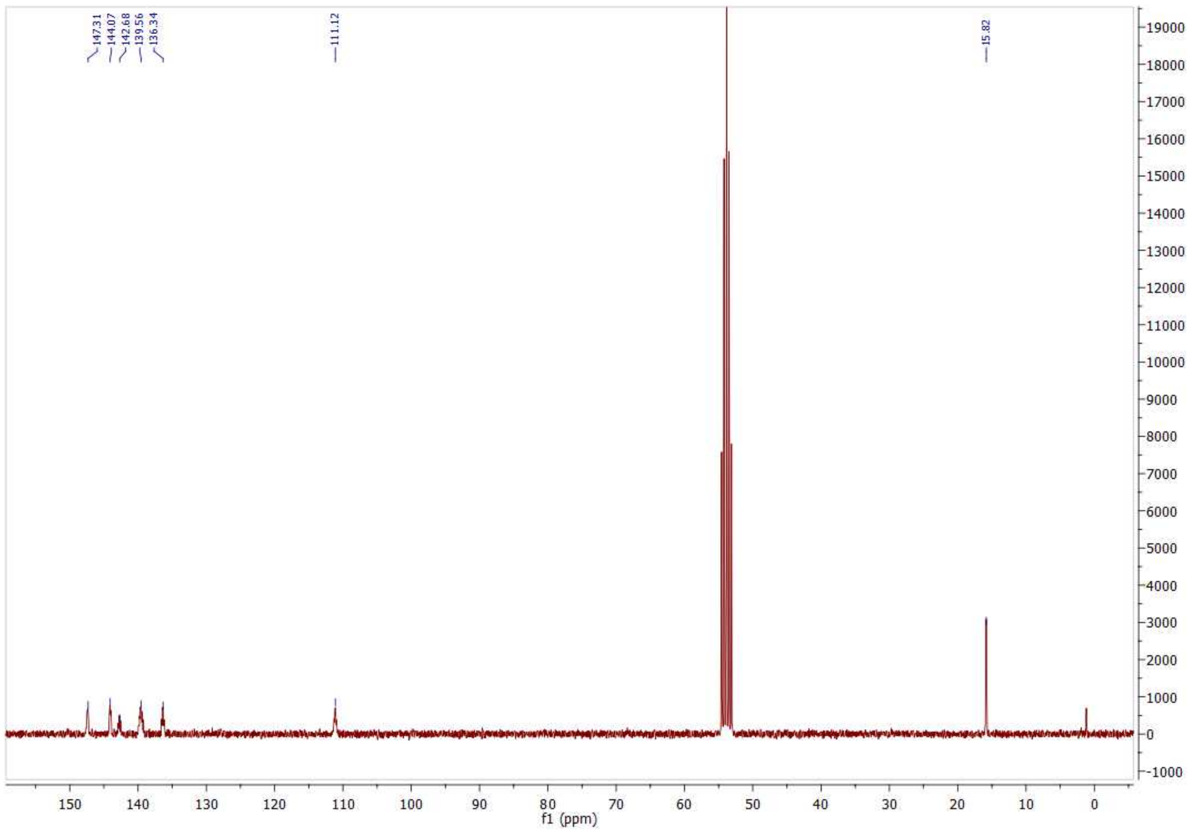


Figure S82. $^{13}C\{^{1}H\}$ NMR spectrum of **4** (76 MHz, 20 °C) in CD_2Cl_2

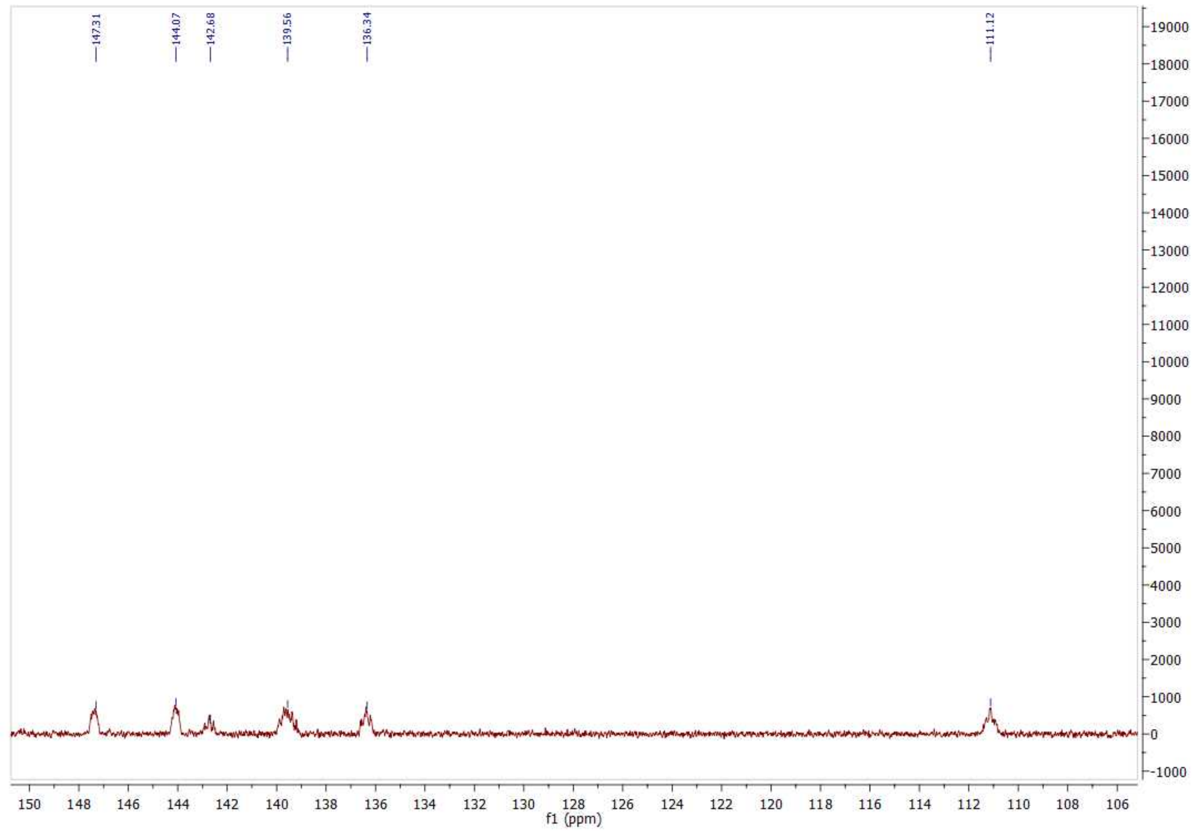


Figure S83. $^{13}C\{^{1}H\}$ NMR spectrum of **4** (76 MHz, 20 °C) in CD_2Cl_2: aromatic region

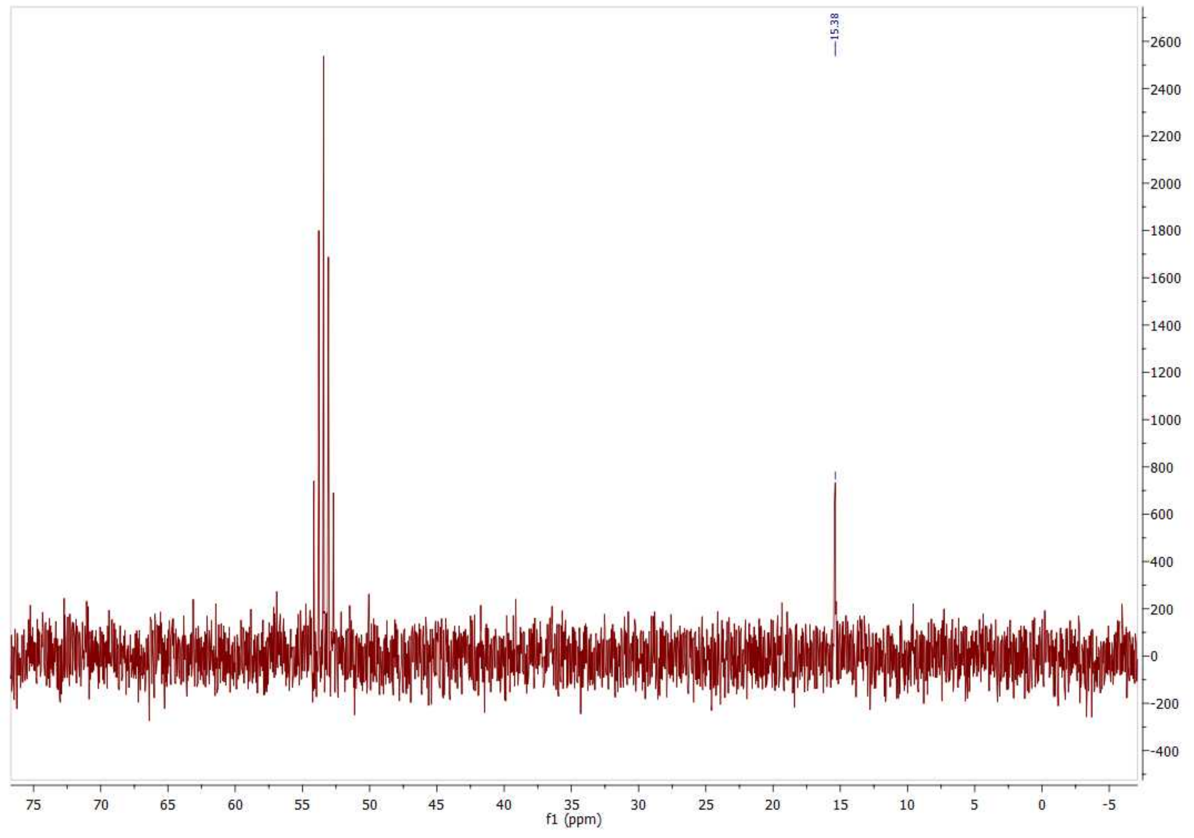


Figure S84. $^{13}C\{^{1}H\}$ NMR spectrum of **4** (76 MHz, 20 °C) in CD_2Cl_2: aliphatic region jmod

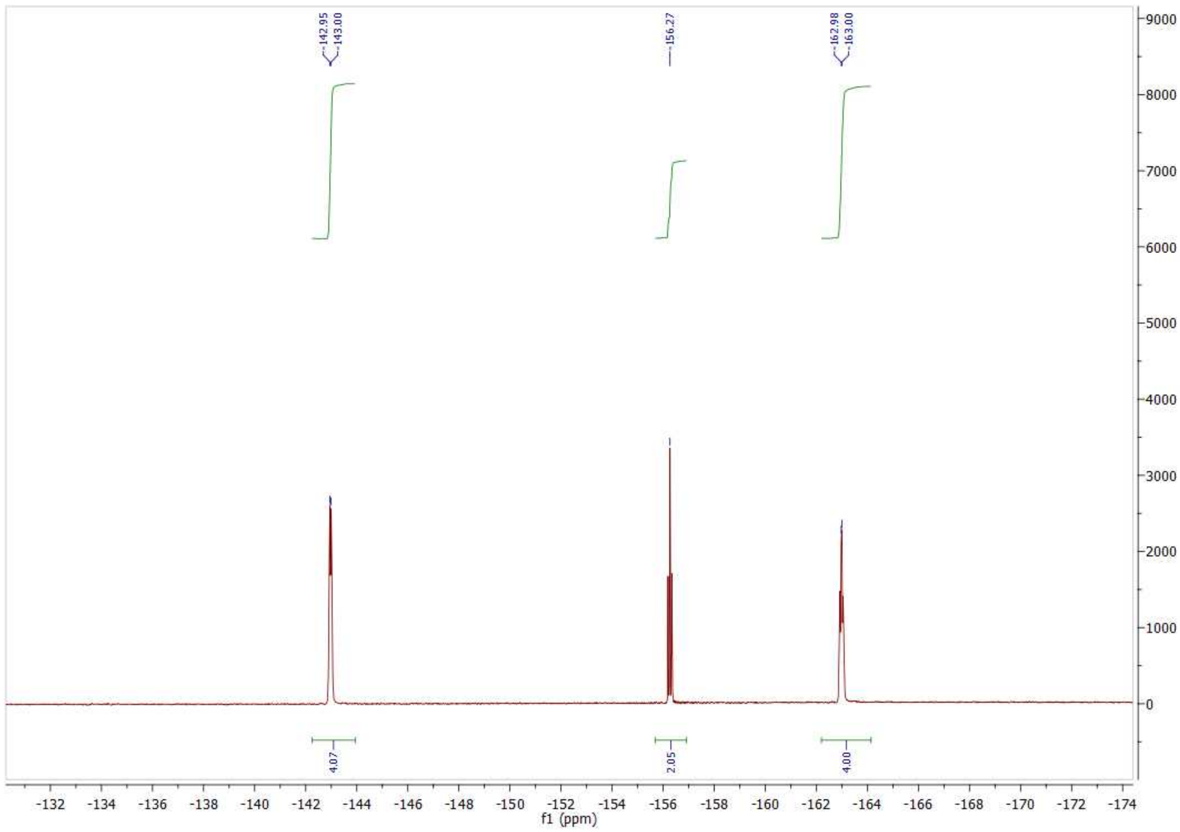


Figure S85. $^{19}F\{^{1}H\}$ NMR spectrum of **4** (282 MHz, 20 °C) in CD_2Cl_2

NMR spectra of ^{13}C-labeled 4

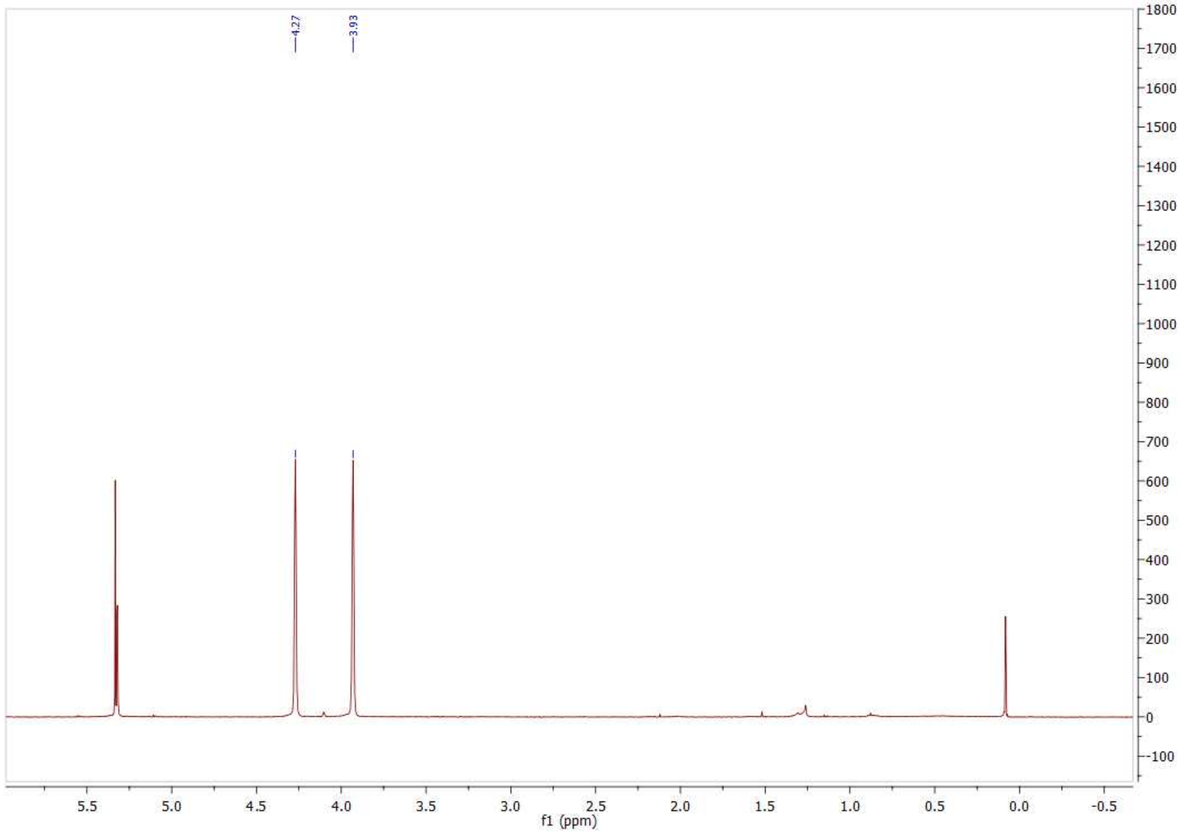


Figure S86. ^{1}H NMR spectrum of ^{13}C-labeled **4** (300 MHz, 20 °C) in CD_2Cl_2

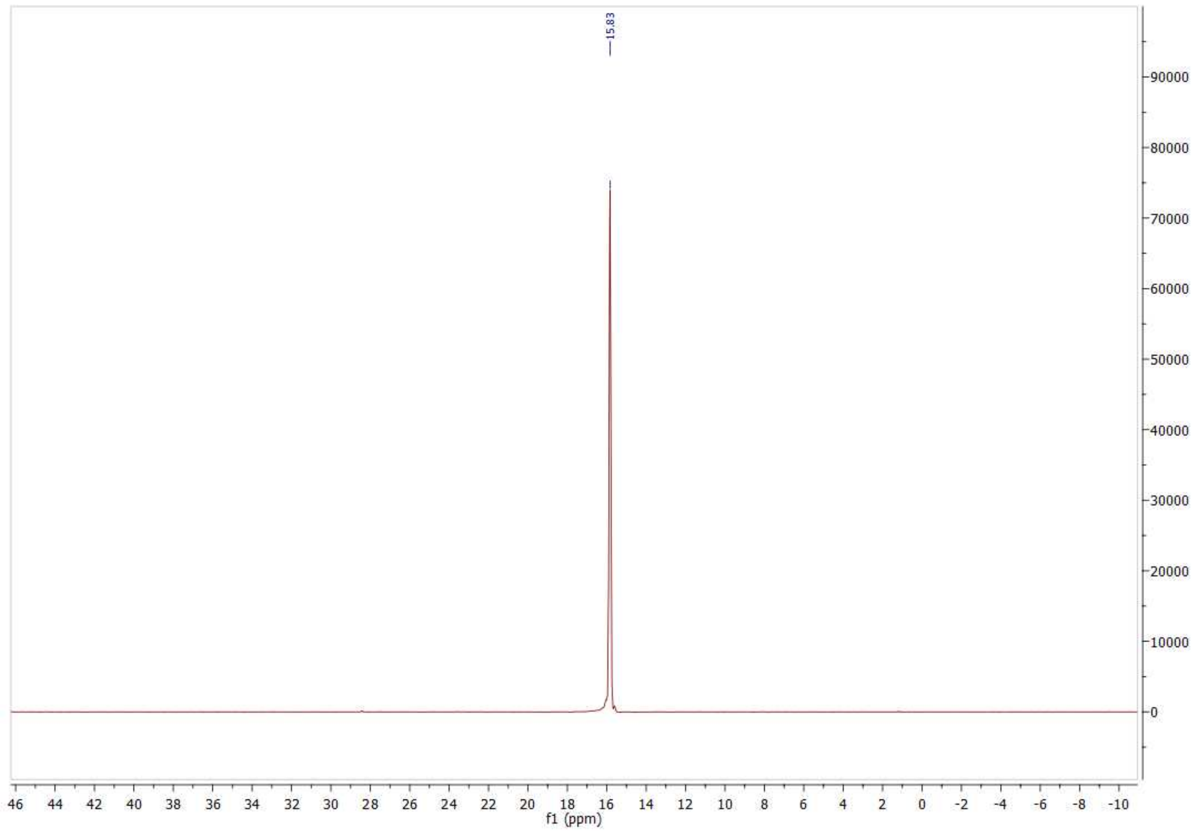


Figure S87. $^{13}C\{^{1}H\}$ NMR spectrum of ^{13}C-labeled **4** (76 MHz, 20 °C) in CD_2Cl_2: aliphatic region

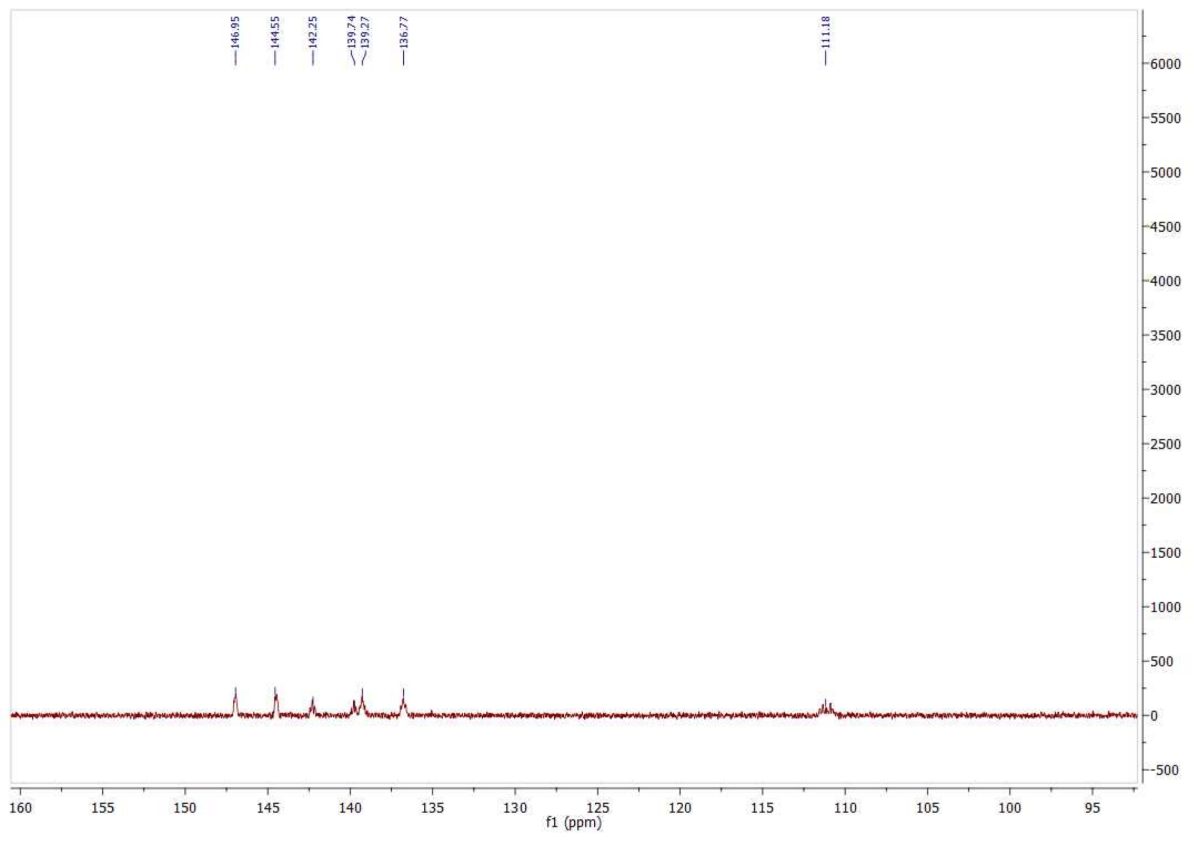


Figure S88. $^{13}C\{^{1}H\}$ NMR spectrum of ^{13}C-labeled **4** (76 MHz, 20 °C) in CD_2Cl_2: aromatic region

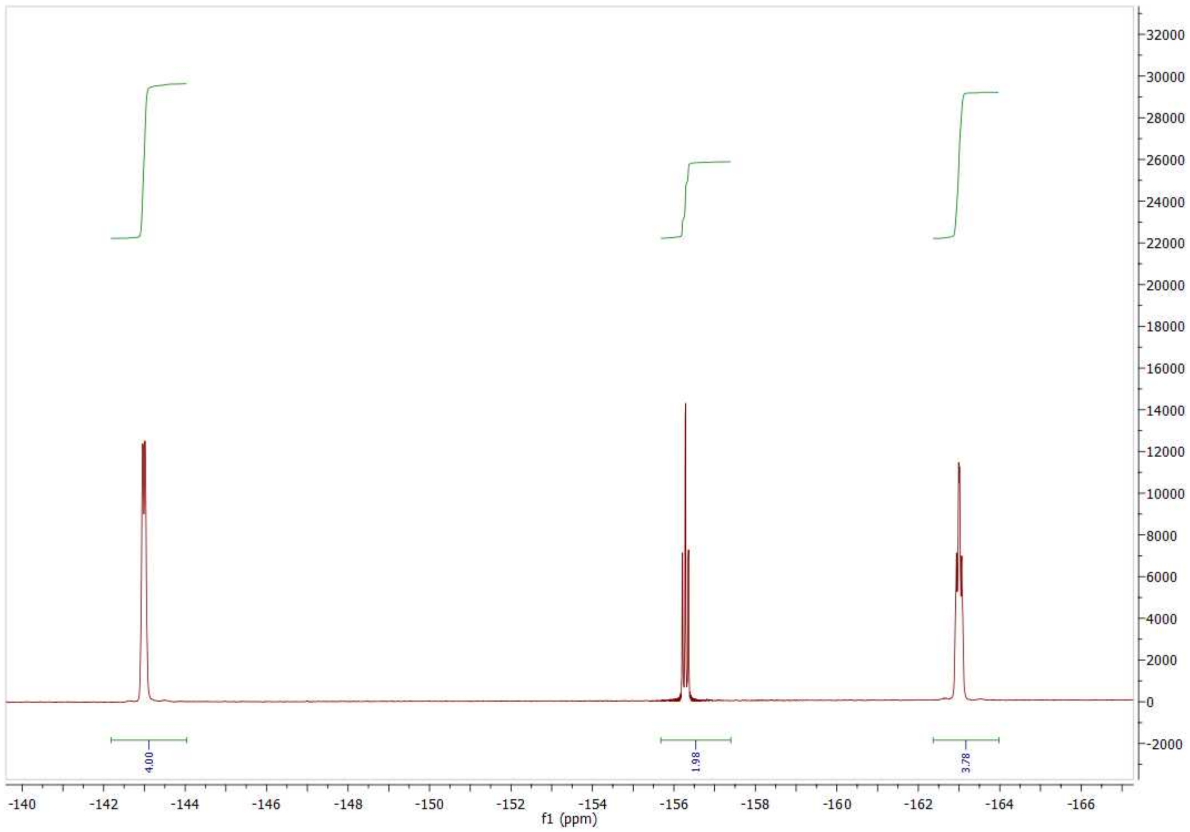
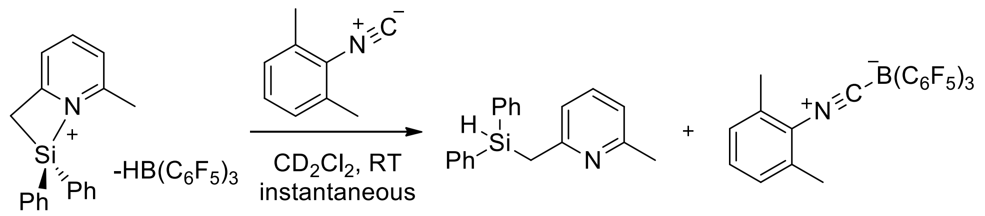


Figure S89. $^{19}F\{^{1}H\}$ NMR spectrum of ^{13}C-labeled **4** (282 MHz, 20 °C) in CD_2Cl_2

Synthesis of 5



2,6-dimethylphenylisocyanide (11.0 mg, 83.3 μmol, 1 eq.) was added to a solution of **1^+-HBCF** (66.8 mg, 83.3 μmol) leading instantaneously to regeneration of silane **1^H** (hydride transfer from boron to silylium) and formation of the isocyanide-borane Lewis pair **5** as the only compounds that could be detected by NMR spectroscopy. The adduct was characterized in situ by multinuclear NMR spectroscopy.

[DMP = 2,6-dimethylphenyl]

^{1}H NMR (300 MHz, CD_2Cl_2, δ): 2.39 (s, 6H, CH_3), 7.23 (m, 2H, $CH_{m\text{-DMP}}$), 7.42 (t, 1H, $CH_{p\text{-DMP}}$).

^{13}C{^{1}H} NMR (76 MHz, CD_2Cl_2, δ): 18.1 (s, 2C, CH_3), 129.3 (s, 2C, $CH_{m\text{-DMP}}$), 133.0 (s, 1C, $CH_{p\text{-DMP}}$), 137.7 (d br., 6C, $^1J_{CF}$ = 245.5 Hz, C-$F_{o\text{-C6F5}}$ or C-$F_{m\text{-C6F5}}$), 137.9 (s, 2C, $C_{o\text{-DMP}}$) 140.8 (d br., 3C, $^1J_{CF}$ = 145.0 Hz, C-$F_{p\text{-C6F5}}$), 148.5 (d br., 6C, $^1J_{CF}$ = 242.2 Hz, C-$F_{p\text{-C6F5}}$). The $C_{ipso\text{-C6F5}}$ was not observed.

^{11}B{^{1}H} NMR (96 MHz, CD_2Cl_2, δ): -20.9 (s).

^{19}F{^{1}H} NMR (282 MHz, CD_2Cl_2, δ): -163.7 (br., 6F, $F_{m\text{-C6F5}}$), -156.6 (t, 3F, $^3J_{FF}$ = 20.0 Hz, $F_{p\text{-C6F5}}$), -132.5 (br., 6F, $F_{o\text{-C6F5}}$).

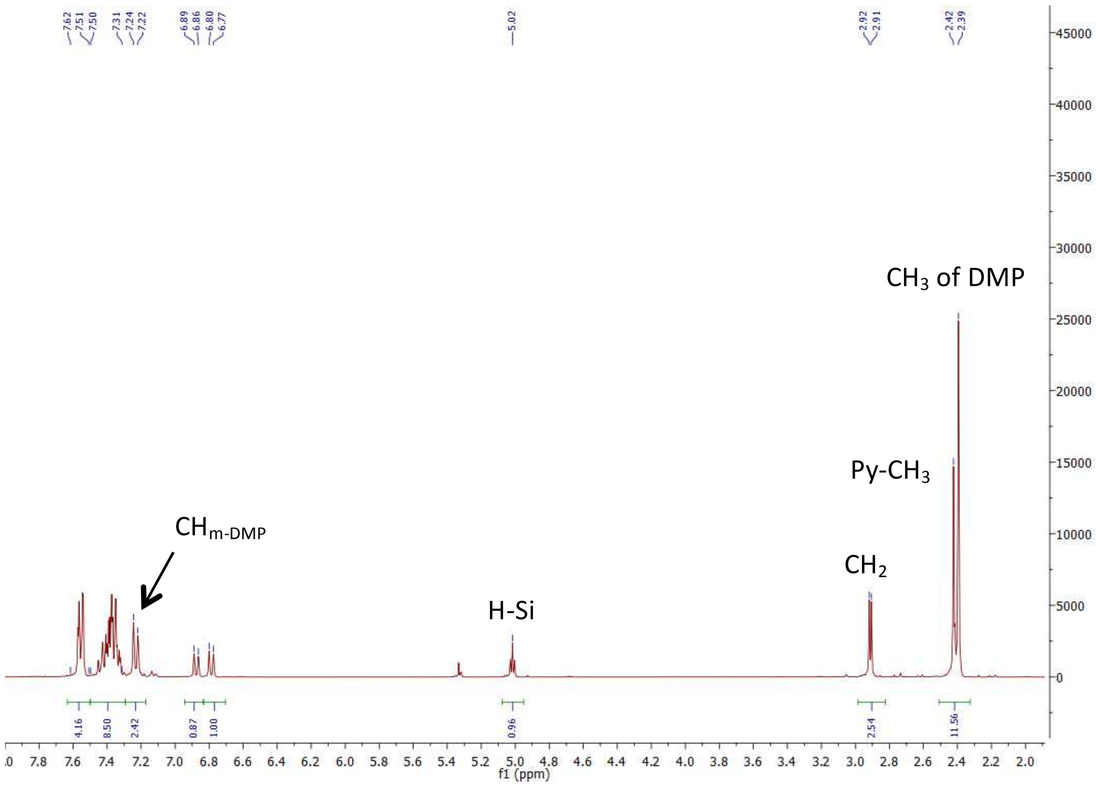


Figure S90. ^{1}H NMR spectrum of the mixture of **5** and **1^H** (300 MHz, 20 °C) in CD_2Cl_2. DMP = 2,6-dimethylphenyl

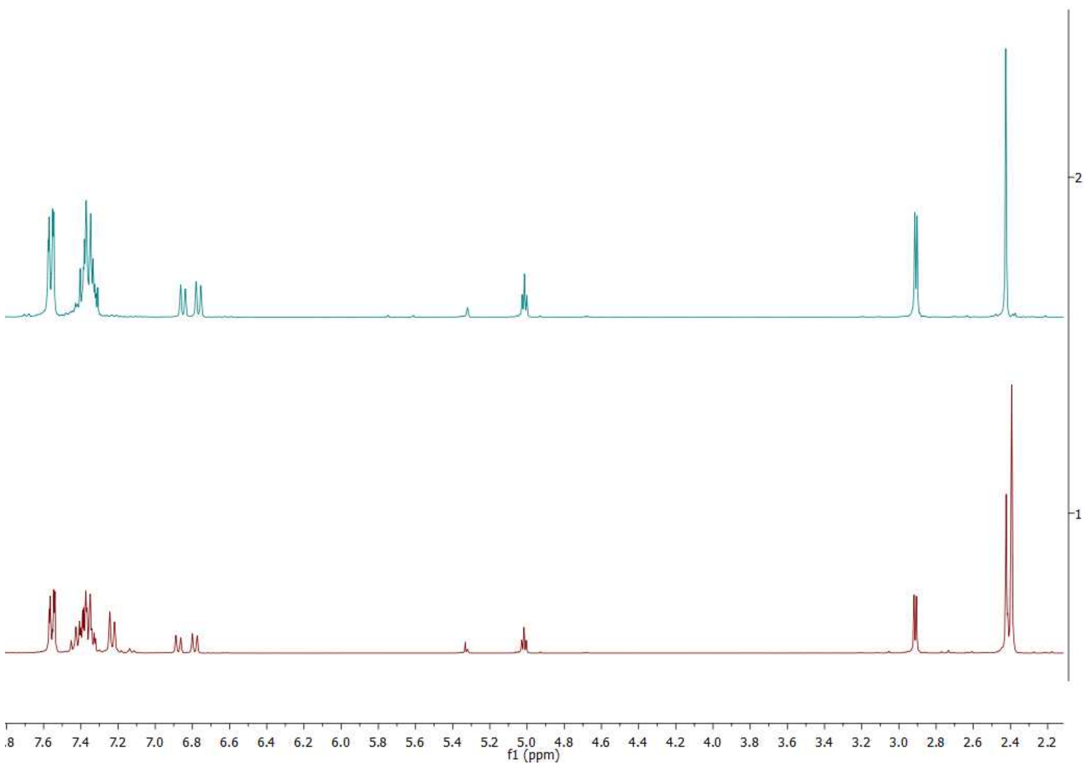


Figure S91. Stacked ^{1}H NMR spectra of **1^H** (top) and of the mixture of **5** and **1^H** (bottom) (300 MHz, 20 °C) in CD_2Cl_2

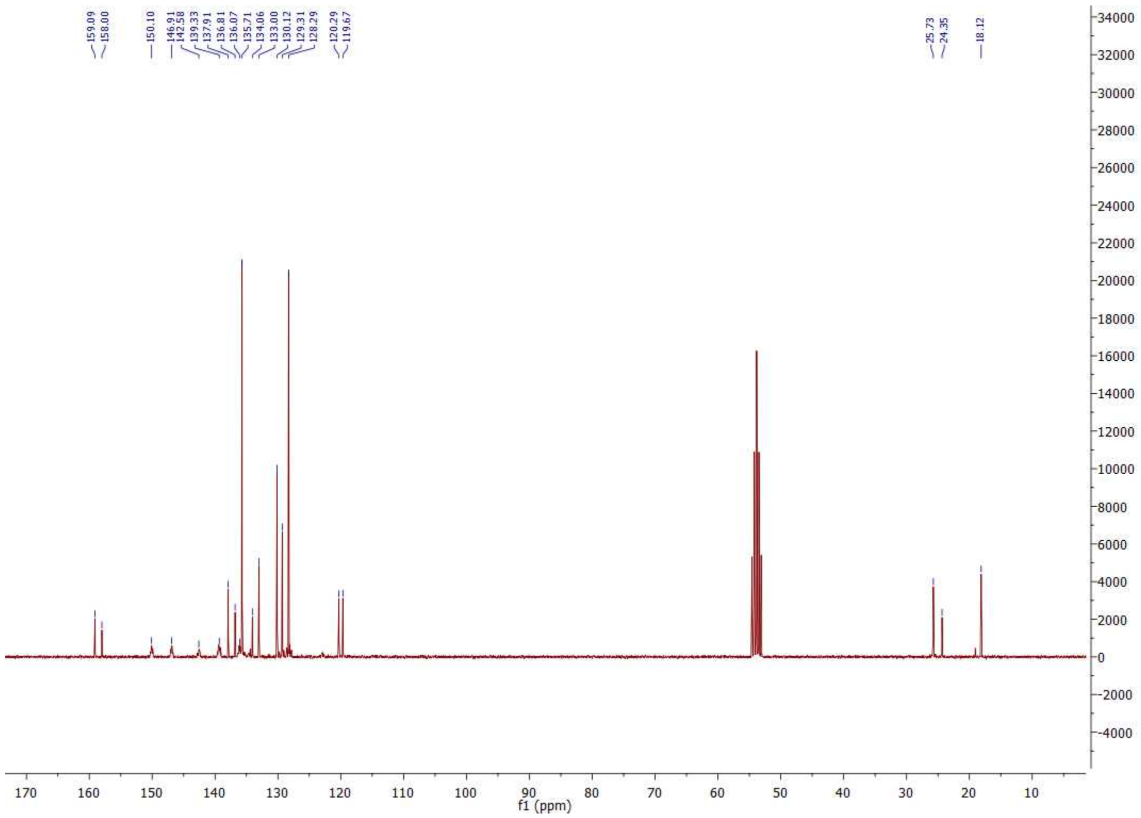


Figure S91. $^{13}C\{^{1}H\}$ NMR spectrum of the mixture of **5** and $\mathbf{1^{H}}$ (76 MHz, 20 °C) in CD_2Cl_2

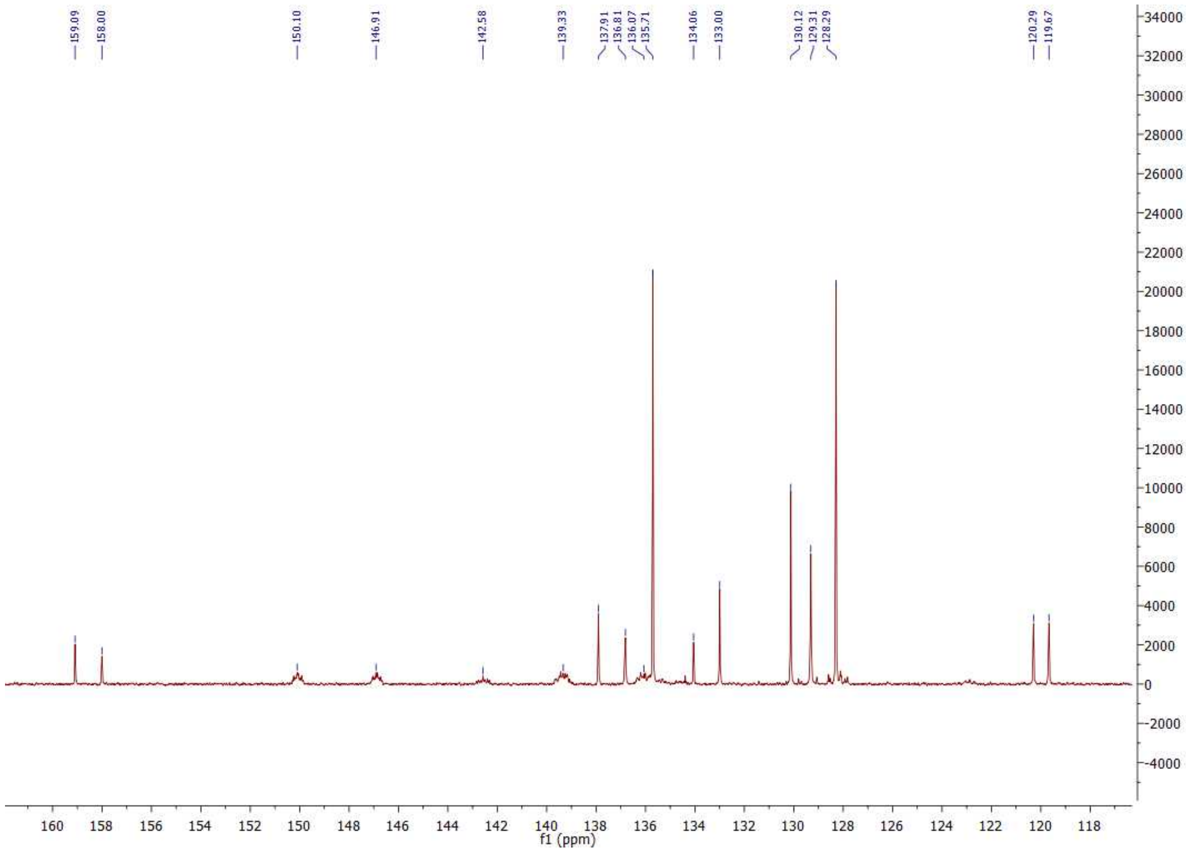


Figure S92. $^{13}C\{^{1}H\}$ NMR spectrum of the mixture of **5** and $\mathbf{1^{H}}$ (76 MHz, 20 °C) in CD_2Cl_2: aromatic region

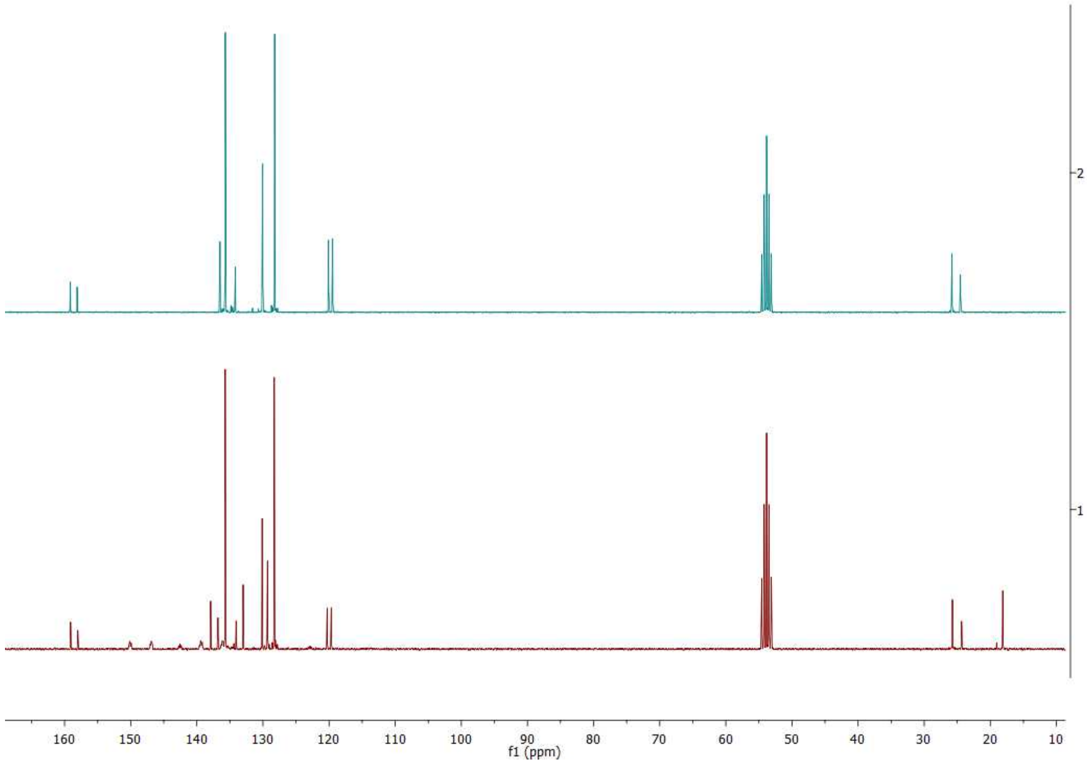


Figure S93. Stacked $^{13}C\{^{1}H\}$ NMR spectra of $\mathbf{1^{H}}$ (top) and of the mixture of **5** and $\mathbf{1^{H}}$ (bottom) (76 MHz, 20 °C) in CD_2Cl_2

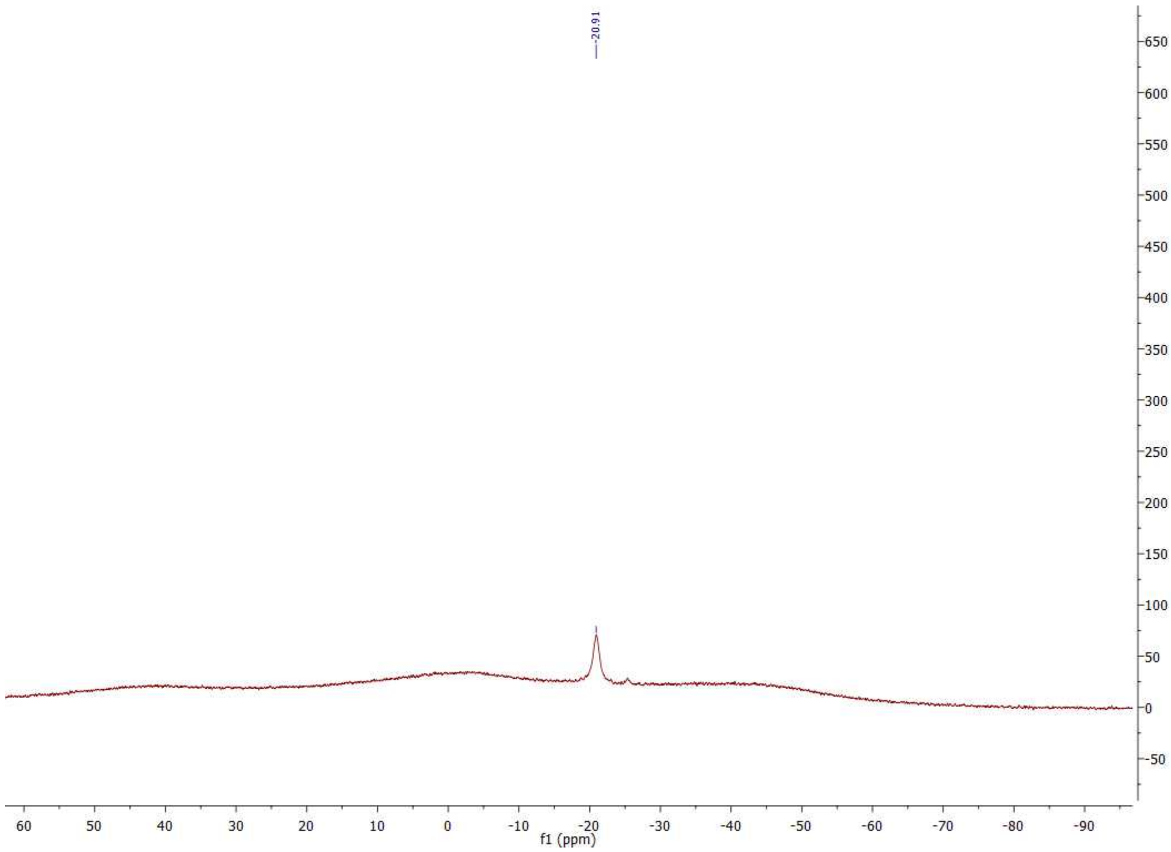


Figure S94. $^{11}B\{^1H\}$ NMR spectrum of the mixture of **5** and $\mathbf{1^H}$ (96 MHz, 20 °C) in CD_2Cl_2

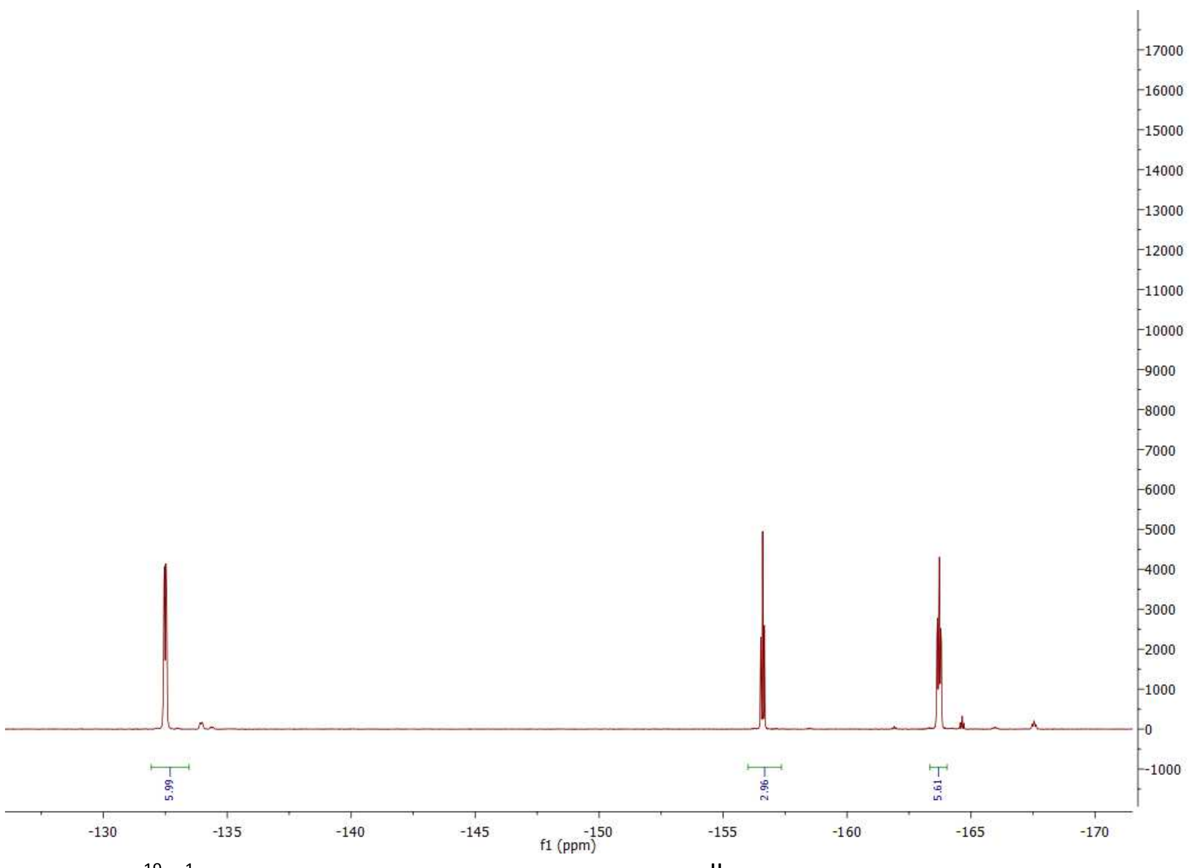
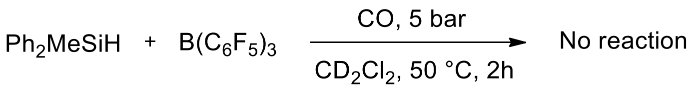


Figure S95. $^{19}F\{^1H\}$ NMR spectrum of the mixture of **5** and $\mathbf{1^H}$ (96 MHz, 20 °C) in CD_2Cl_2

Control experiments to verify the requirement for both 1[H] and BCF as reagents to afford CO activation and triple bond rupture

Control experiment 1



CD_2Cl_2 (0.5 mL) was added to diphenylmethylsilane (4.88 μL, 24.5 μmol) and tris(pentafluorophenyl)borane (12.5 mg, 24.5 μmol, 1 eq.) in a NMR tube suitable for reactions under pressure. Then, the tube was pressurized with 5 bar of carbon monoxide and heated at 50 °C. No reaction was observed after two hours at 50 °C according to multinucleus NMR monitoring.

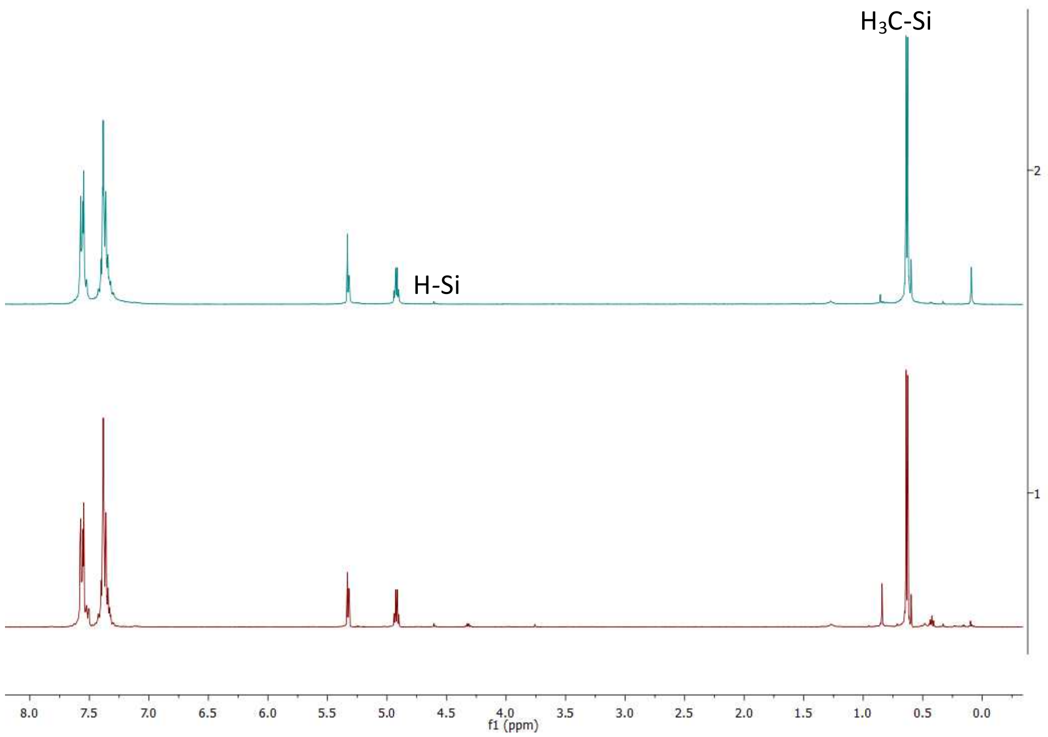


Figure S96. Stacked ^1H NMR spectra before pressurization with CO (top) and after heating for 2 hours in presence of 5 bar of CO (bottom) (300 MHz, 20 °C) in CD_2Cl_2

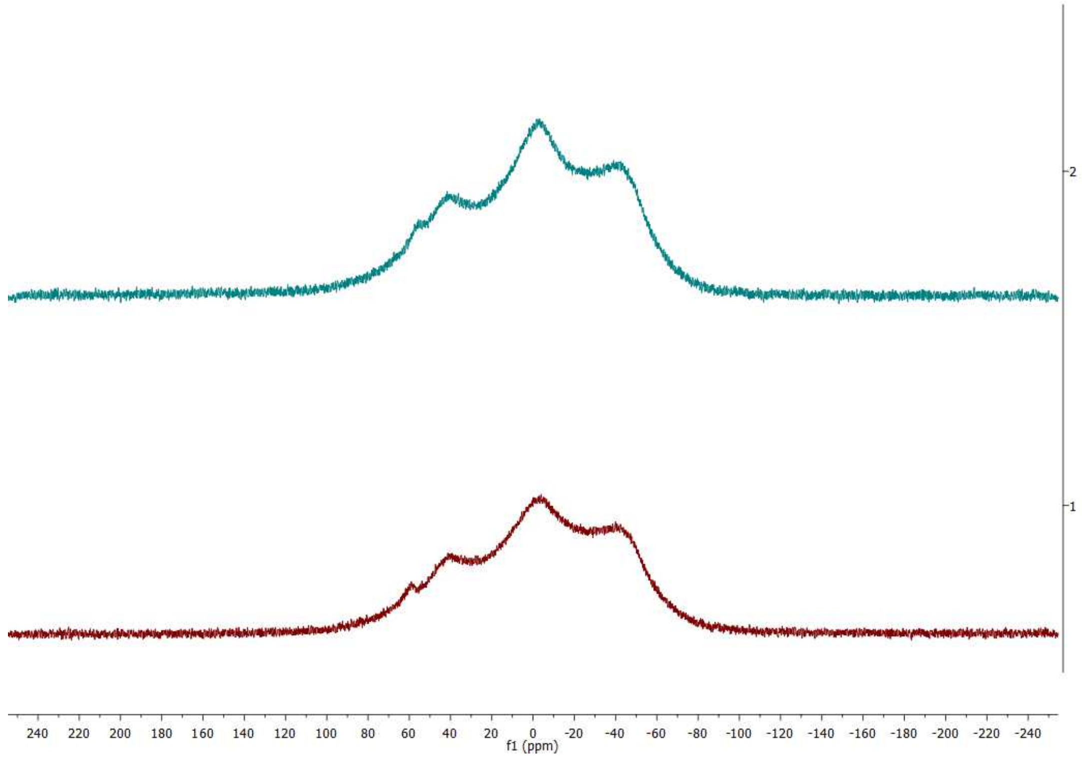


Figure S97. Stacked $^{11}B\{^{1}H\}$ NMR spectra before pressurization with CO (top) and after heating for 2 hours in presence of 5 bar of CO (bottom) (96 MHz, 20 °C) in CD_2Cl_2

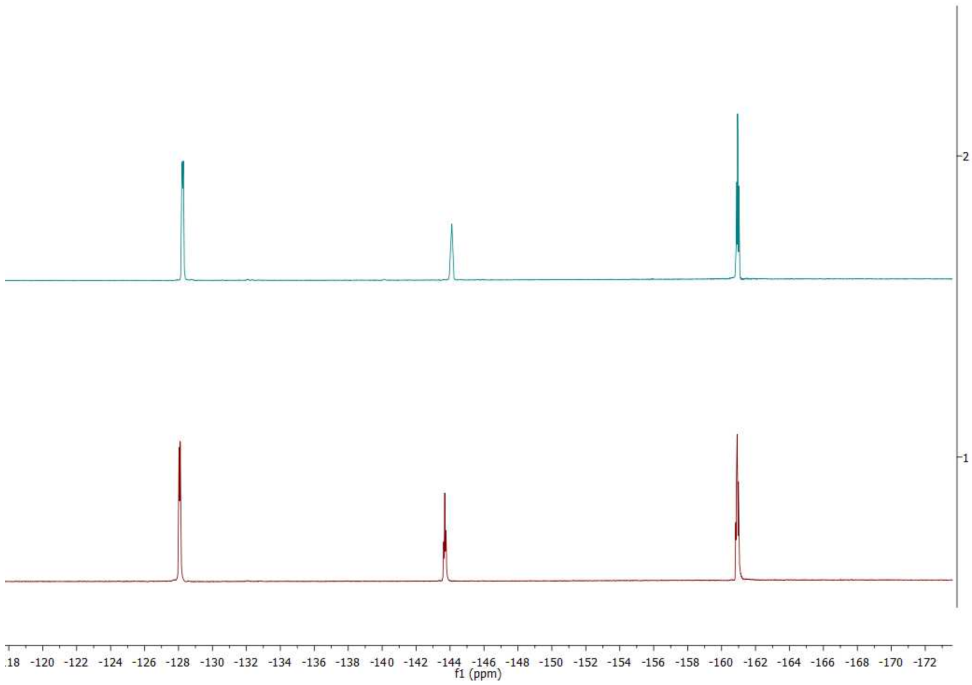
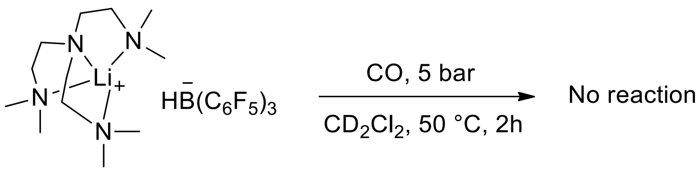


Figure S98. Stacked $^{19}F\{^{1}H\}$ NMR spectra before pressurization with CO (top) and after heating for 2 hours in presence of 5 bar of CO (bottom) (282 MHz, 20 °C) in CD_2Cl_2

Control experiment 2



An NMR tube suitable for reactions under pressure containing a solution of lithium (dimethylamino)ethyl]amine hydridotris(pentafluorophenyl)borate (22.2 mg, 29.6 mmol) in CD_2Cl_2 (0.5 mL) was pressurized with 5 bar of carbon monoxide and heated at 50 °C. Upon monitoring the reaction in time, no reaction was observed even after 2 hours at 50 °C, according to multinuclear NMR spectroscopy.

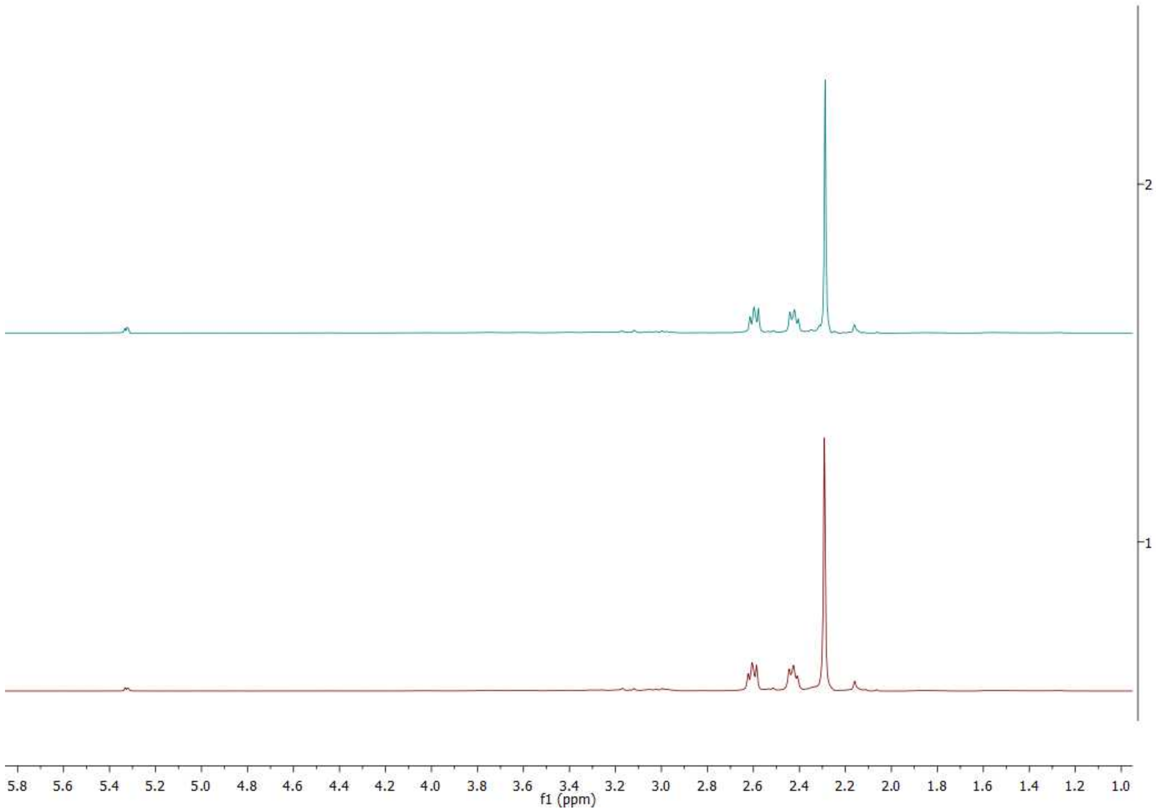


Figure S99. Stacked ^{1}H NMR spectra before pressurization with CO (bottom) and after heating for 2 hours in presence of 5 bar of CO (top) (300 MHz, 20 °C) in CD_2Cl_2

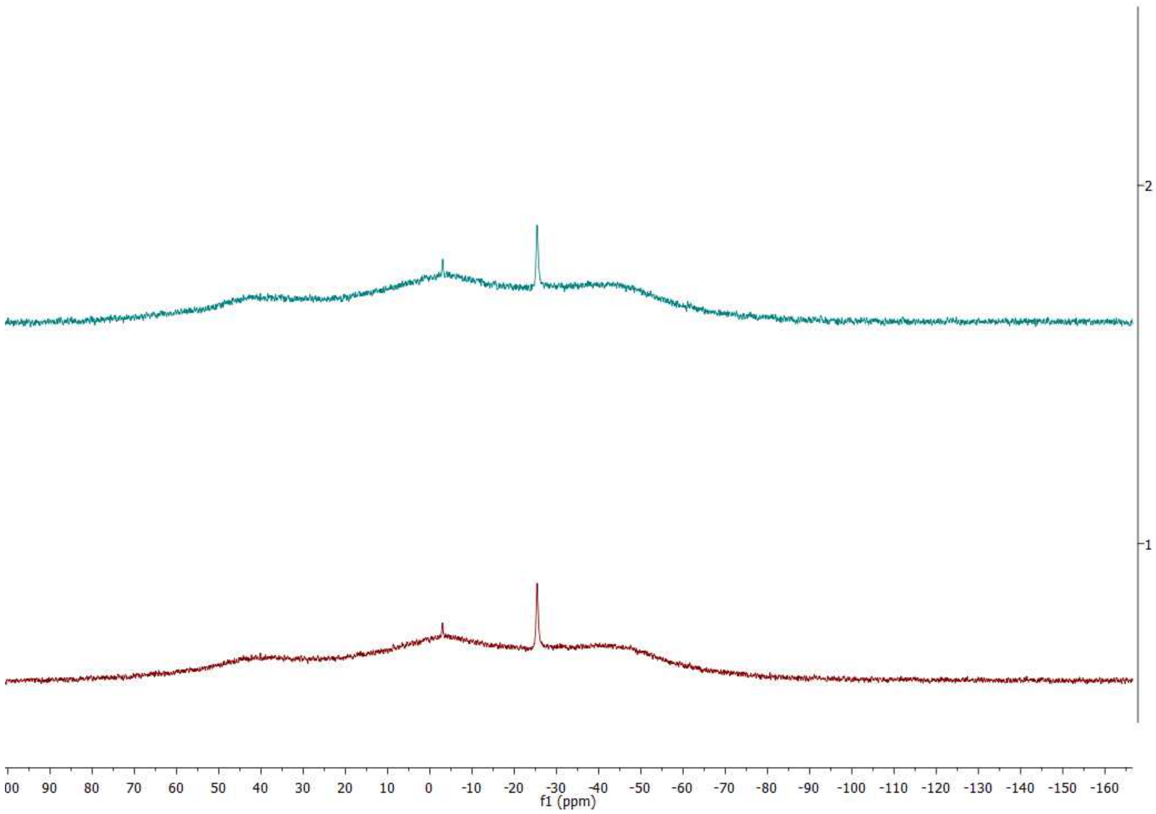


Figure S100. Stacked $^{11}B\{^{1}H\}$ NMR spectra before pressurization with CO (bottom) and after heating for 2 hours in presence of 5 bar of CO (top) (96 MHz, 20 °C) in CD_2Cl_2

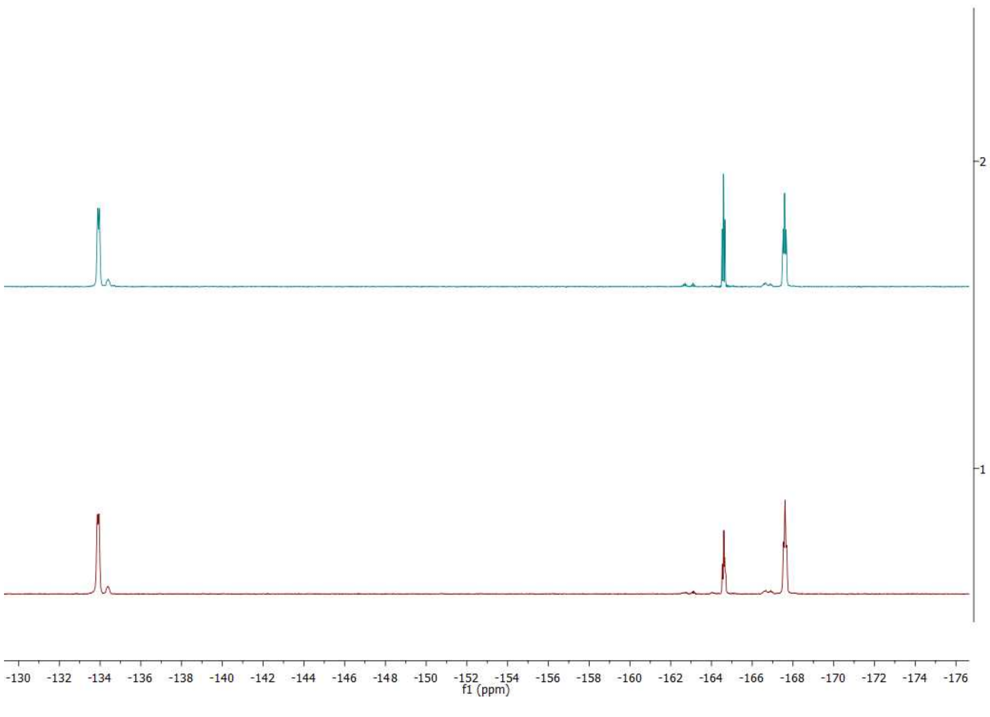
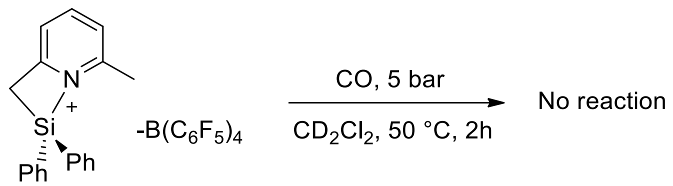


Figure S101. Stacked $^{19}F\{^{1}H\}$ NMR spectra before pressurization with CO (bottom) and after heating for 2 hours in presence of 5 bar of CO (top) (282 MHz, 20 °C) in CD_2Cl_2

Control experiment 3



An NMR tube suitable for reactions under pressure containing a solution of **1^+-BAr$^F_4$** (12.3 mg, 12.7 μmol) in CD_2Cl_2 (0.5 mL) was pressurized with 5 bar of carbon monoxide and heated at 50 °C. Upon monitoring the reaction in time, no reaction was observed even after 2 hours at 50 °C, according to multinuclear NMR spectroscopy.

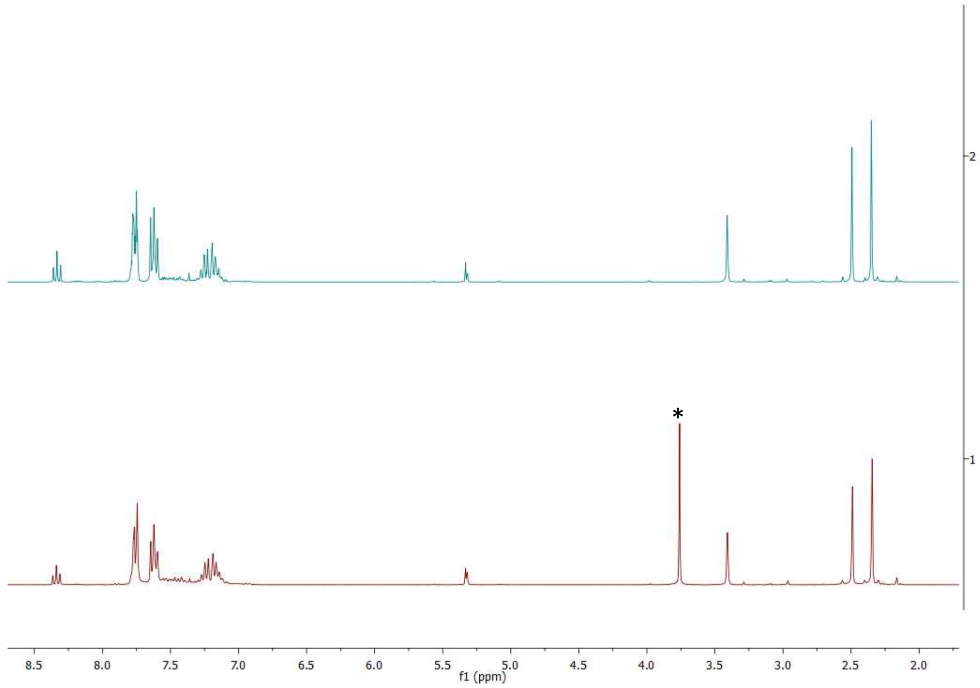
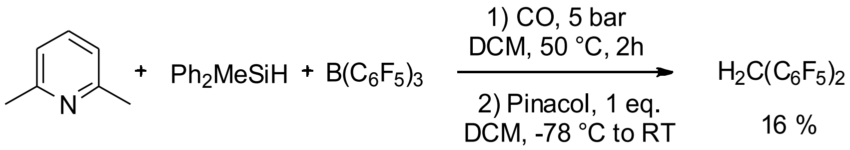


Figure S102. Stacked ^1H NMR before CO pressure (top) and after heating for 2 hours in presence of 5 bar of CO (bottom) (300 MHz, 20 °C) in CD_2Cl_2. ∗Signal of the methylene protons of dichloroethane (internal standard)

Control experiment 4

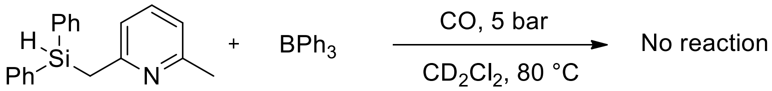


Lutidine (34.1 μL, 0.29 mmol, 1 eq.) in dichloromethane (1 mL) was added to a solution of methyldiphenylsilane (58.6 μL, 0.29 mmol) and tris(pentafluorophenyl)borane (150 mg, 0.29 mmol) in dichloromethane (5 mL) in a flask adapted with a J-Young valve. The flask was pressurized with carbon monoxide (5 bar) and heated at 50 °C for 2h. After release of pressure, a stirring bar was introduced under nitrogen in the valve and the solution was cooled down to -78 °C. Pinacol (34.6 mg, 0.29 mmol, 1 eq) in dichloromethane (2 mL) was added at -78 °C dropwise under stirring and the resulting solution was allowed to warm up to room temperature. After evaporation of the volatiles under reduced pressure, the compound was purified by column chromatography on silica gel and sublimed afterwards (yield: 16%).

Chromatography column on silica gel:

-dimension of the column: 22 cm X 3 cm
-Rf = 0.45
-mass of silica: 70 g
-eluent: pentane
-volume of eluent before the compound goes out: 270 mL
-volume of solvent for the elution of the compound: 55 mL

Control experiment 5



CD_2Cl_2 (0.5 mL) was added to a mixture of $\mathbf{1^H}$ (7.7 mg, 26.7 μmol) and triphenylborane (6.4 mg, 26.7 μmol, 1 eq.) in a NMR pressure tube. The tube was pressurized with 5 bar of carbon monoxide and heated. Upon monitoring the reaction in time, no reaction was observed after 15 hours at 80 °C, according to multinuclear NMR spectroscopy.

Computational details

The mechanism of the CO splitting reaction was explored computationally, using DFT. Full-atom models were used throughout. Geometry optimizations were carried out with the Turbomole program package[S4] coupled to the PQS Baker optimizer[S5] via the BOpt package.[S6] We used unrestricted ri-DFT-D3 calculations at the BP86 level,[S7] in combination with the def2-TZVP basis set,[S8] and a small (m4) grid size. Grimme's dispersion corrections[S9] (version 3, disp3, 'zero damping') were used to include Van der Waals interactions. All minima (no imaginary frequencies) and transition states (one imaginary frequency) were characterized by calculating the Hessian matrix. ZPE and gas-phase thermal corrections (entropy and enthalpy, 298 K, 1 bar) from these analyses were calculated. The nature of the transition states was confirmed by following the intrinsic reaction coordinate. The relative free energies ($\Delta G°_{298K}$ in kcal mol^{-1}) obtained from these calculations are reported in the main text. The energies and entropies ($\Delta G°_{298K}$, $\Delta H°$, $\Delta S°$, SCF+ZPE, SCF) and negative eigenvalues of the transition states and all optimized geometries are provided in the following Tables as well as in a separate archive file.

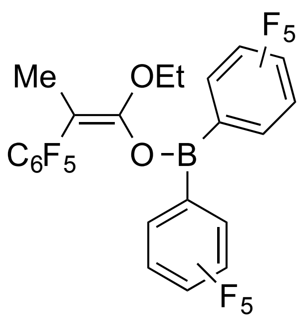
^{11}B NMR chemical shifts were computed with Turbomole using the mpshift module.[S10]

	shielding constant	**referenced to BF_3OEt_2**
BF_3OEt_2	96.15682679	0.0
BH_4-	98.27320507	-2.1
B_ref_3_coord	63.15079858	33.0
B_ref_4_coord	99.73644475	-3.6
3	92.85565169	3.3
3'	57.59533155	**38.6**
Experimental ^{11}B shift of compound **3**		**-25.4**

$\delta_{subst} = \delta_{ref} + \sigma_{ref} - \sigma_{subst}$

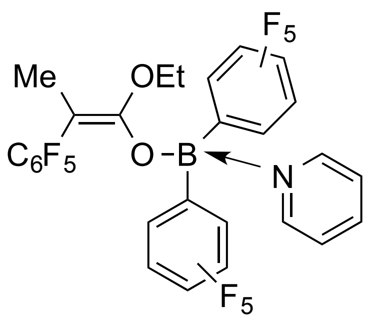
σ = isotropic shielding constant

B_ref_3_coord =



δ ^{11}B 43.9

B_ref_4_coord =



δ ^{11}B 2.5

Both reference compounds have been reported by Stephan et al.[S3]

Table S1. Computed SCF energies and thermal correction factors.

	SCF	ZPE	Enthalpy corr.	Thermal corr.	Neg. eigenv.
	a.u.	a.u	a.u	a.u.	cm^{-1}
CO	*-2209.37291*	*0.14897*	*0.17933*	*0.08688*	-
A_BCF	*-113.36534*	*0.00484*	*0.00815*	*-0.01428*	-
A_Si_H	*-1080.12948*	*0.31527*	*0.33602*	*0.26381*	-
B	*-3289.53605*	*0.46882*	*0.51892*	*0.38425*	-
C	*-3289.52622*	*0.46763*	*0.51901*	*0.37866*	-
D (separ.)	*-2322.75491*	*0.15683*	*0.18957*	*0.09094*	-
D (contact)	*-3402.90685*	*0.47353*	*0.528*	*0.3784*	-
TS1	*-3402.90653*	*0.47333*	*0.52671*	*0.38239*	*-7.55 cm^{-1}*
E	*-3402.91244*	*0.47505*	*0.52825*	*0.38608*	-
F	*-3402.91004*	*0.47726*	*0.53058*	*0.38744*	-
G	*-3402.93205*	*0.47753*	*0.5308*	*0.38679*	-
TS2	*-3402.92314*	*0.47681*	*0.52982*	*0.38294*	*-266.35 cm^{-1}*
H	*-3402.95078*	*0.47944*	*0.53237*	*0.38815*	-
I	*-3402.9475*	*0.4787*	*0.53185*	*0.3862*	-
TS3	*-3402.92894*	*0.47706*	*0.52973*	*0.38667*	*-78.52 cm^{-1}*
J	*-3402.93413*	*0.47771*	*0.53073*	*0.3875*	-
TS4	*-3402.93356*	*0.47783*	*0.52989*	*0.38994*	*-2.03 cm^{-1}*
K	*-3402.98444*	*0.482*	*0.53323*	*0.39595*	-
TS5	*-3402.94733*	*0.47881*	*0.53055*	*0.39187*	*-107.46 cm^{-1}*
3’	*-3403.00554*	*0.47928*	*0.53253*	*0.3851*	-
3	*-3403.0059*	*0.48162*	*0.53324*	*0.39412*	-

Table S2. Relative computed (free) energies and entropies.

	$\Delta G°_{298K}$	$\Delta H°_{298K}$	$\Delta S°_{298K}$	Δ(SCF+ZPE)	ΔSCF
	kcal mol^{-1}	kcal mol^{-1}	cal mol^{-1} K^{-1}	kcal mol^{-1}	kcal mol^{-1}
A	***0.0***	***0.0***	***0.0***	***0.0***	***0.0***
B	***-0.1***	***-18.9***	***-63.1***	***-18.2***	***-21.1***
C	***2.6***	***-12.7***	***-51.2***	***-12.8***	***-15.0***
D (separ.)	***1.1***	***-9.1***	***-34.2***	***-8.6***	***-10.5***
D (contact)	***1.8***	***-21.7***	***-78.9***	***-21.8***	***-24.5***
TS1	***4.5***	***-22.3***	***-90.1***	***-21.7***	***-24.3***
E	***3.1***	***-25.1***	***-94.6***	***-24.3***	***-28.1***
F	***5.5***	***-22.1***	***-92.5***	***-21.4***	***-26.5***
G	***-8.7***	***-35.8***	***-90.7***	***-35.1***	***-40.4***
TS2	***-5.6***	***-30.8***	***-84.7***	***-29.9***	***-34.8***
H	***-19.6***	***-46.5***	***-90.3***	***-45.6***	***-52.1***
I	***-18.8***	***-44.8***	***-87.3***	***-44.0***	***-50.1***
TS3	***-6.9***	***-34.5***	***-92.7***	***-33.4***	***-38.4***
J	***-9.6***	***-37.1***	***-92.4***	***-36.3***	***-41.7***
TS4	***-7.7***	***-37.3***	***-99.3***	***-35.8***	***-41.3***
K	***-35.9***	***-67.1***	***-104.9***	***-65.1***	***-73.2***
TS5	***-15.1***	***-45.5***	***-101.9***	***-43.8***	***-49.9***
3’	***-55.9***	***-80.8***	***-101.8***	***-80.1***	***-86.5***
3	***-50.5***	***-80.6***	***-82.8***	***-78.8***	***-86.7***

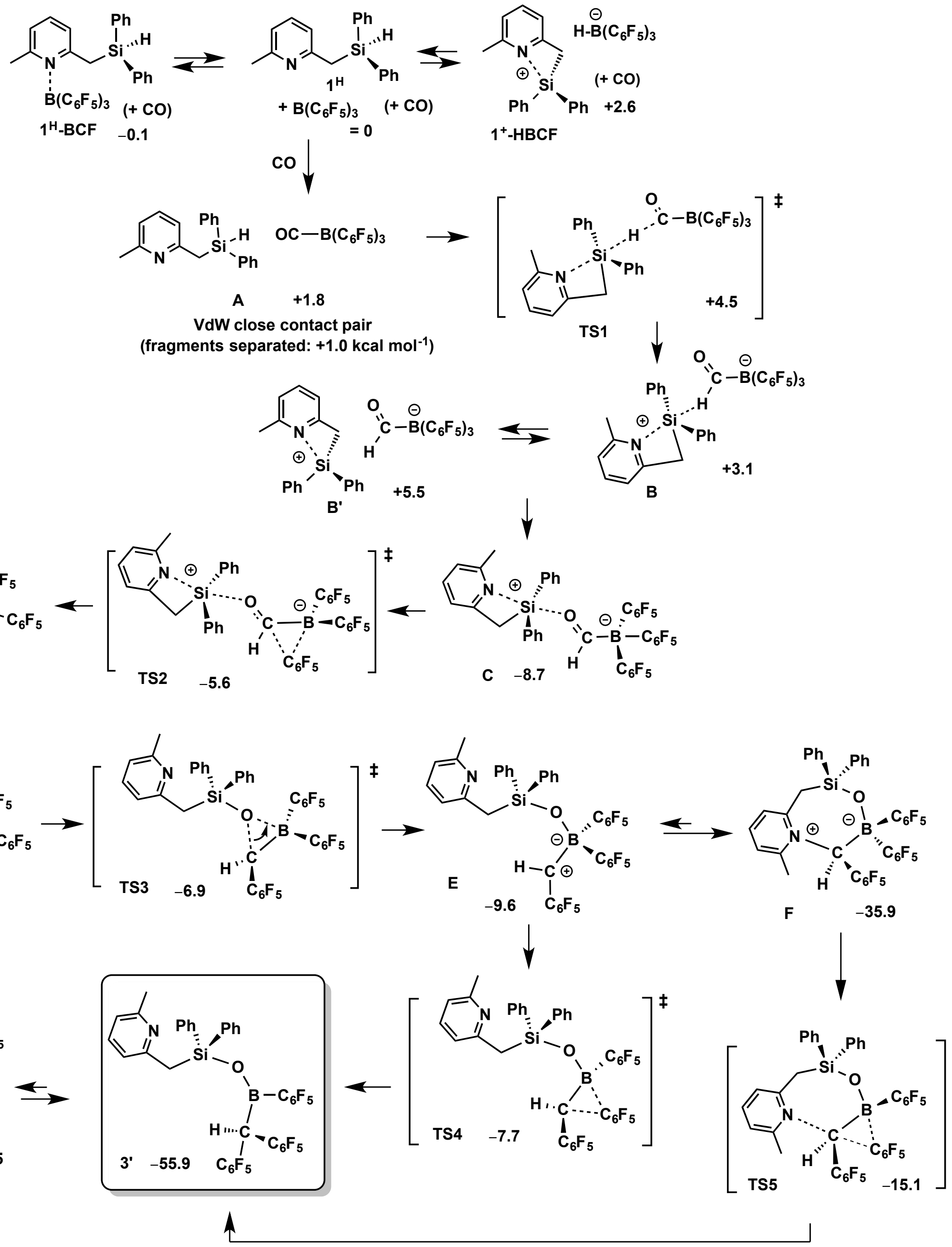


Figure S103. DFT computed reaction pathway (gas-phase free energies ($\Delta G°_{298K}$) in kcal mol^{-1}).

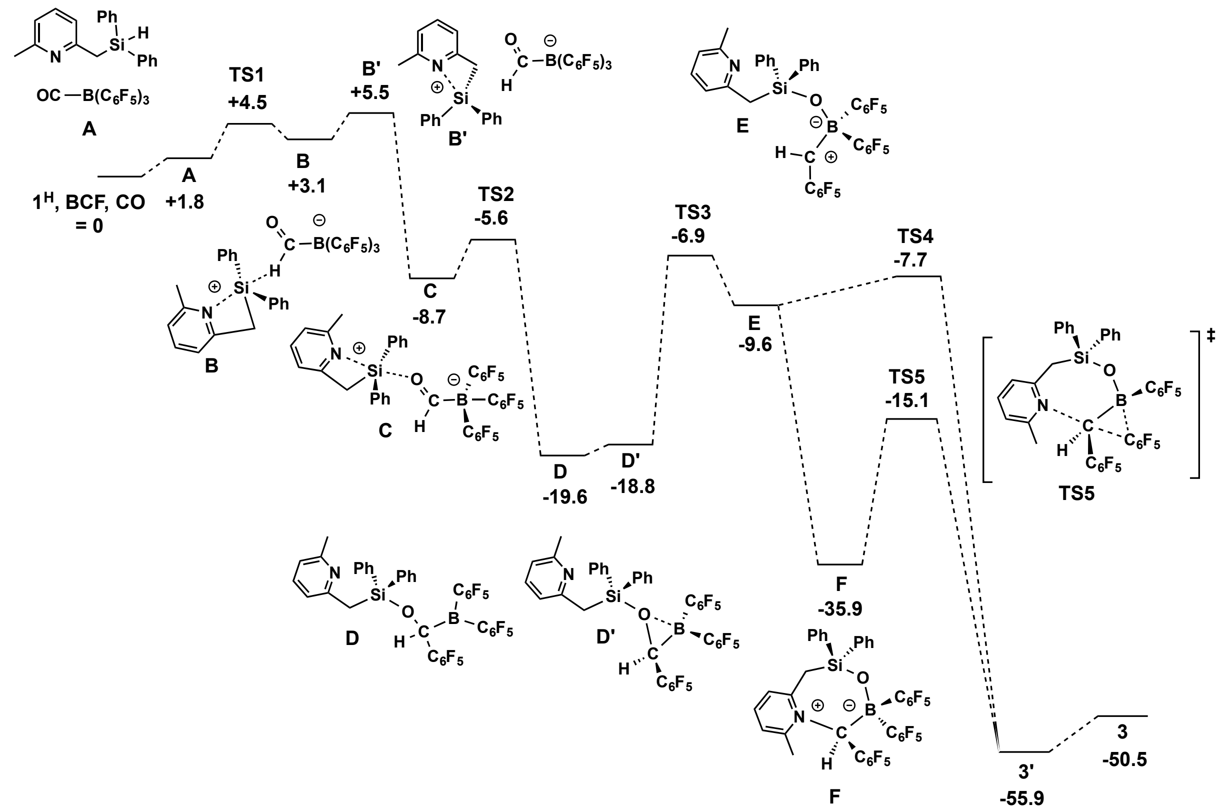


Figure S104. DFT computed gas-phase free energy scheme (ΔG°_{298K} in kcal mol^{-1}).

Optimized geometries:

CO

```
2
C      0.0000000    0.2480000    0.9817788
O      0.0000000    0.2480000    2.1182212
```

A_BCF

```
34
B     -0.9626261   -0.0166523    0.6250863
C     -0.1804839   -0.0800901   -0.7286721
C      1.2450495   -0.1976247   -3.1831317
C      0.7265495    0.9218060   -1.1158194
C     -0.3371785   -1.1434438   -1.6348728
C      0.3439287   -1.2131272   -2.8482856
C      1.4441932    0.8756625   -2.3092042
C     -1.2058483   -1.3247543    1.4481768
C     -1.6530262   -3.7078567    2.9295844
C     -2.4067678   -1.5619696    2.1402252
C     -0.2399124   -2.3426994    1.5385494
C     -0.4361479   -3.5128210    2.2688392
C     -2.6493580   -2.7290586    2.8615385
C     -1.5003241    1.3545510    1.1525169
C     -2.4756409    3.8454760    2.1094280
C     -1.4855201    1.6895759    2.5179421
C     -2.0285513    2.3322827    0.2911675
C     -2.5226708    3.5542338    0.7425611
C     -1.9483372    2.9100687    3.0050911
F     -1.2025972   -2.1421552   -1.3654617
F      0.1493387   -2.2358946   -3.6935167
F      1.9150516   -0.2525488   -4.3375754
F      2.3172367    1.8418368   -2.6296685
F      0.9632005    1.9729127   -0.3046623
F     -2.1075702    2.0977607   -1.0344888
F     -3.0384157    4.4502362   -0.1114440
F     -2.9344874    5.0165521    2.5594053
F     -1.8969340    3.1975093    4.3139589
F     -0.9766610    0.8281117    3.4219728
F      0.9553087   -2.2002908    0.9303686
F      0.5199720   -4.4500282    2.3441583
F     -1.8637009   -4.8285897    3.6253648
F     -3.8183375   -2.9248501    3.4889654
F     -3.4047319   -0.6561209    2.0979026
```

A_Si_H

```
40
Si     3.5809813    1.9363377    4.1642566
H      3.2169955    1.4003300    2.8134677
C      5.4173368    1.6505876    4.4482363
C      8.0811178    1.0431656    5.1434395
C      6.0961785    0.5815815    3.8380547
C      6.1062695    2.4163990    5.4067593
```

C	7.4239697	2.1152103	5.7548416
C	7.4173939	0.2789108	4.1798132
H	5.5860617	-0.0285729	3.0879375
H	5.5981047	3.2498623	5.8970640
H	7.9391329	2.7150873	6.5069278
H	7.9297426	-0.5537505	3.6945039
H	9.1112296	0.8061057	5.4147362
C	3.1638128	3.7648931	4.2358983
C	2.6533438	6.5380378	4.2978271
C	2.7833978	4.4000790	5.4337256
C	3.2809904	4.5487554	3.0722858
C	3.0281436	5.9220321	3.1000118
C	2.5318736	5.7750482	5.4621851
H	2.6939920	3.8105474	6.3508433
H	3.5716628	4.0810725	2.1279576
H	3.1211111	6.5122655	2.1866923
H	2.2374263	6.2523345	6.3987483
H	2.4535476	7.6107242	4.3215079
C	2.6550302	0.9336289	5.5138359
H	2.4710247	-0.0733389	5.1118908
H	1.6857733	1.4151392	5.7064856
C	3.4751032	0.8699505	6.7697602
C	5.1212939	0.9641288	8.9702013
N	3.4090464	1.9328137	7.5916332
C	4.3493947	-0.2024298	7.0165333
C	5.1835742	-0.1468340	8.1273733
C	4.2116841	1.9852131	8.6714613
H	4.3907673	-1.0444652	6.3254291
H	5.8851092	-0.9571410	8.3313819
H	5.7686812	1.0422230	9.8442023
C	4.0818454	3.2152501	9.5299038
H	4.7897828	3.2069438	10.3686133
H	3.0609888	3.2929847	9.9320810
H	4.2580846	4.1178889	8.9264922

B

74

B	0.8112431	1.5068695	3.5410143
C	1.6484388	1.6760241	2.1234060
C	3.0297617	2.1536344	-0.3526213
C	1.5817752	2.8867051	1.4220127
C	2.4762991	0.7236225	1.5108069
C	3.1450424	0.9287788	0.2993564
C	2.2374062	3.1475490	0.2209599
C	0.9302355	0.0099034	4.2588056
C	0.7612440	-2.6455078	5.3381326
C	0.4950094	-1.0985458	3.5127404
C	1.2286051	-0.2908969	5.5927240
C	1.1660378	-1.5781054	6.1355985
C	0.4154697	-2.3981781	4.0088539
C	-0.8300054	1.5715181	3.3597713
C	-3.6794731	1.3014002	3.2123975
C	-1.6490638	1.4371251	4.4909695
C	-1.5235093	1.5415219	2.1437141
C	-2.9149836	1.4145668	2.0532146

C	-3.0348339	1.3127271	4.4512521
F	2.7275059	-0.4752550	2.0915008
F	3.9135702	-0.0372457	-0.2261667
F	3.6816103	2.3792353	-1.5029149
F	2.1169276	4.3424962	-0.3854024
F	0.8274354	3.9066753	1.9060982
F	-0.8792469	1.6260918	0.9589338
F	-3.5207723	1.3918186	0.8532903
F	-5.0137771	1.1832767	3.1417825
F	-3.7551797	1.2192853	5.5842627
F	-1.0881917	1.4720020	5.7289861
F	1.5954225	0.6786050	6.4708240
F	1.4827141	-1.7898788	7.4273616
F	0.6936680	-3.8879883	5.8412381
F	0.0037183	-3.4107692	3.2256219
F	0.1018733	-0.9331192	2.2274837
Si	4.9165450	2.3401268	3.2509961
H	4.2047511	3.2638864	2.3231592
C	5.8176733	0.9961153	2.3153101
C	7.2197696	-0.9613698	0.8543983
C	6.5426855	1.3400068	1.1583948
C	5.8118901	-0.3484276	2.7238265
C	6.5078302	-1.3204255	2.0006509
C	7.2358897	0.3714435	0.4322960
H	6.5553836	2.3763481	0.8111813
H	5.2441762	-0.6530790	3.6049272
H	6.4847199	-2.3611300	2.3270247
H	7.7823338	0.6538221	-0.4686635
H	7.7554670	-1.7213161	0.2837568
C	6.0980204	3.3816266	4.2722761
C	7.7755284	4.9135737	5.9407705
C	5.9170680	4.7707401	4.3975966
C	7.1445214	2.7778572	4.9934946
C	7.9757438	3.5343708	5.8224720
C	6.7473394	5.5324213	5.2245316
H	5.1139698	5.2634558	3.8445153
H	7.3186916	1.7029077	4.8970902
H	8.7845768	3.0507614	6.3723486
H	6.5950319	6.6097422	5.3075889
H	8.4261817	5.5063597	6.5855097
C	3.6525438	1.5313221	4.4554213
H	4.2506077	1.1299580	5.2870792
H	3.1701165	0.6837962	3.9687808
C	2.7172546	2.5552791	4.9972622
C	1.2320288	4.6614542	5.9378939
N	1.4240834	2.7108920	4.5327895
C	3.2342409	3.3972086	5.9890978
C	2.4835219	4.4418248	6.4926834
C	0.7129415	3.8157124	4.9560332
H	4.2469728	3.2126463	6.3414599
H	2.8766698	5.0906070	7.2755758
H	0.6241597	5.5083465	6.2525366
C	-0.6252647	4.2358878	4.4065852
H	-1.4406353	3.8784747	5.0502230
H	-0.8165571	3.8979530	3.3915763
H	-0.6594495	5.3328777	4.4165405

C

74

B	0.8765297	-0.7500718	0.5597044
C	0.5461970	-0.7816874	-1.0359966
C	0.1216633	-0.6227570	-3.8586105
C	0.6094589	0.4182141	-1.7516364
C	0.2595879	-1.9029379	-1.8162112
C	0.0505052	-1.8477060	-3.1986057
C	0.4037707	0.5288791	-3.1232660
C	1.0633018	-2.1979093	1.2876325
C	1.3917198	-4.6345765	2.7397510
C	-0.0189592	-2.9862842	1.6901624
C	2.3121608	-2.7031185	1.6405236
C	2.5036816	-3.8875082	2.3535671
C	0.1145498	-4.1798809	2.4013283
C	-0.1807169	0.1614031	1.4218959
C	-1.8656765	1.8012620	3.0551378
C	0.1788202	0.5913875	2.7005326
C	-1.4517576	0.5775106	1.0129645
C	-2.2879008	1.3837581	1.7925295
C	-0.6137723	1.3956654	3.5179301
F	0.1905450	-3.1394635	-1.2619131
F	-0.1923454	-2.9704767	-3.9073004
F	-0.0421351	-0.5536064	-5.1942455
F	0.5019058	1.7191226	-3.7533666
F	0.9025146	1.5771989	-1.0934866
F	-1.9512022	0.1995756	-0.1870809
F	-3.5013500	1.7599123	1.3429451
F	-2.6554318	2.5792410	3.8183689
F	-0.1864696	1.7841293	4.7408513
F	1.3831388	0.2109010	3.2219195
F	3.4589164	-2.0337979	1.2977593
F	3.7478595	-4.3128794	2.6769745
F	1.5475688	-5.7812027	3.4276925
F	-0.9636548	-4.9018728	2.7636777
F	-1.2775706	-2.6001000	1.3783022
Si	4.3708939	1.7671420	-0.3987237
C	3.9372382	0.7532913	-1.8785284
C	3.3807378	-0.7899796	-4.1573722
C	3.6832884	-0.6274909	-1.7631711
C	3.8922189	1.3499819	-3.1545995
C	3.6067732	0.5840010	-4.2846915
C	3.4239777	-1.3948705	-2.8986365
H	3.6540542	-1.1014038	-0.7818681
H	4.0726460	2.4209212	-3.2675787
H	3.5468996	1.0601766	-5.2635517
H	3.2159636	-2.4597964	-2.7945174
H	3.1466339	-1.3867195	-5.0396927
C	5.0791422	-0.1756857	3.5603193
C	4.0950196	1.1975382	1.8859841
C	5.8947495	-0.2778620	1.2834407
C	5.9462262	-0.7164750	2.6043662
C	4.1433502	0.8010787	3.2147364
H	6.6610874	-1.4900101	2.8797136
H	3.4443455	1.2131631	3.9371534

H	5.1285975	-0.5334276	4.5892928
C	5.6890401	3.0328687	-0.7602881
C	7.7835291	4.8516307	-1.2428338
C	6.6426957	2.7842866	-1.7683315
C	5.8085166	4.2123156	-0.0011390
C	6.8448140	5.1162138	-0.2416949
C	7.6826470	3.6845662	-2.0056430
H	6.5635738	1.8824152	-2.3789885
H	5.0839787	4.4348958	0.7840899
H	6.9190391	6.0292915	0.3502529
H	8.4119811	3.4787931	-2.7901299
H	8.5927249	5.5583766	-1.4315565
C	3.2501568	2.1653611	1.0977203
H	2.2175261	1.8070016	0.9842005
H	3.2393220	3.1855194	1.5009962
N	4.9732961	0.6666332	0.9825374
C	6.7725030	-0.7723918	0.1806577
H	7.3112383	0.0656732	-0.2875319
H	6.1651458	-1.2482478	-0.6036584
H	7.5014852	-1.4996802	0.5537428
H	1.9574904	-0.1884187	0.6480919

D(separated)_CO_BCF

36

B	-0.3121679	0.0935417	0.9879772
C	0.1648636	-0.0454655	-0.5684778
C	0.9736844	-0.1369022	-3.2929195
C	1.0491268	0.8850868	-1.1223798
C	-0.3025172	-1.0307377	-1.4448216
C	0.0845732	-1.0873864	-2.7869128
C	1.4632779	0.8658260	-2.4520383
C	-0.8923470	-1.2795129	1.6568725
C	-1.8340730	-3.7491522	2.7047006
C	-2.2249965	-1.4575521	2.0429912
C	-0.0625996	-2.3927932	1.8193019
C	-0.4950558	-3.6146567	2.3291918
C	-2.7029838	-2.6658560	2.5583314
C	-1.1687071	1.4418792	1.3326386
C	-2.7320191	3.7041046	2.0557615
C	-1.2736705	1.8933256	2.6516963
C	-1.8855884	2.1777764	0.3832957
C	-2.6599050	3.2907104	0.7238466
C	-2.0315106	2.9967887	3.0360620
F	-1.1895082	-1.9626086	-1.0373722
F	-0.3974279	-2.0429000	-3.5960188
F	1.3517430	-0.1834056	-4.5759008
F	2.3137421	1.7880099	-2.9279360
F	1.5334002	1.8843416	-0.3353586
F	-1.8919763	1.8184902	-0.9174299
F	-3.3416950	3.9607915	-0.2173670
F	-3.4696081	4.7688455	2.3923921
F	-2.0966854	3.3811360	4.3198797
F	-0.6160417	1.2191531	3.6340398
F	1.2440409	-2.3013892	1.4494767

F	0.3482001	-4.6499906	2.4602579
F	-2.2814452	-4.9100421	3.1979950
F	-3.9921489	-2.7969679	2.9058326
F	-3.1306351	-0.4674543	1.8985104
C	1.0641866	0.3307552	1.7715058
O	2.0374744	0.5022110	2.3263757

D (close contact)

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B	1.3114905	1.1039616	0.8142428
C	0.6747508	0.7959995	-0.6657235
C	-0.4310926	0.0150541	-3.1655160
C	1.3261701	-0.0871422	-1.5321549
C	-0.5647860	1.2739145	-1.1056183
C	-1.1218729	0.8963477	-2.3311185
C	0.8095853	-0.4860622	-2.7633479
C	1.2176021	-0.2381580	1.7214391
C	0.8970987	-2.5699553	3.3127331
C	-0.0407518	-0.6990842	2.1193702
C	2.3001527	-1.0239773	2.1135568
C	2.1698668	-2.1632960	2.9095033
C	-0.2211335	-1.8356994	2.9067672
C	0.8419322	2.5213219	1.4999404
C	-0.0399872	5.0333381	2.5198522
C	0.3439402	2.6669307	2.7999032
C	0.9151325	3.7083755	0.7582901
C	0.4880214	4.9454776	1.2306529
C	-0.1089762	3.8862067	3.3090817
F	-1.2948927	2.1166468	-0.3486139
F	-2.3180514	1.3712505	-2.7122115
F	-0.9553953	-0.3502233	-4.3424150
F	1.4822527	-1.3354261	-3.5563038
F	2.5323867	-0.5996056	-1.1688128
F	1.4286422	3.6742864	-0.4988450
F	0.5933107	6.0485528	0.4725786
F	-0.4609933	6.2098012	2.9961447
F	-0.5980729	3.9612344	4.5551270
F	0.2705437	1.6168060	3.6456419
F	3.5610876	-0.6979501	1.7224513
F	3.2517257	-2.8694466	3.2826192
F	0.7478870	-3.6616426	4.0750272
F	-1.4485349	-2.2256888	3.2837547
F	-1.1435278	-0.0097833	1.7569689
C	2.8364701	1.4724583	0.5107789
O	3.8392928	1.8996456	0.1930380
Si	3.6053915	1.9739788	4.2430150
H	3.2286302	1.5016789	2.8746915
C	5.4383621	1.6637707	4.4743192
C	8.1147523	1.0272469	5.0752383
C	6.0800831	0.5843911	3.8415788
C	6.1660608	2.4219596	5.4096738
C	7.4917376	2.1054530	5.7111354
C	7.4090242	0.2687686	4.1370966

H	5.5348247	-0.0237785	3.1162206
H	5.6827511	3.2594685	5.9177745
H	8.0399735	2.6986818	6.4447376
H	7.8940718	-0.5710031	3.6364989
H	9.1511113	0.7790475	5.3098634
C	3.1782121	3.7966608	4.3079221
C	2.5367762	6.5397976	4.2715540
C	2.5908932	4.4102082	5.4288725
C	3.4470265	4.5875735	3.1741106
C	3.1319177	5.9471442	3.1531616
C	2.2707342	5.7709705	5.4075000
H	2.3975028	3.8163594	6.3253137
H	3.9026074	4.1350918	2.2891689
H	3.3347002	6.5419091	2.2611243
H	1.8048052	6.2314449	6.2800653
H	2.2742881	7.5983223	4.2525578
C	2.6646768	0.9214930	5.5267903
H	2.4974813	-0.0739377	5.0899033
H	1.6866877	1.3842826	5.7136900
C	3.4785940	0.8465063	6.7851257
C	5.1160698	0.9320284	8.9880433
N	3.4613157	1.9401031	7.5691653
C	4.2988071	-0.2579237	7.0663228
C	5.1297422	-0.2064311	8.1808415
C	4.2591946	1.9876537	8.6523302
H	4.2978191	-1.1236954	6.4039130
H	5.7894044	-1.0430061	8.4160736
H	5.7616507	1.0056437	9.8637297
C	4.1894067	3.2502648	9.4688408
H	4.8620827	3.2165926	10.3353085
H	3.1625218	3.4172883	9.8247826
H	4.4570335	4.1175225	8.8471627

TS1

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B	1.2812207	1.0849236	1.1480827
C	0.8068742	0.7745787	-0.3920669
C	-0.0527426	-0.0184605	-2.9871160
C	1.4840833	-0.1874829	-1.1486073
C	-0.3336421	1.3192065	-0.9935238
C	-0.7685072	0.9392904	-2.2666817
C	1.0883841	-0.5920811	-2.4223002
C	0.9519806	-0.2262232	2.0451371
C	0.2182937	-2.5331662	3.5388823
C	-0.3820484	-0.5482011	2.3137103
C	1.8951494	-1.1352967	2.5210913
C	1.5604844	-2.2655438	3.2695466
C	-0.7651509	-1.6686005	3.0499196
C	0.8254787	2.5423377	1.7487483
C	0.0066609	5.1226824	2.6407538
C	0.2643293	2.7536781	3.0128722
C	1.0067790	3.7010743	0.9817424
C	0.6081948	4.9704042	1.3909845

C	-0.1620808	4.0063749	3.4581580
F	-1.0874774	2.2381687	-0.3560724
F	-1.8723462	1.4852776	-2.8026490
F	-0.4595467	-0.3884948	-4.2091943
F	1.7821394	-1.5200741	-3.1023199
F	2.5894325	-0.7823706	-0.6287467
F	1.6047446	3.6100494	-0.2325464
F	0.8147525	6.0455045	0.6120835
F	-0.3822730	6.3336342	3.0588179
F	-0.7166456	4.1455794	4.6728369
F	0.1062890	1.7366109	3.8906066
F	3.2185967	-0.9490722	2.2721711
F	2.5179266	-3.0915774	3.7312718
F	-0.1260361	-3.6133603	4.2555908
F	-2.0602887	-1.9222172	3.2985083
F	-1.3630805	0.2632781	1.8624792
C	2.8698432	1.3397046	1.0474133
O	3.8938380	1.6699581	0.6681684
Si	3.6046399	1.8371638	4.3741816
H	3.0165383	1.4776046	3.0118145
C	5.4455575	1.5708466	4.1387987
C	8.2160340	1.1501432	3.8380367
C	5.9446423	0.3183014	3.7401525
C	6.3622923	2.6099203	4.3781393
C	7.7351914	2.4041671	4.2278880
C	7.3184833	0.1069808	3.5948070
H	5.2566632	-0.5058751	3.5412674
H	5.9940999	3.5888800	4.6920883
H	8.4325277	3.2224626	4.4158900
H	7.6885526	-0.8727123	3.2882050
H	9.2887245	0.9872115	3.7216949
C	3.1432600	3.6490462	4.5209683
C	2.4995015	6.3941441	4.5864057
C	2.4869113	4.2084280	5.6296151
C	3.4667955	4.4953565	3.4436761
C	3.1585240	5.8571290	3.4769014
C	2.1599131	5.5661952	5.6602411
H	2.2302403	3.5764749	6.4807859
H	3.9709259	4.0868124	2.5638301
H	3.4155072	6.4955917	2.6303338
H	1.6343694	5.9792385	6.5223789
H	2.2408268	7.4533567	4.6083953
C	2.7707992	0.5805871	5.5270890
H	2.8755641	-0.4421752	5.1335540
H	1.6890942	0.7841441	5.5723169
C	3.4275485	0.7405773	6.8689696
C	4.7786194	1.3033048	9.1910863
N	4.1999100	1.8396493	6.9384148
C	3.2915559	-0.1360914	7.9517424
C	3.9809167	0.1581636	9.1276292
C	4.8702817	2.1339285	8.0673132
H	2.6618427	-1.0220641	7.8690607
H	3.8998196	-0.5017566	9.9927937
H	5.3295115	1.5497662	10.0993248
C	5.7205040	3.3714202	8.0261422
H	5.1350228	4.2189798	7.6420891

H	6.5594225	3.2203357	7.3294523
H	6.1242564	3.6262692	9.0137741

E

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B	1.3663030	1.1238874	1.4513796
C	1.1412423	0.8481916	-0.1428088
C	0.7781344	0.1646844	-2.8897642
C	1.9843889	-0.0414736	-0.8179311
C	0.0861548	1.3558040	-0.9081312
C	-0.1051562	1.0383301	-2.2555962
C	1.8339042	-0.3850166	-2.1617074
C	0.8719999	-0.2245083	2.2296743
C	-0.0896060	-2.6227650	3.4431004
C	-0.4912387	-0.5262728	2.3252109
C	1.7235048	-1.2023998	2.7388933
C	1.2791837	-2.3763197	3.3513964
C	-0.9859094	-1.6881770	2.9176373
C	0.7456401	2.5368215	2.0317600
C	-0.1623367	5.0699487	2.9924966
C	0.1458041	2.6996848	3.2836303
C	0.9142009	3.7280736	1.3096622
C	0.4623964	4.9702558	1.7498194
C	-0.3142079	3.9247355	3.7695552
F	-0.8238562	2.1981316	-0.3651380
F	-1.1339703	1.5640423	-2.9481855
F	0.6083963	-0.1522064	-4.1849724
F	2.6829047	-1.2451573	-2.7570721
F	3.0005192	-0.6432306	-0.1516416
F	1.5693297	3.7148626	0.1282047
F	0.6665591	6.0817352	1.0177643
F	-0.5686682	6.2638974	3.4544639
F	-0.8735871	4.0146920	4.9923874
F	-0.0138665	1.6470046	4.1309317
F	3.0766863	-1.0412680	2.6818541
F	2.1604730	-3.2623884	3.8634902
F	-0.5416271	-3.7451410	4.0285085
F	-2.3091332	-1.9177427	2.9977985
F	-1.4005572	0.3456653	1.8375893
C	2.9292611	1.4658256	1.7866711
O	3.8759147	1.8426836	1.1749274
Si	3.7149997	1.8028922	4.7163231
H	3.0525066	1.4851760	3.0446891
C	5.4236606	1.4801807	4.0420152
C	8.0208912	1.0011056	3.0695024
C	5.8397363	0.1765802	3.7189294
C	6.3305979	2.5406466	3.8605457
C	7.6201886	2.3030632	3.3798324
C	7.1285573	-0.0612951	3.2386762
H	5.1490145	-0.6610987	3.8219445
H	6.0259639	3.5642054	4.0880051
H	8.3087284	3.1371450	3.2364112
H	7.4329638	-1.0774366	2.9844851

H	9.0247725	0.8153382	2.6851518
C	3.1391253	3.5840620	4.6913463
C	2.4242607	6.3095946	4.6907982
C	2.4671276	4.1548218	5.7887125
C	3.4274849	4.4034494	3.5837009
C	3.0803507	5.7560305	3.5879874
C	2.1067969	5.5036699	5.7872945
H	2.2108233	3.5423440	6.6556392
H	3.9207670	3.9822886	2.7057358
H	3.3023111	6.3735727	2.7169513
H	1.5682444	5.9233063	6.6377158
H	2.1385641	7.3617339	4.6848445
C	2.6890823	0.3726811	5.4845287
H	2.9349458	-0.6252658	5.0990646
H	1.6022381	0.5065675	5.4130237
C	3.2613365	0.6383465	6.8448790
C	4.6808794	1.6499536	8.9729881
N	4.1159666	1.6800163	6.6873416
C	3.0789313	0.0506103	8.0931667
C	3.8068644	0.5745185	9.1647090
C	4.8316349	2.2103033	7.7014539
H	2.3913287	-0.7843071	8.2174736
H	3.6941366	0.1437581	10.1605638
H	5.2480894	2.0590601	9.8084296
C	5.7311435	3.3596941	7.3791573
H	5.1526666	4.1680008	6.9066367
H	6.4953304	3.0460068	6.6517656
H	6.2268074	3.7457893	8.2767219

F

76

B	0.8839298	-1.6077690	0.7461990
C	0.7676333	-1.4723610	-0.9017643
C	0.6889800	-1.3049811	-3.7643734
C	0.9193540	-0.2701382	-1.6045343
C	0.6525313	-2.5994316	-1.7298854
C	0.6091361	-2.5406845	-3.1255909
C	0.8376161	-0.1560196	-2.9908639
C	0.0769490	-2.8915574	1.3654426
C	-1.4098002	-5.0238643	2.5415332
C	-1.2785158	-3.1029920	1.0956685
C	0.6480440	-3.8014064	2.2577152
C	-0.0596466	-4.8534527	2.8454983
C	-2.0267696	-4.1391914	1.6548773
C	0.4226994	-0.2970942	1.6170411
C	-0.2485496	1.9877788	3.2088125
C	0.9951161	-0.0514416	2.8719883
C	-0.5661454	0.6220203	1.2442270
C	-0.8975958	1.7533674	1.9970633
C	0.6981193	1.0664390	3.6535045
C	2.4905654	-1.8478535	0.7613221
O	3.3751405	-1.0351497	1.0362733
H	2.8175120	-2.8377929	0.3323172

F	0.5754683	-3.8423923	-1.1961947
F	0.4982322	-3.6642766	-3.8614732
F	0.6569408	-1.2234246	-5.1071871
F	0.9233184	1.0489691	-3.5920211
F	1.1656967	0.8959178	-0.9472481
F	-1.2619850	0.4618820	0.0977895
F	-1.8365299	2.6192771	1.5682745
F	-0.5455515	3.0726910	3.9476848
F	1.3208408	1.2664566	4.8418366
F	1.8809663	-0.9249737	3.4095580
F	1.9608110	-3.7042719	2.5994034
F	0.5453195	-5.7037144	3.7002056
F	-2.1101734	-6.0296872	3.0963251
F	-3.3297988	-4.3001243	1.3503227
F	-1.9270408	-2.2803721	0.2365861
Si	4.4431920	1.9358819	-0.4338223
C	4.2936292	0.7997850	-1.8904416
C	4.0022588	-0.8589943	-4.1420236
C	4.4217685	-0.5982808	-1.7725901
C	4.0293415	1.3508179	-3.1602569
C	3.8829120	0.5264265	-4.2766309
C	4.2770255	-1.4190579	-2.8909601
H	4.5943191	-1.0452271	-0.7933840
H	3.9205128	2.4306384	-3.2798093
H	3.6507274	0.9642039	-5.2474996
H	4.3581962	-2.5009652	-2.7814109
H	3.8649850	-1.5036154	-5.0109180
C	5.4827564	0.3222689	3.5955521
C	4.2618473	1.3930097	1.8629562
C	6.4135485	0.4515824	1.3627822
C	6.5120348	0.0364443	2.6871248
C	4.3431814	1.0195851	3.1971041
H	7.3953209	-0.5144339	3.0070897
H	3.5244982	1.2255703	3.8824475
H	5.5711505	-0.0184823	4.6276723
C	5.3545996	3.5043578	-0.8597056
C	6.8483005	5.8212746	-1.4323856
C	6.3347125	3.4987353	-1.8726365
C	5.1400724	4.6956697	-0.1413459
C	5.8780664	5.8459205	-0.4265394
C	7.0773307	4.6466387	-2.1548149
H	6.5104971	2.5898295	-2.4518820
H	4.3858679	4.7322385	0.6468228
H	5.6943359	6.7633727	0.1339036
H	7.8312193	4.6271460	-2.9428816
H	7.4238486	6.7204687	-1.6564988
C	3.2126023	2.0631162	1.0185579
H	2.3282988	1.4219367	0.9190511
H	2.9013513	3.0532559	1.3729871
N	5.2925245	1.1215987	1.0079606
C	7.4441866	0.2158978	0.3061775
H	7.7643745	1.1709343	-0.1374652
H	7.0249101	-0.3962479	-0.5063574
H	8.3218765	-0.2946816	0.7167373

G

76			
B	0.3692287	-0.5489810	0.3661103
C	0.2982302	0.5707040	-0.8393400
C	0.4729901	2.4150185	-3.0139713
C	-0.1995646	1.8716651	-0.7567098
C	0.9282476	0.2681994	-2.0511891
C	1.0215933	1.1377343	-3.1324533
C	-0.1315931	2.7852003	-1.8154861
C	-0.2185934	-2.0344681	-0.0314192
C	-1.2478699	-4.6524818	-0.5390122
C	-1.0834460	-2.3074611	-1.0965017
C	0.0797419	-3.1392128	0.7741479
C	-0.4014294	-4.4285226	0.5473355
C	-1.5938105	-3.5817254	-1.3633308
C	-0.3668298	-0.1283347	1.7702429
C	-1.7606689	0.4596460	4.1811512
C	0.2757746	-0.0380767	3.0016860
C	-1.7513516	0.0671991	1.8037165
C	-2.4542391	0.3618679	2.9715700
C	-0.3813113	0.2552116	4.1982062
C	1.9652347	-0.6708857	0.6145871
O	2.6945090	0.3499979	0.5064078
H	2.4907706	-1.6278214	0.8002231
F	1.5242873	-0.9510846	-2.2014075
F	1.6472714	0.7767466	-4.2691112
F	0.5646752	3.2915856	-4.0300687
F	-0.6158190	4.0359109	-1.6757558
F	-0.7638118	2.3391788	0.3824601
F	-2.4636461	-0.0198742	0.6590958
F	-3.7854332	0.5549846	2.9505145
F	-2.4177104	0.7423157	5.3185492
F	0.2967396	0.3340550	5.3607804
F	1.6227642	-0.2544773	3.0932883
F	0.8724451	-2.9782010	1.8717146
F	-0.0664975	-5.4489917	1.3607522
F	-1.7284576	-5.8833938	-0.7835222
F	-2.4195889	-3.7865600	-2.4065307
F	-1.4874782	-1.3265556	-1.9349270
Si	4.5167273	0.6715640	0.4478731
C	5.1110327	-1.0812933	0.1503404
C	5.9466510	-3.7275584	-0.3477054
C	6.0507742	-1.7108258	0.9856036
C	4.5958017	-1.8088896	-0.9398410
C	5.0133241	-3.1184109	-1.1903904
C	6.4629562	-3.0230673	0.7439834
H	6.4721289	-1.1718090	1.8373449
H	3.8552812	-1.3530595	-1.6011287
H	4.6035155	-3.6642343	-2.0412639
H	7.1860843	-3.4980031	1.4087534
H	6.2684121	-4.7522672	-0.5382034
C	8.1759034	2.7169619	2.6211234
C	6.0080698	1.8620997	2.1042779
C	7.7565135	1.5562929	0.5391515
C	8.6369738	2.2245911	1.3969680

C	6.8414999	2.5376206	2.9933397
H	9.6780858	2.3552702	1.1027786
H	6.4571006	2.9030435	3.9445361
H	8.8633282	3.2393207	3.2880097
C	4.3087395	1.7587559	-1.0608262
C	3.8867313	3.3634441	-3.3369514
C	4.9077000	1.4349344	-2.2904340
C	3.4871870	2.8983216	-0.9966616
C	3.2849158	3.6998972	-2.1212255
C	4.6955370	2.2274837	-3.4213429
H	5.5256396	0.5383932	-2.3748674
H	2.9714107	3.1493478	-0.0675937
H	2.6308236	4.5705018	-2.0584712
H	5.1468599	1.9479476	-4.3742293
H	3.7043803	3.9731855	-4.2222336
C	4.5617412	1.4806984	2.1779507
H	4.3309362	0.7800945	2.9941814
H	3.8795681	2.3360816	2.2875813
N	6.4720793	1.4035929	0.9185204
C	8.1478898	0.9971600	-0.7927429
H	7.7845953	-0.0362402	-0.8894229
H	9.2346741	1.0160817	-0.9337356
H	7.6760738	1.5818604	-1.5968490

TS2

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B	0.1546696	-0.8237288	-0.4215153
C	-0.3948481	0.2189478	-1.4966851
C	-1.2297438	1.9814789	-3.5619064
C	-1.4120799	1.1562319	-1.3051198
C	0.1790678	0.1944674	-2.7735973
C	-0.2139435	1.0531508	-3.8012779
C	-1.8338191	2.0354476	-2.3042631
C	-0.6125453	-2.2137328	-0.2689827
C	-1.9737785	-4.7041505	-0.1624659
C	-1.8798671	-2.3446202	0.3054748
C	-0.0504741	-3.3895304	-0.7810560
C	-0.7056667	-4.6221512	-0.7419439
C	-2.5669344	-3.5569233	0.3707829
C	0.5774510	-0.0908615	1.2259604
C	0.0761652	1.0938172	3.7482402
C	0.4230201	-0.8616414	2.3929263
C	0.5183817	1.3053788	1.3896582
C	0.2595006	1.9000692	2.6208485
C	0.1631521	-0.2985434	3.6378922
C	1.6365335	-0.7711797	-0.0448714
O	2.4941097	0.1278162	-0.5508329
H	2.0970092	-1.6174094	0.4878151
F	1.1468704	-0.7039014	-3.0577689
F	0.3653224	0.9941673	-5.0132877
F	-1.6233421	2.8168222	-4.5359388
F	-2.8022599	2.9381058	-2.0660918
F	-2.0030524	1.2827676	-0.0941714

F	0.7450842	2.1277802	0.3557975
F	0.2032943	3.2348130	2.7421587
F	-0.1626340	1.6539238	4.9359319
F	0.0132897	-1.0629060	4.7292216
F	0.5472566	-2.1980607	2.3342263
F	1.1763372	-3.3684021	-1.3499034
F	-0.1326209	-5.7268046	-1.2511707
F	-2.6172718	-5.8797121	-0.1139045
F	-3.7811458	-3.6360760	0.9423342
F	-2.4760191	-1.2660092	0.8611904
Si	4.1010727	0.4257273	0.0061375
C	4.8127510	-1.2846980	0.2860750
C	5.7565560	-3.9236635	0.5965071
C	5.5100403	-1.6692518	1.4442484
C	4.5944685	-2.2544336	-0.7122508
C	5.0638571	-3.5611748	-0.5617830
C	5.9769811	-2.9763513	1.6009539
H	5.7031907	-0.9351413	2.2279733
H	4.0415955	-1.9872555	-1.6159277
H	4.8834718	-4.2972270	-1.3464393
H	6.5142168	-3.2574153	2.5083580
H	6.1219207	-4.9445369	0.7181856
C	6.7060222	3.3751780	3.2259825
C	5.1817916	2.0108200	1.9743890
C	7.4709127	1.7938152	1.5718785
C	7.7574684	2.7684322	2.5360918
C	5.3941868	2.9954428	2.9464142
H	8.7919559	3.0475724	2.7384481
H	4.5493200	3.4460854	3.4675638
H	6.9108665	4.1381770	3.9785469
C	4.7637951	1.3360368	-1.4817588
C	5.7203077	2.7052618	-3.7471556
C	6.0634603	1.1075920	-1.9630010
C	3.9456272	2.2536709	-2.1648568
C	4.4218211	2.9383213	-3.2858934
C	6.5397213	1.7832388	-3.0878624
H	6.7029822	0.3862598	-1.4515500
H	2.9207635	2.4224844	-1.8272197
H	3.7757266	3.6472982	-3.8059784
H	7.5490106	1.5890067	-3.4550912
H	6.0909203	3.2353112	-4.6259705
C	3.8380389	1.4872973	1.5569738
H	3.3779602	0.8838333	2.3586686
H	3.1335443	2.3047514	1.3391661
N	6.1999347	1.4363626	1.3068548
C	8.5407816	1.1107406	0.7681998
H	8.3211908	0.0379472	0.6802135
H	9.5343454	1.2437315	1.2142913
H	8.5629526	1.5239116	-0.2520873

H

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B	1.5609400	0.2692459	2.6816266

C	2.3009462	-0.0074178	1.3178264
C	3.5180712	-0.2437182	-1.2276364
C	3.6624457	-0.2879554	1.1797674
C	1.5690432	0.1071847	0.1336502
C	2.1469956	0.0101102	-1.1304227
C	4.2789577	-0.4051278	-0.0670810
C	0.5179102	-0.7567736	3.2196028
C	-1.1869445	-2.7154269	4.3985365
C	-0.4268381	-0.4410879	4.2149397
C	0.5459850	-2.1154698	2.8327668
C	-0.2720864	-3.0867919	3.4091195
C	-1.2700592	-1.3800380	4.8020538
C	1.1488712	2.8431715	3.2397452
C	-0.0762277	5.3706876	2.8614017
C	1.1174287	3.4671309	1.9868518
C	0.5481908	3.5392488	4.2965690
C	-0.0643301	4.7801773	4.1252198
C	0.5207367	4.7115223	1.7854269
F	0.2408918	0.3722532	0.2033359
F	1.4110394	0.1618169	-2.2434870
F	4.0995143	-0.3430338	-2.4317468
F	5.5895940	-0.6810865	-0.1627762
F	4.4295928	-0.5253551	2.2652750
F	0.5882059	3.0424356	5.5474781
F	-0.6167978	5.4202156	5.1675279
F	-0.6411401	6.5728866	2.6850892
F	0.5295237	5.2854415	0.5711033
F	1.7240360	2.8950769	0.9269997
F	1.4132169	-2.5569308	1.9053895
F	-0.1916709	-4.3702490	3.0288284
F	-1.9794039	-3.6333423	4.9560391
F	-2.1474942	-1.0242937	5.7522157
F	-0.5558911	0.8245300	4.6424288
C	1.9799824	1.5915229	3.4926294
Si	4.5116347	2.6558709	4.0314818
C	5.8542181	2.9135945	2.7559691
C	7.8673896	3.2894173	0.8207334
C	5.5776219	2.7465783	1.3864233
C	7.1585602	3.2785462	3.1342974
C	8.1582524	3.4656075	2.1769624
C	6.5756333	2.9306675	0.4265500
H	4.5705501	2.4626801	1.0758317
H	7.4033266	3.4190341	4.1906016
H	9.1658543	3.7462737	2.4877100
H	6.3460110	2.7888611	-0.6307296
H	8.6484535	3.4304956	0.0721016
C	3.8094838	4.2777564	4.6528900
C	2.5418162	6.6800998	5.4005925
C	3.3333676	4.4597867	5.9639800
C	3.6461487	5.3278700	3.7271738
C	3.0154294	6.5174440	4.0941965
C	2.7044872	5.6526676	6.3330914
H	3.4164884	3.6450076	6.6873400
H	4.0132537	5.2090829	2.7043539
H	2.8886888	7.3171634	3.3626018
H	2.3270328	5.7747664	7.3494993

H	2.0401583	7.6053825	5.6877074
C	5.1068780	1.5262092	5.4506210
H	5.5036952	2.1505760	6.2637128
H	5.9243644	0.9129739	5.0456219
C	3.9836146	0.6670958	5.9519754
C	1.7624111	-0.7377033	6.7648292
N	3.1557270	1.2177003	6.8599402
C	3.7565599	-0.6184807	5.4251446
C	2.6300306	-1.3216990	5.8400974
C	2.0656113	0.5363881	7.2636884
H	4.4424278	-1.0379487	4.6911149
H	2.4228715	-2.3155869	5.4395931
H	0.8668025	-1.2599529	7.1025422
C	1.1883328	1.2259295	8.2711752
H	0.3133362	0.6192808	8.5356030
H	0.8438603	2.1891095	7.8707875
H	1.7598594	1.4407886	9.1857585
O	3.3456519	1.8527767	3.1465563
H	1.8868697	1.3723293	4.5685849

I

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B	1.7597439	0.9030222	2.5071714
C	3.0217911	0.1610178	1.8726684
C	5.3283468	-1.0365540	0.6955575
C	3.8060765	-0.7872190	2.5450151
C	3.4471875	0.4594965	0.5682231
C	4.5720518	-0.1123860	-0.0246416
C	4.9399158	-1.3815083	1.9896659
C	0.4943455	1.2369545	1.6039195
C	-1.8841157	1.7586675	0.1566335
C	0.2884917	2.4470423	0.9410690
C	-0.5370612	0.3015210	1.5146432
C	-1.7178565	0.5339619	0.8074875
C	-0.8751867	2.7240077	0.2232950
C	0.2340075	1.1033044	4.7643179
C	-2.2729523	1.1353194	6.1023681
C	-0.7043293	2.1229767	4.5457262
C	-0.1337024	0.1096269	5.6867725
C	-1.3610581	0.1059478	6.3470976
C	-1.9373854	2.1484628	5.2035077
F	2.7816683	1.3668594	-0.1750718
F	4.9488827	0.2335018	-1.2665193
F	6.4297437	-1.5747923	0.1543936
F	5.6665794	-2.2691049	2.6905460
F	3.5022224	-1.1762090	3.8085093
F	0.7234115	-0.8998249	5.9463848
F	-1.6677113	-0.8708912	7.2134453
F	-3.4561580	1.1527614	6.7297944
F	-2.8014374	3.1497683	4.9739980
F	-0.4466901	3.1471170	3.7094063
F	-0.4074140	-0.8896560	2.1503429
F	-2.6889193	-0.3947612	0.7507800

F	-3.0100758	2.0093266	-0.5291588
F	-1.0423601	3.9052490	-0.3972752
F	1.2252853	3.4199157	1.0009922
C	1.5362270	0.9324776	4.0711957
Si	3.6183893	2.9513557	3.9541857
C	4.8294130	2.8228588	2.5510874
C	6.5854189	2.6129538	0.3645054
C	4.5792900	3.5283340	1.3576499
C	5.9810150	2.0170134	2.6331773
C	6.8524512	1.9163052	1.5465397
C	5.4477067	3.4198727	0.2707464
H	3.6872132	4.1506400	1.2690959
H	6.2117705	1.4845929	3.5576657
H	7.7377314	1.2826700	1.6191182
H	5.2309815	3.9557140	-0.6538817
H	7.2592571	2.5195324	-0.4881294
C	3.1350653	4.7111449	4.3159414
C	2.5306167	7.3500608	5.0818627
C	1.9310499	5.0089028	4.9796824
C	4.0309205	5.7608491	4.0440264
C	3.7317959	7.0710181	4.4243345
C	1.6281273	6.3177569	5.3579336
H	1.2145448	4.2134658	5.1907657
H	4.9715962	5.5506322	3.5307173
H	4.4355921	7.8753936	4.2052135
H	0.6854452	6.5351318	5.8624258
H	2.2938532	8.3738862	5.3751907
C	4.1705600	2.0819851	5.5369518
H	4.4457365	1.0387394	5.3264652
H	3.3068433	2.0839413	6.2203833
C	5.3424501	2.8061469	6.1477152
C	7.5518058	4.1097859	7.1172778
N	6.5615815	2.3233606	5.8533133
C	5.1601824	3.9550297	6.9348360
C	6.2859302	4.6096811	7.4256721
C	7.6515751	2.9595152	6.3234560
H	4.1564437	4.3298333	7.1371441
H	6.1783139	5.5054911	8.0389024
H	8.4525794	4.6032778	7.4832815
C	8.9799720	2.3672782	5.9375205
H	9.0496487	1.3270933	6.2870967
H	9.8198034	2.9372011	6.3540304
H	9.0772390	2.3446886	4.8420973
O	2.1250876	2.1814044	3.4840188
H	2.2604380	0.4120624	4.6957221

TS3

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B	1.6828462	1.8816683	2.4102341
C	1.7414567	2.4677711	0.8984818
C	1.8819415	3.5259984	-1.7336673
C	2.7789212	2.1444342	0.0245030
C	0.7642057	3.3156328	0.3850210

C	0.8081281	3.8523157	-0.9022878
C	2.8770894	2.6617813	-1.2679831
C	1.1232995	4.1739643	3.8770473
C	1.4138507	6.8372722	4.8114943
C	1.9920629	5.1062862	3.2337375
C	0.4245282	4.6618973	5.0270140
C	0.5481461	5.9648867	5.4821179
C	2.1422467	6.4064452	3.6941562
F	-0.3068686	3.6644158	1.1578785
F	-0.1594374	4.6771789	-1.3469977
F	1.9529871	4.0325640	-2.9755382
F	3.9029119	2.3307821	-2.0734966
F	3.7325967	1.2616057	0.4108243
F	-0.3941906	3.8510380	5.6987993
F	-0.1167327	6.3926321	6.5592370
F	1.5703332	8.0783501	5.2593837
F	2.9972697	7.2471333	3.1057013
F	2.7431729	4.7375726	2.2063166
C	0.9506372	2.8233094	3.5017080
Si	4.1659119	2.0178260	4.2698019
C	5.6503891	2.8949338	3.5393894
C	7.9142395	4.1805346	2.4566559
C	5.6870243	3.2724009	2.1870858
C	6.7711893	3.1849287	4.3428772
C	7.8933091	3.8186851	3.8078966
C	6.8081340	3.9092609	1.6474127
H	4.8305631	3.0597130	1.5487792
H	6.7728638	2.9090613	5.4003199
H	8.7542873	4.0278160	4.4455107
H	6.8185186	4.1890436	0.5926262
H	8.7921209	4.6740603	2.0365362
C	3.5864437	3.0146991	5.7706394
C	2.6067828	4.5831170	7.9130580
C	2.7284784	2.4662274	6.7421238
C	3.9487052	4.3680392	5.9075727
C	3.4644458	5.1459755	6.9639119
C	2.2439462	3.2372105	7.8021916
H	2.4262895	1.4196072	6.6732046
H	4.6260580	4.8186662	5.1786353
H	3.7559538	6.1958710	7.0449587
H	1.5799325	2.7879325	8.5422688
H	2.2273736	5.1892675	8.7377691
C	4.5833678	0.2407790	4.7916688
H	4.7184521	-0.3480541	3.8741277
H	3.7330820	-0.1658343	5.3563770
C	5.8496271	0.2496053	5.5943147
C	8.2435536	0.5196435	6.9137670
N	6.9936815	0.0613903	4.9117310
C	5.8411814	0.5526690	6.9683708
C	7.0576254	0.6863042	7.6310363
C	8.1698000	0.1972525	5.5511200
H	4.8963316	0.7015841	7.4914491
H	7.0829108	0.9292026	8.6946372
H	9.2128772	0.6349671	7.4002104
C	9.4023379	-0.0022161	4.7117139
H	9.3118477	0.5722358	3.7792025

H	10.3143046	0.3038766	5.2409973
H	9.5025675	-1.0618878	4.4307112
O	2.9768245	1.9919461	3.1307301
H	0.3529439	2.2880840	4.2468231
C	1.1056168	0.3334935	2.4802329
C	0.2698633	-2.3991646	2.7350220
C	0.7039534	-0.4415382	1.3834133
C	1.0420842	-0.3424606	3.7049944
C	0.6465707	-1.6691347	3.8632987
C	0.2956839	-1.7766473	1.4876696
F	1.3716445	0.3105436	4.8604468
F	0.6179760	-2.2449669	5.0799922
F	-0.1204308	-3.6769042	2.8518203
F	-0.0745788	-2.4676913	0.3951397
F	0.6819377	0.0661101	0.1300713

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B	1.7765624	2.0945644	2.3348274
C	1.7257051	2.5892989	0.7564210
C	1.7898528	3.5999154	-1.8990141
C	2.7893848	2.3215764	-0.1110718
C	0.7043516	3.3699424	0.2299098
C	0.7042331	3.8810565	-1.0688213
C	2.8403847	2.8144163	-1.4164132
C	0.6264600	4.0030629	3.9194010
C	0.7488648	6.2063513	5.6856157
C	1.6209602	5.0205862	3.7794899
C	-0.3336241	4.1872497	4.9643173
C	-0.2600831	5.2419004	5.8546152
C	1.6690124	6.1141065	4.6336721
F	-0.3773888	3.6908154	1.0083487
F	-0.3119212	4.6397759	-1.5195949
F	1.8231767	4.0771849	-3.1528039
F	3.8808611	2.5324398	-2.2197506
F	3.8136582	1.5396917	0.2845882
F	-1.2889577	3.2731159	5.1458306
F	-1.1145652	5.3584987	6.8759755
F	0.8034860	7.2393602	6.5144977
F	2.5672192	7.0840372	4.4583850
F	2.4612578	5.0029895	2.7571770
C	0.5761492	2.8484192	3.1200229
Si	4.1907354	2.2956814	4.0858999
C	5.8163795	2.9134638	3.3858222
C	8.2523292	3.8502920	2.3119957
C	5.9049769	3.3236905	2.0451769
C	6.9751443	2.9984906	4.1829454
C	8.1815754	3.4574620	3.6525583
C	7.1103993	3.7870498	1.5100649
H	5.0189467	3.2706135	1.4134296
H	6.9411473	2.7024308	5.2337420
H	9.0687266	3.5073084	4.2863521
H	7.1581133	4.0945261	0.4640503

H	9.1957346	4.2071439	1.8952648
C	3.7474184	3.4223312	5.5551674
C	3.0942016	5.1245945	7.7239307
C	2.7508820	3.0701530	6.4880777
C	4.4073397	4.6522170	5.7444202
C	4.0896213	5.4936227	6.8147551
C	2.4244644	3.9068121	7.5578010
H	2.2208644	2.1228540	6.3834700
H	5.1861711	4.9552834	5.0423805
H	4.6172261	6.4407329	6.9368780
H	1.6494964	3.6084375	8.2666075
H	2.8427396	5.7793190	8.5596488
C	4.3235635	0.5116426	4.7386539
H	4.3340139	-0.1579515	3.8677493
H	3.4319329	0.2958051	5.3443586
C	5.5825612	0.3473021	5.5331443
C	8.0062487	0.2532923	6.8232738
N	6.6589600	-0.1045378	4.8641673
C	5.6548547	0.7490459	6.8802228
C	6.8854872	0.6970589	7.5279247
C	7.8502920	-0.1457804	5.4883346
H	4.7634310	1.1141781	7.3914431
H	6.9744598	1.0077369	8.5703546
H	8.9871715	0.2135451	7.2982677
C	9.0137151	-0.6091393	4.6546193
H	9.1851859	0.1053484	3.8351775
H	9.9348977	-0.6971135	5.2450960
H	8.7890749	-1.5800523	4.1915228
O	3.0702993	2.3950424	2.9072468
H	-0.3841563	2.3271130	3.1818975
C	1.4217524	0.4683482	2.5227082
C	1.0126010	-2.2865221	3.1568055
C	1.4600461	-0.5331649	1.5483753
C	1.1288523	0.0152940	3.8090372
C	0.9349092	-1.3175878	4.1592039
C	1.2690075	-1.8889373	1.8443168
F	1.0197303	0.9289411	4.8261227
F	0.6756041	-1.6760959	5.4301210
F	0.8280569	-3.5816200	3.4509391
F	1.3210736	-2.8148510	0.8717249
F	1.6746999	-0.2462061	0.2471263

TS4

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B	1.8041253	2.3559503	2.4877666
C	1.6085925	2.4817051	0.8042092
C	1.8588555	2.4140573	-2.0284126
C	2.3962344	3.4023771	0.0995261
C	0.8521904	1.6079602	0.0118440
C	0.9901849	1.5351418	-1.3755654
C	2.5590602	3.3665327	-1.2852402
C	1.0181661	4.7556694	3.6106210
C	1.2129062	6.7033281	5.6643930

C	2.2673772	5.3563235	3.9637741
C	-0.1389458	5.2877121	4.2688329
C	-0.0464283	6.1952780	5.3124704
C	2.3609374	6.3192774	4.9604420
F	-0.0258600	0.7452324	0.5673858
F	0.3055327	0.6266174	-2.0896211
F	2.0002023	2.3581673	-3.3582837
F	3.3615670	4.2453813	-1.9099038
F	3.0587411	4.3786920	0.7541433
F	-1.3529712	4.8303619	3.9534008
F	-1.1313864	6.5954782	5.9846039
F	1.3118049	7.5833890	6.6530367
F	3.5293391	6.8955186	5.2478627
F	3.3747772	5.0718344	3.2995782
C	0.8482880	3.5581962	2.8764853
Si	4.2839085	2.1648668	4.0153671
C	5.8861983	2.9622436	3.4601264
C	8.2727340	4.1744669	2.5621830
C	5.9723191	3.5289626	2.1769276
C	7.0264927	3.0168880	4.2847002
C	8.2077264	3.6148321	3.8420839
C	7.1517471	4.1301537	1.7298929
H	5.1001033	3.5031893	1.5247997
H	7.0045402	2.5726078	5.2823787
H	9.0806835	3.6399468	4.4965512
H	7.1940982	4.5646603	0.7295546
H	9.1950117	4.6436338	2.2153476
C	3.6686041	2.9697052	5.6180457
C	2.5625091	4.2204432	7.9038405
C	2.4144464	2.5846707	6.1299353
C	4.3622711	3.9879774	6.2956422
C	3.8226232	4.5996089	7.4324569
C	1.8547487	3.2075112	7.2471395
H	1.8581101	1.7838615	5.6408148
H	5.3312582	4.3222082	5.9207845
H	4.3823994	5.3847079	7.9435309
H	0.8725463	2.8975274	7.6082206
H	2.1369890	4.7049455	8.7842812
C	4.4969519	0.3020842	4.3506077
H	4.4823125	-0.2117471	3.3803368
H	3.6463213	-0.0423738	4.9577098
C	5.8121150	0.0764906	5.0295747
C	8.3305955	-0.0477801	6.1208292
N	6.8655609	-0.1309813	4.2177536
C	5.9576371	0.2051018	6.4227496
C	7.2368171	0.1357134	6.9689663
C	8.1020444	-0.1795423	4.7438280
H	5.0831067	0.3787403	7.0505720
H	7.3835462	0.2364765	8.0457289
H	9.3464260	-0.0870278	6.5160943
C	9.2283560	-0.3259459	3.7569848
H	9.2952120	0.5886702	3.1468158
H	10.1945400	-0.4892948	4.2519147
H	9.0285687	-1.1580818	3.0678804
O	3.1930178	2.4094321	2.8179057
H	-0.1959767	3.3757107	2.6044146

C	1.1142466	0.9668284	3.0908245
C	0.2773290	-1.4739808	4.2980225
C	1.6349167	-0.2733060	2.7079467
C	0.1466819	0.9195263	4.0926028
C	-0.2810445	-0.2618749	4.7024259
C	1.2450150	-1.4800980	3.2892179
F	-0.4251448	2.0655146	4.5688692
F	-1.2065082	-0.2388022	5.6790265
F	-0.1116915	-2.6218872	4.8717031
F	1.7807493	-2.6450371	2.8900135
F	2.5609387	-0.3373288	1.7267264

K

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B	1.8627427	1.9683768	2.9660050
C	2.4245465	1.6885824	1.4328517
C	3.8089252	1.5836244	-1.0744924
C	3.0111692	0.5264912	0.9348593
C	2.5793294	2.8055524	0.5967549
C	3.2410030	2.7774210	-0.6291253
C	3.6926182	0.4464069	-0.2824512
C	1.1573023	-0.8017911	3.6741296
C	0.0684597	-3.3956752	3.2450978
C	0.1216942	-1.0269412	2.7646968
C	1.6319736	-1.9376796	4.3470666
C	1.1090851	-3.2155197	4.1597090
C	-0.4239767	-2.2946201	2.5430485
C	0.4562604	2.8372033	3.0177336
C	-1.9368317	4.4197436	3.1644354
C	-0.4829310	2.9007763	1.9786817
C	0.1369941	3.6466496	4.1171341
C	-1.0230668	4.4167623	4.2168462
C	-1.6577836	3.6571839	2.0314200
F	2.1033868	4.0140828	0.9806720
F	3.3722926	3.8933367	-1.3729605
F	4.4861736	1.5415983	-2.2346075
F	4.2614102	-0.7092782	-0.6789574
F	2.9979566	-0.6358504	1.6545178
F	0.9505821	3.7125201	5.2090818
F	-1.2732963	5.1476796	5.3236406
F	-3.0618655	5.1502868	3.2387445
F	-2.5156691	3.6699787	0.9944646
F	-0.2843355	2.2369435	0.8177233
F	2.6644102	-1.8094628	5.2154620
F	1.6036291	-4.2671559	4.8323836
F	-0.4500307	-4.6137083	3.0445356
F	-1.4283704	-2.4556898	1.6687786
F	-0.4136031	-0.0063782	2.0802798
C	1.8578974	0.5234078	3.9191981
Si	4.4201075	2.4940450	4.0941411
H	2.9074259	0.2451658	3.8003757
C	5.5614509	1.9280723	2.7202274
C	7.0964651	1.1675646	0.4784218

C	5.8738058	2.8557241	1.7065562
C	6.0447958	0.6151722	2.5854679
C	6.8051609	0.2349631	1.4763520
C	6.6309069	2.4807689	0.5957973
H	5.5033349	3.8812698	1.7782255
H	5.8183976	-0.1373238	3.3439063
H	7.1577344	-0.7930815	1.3838343
H	6.8457761	3.2092127	-0.1874625
H	7.6755112	0.8694327	-0.3965026
C	5.0628449	4.0024500	4.9827934
C	5.9956726	6.2138457	6.4527326
C	6.4414772	4.2179586	5.1594485
C	4.1583209	4.9186737	5.5514745
C	4.6220257	6.0165038	6.2811788
C	6.9066825	5.3151138	5.8887845
H	7.1602520	3.5286840	4.7083281
H	3.0870821	4.7723212	5.4036234
H	3.9106961	6.7240283	6.7108631
H	7.9792956	5.4747088	6.0114794
H	6.3575502	7.0736932	7.0190302
C	4.2454422	1.0698722	5.3975479
H	5.0367721	1.1652238	6.1511632
H	4.3626799	0.0902322	4.9131758
C	2.9233956	1.1991800	6.0568671
C	0.4656910	1.4619077	7.3095928
N	1.7561076	0.8992222	5.3792573
C	2.8412045	1.6845823	7.3651090
C	1.6178558	1.8179359	8.0005425
C	0.5318967	1.0184881	5.9932712
H	3.7692374	1.9478691	7.8688835
H	1.5602710	2.1933737	9.0222454
H	-0.5158885	1.5542518	7.7704520
C	-0.7407131	0.6929674	5.2720017
H	-0.9266796	-0.3908880	5.2728517
H	-0.7358763	1.0412275	4.2349825
H	-1.5739816	1.1821004	5.7890707
O	2.8997310	2.8146285	3.6095506

TS5

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B	2.0885055	1.9303352	2.5748432
C	2.2543884	1.0762338	1.0820988
C	2.6942572	-0.0596481	-1.4911000
C	3.4582716	0.4425824	0.7367103
C	1.2547663	1.0374662	0.0991507
C	1.4564006	0.5076461	-1.1731894
C	3.7034765	-0.0956310	-0.5268634
C	0.6615265	-0.4575113	2.9746883
C	-1.3720855	-2.4069802	2.5968345
C	-0.6865570	-0.0970719	2.7696590
C	0.9345897	-1.8460643	2.9872822
C	-0.0490855	-2.8125028	2.8071146
C	-1.6893448	-1.0455726	2.5786702

C	1.0482670	3.1815155	2.5292550
C	-0.4442431	5.6097234	2.6164352
C	0.2766282	3.5502660	3.6278174
C	1.0677133	4.1110763	1.4863795
C	0.3358461	5.2999393	1.5007311
C	-0.4702949	4.7263950	3.6959768
F	0.0284831	1.5412276	0.3506079
F	0.4803848	0.5310991	-2.0960405
F	2.9027861	-0.5823423	-2.7054481
F	4.8808426	-0.6741916	-0.8155668
F	4.4533092	0.3004998	1.6407871
F	1.8354982	3.8914573	0.3899235
F	0.3816009	6.1542631	0.4617226
F	-1.1527142	6.7503313	2.6545608
F	-1.2010988	5.0211445	4.7895290
F	0.2381644	2.7524373	4.7309392
F	2.1939895	-2.2751583	3.1752497
F	0.2536530	-4.1180395	2.8190163
F	-2.3292471	-3.3196701	2.4184587
F	-2.9613548	-0.6642467	2.4044255
F	-1.0697318	1.1811764	2.8160443
C	1.7666933	0.4709608	3.1645665
Si	4.5757540	2.3870351	4.0352914
H	2.6963397	-0.0852145	3.2590452
C	6.2003716	2.4967543	3.1141679
C	8.6168839	2.7198834	1.6794845
C	6.2051478	2.9062513	1.7686744
C	7.4326578	2.2012386	3.7240885
C	8.6323244	2.3106819	3.0157990
C	7.4012417	3.0174301	1.0565925
H	5.2563474	3.1335134	1.2781703
H	7.4646490	1.8783352	4.7683849
H	9.5789664	2.0741426	3.5044984
H	7.3859675	3.3350208	0.0126520
H	9.5518705	2.8044620	1.1233888
C	4.4289177	3.7424237	5.3247457
C	4.1434173	5.7071185	7.3291017
C	5.5334400	4.4959117	5.7592746
C	3.1761301	3.9997525	5.9146301
C	3.0313368	4.9728716	6.9046195
C	5.3947468	5.4681291	6.7546544
H	6.5132728	4.3328417	5.3045905
H	2.2997783	3.4325143	5.5976987
H	2.0496610	5.1603422	7.3427698
H	6.2628403	6.0464416	7.0758682
H	4.0329692	6.4701398	8.1014994
C	4.4678496	0.7047055	4.9471607
H	5.4190659	0.5583341	5.4784602
H	4.3974685	-0.0829148	4.1859569
C	3.3416073	0.6678181	5.9259412
C	1.2870876	0.6743689	7.7621362
N	2.0758287	0.4147223	5.5132752
C	3.6082771	0.9646802	7.2753856
C	2.5733655	0.9866732	8.1958176
C	1.0641805	0.3809565	6.4131817
H	4.6306036	1.1966703	7.5715794

H	2.7642931	1.2349576	9.2404961
H	0.4487299	0.6518831	8.4577928
C	-0.3158851	-0.0025667	5.9596217
H	-0.3093100	-0.9890979	5.4761752
H	-0.7126491	0.7286252	5.2466462
H	-0.9983439	-0.0470886	6.8163667
O	3.3545144	2.4841065	2.9680469

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B	2.5869022	1.4559148	3.3888920
C	2.9823898	1.7334614	1.8682707
C	3.7259826	2.4421740	-0.7668048
C	3.3402080	0.7715752	0.9268229
C	3.0040371	3.0609342	1.4375090
C	3.3552189	3.4348790	0.1427529
C	3.7242474	1.1027665	-0.3732779
C	0.6342694	-0.3388896	3.5311789
C	-0.0684252	-3.0662091	3.1283400
C	-0.6881235	-0.7360193	3.2930723
C	1.5750199	-1.3730813	3.6041202
C	1.2547300	-2.7146116	3.4011502
C	-1.0447489	-2.0696057	3.0791491
C	0.2362480	2.1918659	3.1581989
C	-1.0575578	4.4106685	1.9521266
C	-0.1407731	2.1839143	1.8090036
C	-0.0538514	3.3588781	3.8750280
C	-0.6921324	4.4576253	3.2986326
C	-0.7808668	3.2639486	1.2032922
F	2.6918548	4.0480039	2.3165966
F	3.3746354	4.7267846	-0.2267788
F	4.1073610	2.7765999	-2.0075724
F	4.1005634	0.1519891	-1.2431710
F	3.3474734	-0.5373357	1.2600359
F	0.3106681	3.4546451	5.1736692
F	-0.9459533	5.5576303	4.0249041
F	-1.6667340	5.4581468	1.3804953
F	-1.1261941	3.2110488	-0.0924654
F	0.1113531	1.0977642	1.0479074
F	2.8623478	-1.0789194	3.9037372
F	2.2025853	-3.6614685	3.4729535
F	-0.4002654	-4.3490103	2.9295956
F	-2.3239322	-2.3990079	2.8410013
F	-1.6835517	0.1743548	3.2767853
C	1.0601236	1.0934560	3.7995682
Si	5.1096625	1.9789388	4.5645839
C	6.0143928	1.6984152	2.9541481
C	7.1723218	1.2764021	0.4209988
C	6.2346805	2.7737532	2.0726159
C	6.4040311	0.4088635	2.5468679
C	6.9752689	0.1993207	1.2898709
C	6.8066384	2.5667570	0.8158848
H	5.9430722	3.7839554	2.3689901

H	6.2779144	-0.4374976	3.2220206
H	7.2633209	-0.8078027	0.9853365
H	6.9583642	3.4101707	0.1404027
H	7.6091506	1.1109425	-0.5649987
C	5.2981187	3.7378973	5.1541885
C	5.6371759	6.3599325	6.1245221
C	6.5823632	4.3063884	5.2623633
C	4.1874749	4.5126407	5.5343419
C	4.3549351	5.8142869	6.0146025
C	6.7519621	5.6052403	5.7461605
H	7.4598164	3.7279244	4.9643934
H	3.1814131	4.0972238	5.4481202
H	3.4831455	6.4046328	6.3012404
H	7.7537338	6.0306673	5.8253052
H	5.7681339	7.3760150	6.5006019
C	5.6024883	0.7250468	5.8915247
H	5.3288719	-0.2775440	5.5319676
H	4.9972347	0.9512996	6.7817850
C	7.0739672	0.7886856	6.1828543
C	9.7949249	0.9376002	6.5177660
N	7.8671098	0.0146409	5.4201643
C	7.5928208	1.6631376	7.1528556
C	8.9732252	1.7315043	7.3190738
C	9.2018995	0.0856879	5.5757817
H	6.9217131	2.2833897	7.7473460
H	9.4063489	2.4017146	8.0633123
H	10.8800197	0.9740628	6.6191378
C	10.0181132	-0.7987783	4.6720563
H	11.0961425	-0.6485039	4.8134001
H	9.7637478	-0.5952469	3.6217271
H	9.7819584	-1.8564351	4.8606410
O	3.4439655	1.7233289	4.3892827
H	1.0202485	1.2434704	4.8900427

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B	2.3816777	0.9671366	3.6379203
C	2.9865691	-0.1984540	2.6526624
C	4.1123829	-2.1791296	0.9223270
C	3.0646508	-1.5516051	2.9962962
C	3.4920755	0.1051421	1.3827786
C	4.0464041	-0.8449728	0.5213323
C	3.6134366	-2.5363171	2.1755132
C	-0.4914762	0.5313878	3.2716136
C	-2.9772507	-0.8626782	3.0366592
C	-1.6998666	1.0321067	3.7900403
C	-0.5964829	-0.7032851	2.6203908
C	-1.8069975	-1.3963596	2.5008850
C	-2.9213213	0.3693111	3.6907601
C	0.7096589	2.4870471	2.3715833
C	0.7989438	4.5541775	0.4251202
C	0.6814173	2.2153116	1.0015086
C	0.7549115	3.8411818	2.7285056

C	0.8081451	4.8678869	1.7863940
C	0.7285251	3.2181826	0.0311668
F	3.4675094	1.3743974	0.9142221
F	4.5153334	-0.4877141	-0.6870346
F	4.6381301	-3.1091645	0.1102234
F	3.6494660	-3.8234229	2.5682689
F	2.5519484	-1.9928816	4.1783633
F	0.7772868	4.1965730	4.0307736
F	0.8744447	6.1531958	2.1752368
F	0.8551075	5.5306612	-0.4953213
F	0.7187628	2.9032006	-1.2750560
F	0.6377697	0.9390823	0.5641921
F	0.4773884	-1.3046663	2.0803744
F	-1.8430942	-2.5809347	1.8689985
F	-4.1397406	-1.5218959	2.9284650
F	-4.0366454	0.9012677	4.2186611
F	-1.7007449	2.2176654	4.4436679
C	0.7516320	1.4010924	3.4452412
Si	4.5146425	2.7599608	3.9270318
C	5.4070102	3.5525912	2.4996726
C	6.6528744	4.9111910	0.3734492
C	4.6455855	4.0891921	1.4450245
C	6.8042982	3.7065113	2.4661471
C	7.4246969	4.3803394	1.4108986
C	5.2627944	4.7627234	0.3900665
H	3.5614659	3.9618445	1.4462533
H	7.4229624	3.2927081	3.2672587
H	8.5102377	4.4902490	1.3962986
H	4.6582505	5.1696154	-0.4217994
H	7.1360487	5.4372742	-0.4512369
C	4.4156266	3.8938083	5.4136457
C	4.2867853	5.4337595	7.7707393
C	5.4708407	4.7508907	5.7733435
C	3.2880008	3.8359892	6.2535409
C	3.2215064	4.5988919	7.4210640
C	5.4111062	5.5121588	6.9433949
H	6.3461911	4.8378374	5.1244573
H	2.4453845	3.2003702	5.9753724
H	2.3345662	4.5494950	8.0550463
H	6.2374453	6.1745682	7.2062985
H	4.2361297	6.0323331	8.6816923
C	5.1859797	1.0701061	4.4977638
H	6.2009702	1.0757529	4.9091872
H	5.1583505	0.4297900	3.6050449
C	4.2122947	0.6348632	5.5395306
C	2.4812174	-0.0612468	7.5637167
N	2.8702196	0.4775748	5.2482000
C	4.6789057	0.4925180	6.8522472
C	3.8123639	0.1730967	7.8823028
C	2.0320381	0.0683976	6.2493441
H	5.7391865	0.6516415	7.0397913
H	4.1696516	0.0821057	8.9083021
H	1.7680687	-0.3683050	8.3271505
C	0.6101768	-0.2981354	5.9632803
H	0.2306956	-0.9357940	6.7697835
H	0.5232380	-0.8481577	5.0232397

H	-0.0384393	0.5860285	5.9129107
O	3.0151968	2.2617543	3.5110671
H	0.5764783	1.9581806	4.3767436

X-Ray Crystallography

X-ray Crystal Structure Determination of complex 2^H-BCF: X-ray intensities were measured on a Bruker D8 Quest Eco diffractometer equipped with a Triumph monochromator (λ = 0.71073 Å) and a CMOS Photon 50 detector at a temperature of 150(2) K. Intensity data were integrated with the Bruker APEX2 software.[S11] Absorption correction and scaling was performed with SADABS.[S12] The structures were solved using intrinsic phasing with the program SHELXT.[S11] Least-squares refinement was performed with SHELXL-2013[S13] against F^2 of all reflections. Non-hydrogen atoms were refined with anisotropic displacement parameters. The H atoms were placed at calculated positions using the instructions AFIX 13, AFIX 43 or AFIX 137 with isotropic displacement parameters having values 1.2 or 1.5 times *U*eq of the attached C atoms.

X-ray Crystal Structure Determination of complex 3O: All reflection intensities were measured at 110(2) K using a SuperNova diffractometer (equipped with Atlas detector) with Cu *K*α radiation (λ = 1.54178 Å) under the program CrysAlisPro (Version 1.171.36.32 Agilent Technologies, 2013). The same program was used to refine the cell dimensions and for data reduction. The structure was solved with the program SHELXS-2014/7 (Sheldrick, 2015) and was refined on F^2 with SHELXL-2014/7 (Sheldrick, 2015). Analytical numeric absorption correction using a multifaceted crystal model was applied using CrysAlisPro. The temperature of the data collection was controlled using the system Cryojet (manufactured by Oxford Instruments). The H atoms were placed at calculated positions (unless otherwise specified) using the instructions AFIX 13, AFIX 23, AFIX 43 or AFIX 137 with isotropic displacement parameters having values 1.2 or 1.5 *U*eq of the attached C atoms. The structure is partly disordered. The phenyl ring C13→C18 is disordered over 2 orientations, and the occupancy factor of the major component of the disorder refines to 0.64(2). The lattice pentane solvent molecule is found at sites of inversion symmetry, and thus is disordered over two orientations. Its occupancy factor was constrained to be 0.5.

CCDC 1538414 (**2^H-BCF**) and 1538261 (**3O**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_ request/cif.

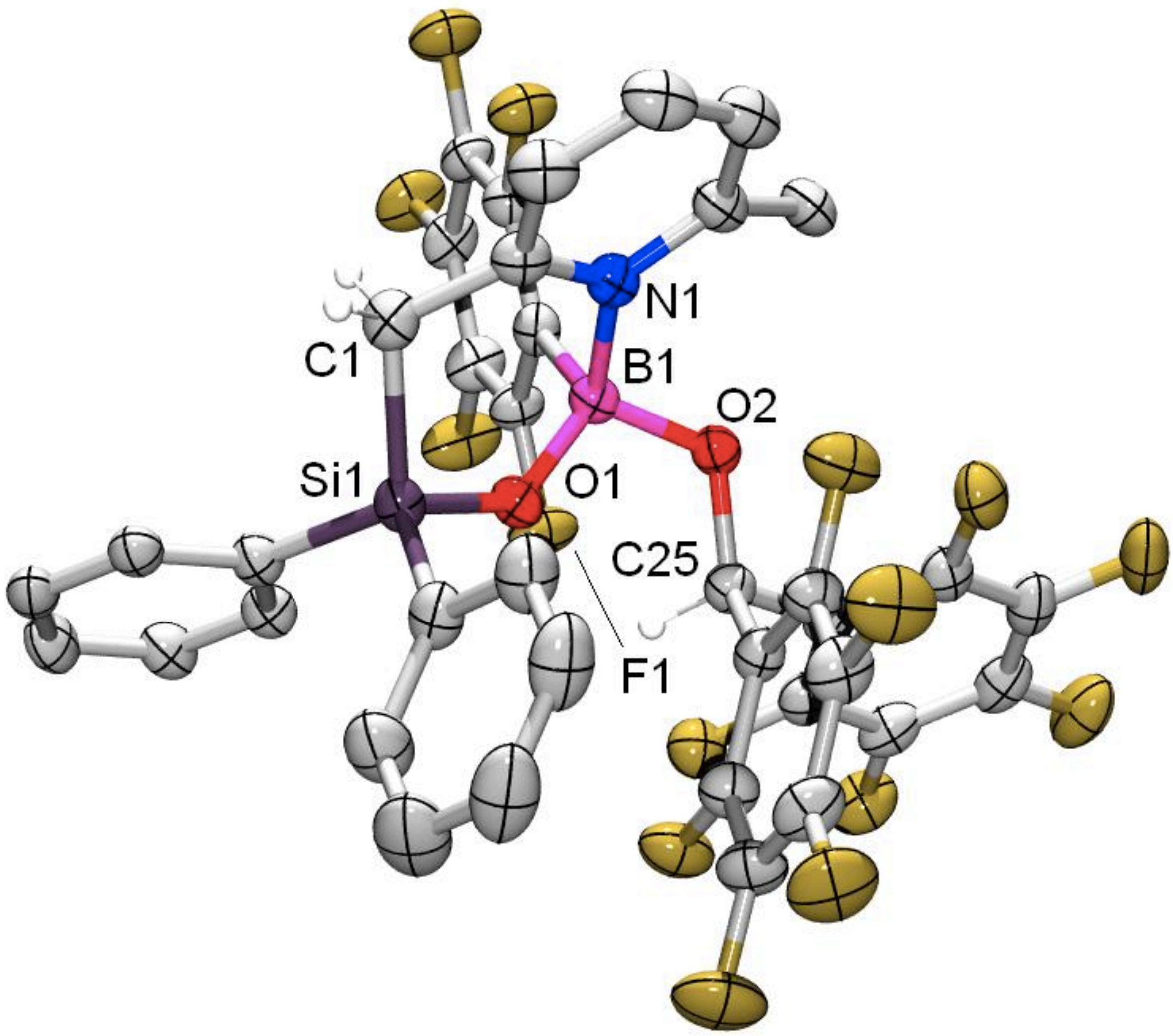

Figure S105. Displacement ellipsoid plot for **3O**

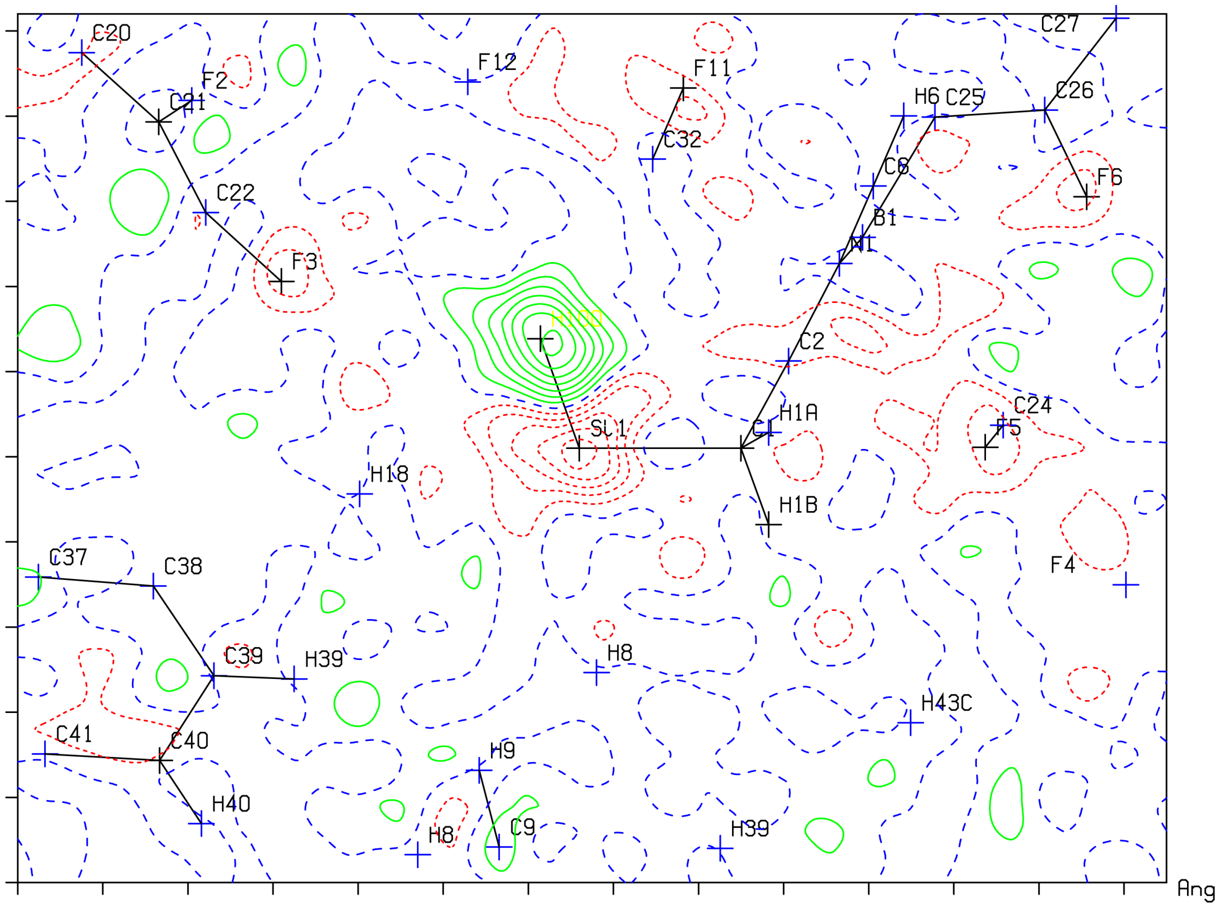

Figure S106. Contour difference Fourier map for **2H-BCF**

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