Supplementary information for

Imine-Stabilized Silylium Ions: Synthesis, Structure and Application in Catalysis.

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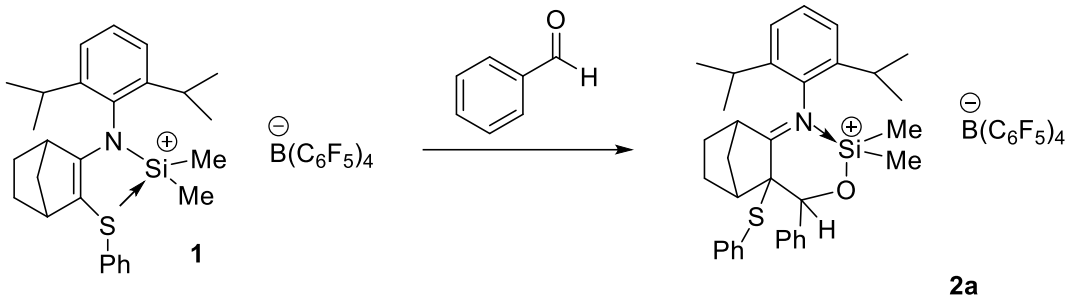
1-General

All manipulations were performed under inert atmosphere of argon by using Schlenk or high-pressure NMR tube techniques. Dry, oxygen-free solvents were employed. ^{1}H, ^{11}B, ^{13}C, ^{19}F and ^{29}Si NMR spectra were recorded on Bruker Avance II 300MHz, Avance III HD 400 MHz and Avance I and III HD 500 MHz spectrometers. ^{1}H, ^{29}Si and ^{13}C NMR chemical shifts are reported in ppm relative to $SiMe_4$ as internal standard. The following abbreviations and their combinations are used: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; sept, septuplet; m, multiplet. ^{1}H and ^{13}C resonance signals were attributed by means of 2D COSY, HSQC and HMBC experiments. The sulfide-stabilized silylium **1a** was synthesized as previously reported.[1]

2-Experimental procedures and characterization data



Synthesis of 2a: To a solution of **1** (150 mg, 0.13 mmol) in benzene (2.0 mL) was added benzaldehyde (13.7 µL, 0.13 mmol). Reaction mixture was stirred overnight and two phases were formed, the upper phase was removed and the lower phase washed twice with benzene (0.3 mL). Lower phase was dried under vacuum to obtained the adduct **2a** as a yellow-orange powder (71.6 mg, 44 %). **M.p.** = 74 °C (Decomposition)

Major isomer (75 %):

^{1}H NMR (500 MHz, CD_2Cl_2): δ = 0.48 (s, 3H, Si-CH_3), 1.17 (s, 3H, Si-CH_3), 1.28 (d, $^{3}J_{H\text{-}H}$ = 6.8 Hz, 3H, CH_{3iPr}), 1.31 (d, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 3H, CH_{3iPr}), 1.40 (d, $^{3}J_{HH}$ = 6.8 Hz, 3H, CH_{3iPr}), 1.42 (d, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 3H, CH_{3iPr}), 1.83-1.65 (m, 1H, CH_2), 2.17-1.86 (m, 3H, 3 CH_2), 2.43-2.31 (m, 2H, 2 CH_2), 2.47 (sept, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 1H, CH_{iPr}), 2.99-2.85 (sept, 1H, CH_{iPr} overlapped by signals of minor isomer), 3.34-3.27 (m, 2H, 2 C$H_{bridgehead}$), 5.60 (s, 1H, CHO), 6.39-6.33 (m, 2H, CH_{PhCHO}), 7.01-6.97 (m, 2H, CH_{PhCHO}), 7.13-7.06 (m, 1H, CH_{PhCHO}), 7.73-7.28 (m, 8H, 5 S(C_6H_5) and 3 CH_{dipp}).

^{13}C NMR (126 MHz, CD_2Cl_2): δ = 0.2 (s, Si-CH$_3$), 3.3 (s, Si-CH$_3$), 24.5 (s, CH$_{3iPr}$), 24.7 (s, CH$_{3iPr}$), 25.4 (s, CH$_2$), 25.8 (s, CH$_{3iPr}$), 26.1 (s, CH$_{3iPr}$), 26.7 (s, CH$_2$), 28.6 (s, CH$_{iPr}$), 29.7 (s, CH$_{iPr}$), 40.6 (s, CH$_2$), 43.6 (s, CH$_{bridgehead}$), 49.3 (s, CH$_{bridgehead}$), 68.5 (s, C-S), 76.9 (s, CH-O), 124.6 (br, *i* of BAr), 127.2 (s, CH$_{dipp}$), 127.3 (s, CH$_{dipp}$), 127.3 (s, CH$_{Ph}$), 128.2 (s, CH$_{Ph}$), 128.7 (s, CH$_{Ph}$), 129.2 (s, CH$_{Ph}$), 129.8 (s, CH$_{Ph}$),

[1] A. Dajnak, G. A. Özpınar, R. Lenk, N. Saffon-Merceron, A. Baceiredo, T. Kato, T. Müller, E. Maerten, Norbornene Based-Sulfide-Stabilized Silylium Ions: Synthesis, Structure and Application in Catalysis. Dalton Transactions, 2022, 51, 1407 – 1414.

130.3 (s, *C*H$_{Ph}$), 131.9 (s, *C*$_{Ph}$), 132.2 (s, *C*H$_{dipp}$), 132.6 (s, N-*C*$_{Dipp}$), 135.5 (s, *C*$_{Ph}$), 135.5 (s, *C*$_{PhCHO}$), 136.6 (br d, $J_{C\text{-}F}$ = 244.8 Hz, Ar*C*-F), 138.6 (br d, $J_{C\text{-}F}$ = 244.8 Hz, Ar*C*-F), 142.2 (s, *C*$_{iPr}$), 143.8 (s, *C*$_{iPr}$), 148.5 (br d, $J_{C\text{-}F}$ = 241.3 Hz, Ar*C*-F), 212.0 (s, N-*C*).

^{29}Si NMR (99 MHz, CD_2Cl_2): δ = 12.3 (s, *Si*-CH_3)

Minor isomer (25 %):

All signals marked with * are overlapped by signals of the major isomer.

^{1}H NMR (500 MHz, CD_2Cl_2): δ = 0.62 (s, 3H, Si-C*H*$_3$), 1.00 (d, $^3J_{H\text{-}H}$ = 6.7 Hz, 3H, C*H*$_{3iPr}$), 1.25-1.21 (m, 1H, C*H*$_2$*), 1.26 (d, 3H, C*H*$_{3iPr}$*), 1.33 (s, 3H, Si-C*H*$_3$*), 1.40 (d, 3H, C*H*$_{3iPr}$*), 1.48 (d, $^3J_{HH}$ = 6.6 Hz, 3H, C*H*$_{3iPr}$), 1.83-1.65 (m, 3H , C*H*$_2$*), 2.17-1.86 (m, 2H , C*H*$_2$*), 2.66 (sept, $^3J_{H\text{-}H}$ = 6.6 Hz, 1H, C*H*$_{iPr}$), 2.99-2.85 (m, 4H, 2 C*H*$_{bridgehead}$ + C*H*$_{iPr}$ + 1H C*H*$_2$*), 5.44 (s, 1H, C*H*O), 7.14-7.06 (m, 1H, C*H*$_{PhCHO}$*),7.73-7.28 (m, 12H, all Ar* signal excepted for 1H C*H*$_{PhCHO}$).

^{13}C NMR (126 MHz, CD_2Cl_2): δ = 0.8 (s, Si-*C*H$_3$), 4.8 (s, Si-*C*H$_3$), 24.6 (s, *C*H$_{3iPr}$), 24.7 (s, *C*H$_{3iPr}$), 24.7 (s, *C*H$_{3iPr}$), 25.0 (s, *C*H$_{3iPr}$), 25.2 (s, *C*H$_2$), 25.9 (s, *C*H$_{3iPr}$), 27.6 (s, *C*H$_2$), 28.8 (s, *C*H$_{iPr}$), 29.1 (s, *C*H$_{iPr}$), 38.3 (s, *C*H$_2$), 44.8 (s, *C*H$_{bridgehead}$), 46.6 (s, *C*H$_{bridgehead}$), 68.8 (s, *C*-S), 80.4 (s, *C*H-O), 124.6 (br, *i* of BAr), 127.2 (s, *C*H$_{dipp}$), 127.2 (s, *C*H$_{dipp}$), 128.1(s, *C*H$_{Ph}$), 129.2 (s, *C*H$_{Ph}$), 130.4 (s, *C*H$_{Ph}$), 131.1 (s, *C*H$_{Ph}$), 132.1 (s, *C*H$_{dipp}$), 132.1 (s, *C*H$_{dipp}$), 133.4 (s, N-*C*$_{Dipp}$), 136.6 (br d, $J_{C\text{-}F}$ = 244.8 Hz, Ar*C*-F), 136.7 (s, *C*$_{PhCHO}$), 138.6 (br d, $J_{C\text{-}F}$ = 244.8 Hz, Ar*C*-F), 141.5 (s, *C*$_{iPr}$), 143.6 (s, *C*$_{iPr}$), 148.5 (br d, $J_{C\text{-}F}$ = 241.3 Hz, Ar*C*-F), 212.9 (s, N-*C*).

Signal of 3 C$_{Ph}$ could not be detected due to overlapping

^{19}F NMR (471 MHz, CD_2Cl_2): δ = -167.6 (t, J_{FF} = 19.2 Hz, *m* of ArC-*F*), -163.7 (t, J_{FF} = 20.4 Hz, *p* of ArC-*F*), -133.1 (br, o of ArC-*F*).

^{11}B NMR (160 MHz, CD_2Cl_2): δ = -16.7 (s, *B*Ar).

^{29}Si NMR (99 MHz, CD_2Cl_2): δ = 7.4 (s, *Si*-CH_3).

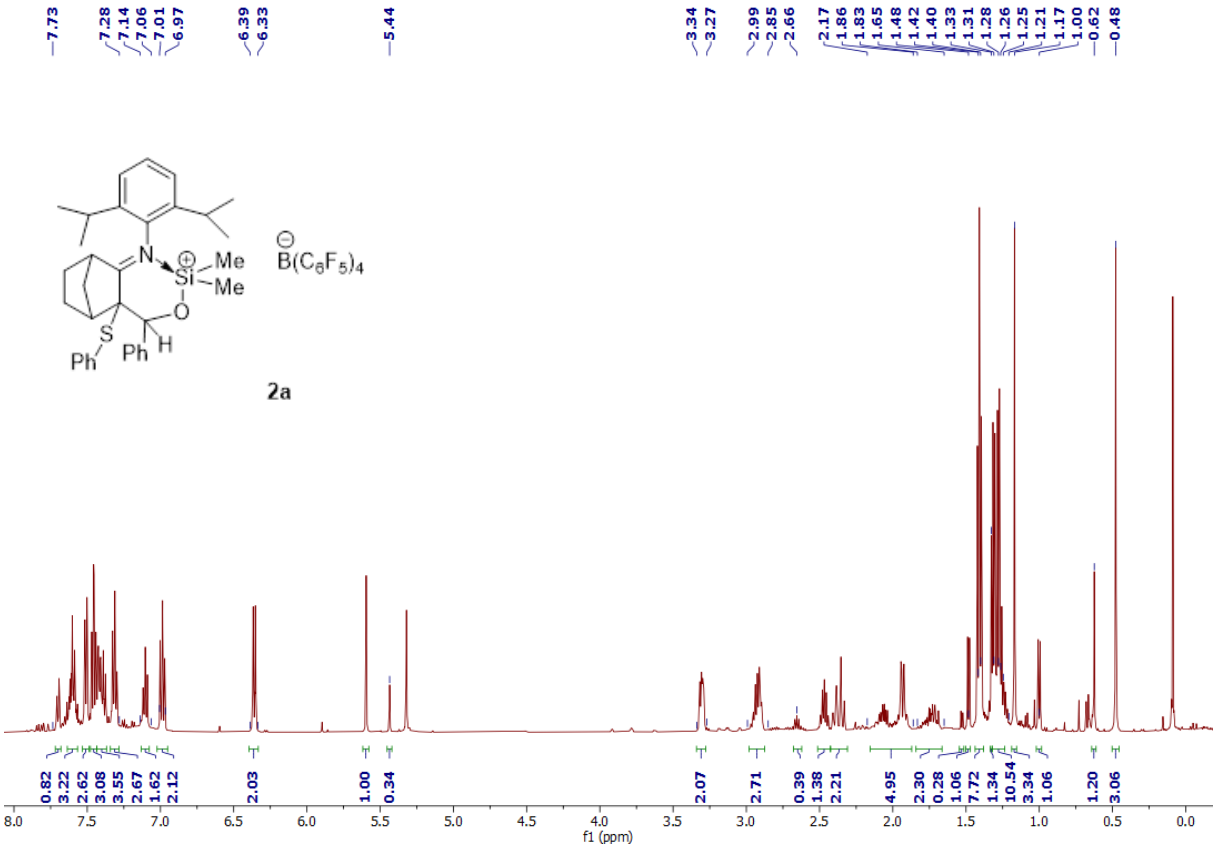


Figure S1: ^{1}H NMR (500 MHz, CD_2Cl_2) of 2a

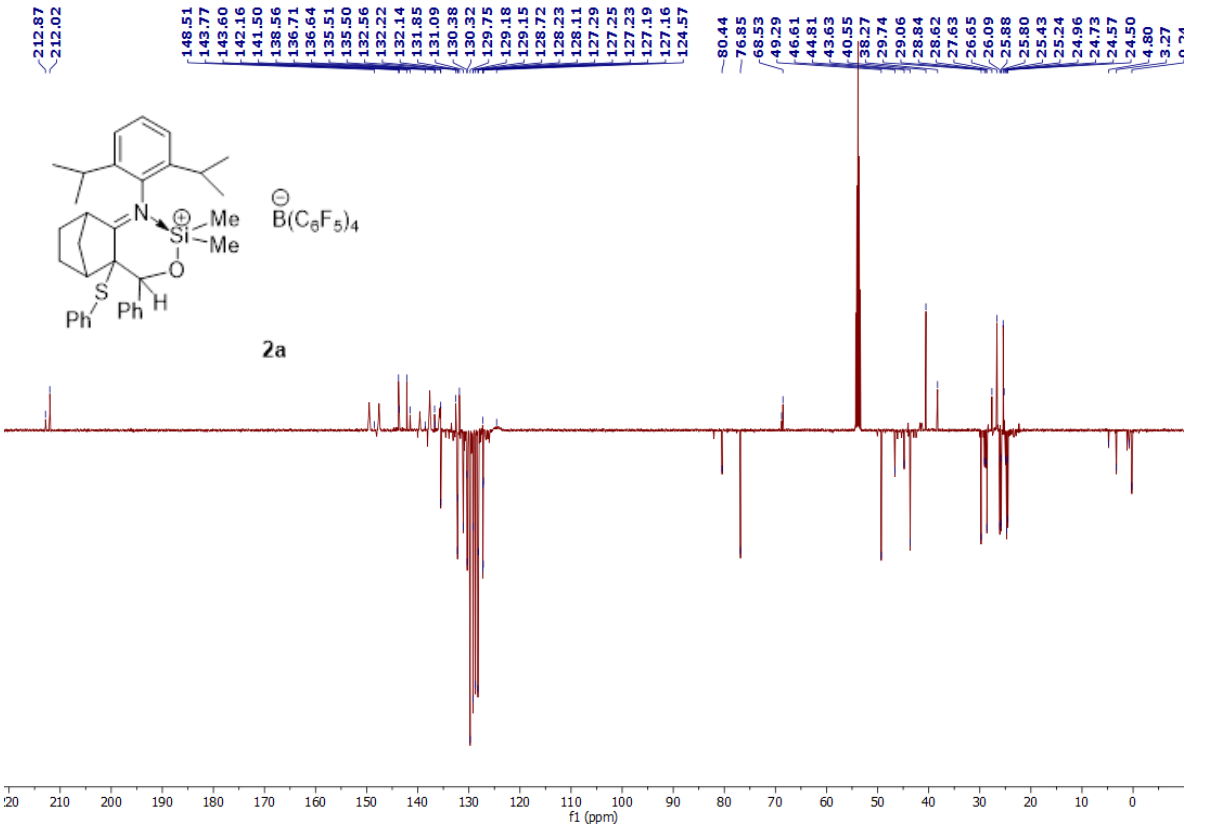


Figure S2: $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_2Cl_2) of 2a

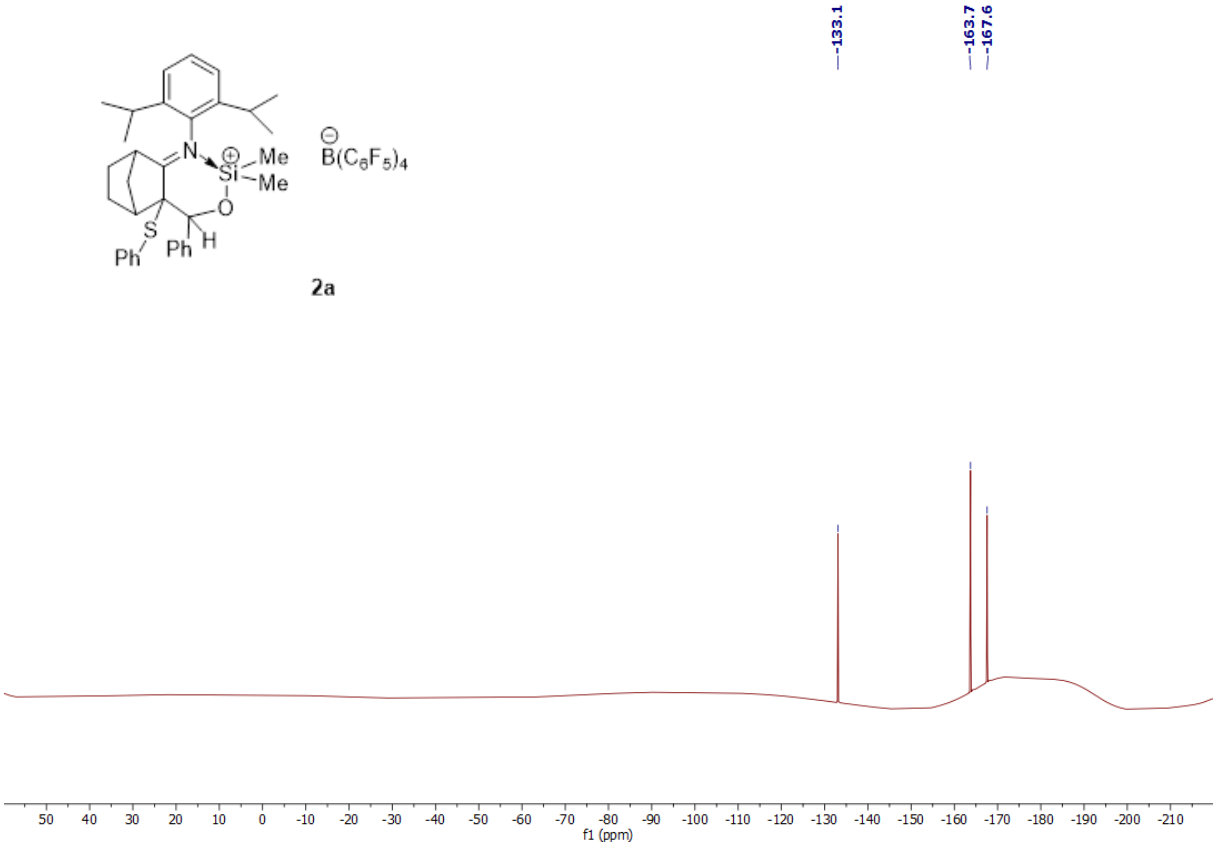


Figure S3: ^{19}F NMR (471 MHz, CD_2Cl_2) of 2a

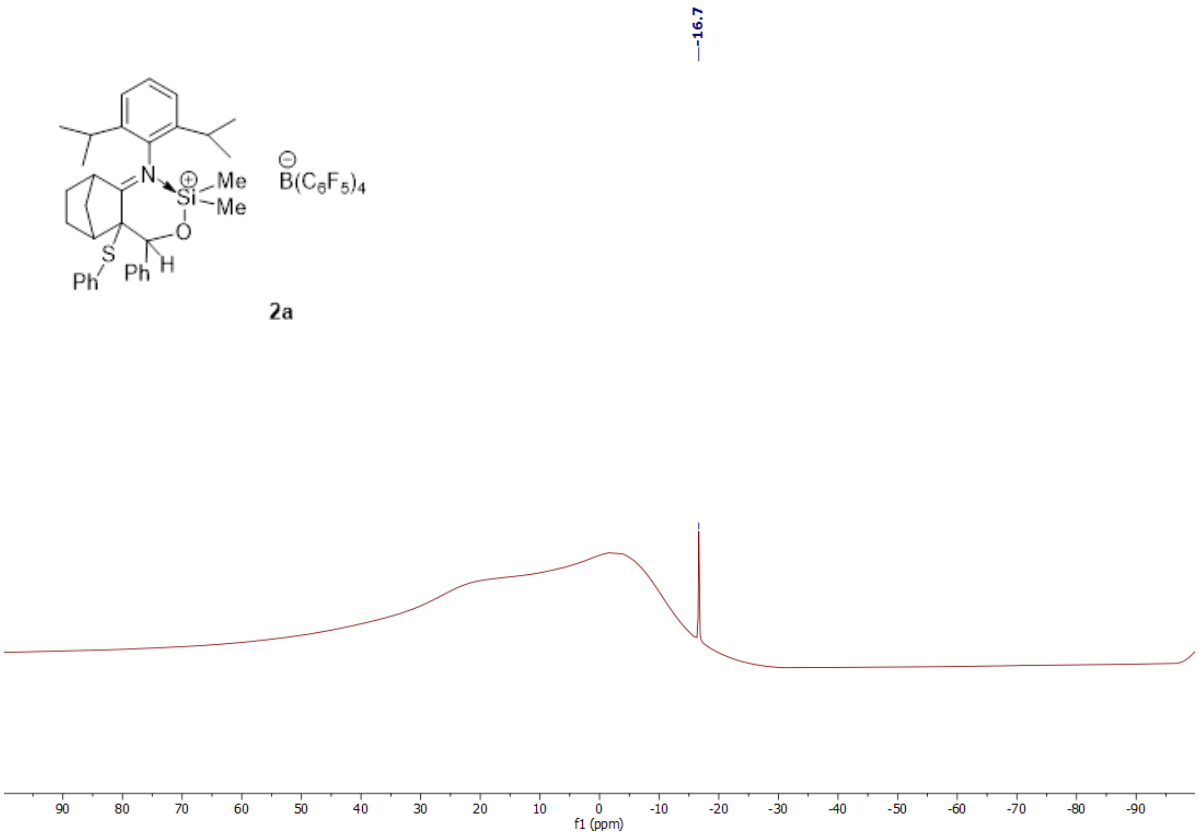


Figure S4: ^{11}B NMR (160 MHz, CD_2Cl_2) of 2a

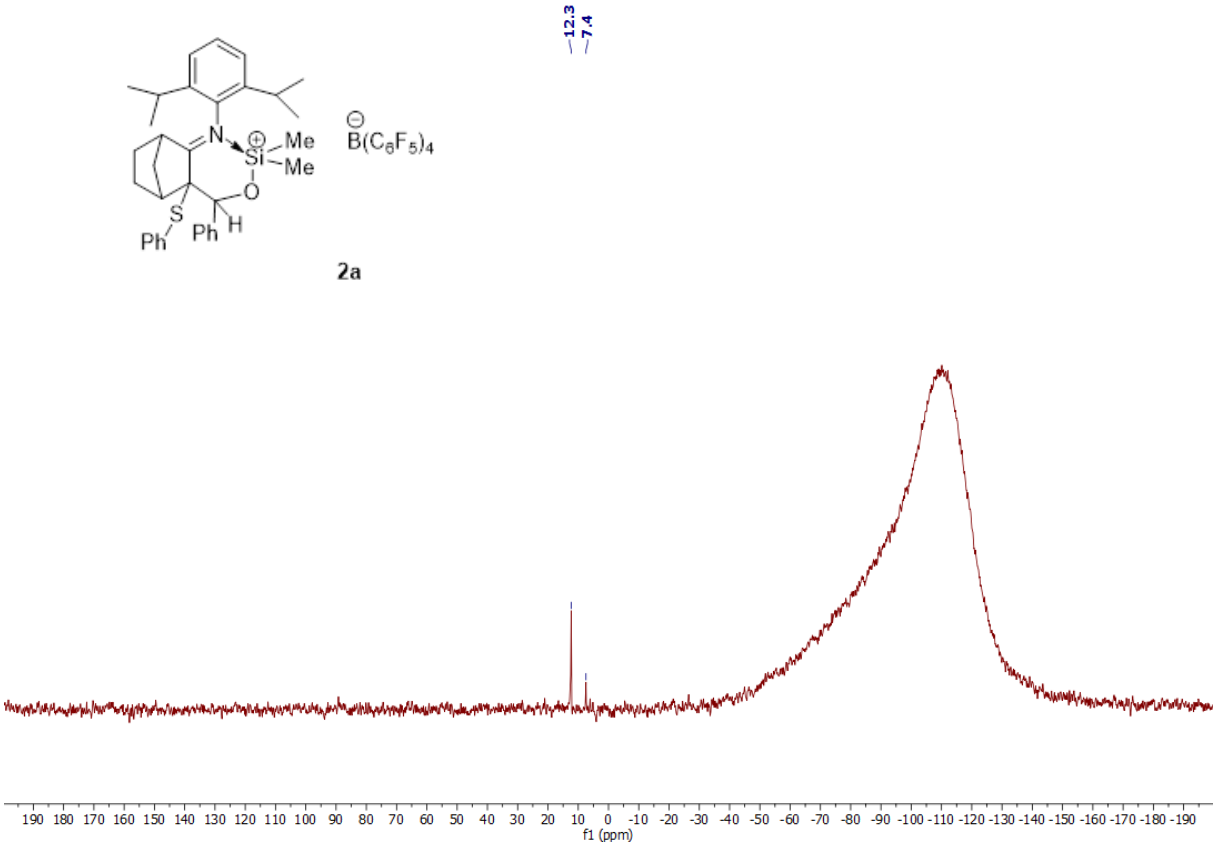
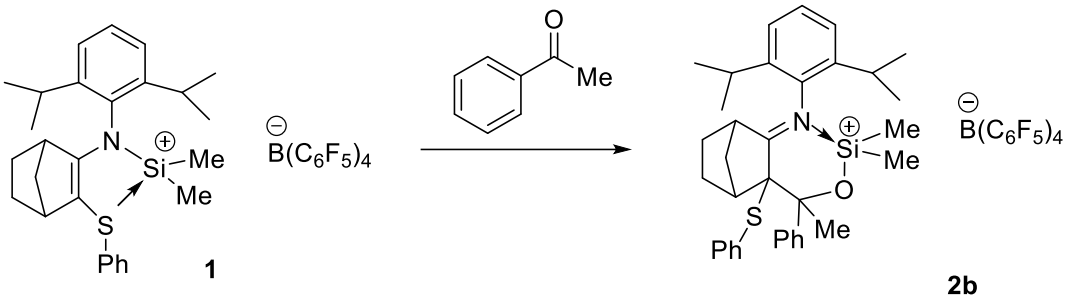


Figure S5: $^{29}Si\{^{1}H\}$ NMR (99 MHz, CD_2Cl_2) of 2a



Synthesis of 2b: To a solution of **1** (150 mg, 0.13 mmol) in benzene (2.0 mL) was added acetophenone (15.7 µL, 0.13 mmol). Reaction mixture was stirred overnight and two phases were formed, the upper phase was removed and the lower phase washed twice with benzene (0.3 mL). Lower phase was dried under vacuum to obtained the adduct **2b** as a yellow powder (88.1 mg, 53 %). **M.p.** = 70°C (Decomposition).

^{1}H NMR (300 MHz, CD_2Cl_2): δ = 0.56 (s, 3H, Si-CH_3), 1.07 (s, 3H, Si-CH_3), 1.30 (d, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 3H, CH_{3iPr}), 1.31 (d, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 3H, CH_{3iPr}), 1.43 (d, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 3H, CH_{3iPr}), 1.42 (d, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 3H, CH_{3iPr}), 2.12 (s, 3H, PhCOCH_3), 2.22-1.64 (m, 5H, 3 CH_2), 2.38-2.26 (m, 1H, CH_2), 2.67 (sept, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 1H, CH_{iPr}), 3.14 (sept, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 1H, CH_{iPr}), 3.23 (m, 1H, C$H_{bridgehead}$), 3.46 (m, 1H, C$H_{bridgehead}$), 6.31-6.17 (m, 2H, 2 C$H_{PhCOCH3}$), 7.68-6.89 (m, 11H, S(C$_6H_5$) + 3 CH_{dipp} + 3 C$H_{PhCOCH3}$).

^{13}C NMR (75 MHz, CD_2Cl_2): δ =1.0 (s, Si-CH$_3$), 2.4 (s, Si-CH$_3$), 24.3 (s, CH$_{3iPr}$), 24.5 (s, CH$_{3iPr}$), 25.7 (s, CH$_{3iPr}$), 26.3 (s, CH$_{3iPr}$), 28.0 (s, CH$_2$), 28.2 (s, CH$_2$), 28.3 (s, CH$_{iPr}$), 30.1 (s, CH$_{iPr}$), 42.4 (s, CH$_2$), 44.3 (s, CH$_{bridgehead}$), 47.5 (s, CH$_{bridgehead}$), 58.5 (s, PhCOCH$_3$), 73.5 (s, C-S), 83.1 (s, PhCOCH$_3$), 127.2 (s, CH$_{dipp}$), 127.5 (s, CH$_{dipp}$), 127.6 (s, 2 C_{Ph} overlapped), 129.6 (s, C_{Ph}), 129.7 (s, C_{Ph}), 130.7 (s, C_{Ph}), 132.2 (s, CH$_{dipp}$), 132.3 (s, C_{Ph}), 132.5 (s, C_{Ph}), 133.7 (s, N-C_{Dipp}), 136.6 (br d, $J_{C\text{-}F}$ = 245.2 Hz, ArC-F), 138.8 (br d, $J_{C\text{-}F}$ = 245.4 Hz, ArC-F), 141.0 (s, C_{Ph}), 142.5 (s, C_{iPr}), 144.7 (s, C_{iPr}), 148.5 (br d, $J_{C\text{-}F}$ = 241.2 Hz, ArC-F), 212.2 (s, N-C).

^{19}F NMR (471 MHz, CD_2Cl_2): δ = -167.6 (t, J_{FF} = 19.2 Hz, *m* of ArC-*F*), -163.7 (t, J_{FF} = 20.4 Hz, *p* of ArC-*F*), -133.1 (br, o of ArC-*F*).

^{11}B NMR (160 MHz, CD_2Cl_2): δ = -16.7 (s, *B*Ar).

^{29}Si NMR (99 MHz, CD_2Cl_2): δ = 8.3 (s, *Si*-CH$_3$).

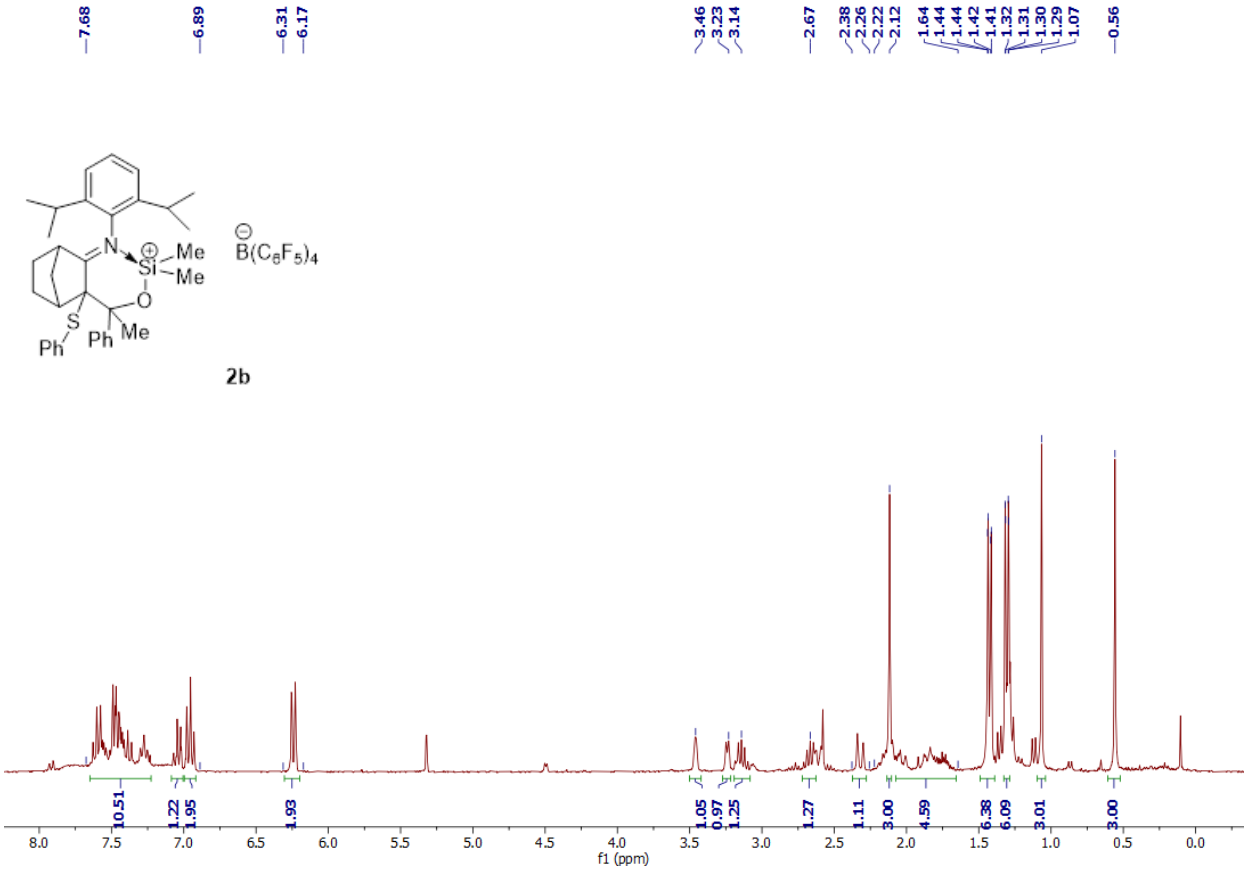


Figure S6: ^{1}H NMR (300 MHz, CD_2Cl_2) of 2b

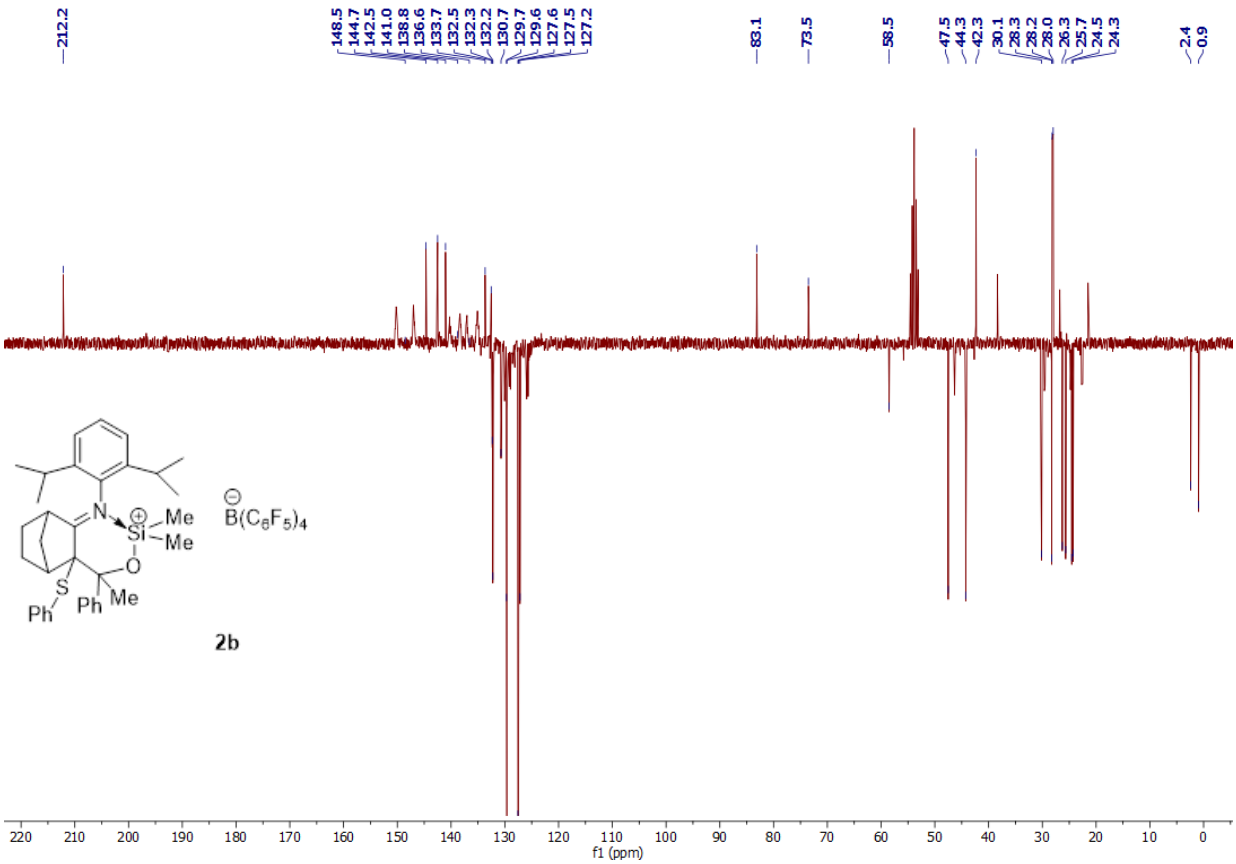


Figure S7: $^{13}C\{^{1}H\}$ NMR (75 MHz, CD_2Cl_2) of 2b

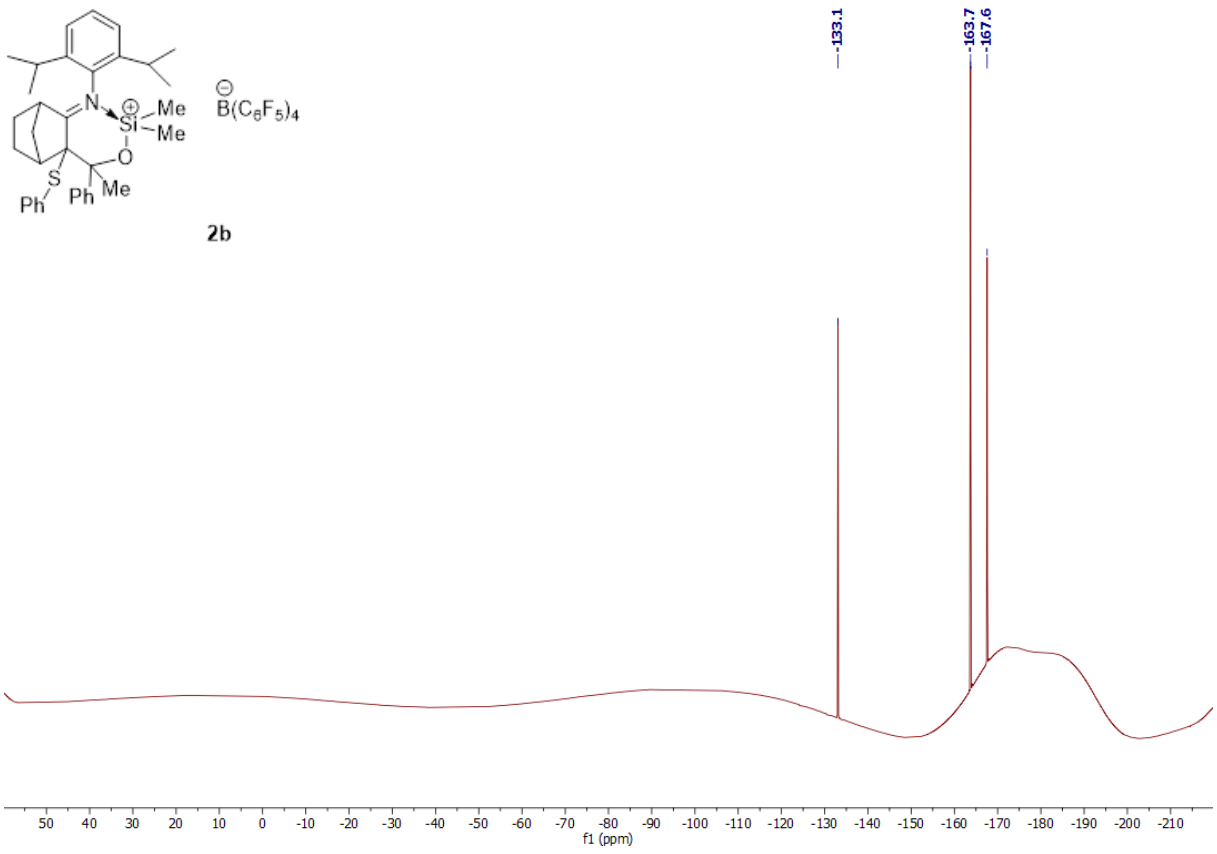


Figure S8: ^{19}F NMR (471 MHz, CD_2Cl_2) of 2b

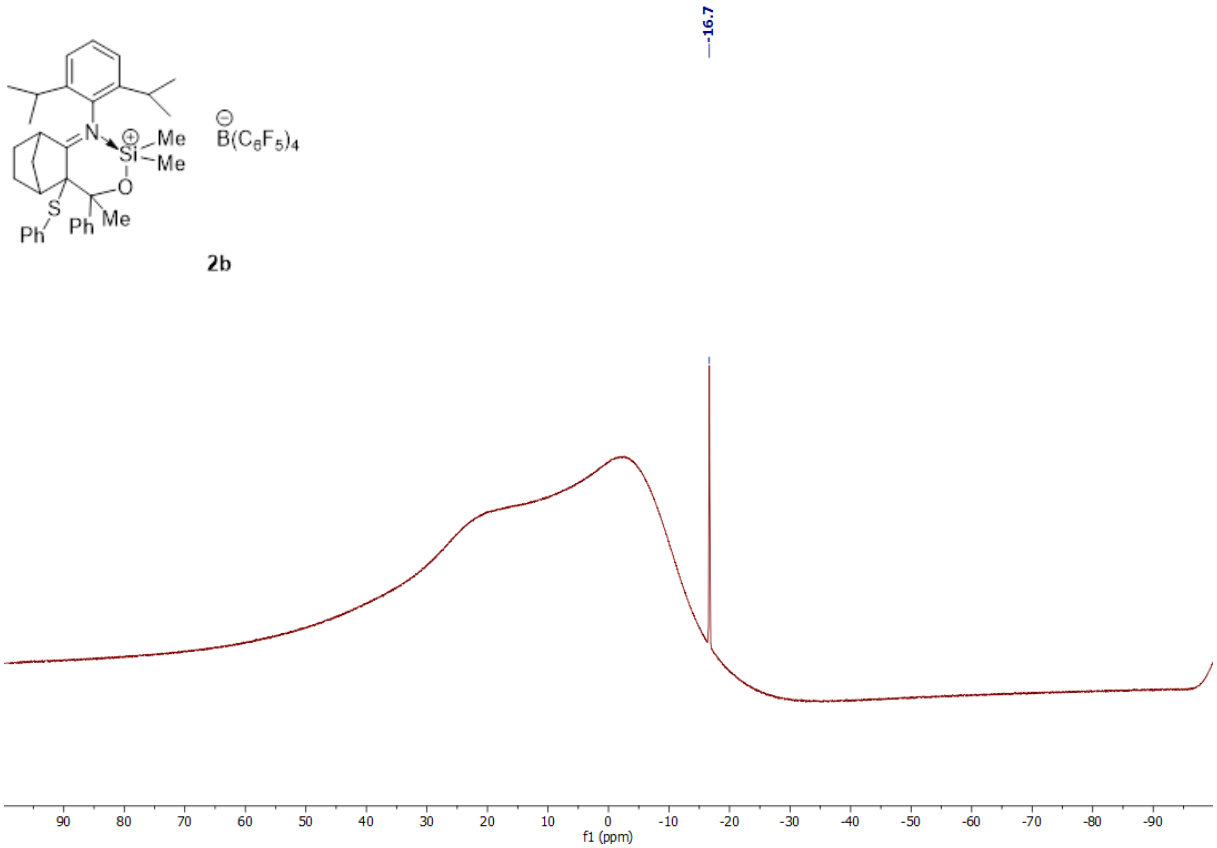


Figure S9: ^{11}B NMR (160 MHz, CD_2Cl_2) of 2b

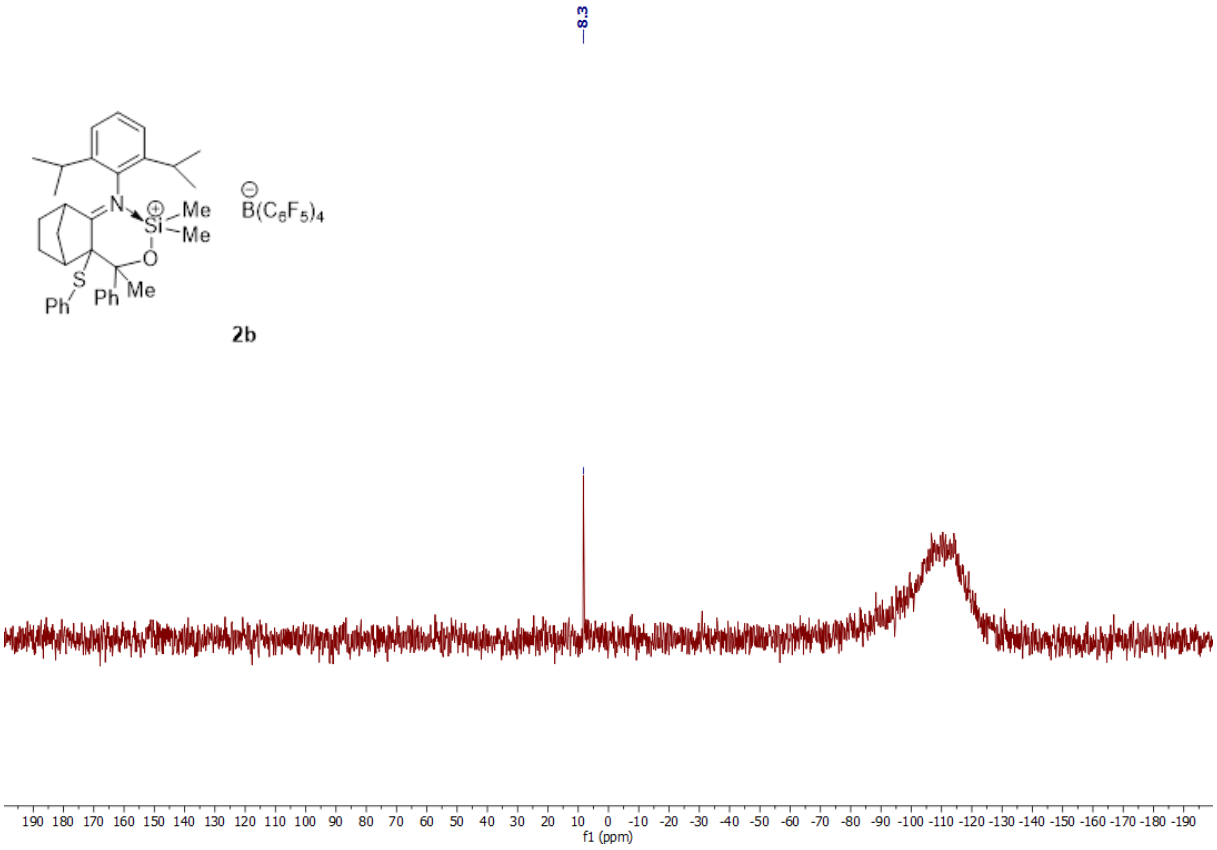
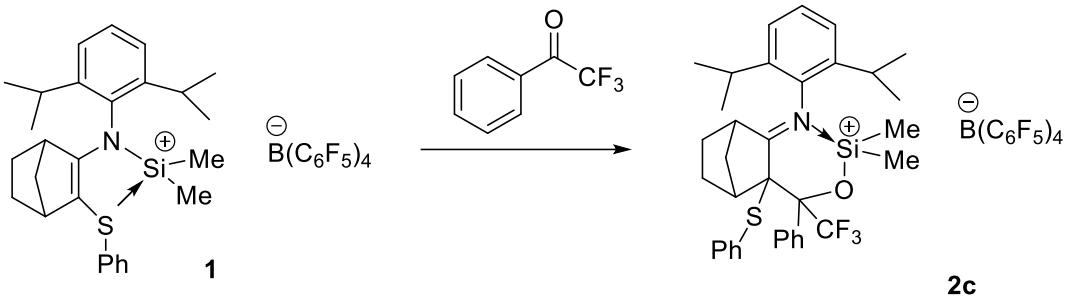


Figure S10: $^{29}Si\{^{1}H\}$ NMR (99 MHz, CD_2Cl_2) of 2b



Synthesis of 2c: To a solution of **1** (150 mg, 0.13 mmol) in benzene (2.0 mL) was added α,α,α-trifluoroacetophenone (18.9 µL, 0.13 mmol). Reaction mixture was stirred overnight and two phases were formed, the upper phase was removed and the lower phase washed twice with benzene (0.3 mL). Lower phase was dried under vacuum to obtained the adduct **2c** as a pale brown powder (131.2 mg, 76 %). **M.p.** = 71 °C (Decomposition).

Major isomer (70 %):

^{1}H NMR (300 MHz, CD_2Cl_2): δ = 0.68 (s, 3H, Si-CH_3), 1.24 (s, 3H, Si-CH_3), 1.49-1.27 (m, 12H, CH_{3iPr}), 2.28-1.88 (m, 5H, 3 CH_2), 2.47-2.33 (m, 1H, CH_2), 2.72 (sept, $^{3}J_{H-H}$ = 6.7 Hz, 1H, CH_{iPr}), 3.24 (sept, $^{3}J_{H-H}$ = 6.7 Hz, 1H, CH_{iPr}), 3.37 (m, 1H, C$H_{bridgehead}$), 3.83 (m, 1H, C$H_{bridgehead}$), 6.55-6.48 (m, 2H, 2 C$H_{PhCOCF3}$), 7.96-6.95 (m, 11H, S(C_6H_5) + 3 CH_{dipp} + 3 C$H_{PhCOCF3}$).

^{13}C NMR (75 MHz, CD_2Cl_2): δ = -0.5 (s, Si-CH$_3$), 2.8 (s, Si-CH$_3$), 23.9 (s, CH$_{3iPr}$), 24.4 (s, CH$_{3iPr}$), 24.9 (s, CH$_{3iPr}$), 25.8 (s, CH$_{3iPr}$), 27.4 (s, CH$_2$), 27.6 (s, CH$_{iPr}$), 27.8 (s, CH$_{iPr}$), 28.2 (s, CH$_2$), 41.2 (s, CH$_2$), 44.2 (s, CH$_{bridgehead}$), 47.4 (s, CH$_{bridgehead}$), 72.6 (s, C-S), 84.2 (q, J_{C-F} = 28.3 Hz, PhCOCF$_3$), 123.8 (br, *i* of BAr), 127.2 (s, CH$_{dipp}$), 127.3 (s, CH$_{dipp}$), 128.3 (s, SC_{Ph}), 128.7 (s, CH$_{PhCOCF3}$), 129.3 (s, CH$_{PhCOCF3}$), 129.9 (s, SC_{Ph}), 130.8 (s, SC_{Ph}), 131.3 (s, SC_{Ph}), 132.1 (s, CH$_{dipp}$), 132.2 (s, N-C_{Dipp}), 136.3 (br d, J_{C-F} = 244.2 Hz, ArC-F), 136.9 (br d, J_{C-F} = 244.5 Hz, ArC-F), 138.3 (s, CH$_{PhCOCF3}$), 142.7 (s, C_{iPr}), 144.3 (s, C_{iPr}), 148.1 (br d, J_{C-F} = 241.1 Hz, ArC-F), 211.4 (s, N-C).

Signal of carbon *ipso* of *Ph*COCF$_3$ and PhCOCF$_3$ are not visible.

^{19}F NMR (282 MHz, CD_2Cl_2): δ = -167.5 (t, J_{FF} = 19.2 Hz, *m* of ArC-*F*), -163.6 (t, J_{FF} = 20.4 Hz, *p* of ArC-*F*), -133.0 (br, o of ArC-*F*), -68.6 (br, CF_3).

^{11}B NMR (96 MHz, CD_2Cl_2): δ = -16.6 (s, *B*Ar).

^{29}Si NMR (99 MHz, CD_2Cl_2): δ = 10.5 (s, *Si*-CH$_3$).

Minor isomer (30 %):

^{1}H NMR (300 MHz, CD_2Cl_2): δ = 0.76 (s, 3H, Si-CH_3), 0.94 (s, 3H, Si-CH_3), 1.49-1.27 (m, 12H, CH_{3iPr}), 1.72-1.63 (m, 1H, CH_2), 2.28-1.88 (m, 5H, 3 CH_2), 2.68 (m, 1H, C$H_{bridgehead}$), 2.75 (sept, 1H, CH_{iPr}

overlapped by CH_{iPr} of major isomer), 3.41 (m, 1H, C$H_{bridgehead}$), 3.64 (sept, $^{3}J_{H-H}$ = 6.7 Hz, 1H, CH_{iPr}), 6.37-6.31 (m, 2H, 2 C$H_{PhCOCF3}$), 7.96-6.95 (m, 11H, S(C_6H_5) + 3 CH_{dipp} + 3 C$H_{PhCOCF3}$).

^{13}C NMR (75 MHz, CD_2Cl_2): δ =-0.3 (s, Si-CH_3), 0.5 (s, Si-CH_3), 22.8 (s, CH_{3iPr}), 23.8 (s, CH_{3iPr}), 25.9 (s, CH_{3iPr}), 26.9 (s, CH_{3iPr}), 27.6 (s, CH_2), 27.7 (s, CH_{iPr}), 27.9 (s, CH_{iPr}), 28.5 (s, CH_2), 40.2 (s, CH_2), 45.6 (s, $CH_{bridgehead}$), 47.9 (s, $CH_{bridgehead}$), 73.7 (s, *C*-S), 84.2 (Ph*C*OCF_3 overlapped with major isomer), 123.8 (br, *i* of BAr), 127.1 (s, CH_{dipp}), 127.2 (s, CH_{dipp}), 128.2 (s, SCH_{Ph}), 128.6 (s, $CH_{PhCOCF3}$), 129.4 (s, $CH_{PhCOCF3}$), 129.8 (s, SCH_{Ph}), 130.8 (s, SCH_{Ph} overlapped by major isomer), 131.1 (s, SC_{Ph}), 131.9 (s, $CH_{PhCOCF3}$), 132.0 (s, CH_{dipp}), 132.4 (s, N-C_{Dipp}), 136.3 (br d, J_{C-F} = 244.2 Hz, Ar*C*-F), 138.3 (br d, J_{C-F} = 244.5 Hz, Ar*C*-F), 143.8 (s, C_{iPr}), 144.7 (s, C_{iPr}), 148.1 (br d, J_{C-F} = 241.1 Hz, Ar*C*-F), 210.5 (s, N-*C*).

Signal of carbon *ipso* of *Ph*$COCF_3$ and PhCO*C*F_3 are not visible.

^{19}F NMR (282 MHz, CD_2Cl_2): δ = -167.5 (t, J_{FF} = 19.2 Hz, *m* of ArC-*F*), -163.6 (t, J_{FF} = 20.4 Hz, *p* of ArC-*F*), -133.0 (br, o of ArC-*F*), -68.1 (s, CF_3).

^{11}B NMR (96 MHz, CD_2Cl_2): δ = -16.6 (s, *B*Ar).

^{29}Si NMR (99 MHz, CD_2Cl_2): δ = 11.1 (s, *Si*-CH_3).

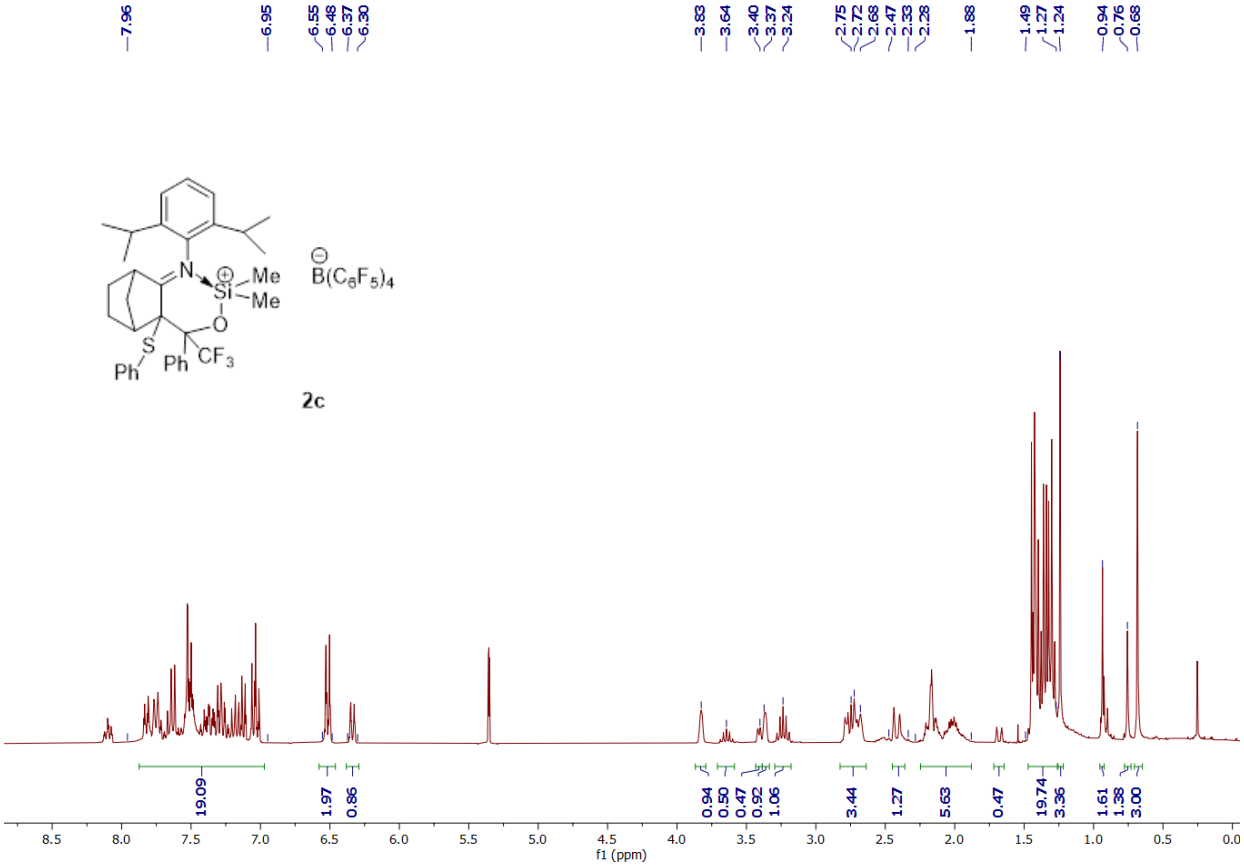


Figure S11: ^{1}H NMR (300 MHz, CD_2Cl_2) of 2c

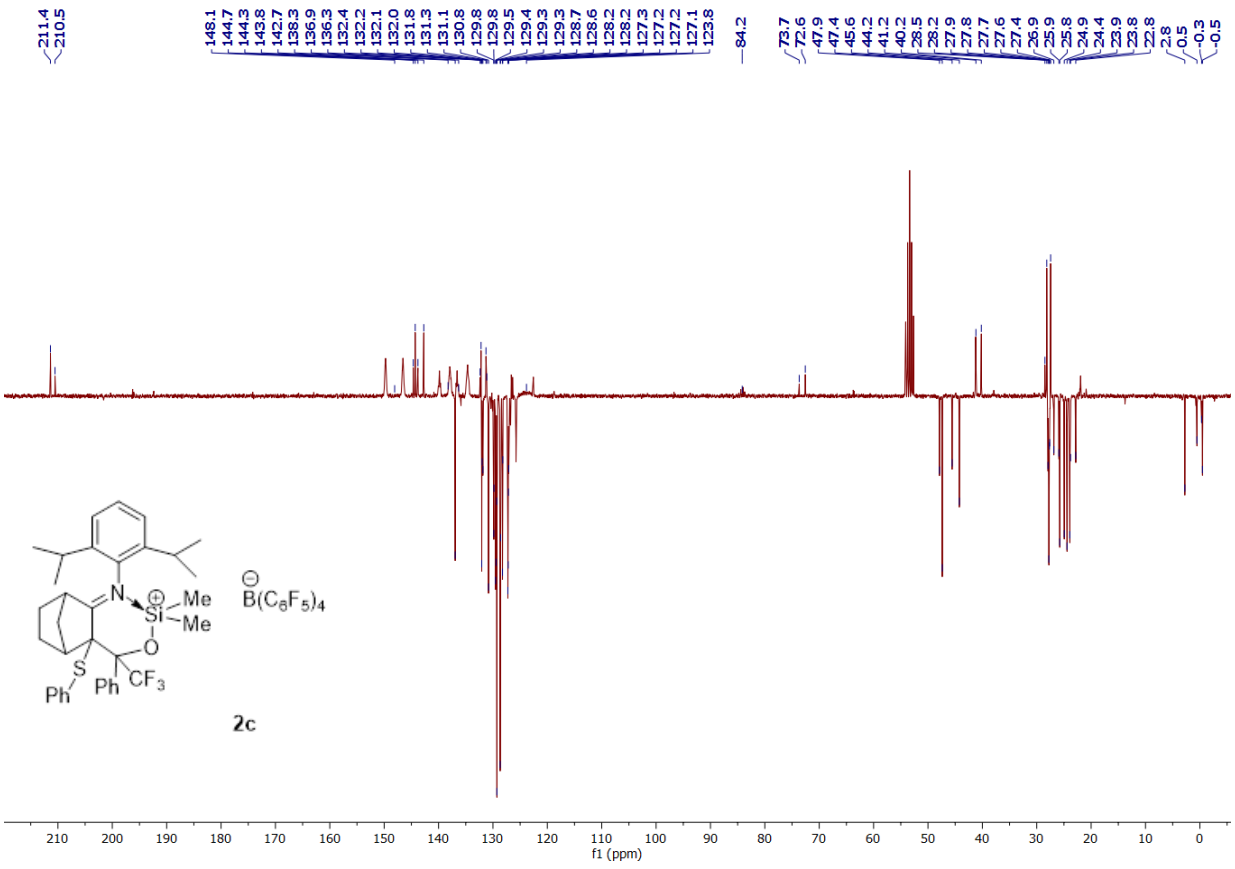


Figure S12: $^{13}C\{^{1}H\}$ NMR (75 MHz, CD_2Cl_2) of 2c

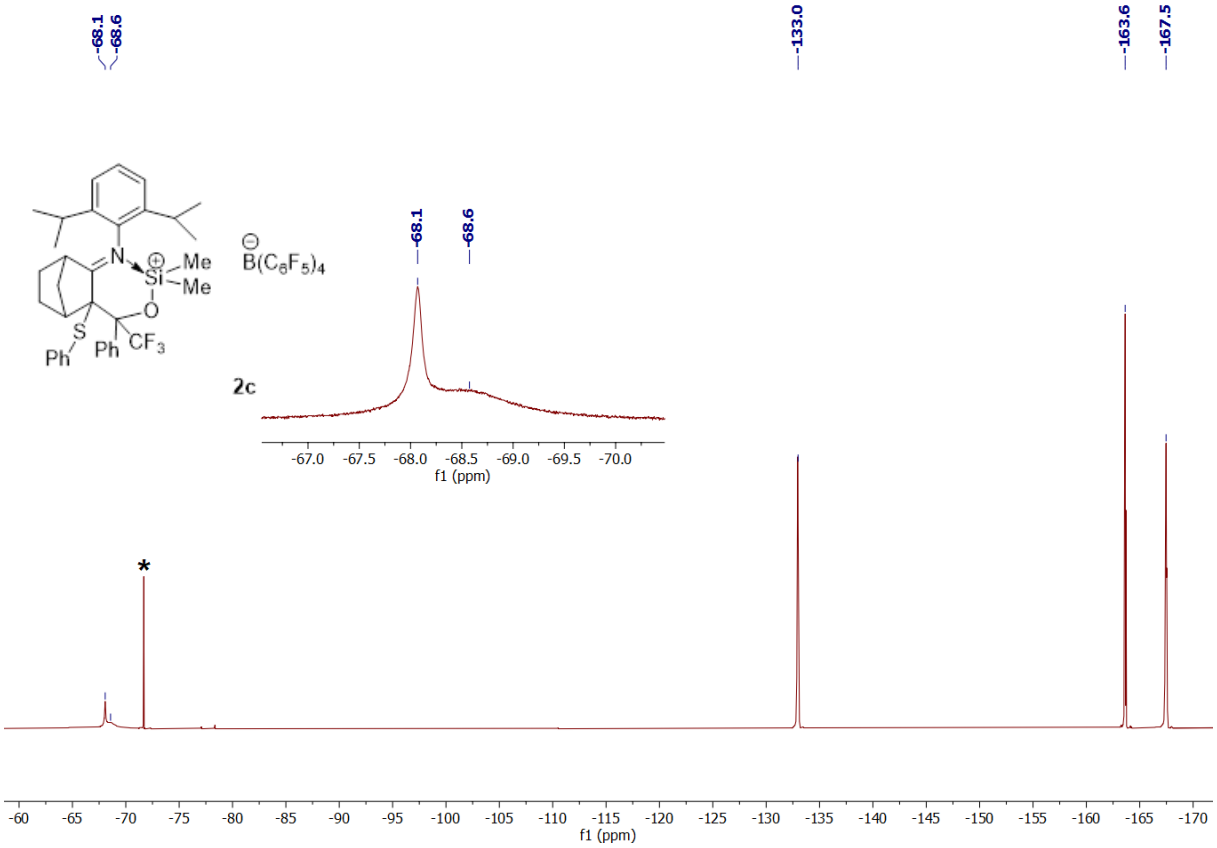


Figure S13: ^{19}F NMR (282 MHz, CD_2Cl_2) of 2c (* trifluoroacétophénone)

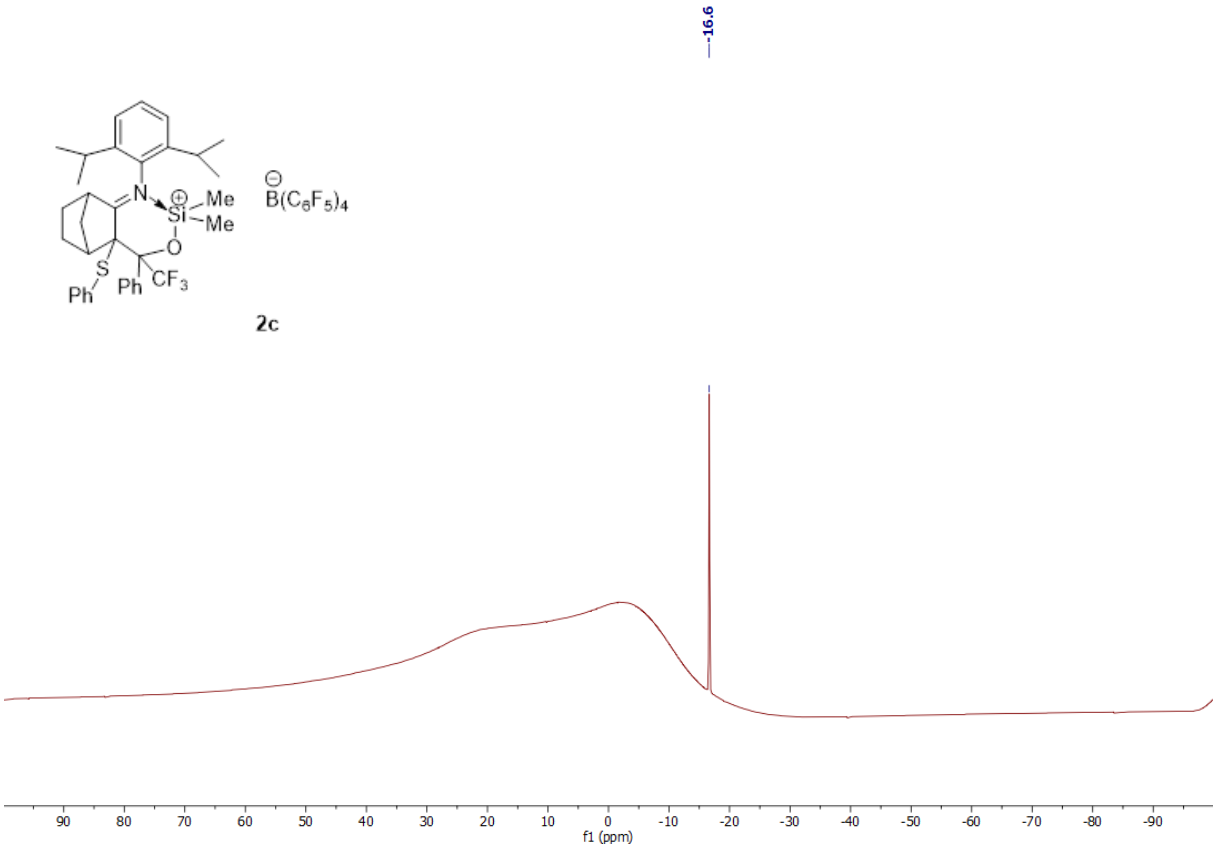


Figure S14: ^{11}B NMR (96 MHz, CD_2Cl_2) of 2c

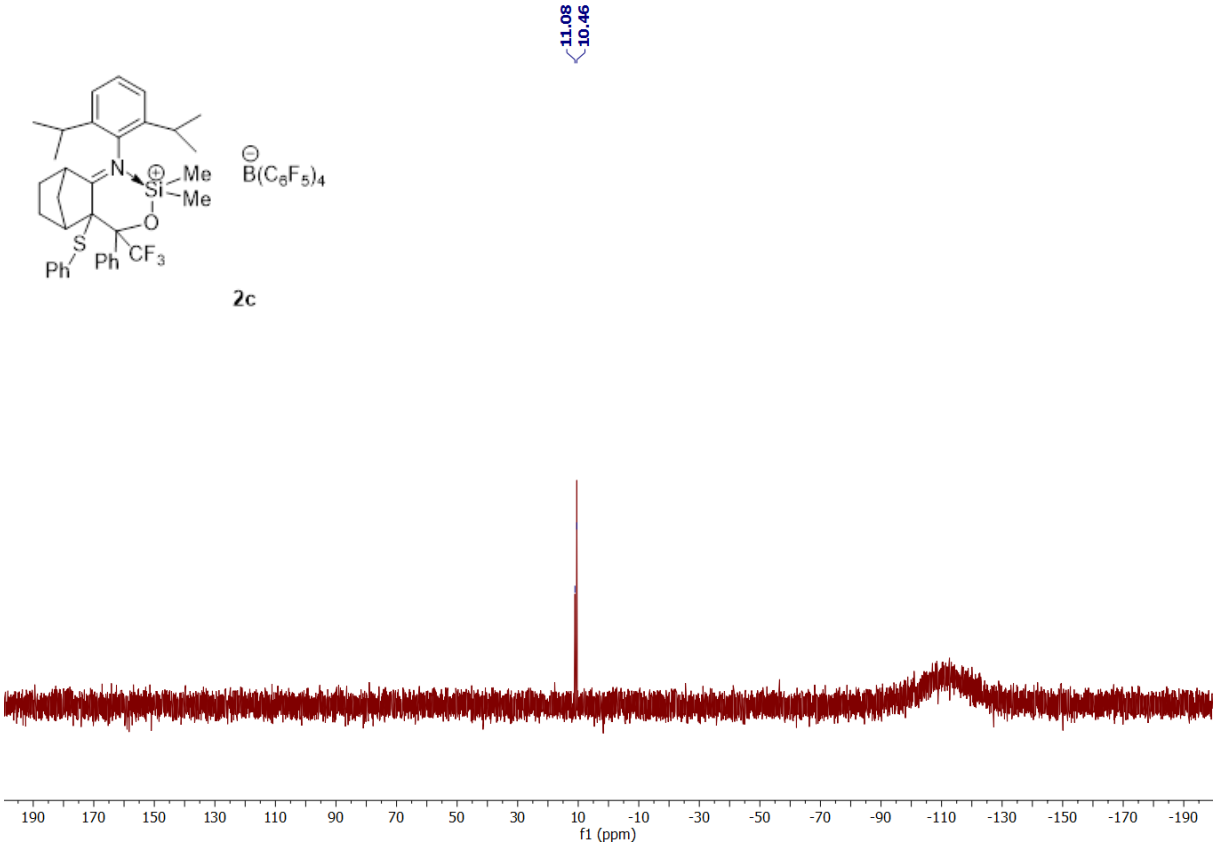


Figure S15: $^{29}Si\{^{1}H\}$ NMR (99 MHz, CD_2Cl_2) of 2c

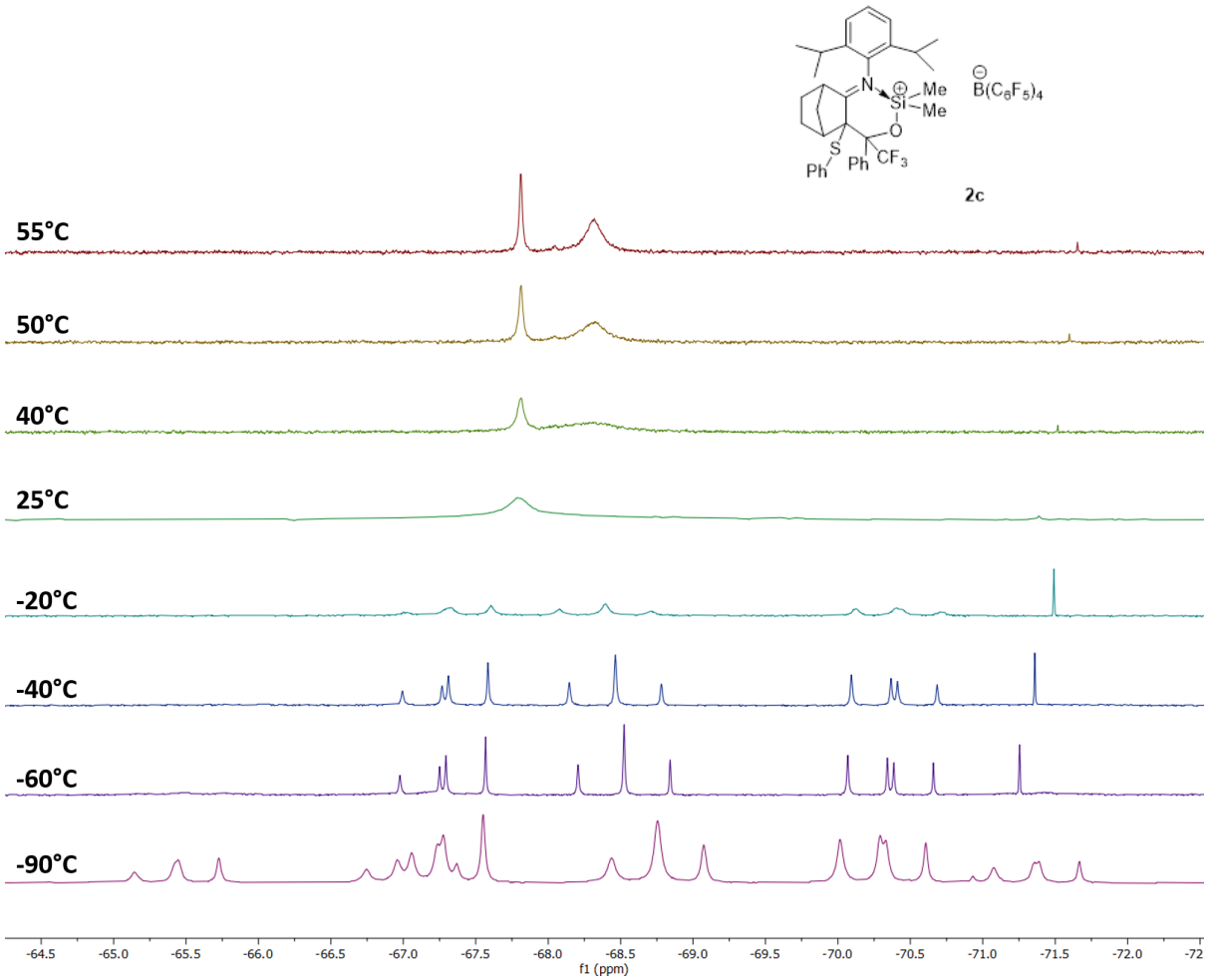
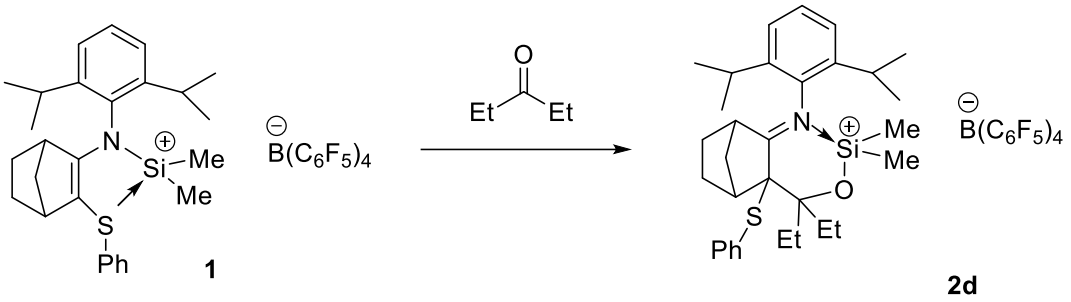


Figure S16: Variable Temperature ^{19}F NMR (376 MHz): 25°C to 60°C in $CDCl_3$ and -20°C to -90°C in CD_2Cl_2



1 2d

Synthesis of 2d: To a solution of **1** (300 mg, 0.27 mmol) in benzene (2.0 mL) was added 3-pentanone (28.5 µL, 0.27 mmol). Reaction mixture was stirred overnight and two phases were formed, the upper phase was removed and the lower phase washed twice with benzene (0.3 mL). Lower phase was dried under vacuum to obtained the adduct **2d** as an orange powder (263 mg, 81 %). **M.p.** = 69 °C (Decomposition).

^{1}H NMR (500 MHz, CD_2Cl_2): δ = 0.43 (s, 3H, Si-CH_3), 0.87 (s, 3H, Si-CH_3), 0.93 (t, $^{3}J_{H\text{-}H}$ = 7.7 Hz, 3H, CH_{3Et}), 1.15 (t, $^{3}J_{H\text{-}H}$ = 7.3 Hz, 3H, CH_{3Et}), 1.23 (d, $^{3}J_{H\text{-}H}$ = 6.7 Hz, 3H, CH_{3iPr}), 1.28 (d, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 3H, CH_{3iPr}), 1.36 (d, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 3H, CH_{3iPr}), 1.37 (d, $^{3}J_{H\text{-}H}$ = 6.7 Hz, 3H, CH_{3iPr}), 2.18-1.75 (m, 8H, 2 CH_{2Et} and 2 CH_2), 2.29-2.20 (m, 1H, CH_2), 2.43-2.31 (m, 2H, CH_2), 2.55 (sept, $^{3}J_{H\text{-}H}$ = 6.7 Hz, 1H, CH_{iPr}), 3.03 (sept, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 1H, CH_{iPr}), 3.12 (br, 1H, C$H_{bridgehead}$), 3.37 (br, 1H, C$H_{bridgehead}$), 7.61-7.37 (m, 8H, CH_{Ph}).

^{13}C NMR (126 MHz, CD_2Cl_2): δ = 0.8 (s, Si-CH$_3$), 2.5 (s, Si-CH$_3$), 8.9 (s, CH$_3$), 9.2 (s, CH$_3$), 24.2 (s, CH$_{3iPr}$), 24.6 (s, CH$_{3iPr}$), 25.6 (s, CH$_{3iPr}$), 26.3 (s, CH$_{3iPr}$), 27.4 (s, CH$_2$), 28.2 (s, CH$_{iPr}$), 29.3 (s, CH$_2$), 29.7 (s, CH$_{2Et}$), 30.0 (s, CH$_{iPr}$), 32.8 (s, CH$_{2Et}$), 41.4 (s, CH$_2$), 44.3 (s, CH$_{bridgehead}$), 46.8 (s, CH$_{bridgehead}$), 75.6 (s, C-S), 87.4 (s, CEt$_2$), 124.3 (br, *i* of BAr), 127.1 (s, CH$_{dipp}$), 127.5 (s, CH$_{dipp}$), 128.9 (s, SC_{Ph}), 129.4 (s, SC_{Ph}), 130.2 (s, SC_{Ph}), 132.1 (s, CH$_{dipp}$), 132.7(s, N-C_{Dipp}), 134.6 (s, CH$_{Ph}$), 136.7 (br d, $J_{C\text{-}F}$ = 244.5 Hz, ArC-F), 138.6 (br d, $J_{C\text{-}F}$ = 244.5 Hz, ArC-F), 144.3 (s, C_{iPr}), 142.3 (s, C_{iPr}), 148.6 (br d, $J_{C\text{-}F}$ = 240.5 Hz, ArC-F), 212.9 (s, N-C).

^{19}F NMR (471 MHz, CD_2Cl_2): δ = -167.6 (t, J_{FF} = 19.2 Hz, *m* of ArC-*F*), -163.7 (t, J_{FF} = 20.4 Hz, *p* of ArC-*F*), -133.1 (br, o of ArC-*F*).

^{11}B NMR (160 MHz, CD_2Cl_2): δ = -16.7 (s, *B*Ar).

^{29}Si NMR (99 MHz, CD_2Cl_2): δ = 6.4 (s, *Si*-CH_3).

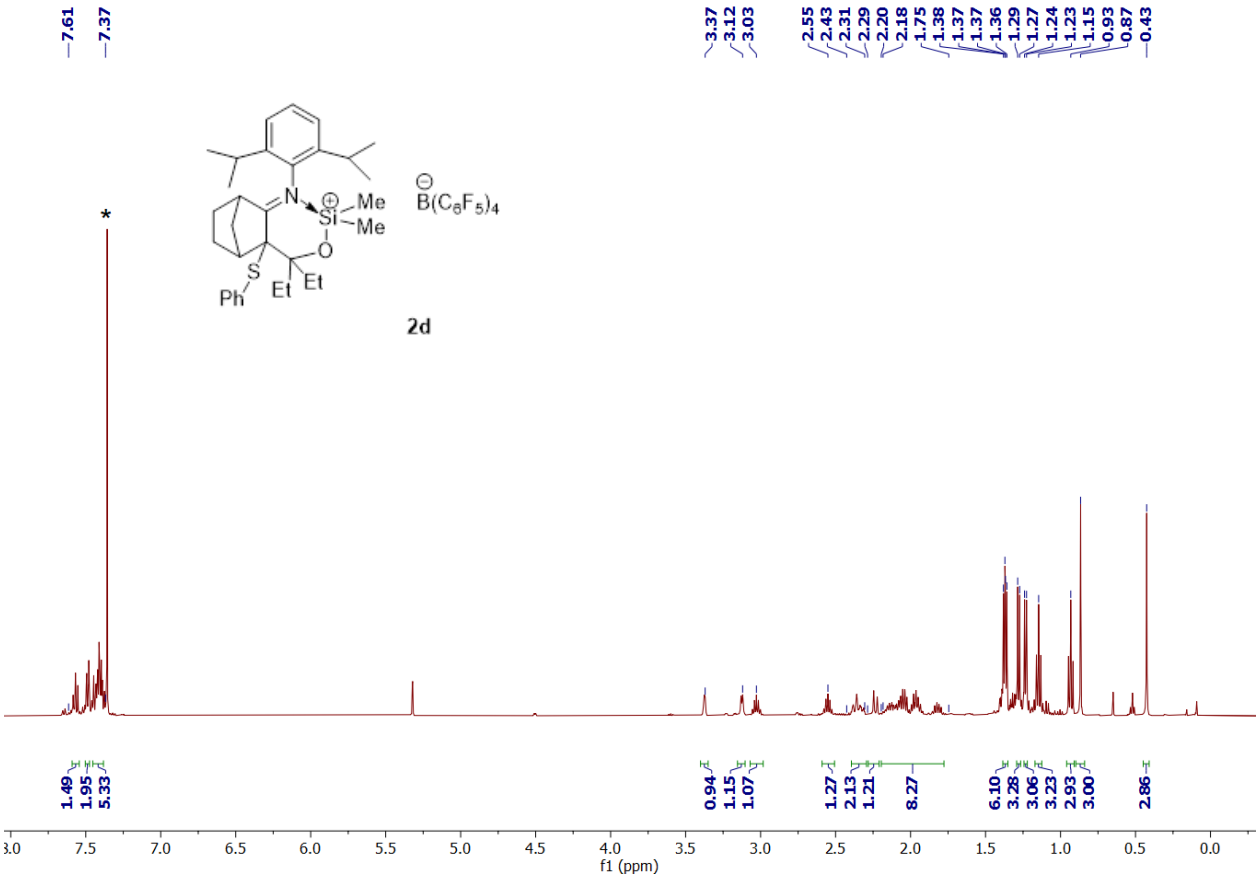


Figure S17: ^{1}H NMR (500 MHz, CD_2Cl_2) of 2d (* benzene)

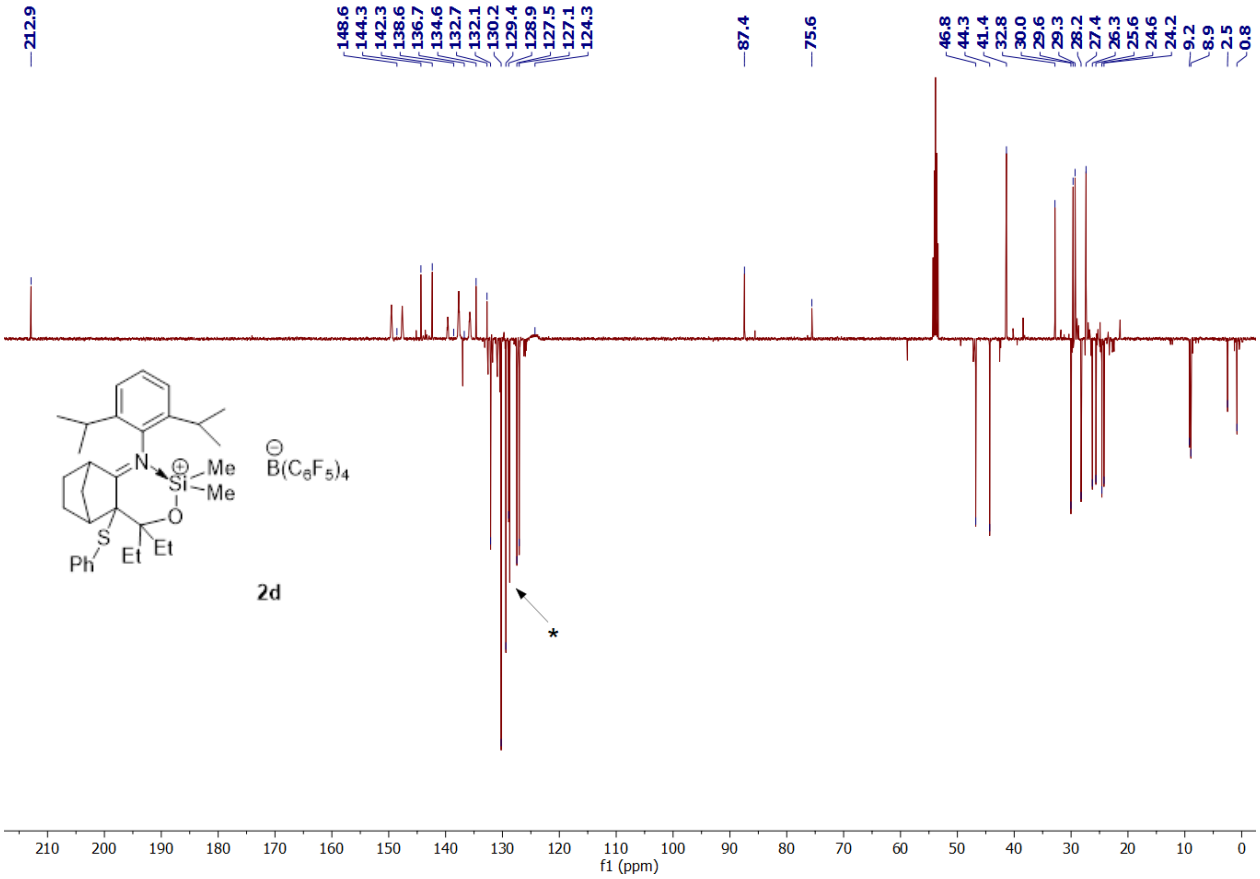


Figure S18: $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_2Cl_2) of 2d (*benzene)

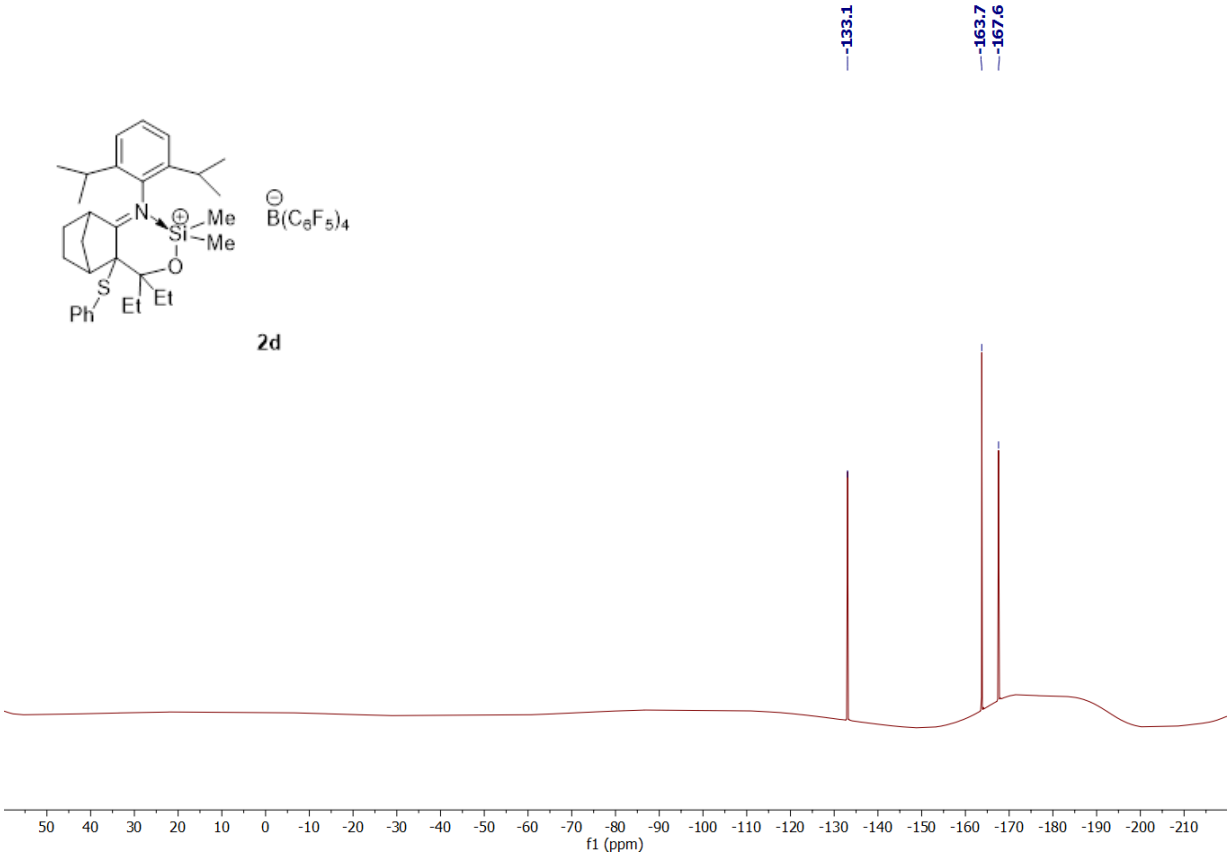


Figure S19: ^{19}F NMR (471 MHz, CD_2Cl_2) of 2d

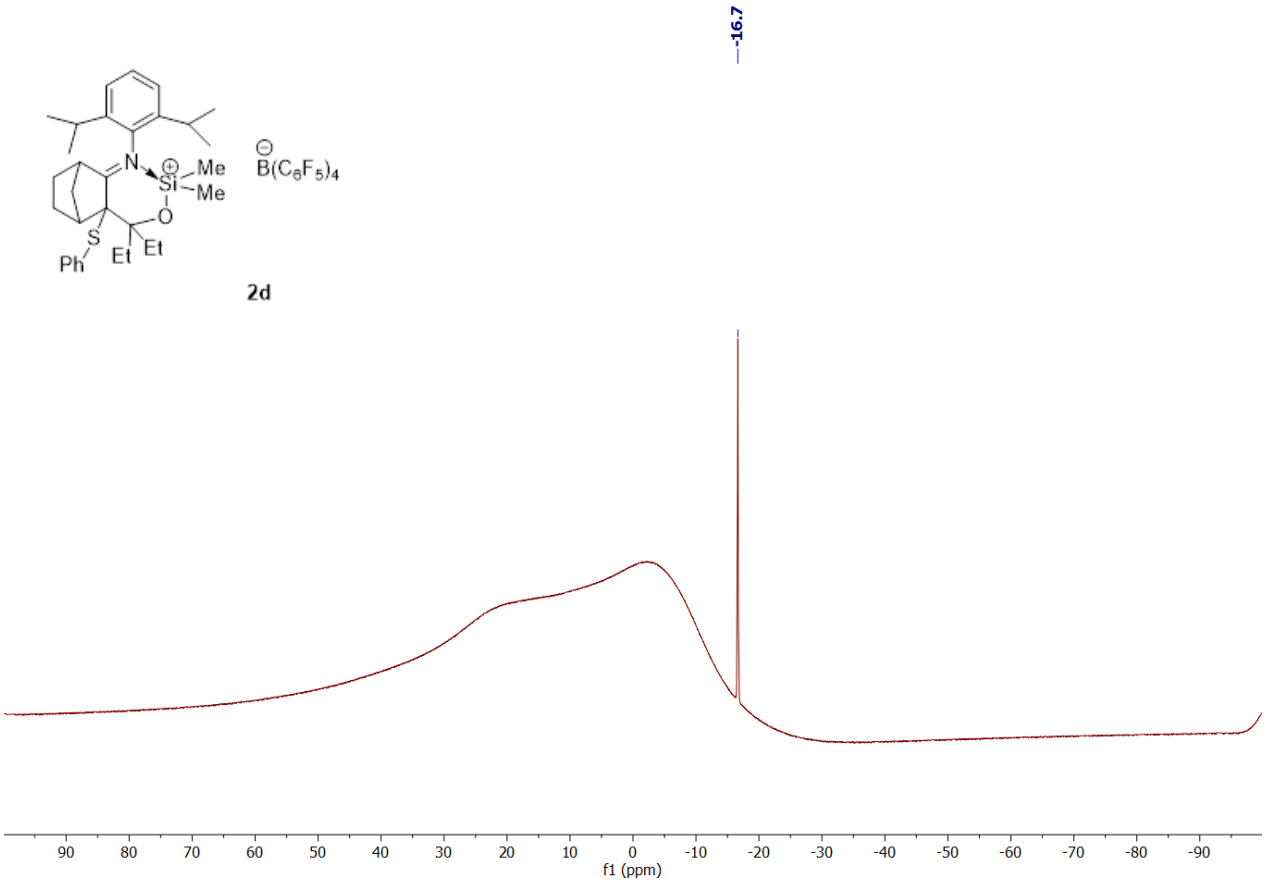


Figure S20: ^{11}B NMR (160 MHz, CD_2Cl_2) of 2d

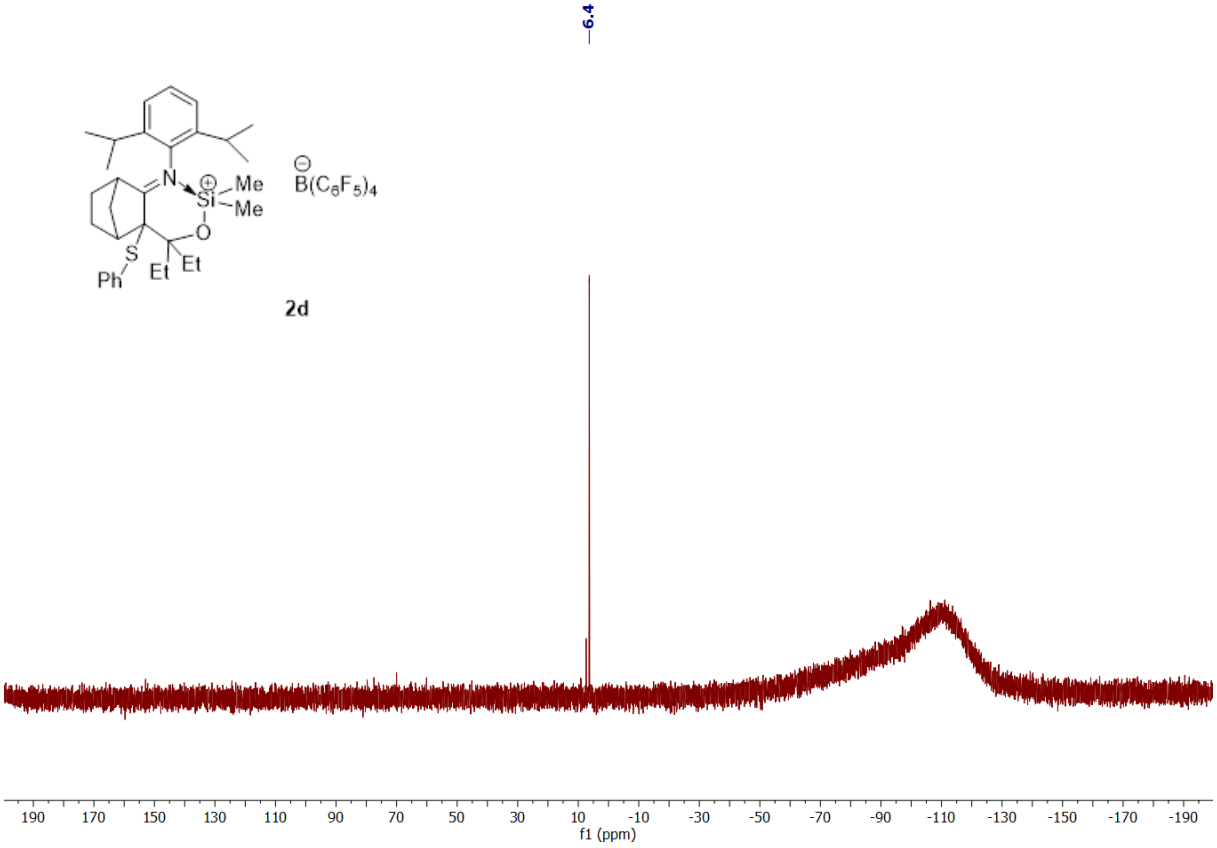
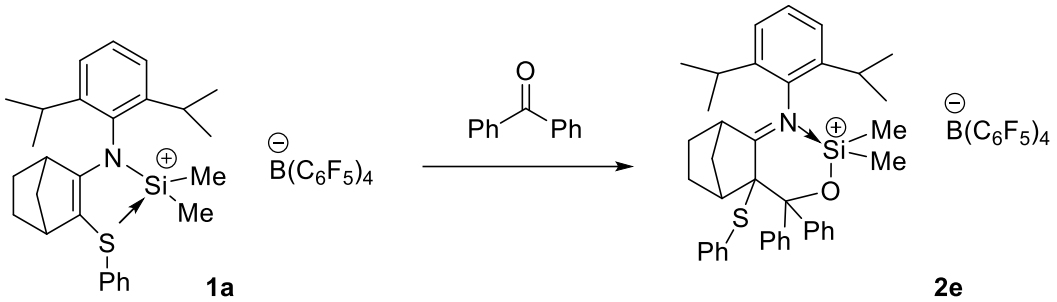


Figure S21: $^{29}Si\{^{1}H\}$ NMR (99 MHz, CD_2Cl_2) of 2d



Synthesis of 2e: To a solution of **1** (300.0 mg, 0.27 mmol) in benzene (2.0 mL) was added benzophenone (4.91 mg, 0.27 mmol). Reaction mixture was stirred overnight and precipitate was formed, solvent was removed by filtration and the solid washed twice with benzene (0.5 mL). Solid was dried under vacuum to obtained the adduct **2e** as a yellow powder (295.0 mg, 85 %). Crystals were obtained from a chloroform solution at -30°C. **M.p.** = 70 °C (Decomposition).

^{1}H NMR (500 MHz, CD_2Cl_2): δ = 0.77 (d, $^{3}J_{H\text{-}H}$ = 6.5 Hz, 3H, CH_{3iPr}), 0.78 (s, 3H, Si-CH_3), 1.26 (d, $^{3}J_{H\text{-}H}$ = 6.7 Hz, 3H, CH_{3iPr}), 1.33 (d, $^{3}J_{H\text{-}H}$ = 6.5 Hz, 4H, CH_{3iPr} + CH_2), 1.36 (s, 3H, Si-CH_3), 1.37 (d, $^{3}J_{H\text{-}H}$ = 6.7 Hz, 3H, CH_{3iPr}), 2.20-1.95 (m, 4H, CH_2), 2.24 (sept, $^{3}J_{H\text{-}H}$ = 6.5 Hz, 1H, CH_{iPr}), 2.84-2.75 (m, 1H, CH_2), 2.93 (br, 1H, C$H_{bridgehead}$), 3.10 (sept, $^{3}J_{H\text{-}H}$ = 6.7 Hz, 1H, CH_{iPr}), 4.08 (br, 1H, C$H_{bridgehead}$), 7.06-6.93 (m, 6H, CH_{Ph}), 7.18 (m, 1H, CH_{Ph}), 7.75-7.34 (m, 10H, CH_{Ph}).

^{13}C NMR (126 MHz, CD_2Cl_2): δ = 1.2 (s, Si-CH$_3$), 5.8 (s, Si-CH$_3$), 24.6 (s, CH$_{3iPr}$), 24.9 (s, CH$_{3iPr}$), 24.9 (s, CH$_{3iPr}$), 25.8 (s, CH$_{3iPr}$), 27.1 (s, CH$_2$), 28.6 (s, CH$_{iPr}$), 28.6 (s, CH$_{iPr}$), 29.2 (s, CH$_2$), 40.6 (s, CH$_2$), 45.8 (s, CH$_{bridgehead}$), 47.1 (s, CH$_{bridgehead}$), 76.9 (s, C-S), 89.3 (s, CPh$_2$), 124.4 (br, *i* of BAr), 127.0 (s, CH$_{Ph}$), 127.2 (s, CH$_{dipp}$), 127.4 (s, CH$_{dipp}$), 127.6 (s, CH$_{Ph}$), 128.4 (br, CH$_{Ph}$), 128.8 (s, CH$_{Ph}$), 128.9 (s, CH$_{Ph}$), 129.6 (s, CH$_{Ph}$), 129.6 (s, CH$_{Ph}$), 129.7 (s, CH$_{Ph}$), 131.0 (s, SC_{Ph}), 132.1 (s, CH$_{dipp}$), 133.4 (s, N-C_{Dipp}), 133.5 (s, CH$_{Ph}$), 136.6 (br d, $J_{C\text{-}F}$ = 244.5 Hz, ArC-F), 138.7 (br d, $J_{C\text{-}F}$ = 244.5 Hz, ArC-F), 140.5 (s, CPh), 141.9 (s, CPh), 142.2 (s, C_{iPr}), 143.7 (s, C_{iPr}), 148.5 (br d, $J_{C\text{-}F}$ = 240.5 Hz, ArC-F), 213.2 (s, N-C).

^{19}F NMR (471 MHz, CD_2Cl_2): δ = -167.5 (t, J_{FF} = 19.2 Hz, *m* of ArC-*F*), -163.7 (t, J_{FF} = 20.4 Hz, *p* of ArC-*F*), -133.0 (br, o of ArC-*F*).

^{11}B NMR (160 MHz, CD_2Cl_2): δ = -16.6 (s, BAr).

^{29}Si NMR (99 MHz, CD_2Cl_2): δ = 5.5 (s, *Si*-CH_3).

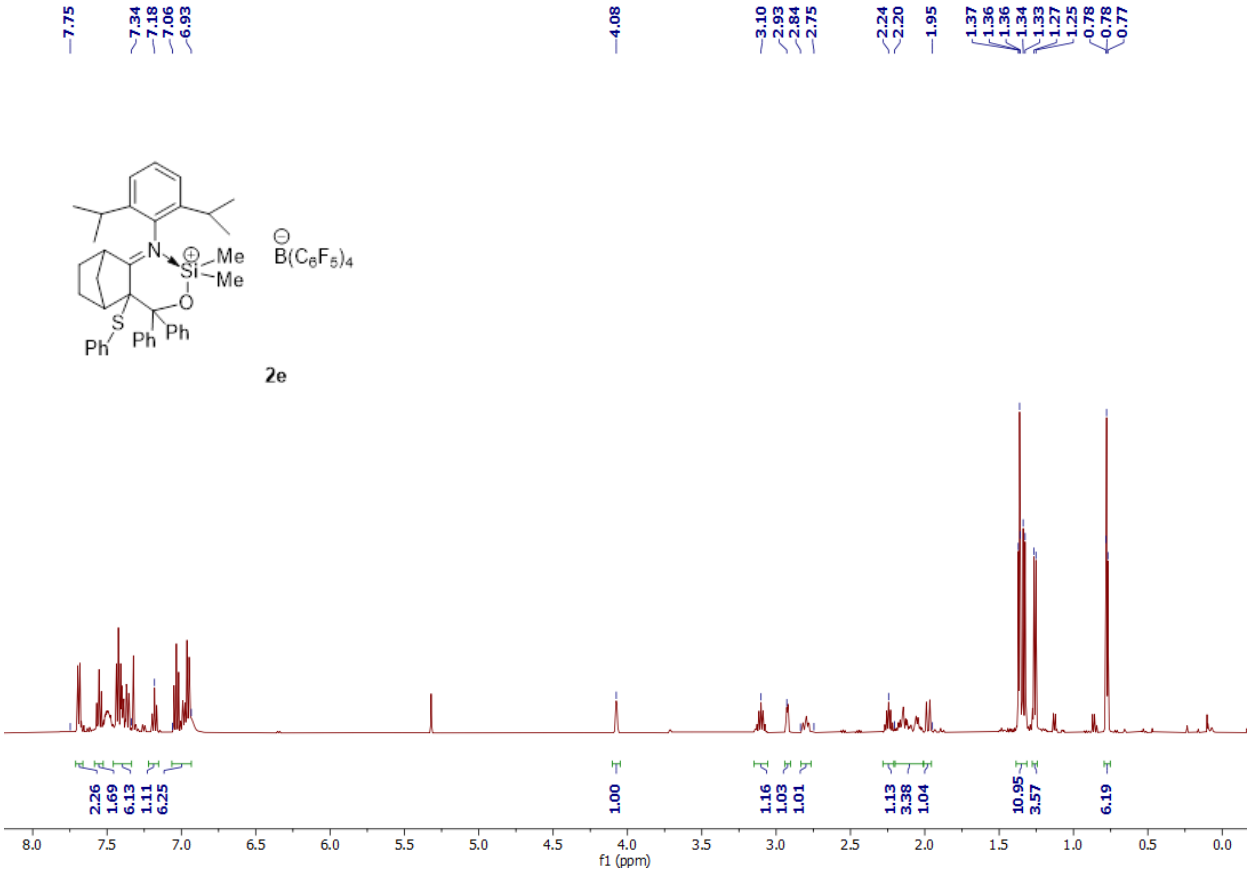


Figure S22: ^{1}H NMR (500 MHz, CD_2Cl_2) of 2e

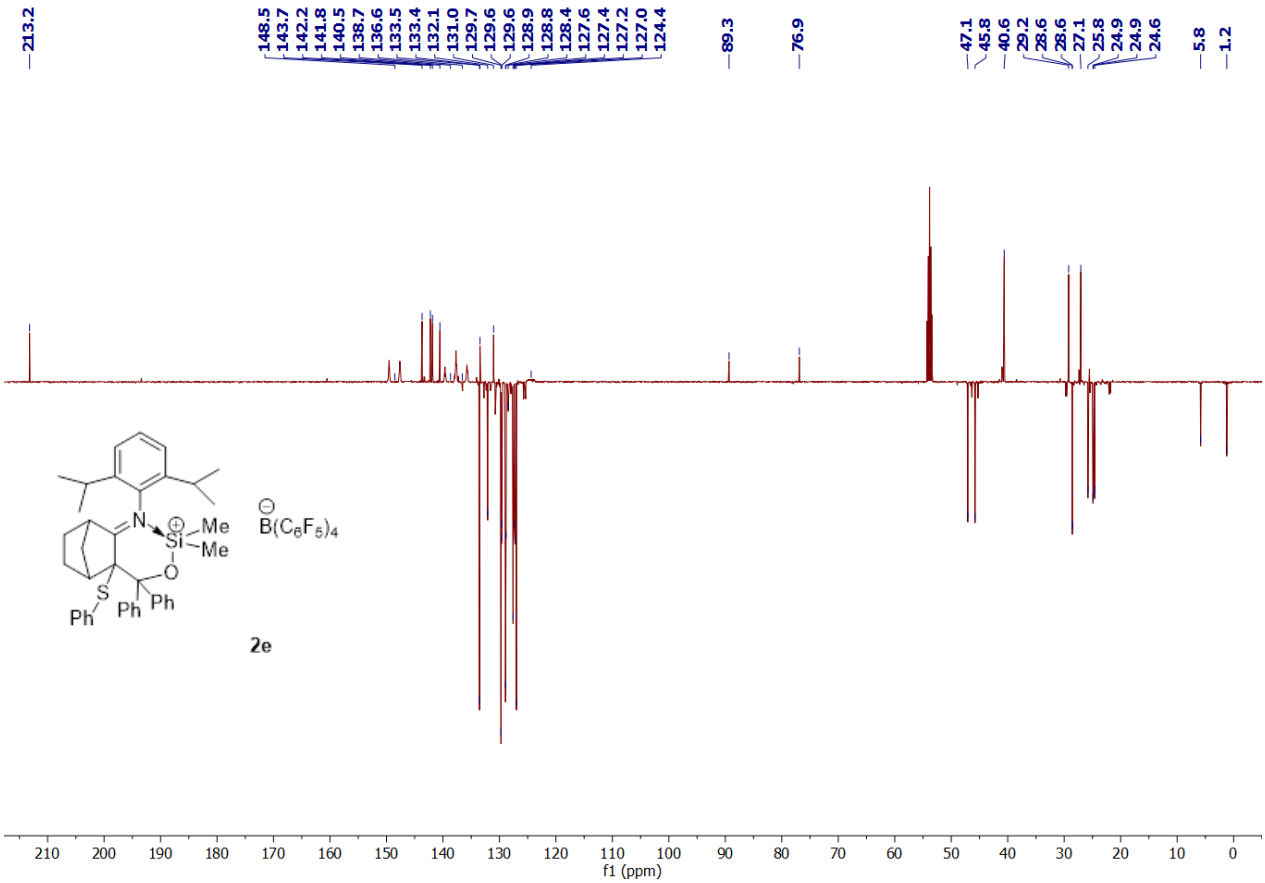


Figure S23: $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_2Cl_2) of 2e Figure S24: ^{19}F NMR (471 MHz, CD2Cl2) of 2e

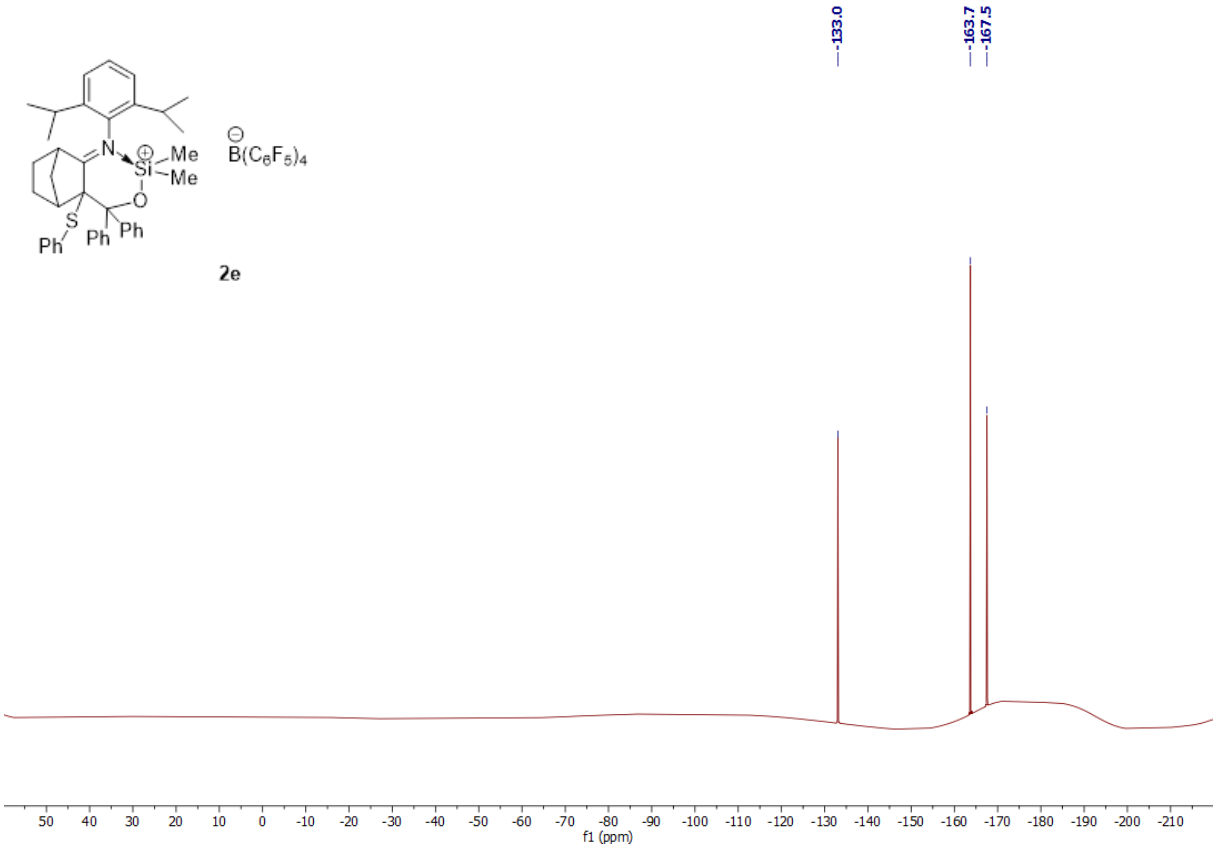


Figure S24: ^{19}F NMR (471 MHz, CD_2Cl_2) of 2d

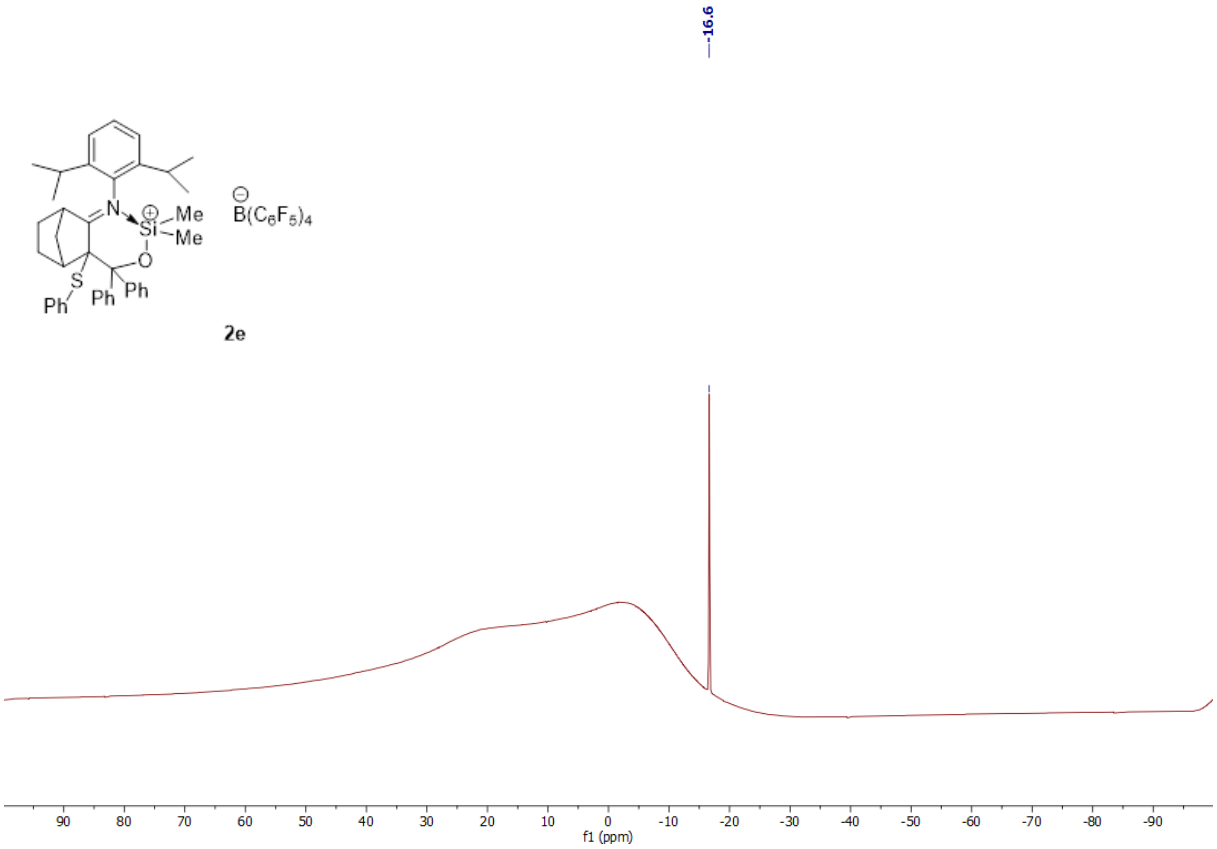


Figure S25: ^{11}B NMR (160 MHz, CD_2Cl_2) of 2e

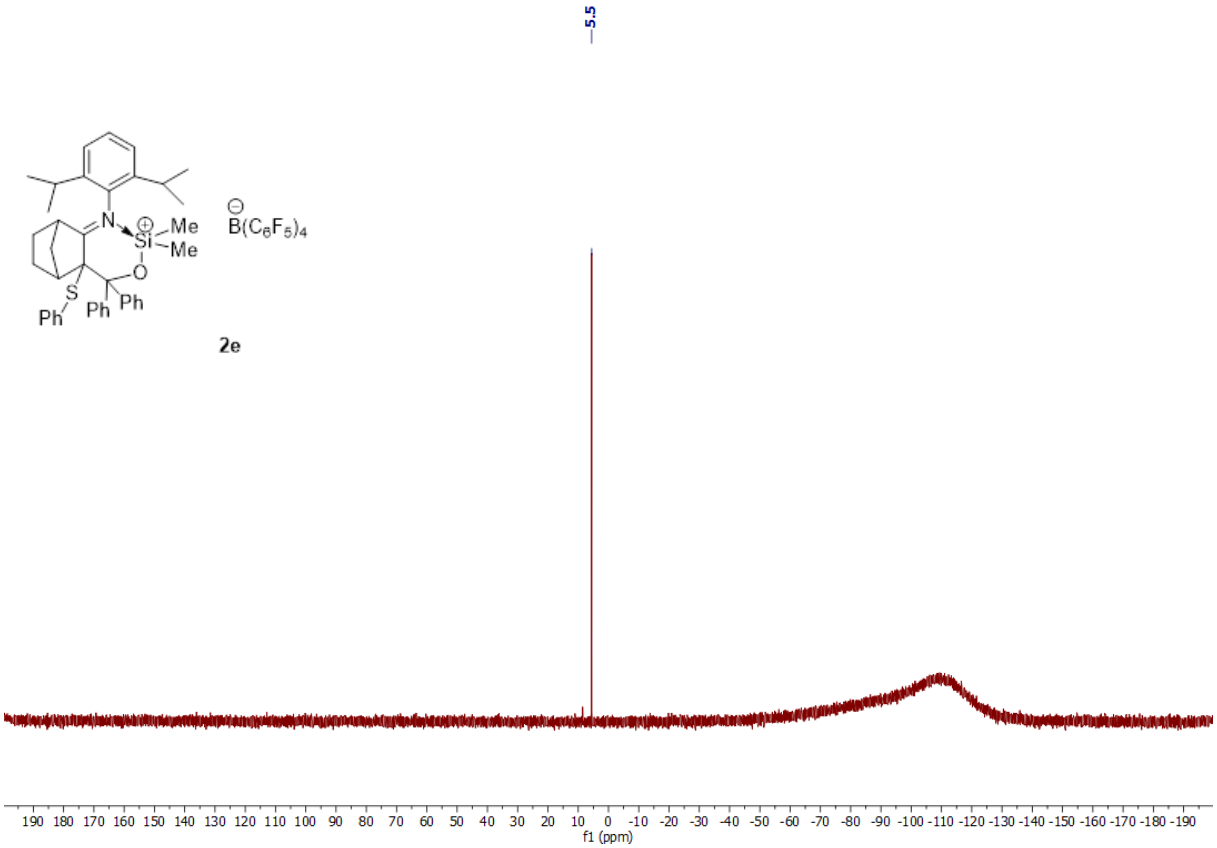
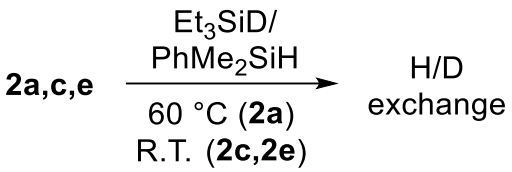
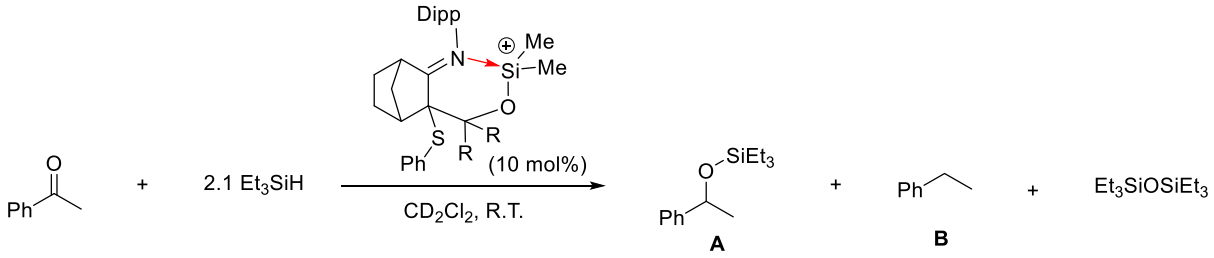


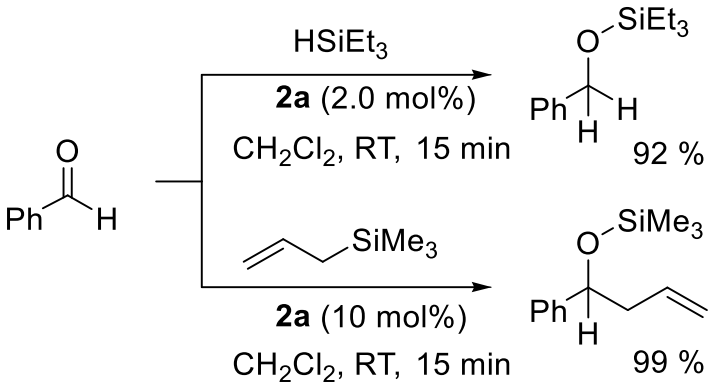
Figure S26: $^{29}Si\{^{1}H\}$ NMR (99 MHz, CD_2Cl_2) of 2e



Scrambling H/D reaction: In a J. Young NMR tube, to a solution of **2a** or **2c** (10 mol%) in CD_2Cl_2 was added D_1-triethylsilane (0.082 mmol, 13.1 µL) and dimethylphenylsilane (0.082 mmol, 12.6 µL) successively. Exchange reactions were monitored by ^1H NMR at different temperature (relaxation time D_1 = 10 sec).



Hydrosilylation of acetophenone: In a J. Young NMR tube, to **2a-2e** (10 mol%) was added a solution of CD_2Cl_2 containing acetophenone (0.025 mmol), triethylsilane (0.053 mmol) and hexamethylbenzene as internal standard (0.0041 mmol). Reaction was monitored by ^1H NMR (relaxation time D_1 = 10 sec). Conversions and selectivities were determined by ^1H NMR analysis of the crude samples.



Hydrosilylation of benzaldehyde: In a J. Young NMR tube, to a solution of **2a** (2.0 mol%) in CD_2Cl_2 was added benzaldehyde (0.41 mmol, 41.8 µL) and triethylsilane (0.41 mmol, 47.6 µL) successively. NMR was realized 15 minutes after and full conversion was observed.

Allylation of benzaldehyde: In a J. Young NMR tube, to a solution of **2a** (10 mol%) in CD_2Cl_2 was added benzaldehyde (0.082 mmol, 8.37 µL) and allylsilane (0.082 mmol, 13.0 µL) successively. NMR was realized 15 minutes after and full conversion was observed.

X-ray analysis

Crystallographic data for **2e** was collected at 193 K on a Bruker-AXS D8-Venture diffractometer equipped with a MoKα sealed tube (wavelength = 0.71073 Å), a multilayer TRIUMPH X-ray mirror, a Photon III-C14 detector and an Oxford Instruments Cryostream 700+ Series low-temperature device. Phi- and omega-scans were used. The data were integrated with SAINT, and an empirical absorption correction with SADABS was applied.[2] The structure was solved using an intrinsic phasing method (ShelXT)[3] and refined using the least–squares method on F^2 (ShelXL-2018).[4] All non-H atoms were treated anisotropically. All H atoms attached to C atoms were fixed geometrically and treated as riding on their parent atoms with C-H = 0.95 Å (aromatic), 0.98 Å (CH_3), 0.99 Å (CH_2) or 1.0 Å (CH) with $U_{iso}(H) = 1.2U_{eq}(CH, CH_2)$ or $U_{iso}(H) = 1.5U_{eq}(CH_3)$. Some parts of the molecule (2 phenyls groups) and the solvent molecule ($CHCl_3$) were found to be disordered over 2 positions, several restraints (SAME, SADI, SIMU, DELU) were applied to refine these disorders and to avoid the collapse of the structure during the least-squares refinement by the large anisotropic displacement parameters.

Supplementary crystallographic data for CCDC-2234864 (**2e**) can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/.

The details of data collection and crystal structures refinement are summarized in Table S1.

[2] SADABS, Program for data correction, Bruker−AXS.
[3] ShelXT, G. M. Sheldrick, Acta Crystallogr. Sect. A, 2015, 71, 3-8.
[4] ShelXL, G. M. Sheldrick, Acta Crystallogr. Sect. C, 2015, 71, 3-8.

Table S1. Crystallographic data for the compound 2e

Compound	**2e**
Chemical formula	$C_{40}H_{46}NOSSi$, $C_{24}BF_{20}$, $CHCl_3$
M_r	1415.34
Crystal system	Orthorhombic
Space group	*P bca*
a [Å]	18.2031(10)
b [Å]	24.9358(16)
c [Å]	26.8374(17)
α [°]	90
β [°]	90
γ [°]	90
V [Å^3]	12181.7(13)
Z	8
ρ [g cm^{-3}]	1.543
μ($Mo_{K\alpha}$) [mm^{-1}]	0.311
Reflections collected	500249
Independent reflections	10369 R(int)=0.1758
Data/ restraints/ parameters	10369/548/955
Crystal size [mm^3]	0.200x0.160x0.130
GOOF on F^2	1.057
R (I > 2σ(I))	0.0661
wR2 (all data)	0.1764
Largest difference peak and hole, [e Å^{-3}]	1.119 and -0.633
CCDC number	2234864

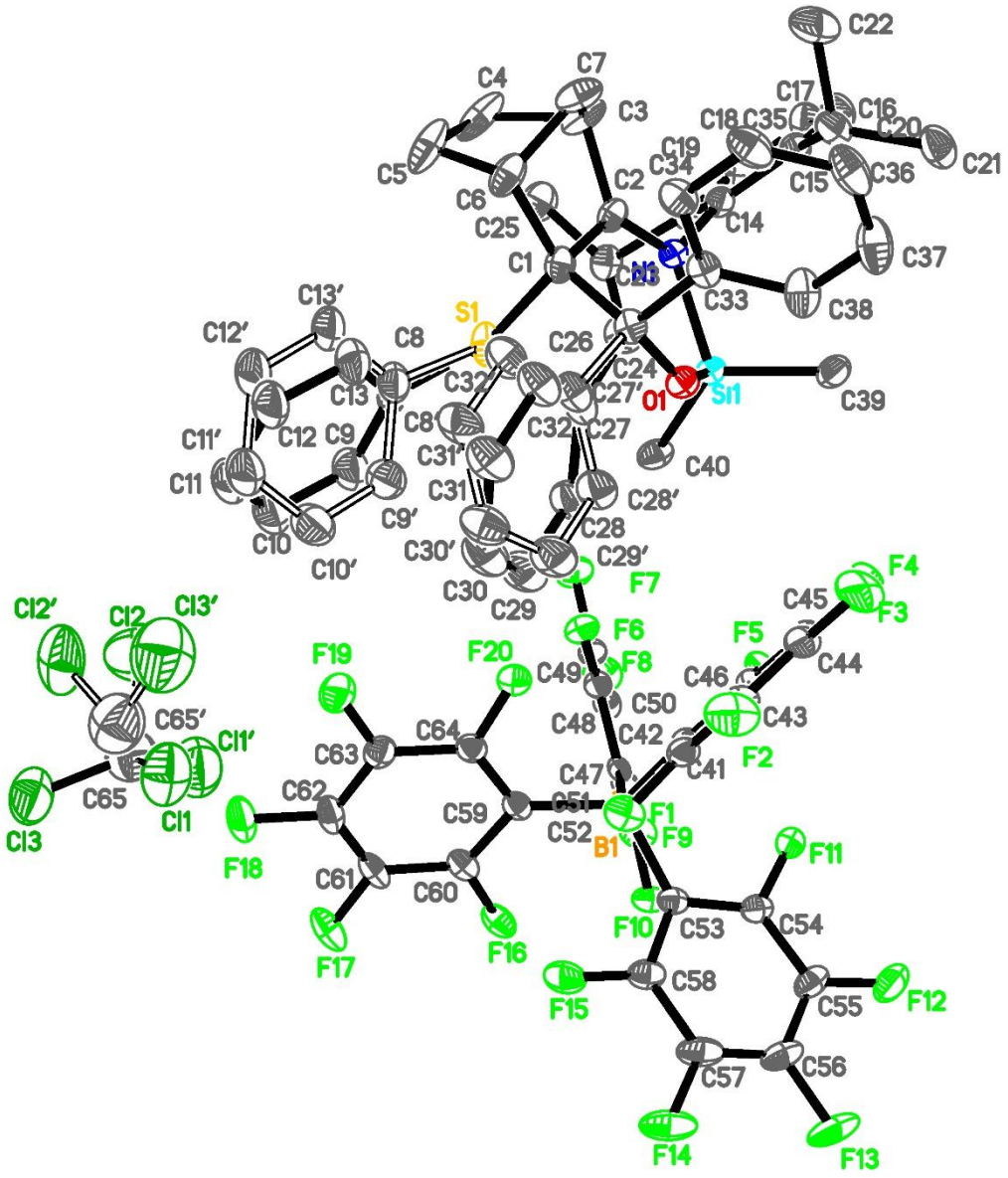


Figure S27: asymmetric unit of **2e**

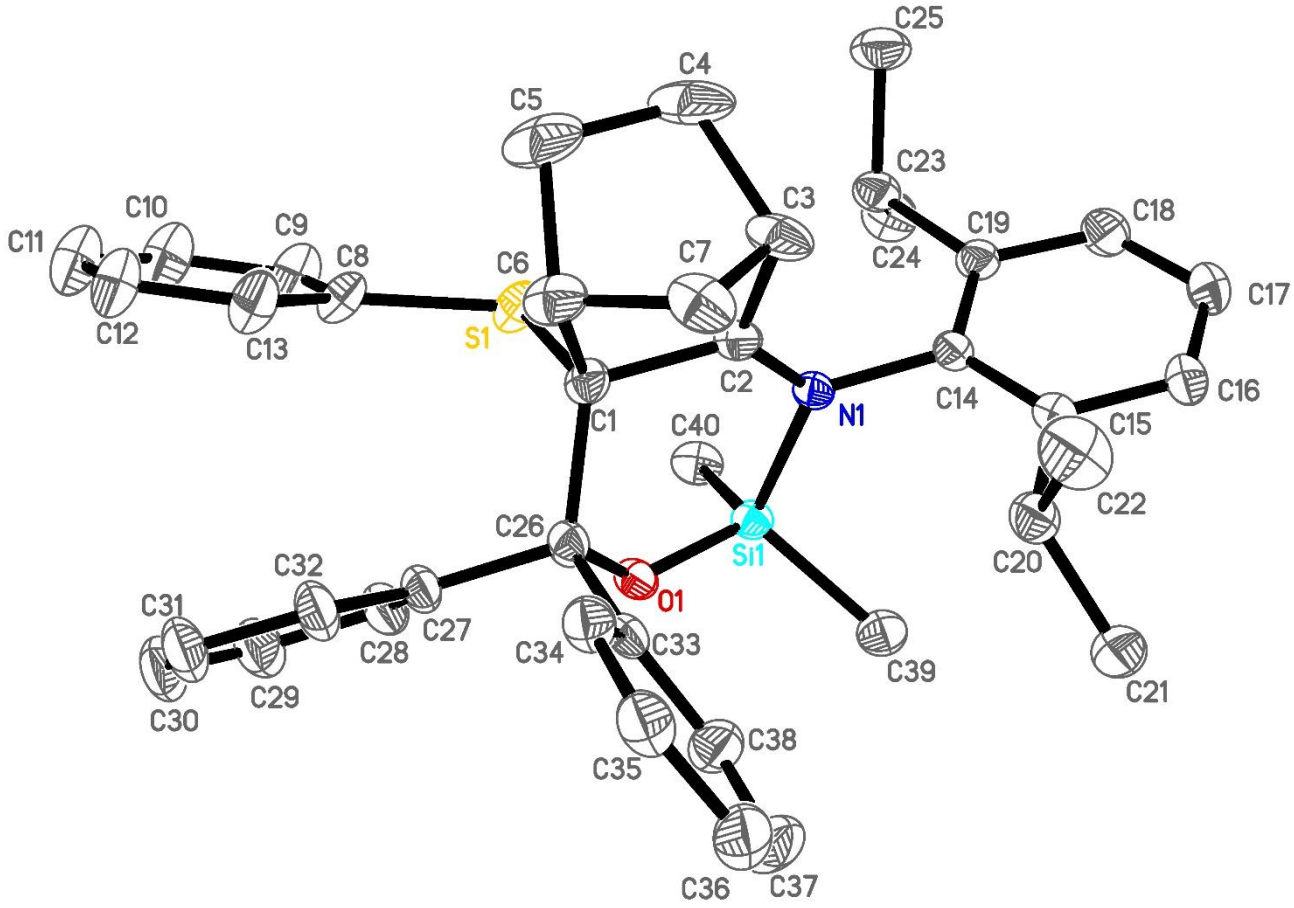


Figure S28 : Molecular view of the cationic part of molecule **2e**. Thermal ellipsoids represent 30 % probability. H and disordered atoms, counterion $[B(C_6F_5)_4]^-$ and solvent molecule were omitted for clarity. Selected bond lengths [Å] and angles [°]: N1−Si1 1.839(3), Si1−O1 1.614(3), C26-O1 1.428(5), S1−C1 1.857(4), C1−C2 1.550(6), C2−N1 1.292(5), N1−C14 1.484(5), S1−C8 1.804(4), C26-C33 1.542(6), C26-C27 1.559(9), Si1−C39 1.823(4), Si1−C40 1.838(4); N1−Si1−O1 99.8(1), Si1−O1−C26 135.4(2), C26−C1−C2 111.6(3), C1−C2−N1 124.3(4), C2−N1−Si1 120.0(3), O1−C26−C1 105.8(3), C2−N1−C14 120.9(3), C14−N1−Si1 118.8(2), O1−Si1−C39 111.8(2), O1−Si1−C40 112.4(2).

Computational details

All computations were carried out using Gaussain09[5] and Gaussian16.[6] The structures were optimized at the M06-2X/def-2tzvp level.[7] Frequency computations were also performed to characterize the nature of the local minima (no imaginary frequency) at the same computational level. The natural bond orbital (NBO) analysis of **2'** was done at the M06-2X/def-2tzvp level.

[5] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J.A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision D.01, Inc., Wallingford CT, **2013**.

[6] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian 16, Revision A.03, Inc., Wallingford CT, **2016**.

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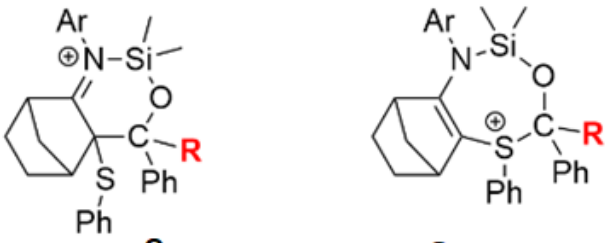
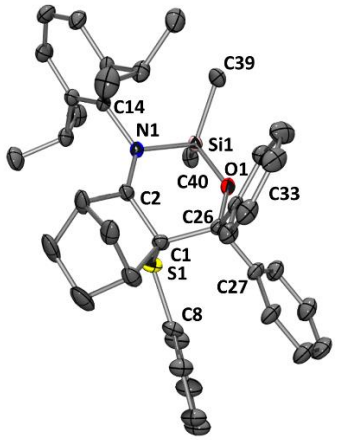


Table S2. Electronic energy difference in kJ mol^{-1}.

	2	**C**
R = H	0	80
R = Ph	0	58
R = CF_3	0	95

Table S3. Comparison of calculated geometric parameters of **2e** with the X-Ray data.



Bond lengths [100 pm]	**Exp.**	**M06-2X/ def-2tzvp**	**Unsigned Error (UE)**
N1-Si1	1.839	1.847	0.008
Si1-O1	1.614	1.627	0.013
C26-O1	1.428	1.415	0.013
S1-C1	1.857	1.880	0.023
C1-C2	1.542	1.542	0.000
C2-N1	1.292	1.288	0.004
N1-C14	1.484	1.466	0.018

S1-C8	1.804	1.776	0.028
C26-C33	1.542	1.541	0.001
C26-C27	1.559	1.534	0.025
Si1-C39	1.823	1.849	0.026
Si1-C40	1.838	1.846	0.008
			(Mean UE) = 0.014
Angles [°]			
N1-Si1-O1	99.79	99.7	0.1
Si1-O1-C26	135.5	135.6	0.1
C26-C1-C2	111.6	112.3	0.7
C1-C2-N1	124.3	124.7	0.4
C2-N1-Si1	120.0	118.8	1.2
O1-C26-C1	105.8	107.0	1.2
C2-N1-C14	120.9	120.5	0.4
C14-N1-Si1	118.8	120.4	1.6
O1-Si1-C39	111.84	114.9	3.1
O1-Si1-C40	112.39	111.7	0.7
			(Mean UE) = 0.9

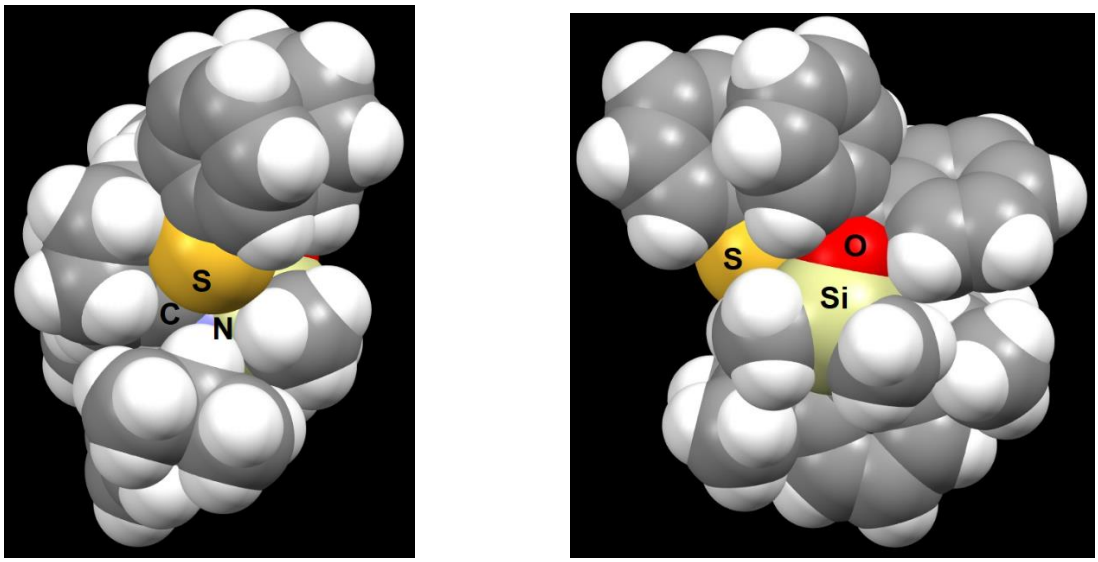
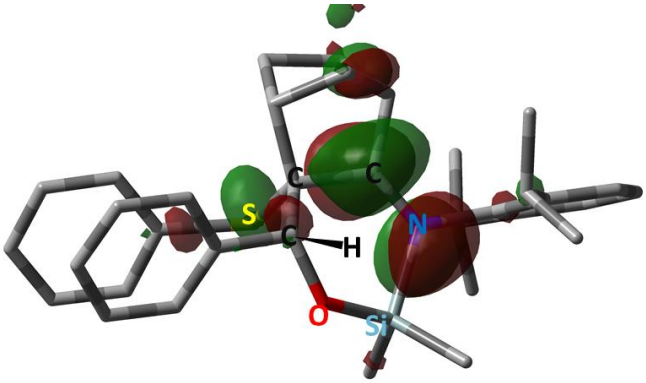
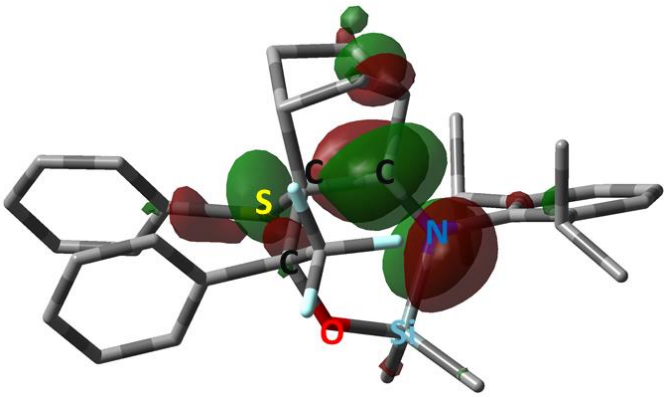


Figure S29 :. Spacefill representation of 2e (R = R' = Ph)

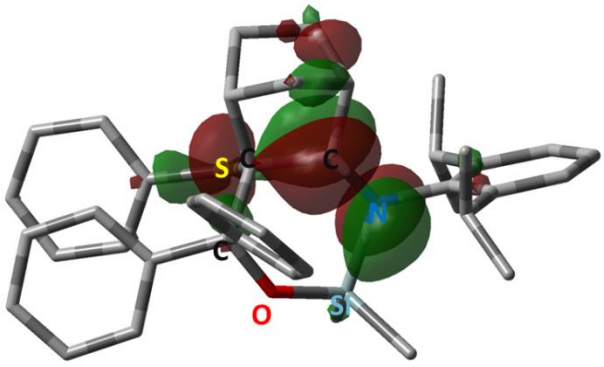
The Optimized geometry of 2a, 2c and 2e (R = H, CF_3, Ph, respectively) and LUMO and MO and energy level.



2a (R = H) -4.24 eV



2c (R = CF_3) -4.37 eV



2e (R = Ph) -4.22 eV

Figure S30 : Surface diagram of the LUMO of **2a**, **2c**, and **2e** calculated at the M062X/def2-TZVP level (isodensity value = 0.04). Hydrogen atoms were omitted for clarity.

Electrostatic potential map 2a (R=H)

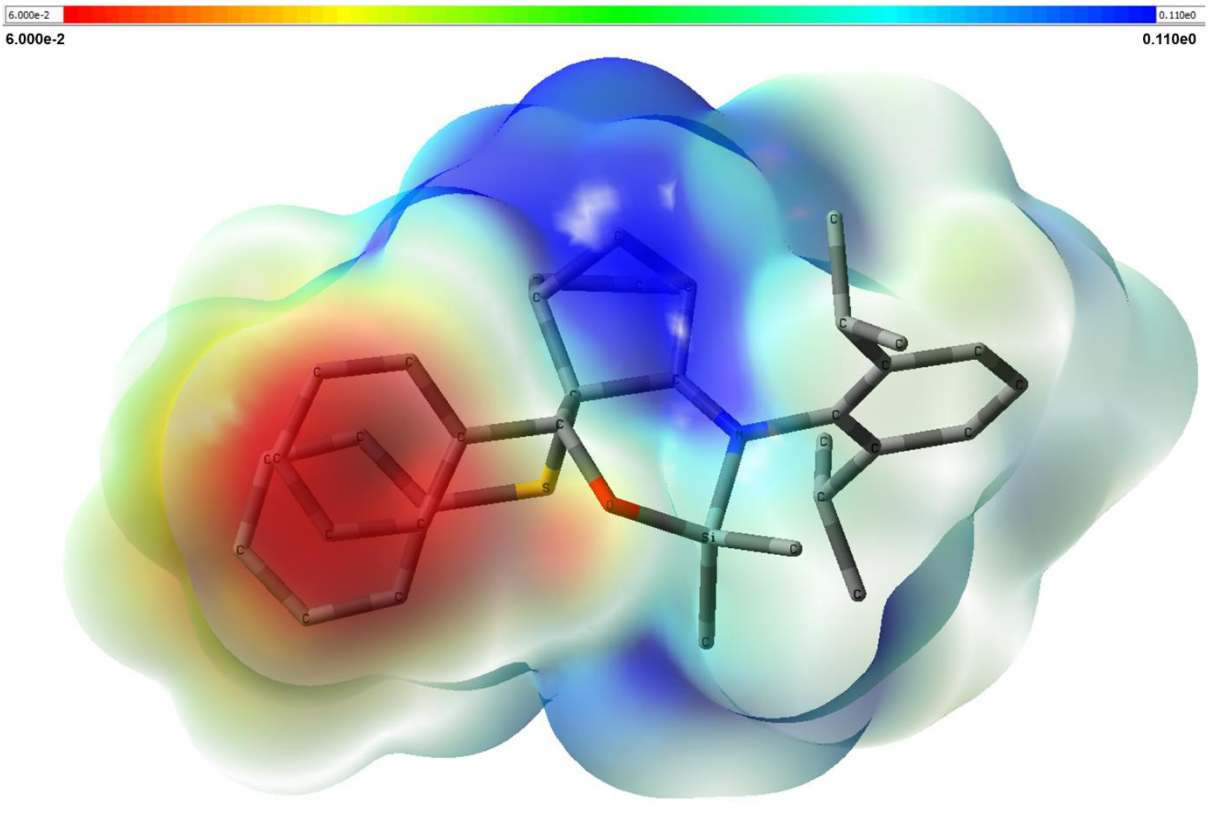


Figure S31. Electrostatic potential surface of **2a** (R=H) calculated at the M062X/def2-TZVP level (isodensity value = 0.0004). Hydrogen atoms were omitted for clarity .

Table S4. Absolute energies (au) of optimized geometries (2a, 2c, and 2e) calculated at the M06-2X/def2-TZVP level.

	E	**G**
2a	-2137.666423	-2137.732865
2c	-2474.738909	-2474.807751
2e	-2368.610446	-2368.680900

Cartesian Coordinates

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Molecule Name: 2a

C	1.174400	-0.100700	2.203400
C	-1.055700	-0.540200	2.188000
C	-0.747800	-0.204100	0.694800
C	0.235300	-1.260400	2.621500
H	0.276900	-1.442800	3.694500
H	0.435300	-2.194000	2.094600
C	0.527400	1.111800	2.932400
H	1.005500	1.227800	3.903400
H	0.665400	2.038300	2.377000
C	-0.965200	0.724000	3.052400
H	-1.222200	0.470200	4.080300
H	-1.625400	1.523600	2.727800
H	2.241900	-0.212100	2.364000
H	-1.972300	-1.108100	2.306900
C	-1.068800	-1.368000	-0.300700
S	-1.293700	1.438100	0.073400
C	0.773600	-0.051300	0.774300
Si	0.850900	-0.296000	-1.953100
O	-0.532400	-1.064600	-1.566500
N	1.546100	-0.027600	-0.254400
C	-3.070400	1.486600	0.101100
C	-3.652300	2.186400	-0.952200
C	-3.868900	0.939500	1.098700
C	-5.029700	2.336900	-1.006200
H	-3.028000	2.600200	-1.734600
C	-5.247400	1.068000	1.018000

H	-3.438200	0.397800	1.926500
C	-5.832000	1.768700	-0.027700
H	-5.474100	2.887400	-1.824900
H	-5.865900	0.620300	1.784700
H	-6.907500	1.871700	-0.078200
C	-2.537300	-1.688600	-0.427500
C	-3.139100	-2.546100	0.487100
C	-3.299900	-1.132900	-1.447500
C	-4.501300	-2.802200	0.418500
H	-2.540500	-3.035400	1.248100
C	-4.660100	-1.389300	-1.518300
H	-2.825500	-0.490400	-2.177000
C	-5.265200	-2.214600	-0.579600
H	-4.960800	-3.473100	1.132200
H	-5.249600	-0.943400	-2.308600
H	-6.327000	-2.414600	-0.637500
C	1.984700	-1.408800	-2.883500
H	1.647000	-1.420300	-3.923100
H	3.012900	-1.042500	-2.876100
H	1.962100	-2.432600	-2.515300
C	0.617000	1.306400	-2.839700
H	-0.287600	1.206000	-3.446500
H	0.481500	2.165200	-2.187100
H	1.452100	1.493100	-3.516000
C	2.992100	0.107200	-0.099700
C	3.533100	1.396700	-0.102700
C	3.774900	-1.050300	0.015100
C	4.919800	1.505800	-0.020100
C	5.152000	-0.876700	0.101800

C	5.722900	0.385000	0.074000
H	5.371700	2.489400	-0.021600
H	5.788500	-1.746900	0.195700
H	6.797600	0.492800	0.136600
C	3.203400	-2.454700	0.107100
H	2.145700	-2.425500	-0.170000
C	2.697100	2.661700	-0.139800
H	1.640200	2.390000	-0.186200
C	3.914600	-3.434100	-0.833300
H	4.911000	-3.672900	-0.460300
H	3.357900	-4.370400	-0.886700
H	4.022800	-3.037100	-1.841000
C	3.303000	-2.984900	1.543500
H	2.793200	-2.345400	2.262600
H	2.870900	-3.984800	1.606700
H	4.349500	-3.052400	1.844700
C	3.020100	3.512700	-1.370100
H	2.353900	4.374900	-1.417900
H	4.043800	3.886900	-1.323000
H	2.915500	2.944200	-2.293700
C	2.908000	3.477200	1.140500
H	3.922600	3.875900	1.181800
H	2.217000	4.320600	1.169700
H	2.755600	2.871300	2.034500
H	-0.562500	-2.259100	0.092400

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Molecule Name: 2c

C	1.203300	0.292100	2.203700
C	-0.976400	-0.353700	2.235900
C	-0.682900	-0.171900	0.708400
C	0.371900	-0.882100	2.774100
H	0.399800	-0.893100	3.862900
H	0.676200	-1.855900	2.404100
C	0.443400	1.513900	2.792000
H	0.896800	1.766200	3.749200
H	0.504300	2.386100	2.146800
C	-1.010600	1.010100	2.944900
H	-1.261600	0.848000	3.992600
H	-1.732500	1.709600	2.536400
H	2.275100	0.300500	2.375700
H	-1.838000	-0.986000	2.425500
C	-1.075100	-1.350900	-0.268700
S	-1.231200	1.425200	-0.060000
C	0.834500	0.107500	0.773000
Si	0.996500	-0.424700	-1.899300
O	-0.411700	-1.147300	-1.485700
N	1.623400	0.114900	-0.245500
C	-2.980000	1.684600	0.126600
C	-3.493600	2.593600	-0.797900
C	-3.808700	1.131900	1.092000
C	-4.830400	2.951900	-0.745000
H	-2.849800	3.012900	-1.561500
C	-5.152100	1.482000	1.120600
H	-3.435200	0.416000	1.807200

C	-5.666500	2.393400	0.212100
H	-5.219300	3.661900	-1.462900
H	-5.796900	1.033800	1.865200
H	-6.712700	2.665100	0.246800
C	-2.580500	-1.417400	-0.522600
C	-3.465900	-2.013900	0.373900
C	-3.083200	-0.842000	-1.684300
C	-4.828600	-2.013300	0.116000
H	-3.117900	-2.492300	1.276900
C	-4.447200	-0.828900	-1.931000
H	-2.404500	-0.386700	-2.391000
C	-5.325300	-1.412400	-1.030300
H	-5.502100	-2.486900	0.818000
H	-4.822100	-0.364200	-2.833200
H	-6.389500	-1.406500	-1.225100
C	2.161700	-1.626500	-2.663600
H	1.846200	-1.760200	-3.701600
H	3.178700	-1.231000	-2.680100
H	2.160200	-2.602300	-2.181400
C	0.756800	1.034700	-2.997300
H	0.048600	0.737100	-3.776100
H	0.358800	1.913200	-2.495400
H	1.694800	1.290500	-3.492400
C	3.027800	0.534800	-0.125800
C	3.319400	1.903000	-0.219000
C	4.026900	-0.438500	0.037200
C	4.661200	2.276300	-0.167800
C	5.345300	-0.000300	0.092200
C	5.666100	1.341400	-0.017600

H	4.914900	3.326000	-0.239500
H	6.134700	-0.728000	0.224500
H	6.700200	1.656800	0.021300
C	3.738700	-1.915500	0.213500
H	2.734600	-2.108900	-0.145600
C	2.280300	3.002400	-0.322400
H	1.285300	2.556200	-0.334700
C	4.695400	-2.808500	-0.580500
H	5.689100	-2.825600	-0.131600
H	4.324700	-3.834100	-0.578400
H	4.799400	-2.484300	-1.615500
C	3.784300	-2.306500	1.694800
H	3.058900	-1.752500	2.290100
H	3.570700	-3.370200	1.807700
H	4.775700	-2.112500	2.108300
C	2.445700	3.824400	-1.604000
H	1.638100	4.553100	-1.687900
H	3.386700	4.375700	-1.589600
H	2.440500	3.200000	-2.495400
C	2.366900	3.930700	0.896300
H	3.268700	4.542400	0.848100
H	1.509800	4.605300	0.920200
H	2.400000	3.373700	1.832400
C	-0.580600	-2.747600	0.189000
F	0.764700	-2.764900	0.265700
F	-0.931900	-3.670900	-0.687000
F	-1.028800	-3.120600	1.388300

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Molecule Name: 2e

C	1.375800	-0.026600	-2.174500
C	-0.827400	0.491600	-2.287000
C	-0.658200	0.043200	-0.791500
C	0.519600	1.187700	-2.583700
H	0.634600	1.422600	-3.641400
H	0.717800	2.080100	-1.993200
C	0.755700	-1.164000	-3.034200
H	1.303400	-1.222900	-3.973200
H	0.822300	-2.132300	-2.541400
C	-0.708100	-0.710500	-3.234000
H	-0.876600	-0.369700	-4.254800
H	-1.413300	-1.505500	-3.023600
H	2.455200	0.047500	-2.243600
H	-1.700700	1.103900	-2.465600
C	-1.132900	1.062700	0.332900
S	-1.143200	-1.721500	-0.361600
C	0.869600	-0.167600	-0.783600
Si	0.775400	-0.261400	1.926900
O	-0.493200	0.678300	1.535100
N	1.570300	-0.421400	0.266900
C	-2.902100	-1.957800	-0.289900
C	-3.507800	-1.977100	0.964100
C	-3.643600	-2.260800	-1.427000
C	-4.858100	-2.264200	1.074300
H	-2.921100	-1.746500	1.843200
C	-4.997900	-2.539100	-1.311200
H	-3.173400	-2.289700	-2.399400

C	-5.606200	-2.536700	-0.063800
H	-5.327100	-2.268500	2.049200
H	-5.574200	-2.771300	-2.197000
H	-6.661800	-2.757900	0.022800
C	-2.644300	1.054300	0.592900
C	-3.597000	0.911900	-0.411500
C	-3.081000	1.296700	1.891600
C	-4.950900	0.991900	-0.123600
H	-3.307800	0.688400	-1.427800
C	-4.435700	1.377300	2.181700
H	-2.356300	1.426500	2.682400
C	-5.377100	1.226100	1.175400
H	-5.672600	0.856800	-0.918600
H	-4.752800	1.566300	3.198900
H	-6.433600	1.288500	1.400200
C	-0.737500	2.516200	0.009500
C	0.311300	3.133600	0.679000
C	-1.441100	3.262700	-0.937800
C	0.706000	4.427800	0.357400
H	0.805500	2.620400	1.488400
C	-1.046600	4.548700	-1.265800
H	-2.321400	2.854800	-1.413300
C	0.042900	5.133500	-0.631800
H	1.521900	4.888100	0.900100
H	-1.605300	5.104700	-2.007000
H	0.345900	6.140900	-0.883900
C	1.969600	0.626400	3.018600
H	1.538800	0.657500	4.022800
H	2.904200	0.063600	3.084200

H	2.200100	1.645400	2.719500
C	0.335800	-1.871700	2.722000
H	-0.608100	-1.706000	3.249900
H	0.188500	-2.701500	2.037300
H	1.085400	-2.142300	3.466400
C	3.003500	-0.708400	0.155200
C	3.399800	-2.049500	0.101900
C	3.919500	0.353400	0.113500
C	4.766000	-2.311000	0.019200
C	5.268800	0.029000	0.022000
C	5.693600	-1.287800	-0.019800
H	5.101800	-3.339300	-0.021700
H	5.998600	0.827500	-0.017000
H	6.749300	-1.514800	-0.087000
C	3.520900	1.815400	0.143600
H	2.455900	1.877400	0.359600
C	2.435600	-3.219300	0.110200
H	1.414500	-2.836500	0.128600
C	4.276600	2.587900	1.231000
H	5.311500	2.762600	0.933900
H	3.815300	3.565700	1.381200
H	4.290600	2.059300	2.182800
C	3.754900	2.503400	-1.206100
H	3.200000	2.036700	-2.018500
H	3.442500	3.547400	-1.145400
H	4.814500	2.481500	-1.466800
C	2.642800	-4.090100	1.352500
H	1.882400	-4.870900	1.400100
H	3.618700	-4.576900	1.321600

H	2.593600	-3.503700	2.269600
C	2.586200	-4.066700	-1.157300
H	3.546900	-4.583100	-1.168500
H	1.802200	-4.823700	-1.198000
H	2.528800	-3.458600	-2.060300