Supporting Information

CO_2 Hydrosilylation Catalyzed by an N-Heterocyclic Carbene (NHC)-stabilized stannyliumylidene

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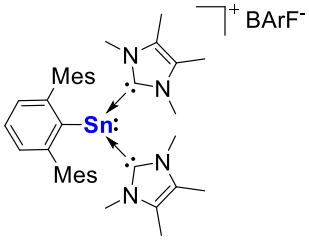
1. Experimental Details

1.1 General Methods and Instrumentation

All experiments and manipulations were carried out under a dry oxygen-free argon atmosphere using standard Schlenk techniques or in a glovebox. All glass junctions were coated with PTFE-based grease Merkel Triboflon III. Solvents were dried by standard methods (withdrawn from MBraun Solvent Purification System (SPS) over molecular (3 Å)) or distilled from sodium/benzophenone or CaH_2 under argon atmosphere and degassed via freeze-pump-thaw cycling). The ^{1}H, $^{13}C\{^{1}H\}$, $^{119}Sn\{^{1}H\}$, $^{11}B\{^{1}H\}$ and $^{19}F\{^{1}H\}$ NMR spectra of the compounds were measured on Bruker 400 MHz and 300 MHz spectrometer. Chemical shifts are referenced to (residual) solvent signals (^{1}H and $^{13}C\{^{1}H\}$ NMR). Deuterated benzene (C_6D_6), deuterated toluene (toluene-d_8) and deuterated tetrahydrofuran (THF-d_8) were obtained from Sigma-Aldrich Deutero Chemie GmbH, stored over 4 Å molecular sieves in the glovebox. Carbon dioxide (5.0) was purchased from Westfalen AG and used as received. Unless otherwise stated, all reagents were purchased from commercial sources and used as received. Abbreviations: s = singlet, br = broadened, d = doublet, t = triplet, m = multiplet, dec = decompose. Some NMR spectra include resonances for silicone grease (C_6D_6: $\delta(^{1}H)$ = 0.29 ppm, $\delta(^{13}C)$ = 1.4 ppm; δ = THF-d_8: $\delta(^{1}H)$ = 0.11 ppm, $\delta(^{13}C)$ = 1.2 ppm). Liquid Injection Field Desorption Ionization Mass Spectrometry (LIFDI-MS) were measured directly from an inert atmosphere glovebox with a Thermo Fisher Scientific Exactive Plus Orbitrap equipped with an ion source from Linden CMS. The UV-vis spectra were taken on a *Agilent Cary 50* spectrophotometer with a *Schlenk* quartz cuvette as the Central Anlytic Department at the TUM Catalysis Research Center. Quantitative elemental analyses (EA) were carried out using an EURO EA (HEKA tech) instrument equipped with a CHNS combustion analyzer at the Laboratory for Microanalysis at the TUM Catalysis Research Center. For fluoride determination, the sample is digested in an alkaline medium. Fluoride content is then measured directly by potentiometry using a Titrando 904 (Metrohm). For tin determination, the sample is acid digested. Measurements are conducted at a wavelength of 235.5 nm in an acetylene/nitrous oxide flame using atomic absorption spectroscopy (Agilent 280 FS-AA). Melting Points (m.p.) were determined in sealed glass capillaries under inter gas by a Büchi M-540. IMe_4 (1,3,4,5-tetramethylimidazaol-2-ylidene), Chlorostannylene [^{Mes}TerSnCl] (**1**), Sodium tetrakis [3,5-bis(trifluoromethyl)phenyl] borate (NaBArF), and Li[Al(OC(CF_3)$_3$)$_4$] were synthesized according to the literature procedures.[S1]

1.2 Synthesis of Stannyliumylidene [**2**]$^{+}$

1.2.1 Synthesis of [**2**][BArF]



[**2**][**BArF**]: A solution of IMe_4 (2.00 eq, 531.0 mg, 4.28 mmol) in toluene (3 mL) was added dropwise to [^{Mes}TerSnCl] (1.00 eq, 1.00 g, 2.14 mmol) dissolved in toluene (10 mL) at room temperature. After stirring for 10 minutes, NaBArF ([BArF] = 1,3-bis(trifluoromethyl)-boron) (1.00 eq, 1.90 g, 2.14 mmol) was introduced, resulting in the immediate formation of a brown precipitate. Following this, fluorobenzene (C_6H_5F) (3 mL) was

added, and the reaction was allowed to stir overnight at room temperature. The mixture was then filtered, and the filtrate was concentrated to a volume of 5 mL. After 2 days at −35 ºC, colourless crystals suitable for XRD analysis were obtained. Yield: 2.65 g (1.72 mmol, 80.4%).

^{1}H NMR (400 MHz, 298 K, THF-d$_8$): δ[ppm] = 2.08 (s, 12 H, 4xC-C*H*$_3$, NHC), 2.09 (s, 6 H, 2xC^4-C*H*$_3$, Mes), 2.15 (s, 12H, 2xC^{2,6}-C*H*$_3$, Mes), 3.41 (s, 12 H, 4xN-C*H*$_3$, NHC), 6.69 (s, 4 H, 2xC^{3,5}-*H*, Mes), 7.04 (d, $^{3}J_{H-H}$ = 8 Hz, 2 H, C^{3,5}-*H*, C$_6$H$_3$), 7.38 (t, $^{3}J_{H-H}$ = 8 Hz, 1 H, C^4-*H*, C$_6$H$_3$), 7.59, 7.79 (s, 12 H, 4x*C*^{2,4,6}, 4C$_6$H$_3$(CF$_3$)$_2$).

^{13}C{^{1}H} NMR (101 MHz, 298 K, THF-d$_8$): δ[ppm] = 8.68 (2xC^{4,5}-*C*H$_3$, NHC), 20.99 (C^4-*C*H$_3$, Mes), 21.81 (C^{2,6}-*C*H$_3$, Mes), 36.38 (4xN-*C*H$_3$, NHC), 118.13 (*p*-*C*H$_{B-Ar}$), 121.52, 124.22, 126.93 (*C*, BArF), 128.01 (*C*^{4,5}-*C*H$_3$, NHC), 128.50 (*C*^{4}-H, C$_6$H$_3$), 128.56 (4x*C*^{3,5}-H, Mes), 129.61 (*C*^{3,5}-H, C$_6$H$_3$), 129.95-130.54 (m-*C*$_{B-Ar}$), 135.66 (o-CH$_{B-Ar}$), 136.52 (2x*C*^{1}-Mes), 137.22 (2x*C*^{4}-Mes), 141.73 (2x*C*^{2,6}-Mes), 150.00 (2xC^{2,6}-C$_6$H$_3$),159.66 (Sn-*C*, C$_6$H$_3$), 159.66-163.62 (ipso-CB-Ar), 170.18 (Sn-*C*, NHC).

^{119}Sn{^{1}H} NMR (150 MHz, 298 K, THF-d$_8$): δ[ppm] = −235.72 (Sn).

^{11}B{^{1}H} NMR (128 MHz, 298 K, THF-d$_8$): δ[ppm] = −6.52 (B, BArF).

^{19}F{^{1}H} NMR (376 MHz, 298 K, THF-d$_8$): δ[ppm] = −63.45 (C*F*$_3$, BArF).

LIFDI-MS m/z $C_{38}H_{49}N_4Sn$ calcd: 681.2979; found: 681.2932.

Elemental analysis (%) calcd for $C_{70}H_{61}BF_{24}N_4Sn$: C 54.46, H 3.98, N 3.63, F 29.54, Sn 7.69; found: C 54.42, H 4.25, N 3.72, F 26.5, Sn 7.3.

m.p.: 126 ºC.

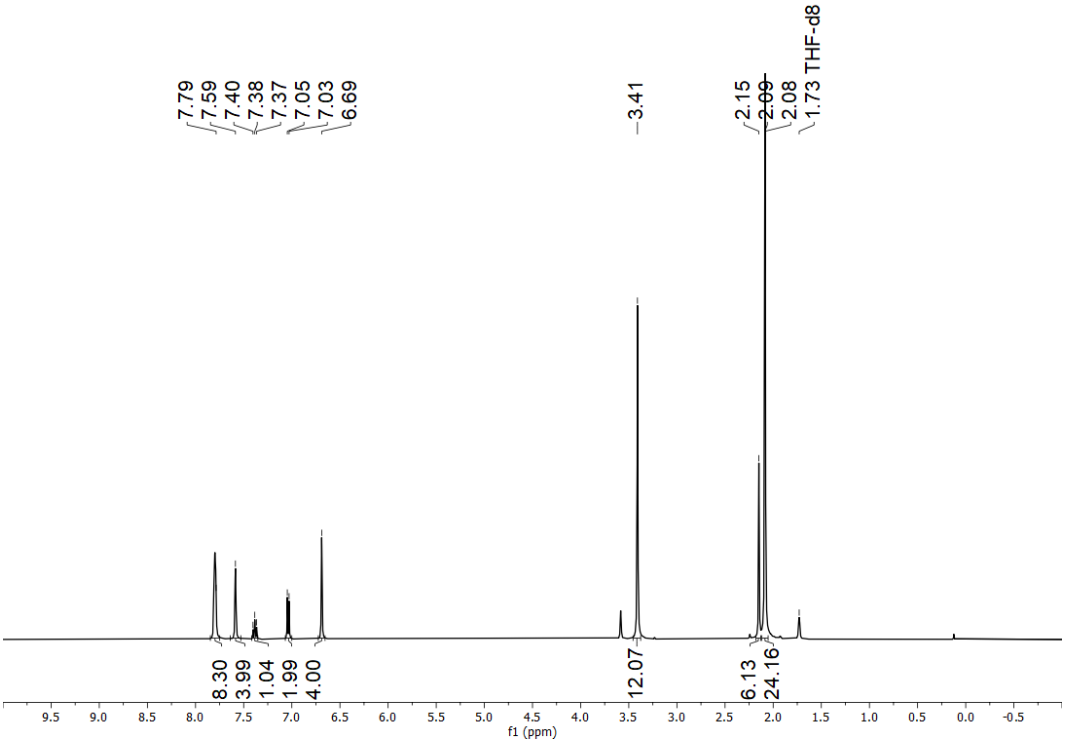


Figure S1. ^{1}H NMR spectrum of [**2**][**BArF**] in THF-d$_8$ at 298 K.

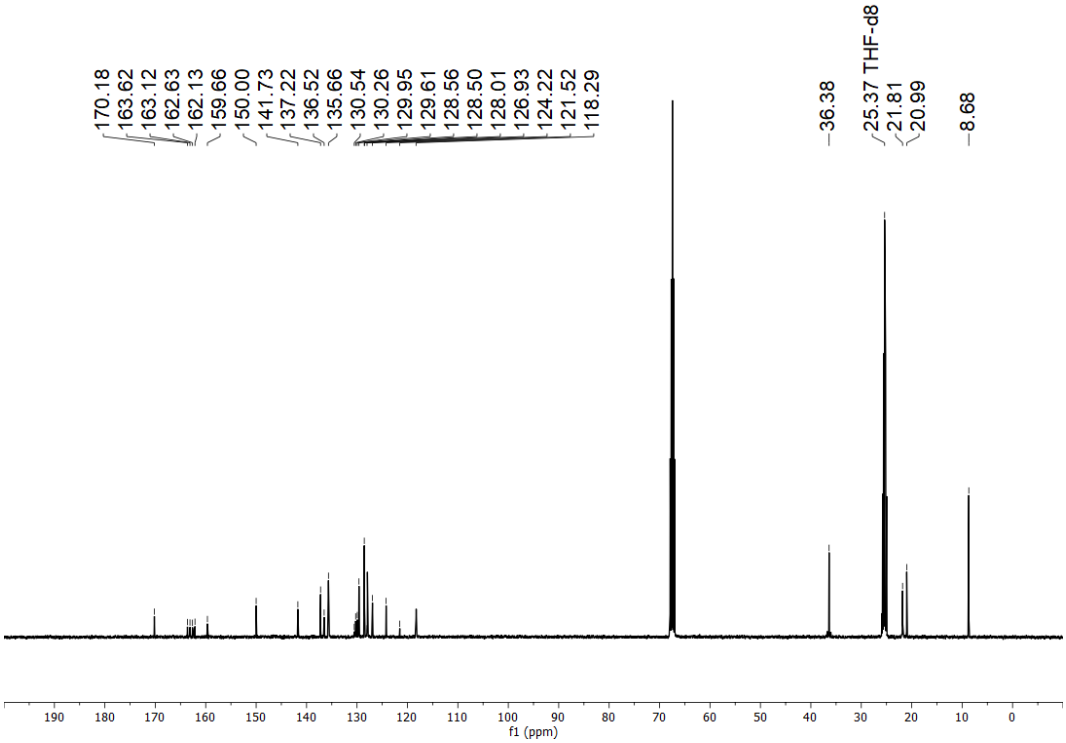


Figure S2. ^{13}C{^{1}H} NMR spectrum of [**2**][**BArF**] in THF-d$_8$ at 298 K.

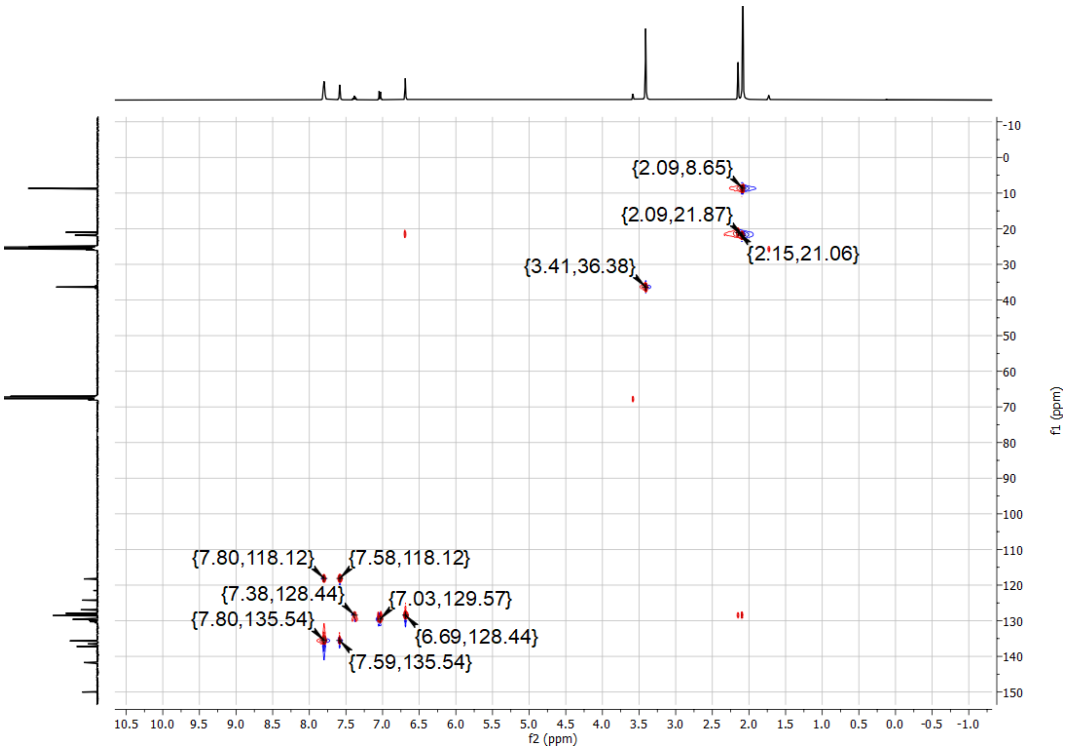


Figure S3. $^{1}H/^{13}C$ NMR HSQC spectrum of [**2**][**BArF**] in THF-d_8 at 298 K.

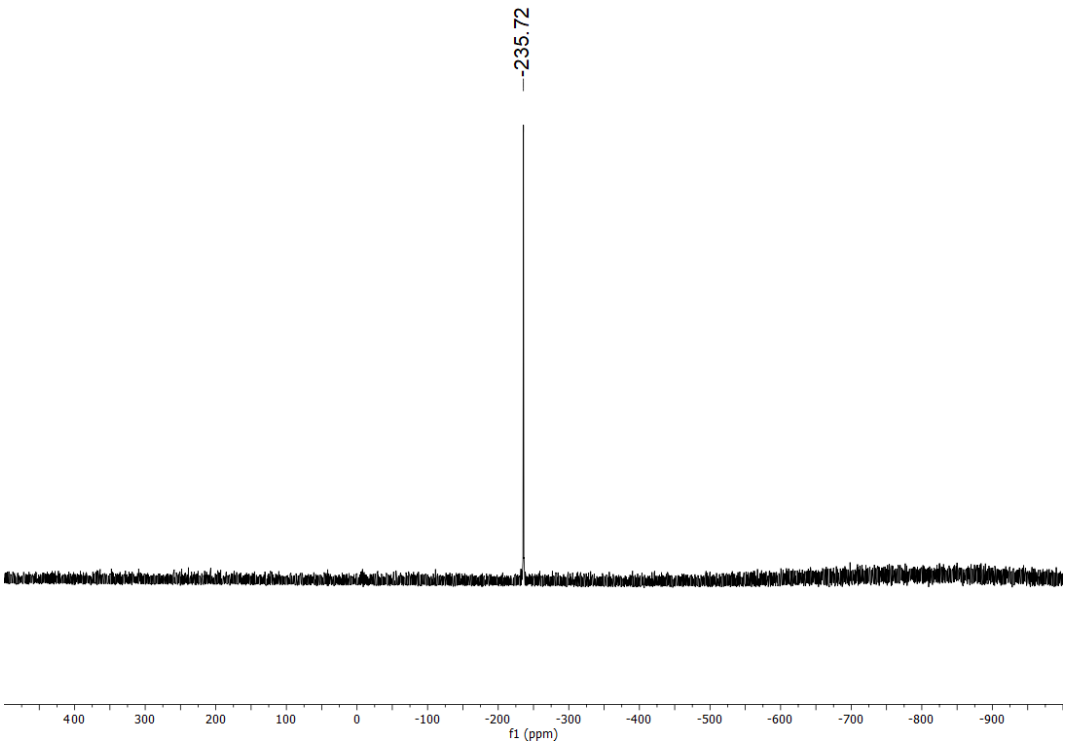


Figure S4. $^{119}Sn\{^{1}H\}$ NMR spectrum of [**2**][**BArF**] in THF-d_8 at 298 K.

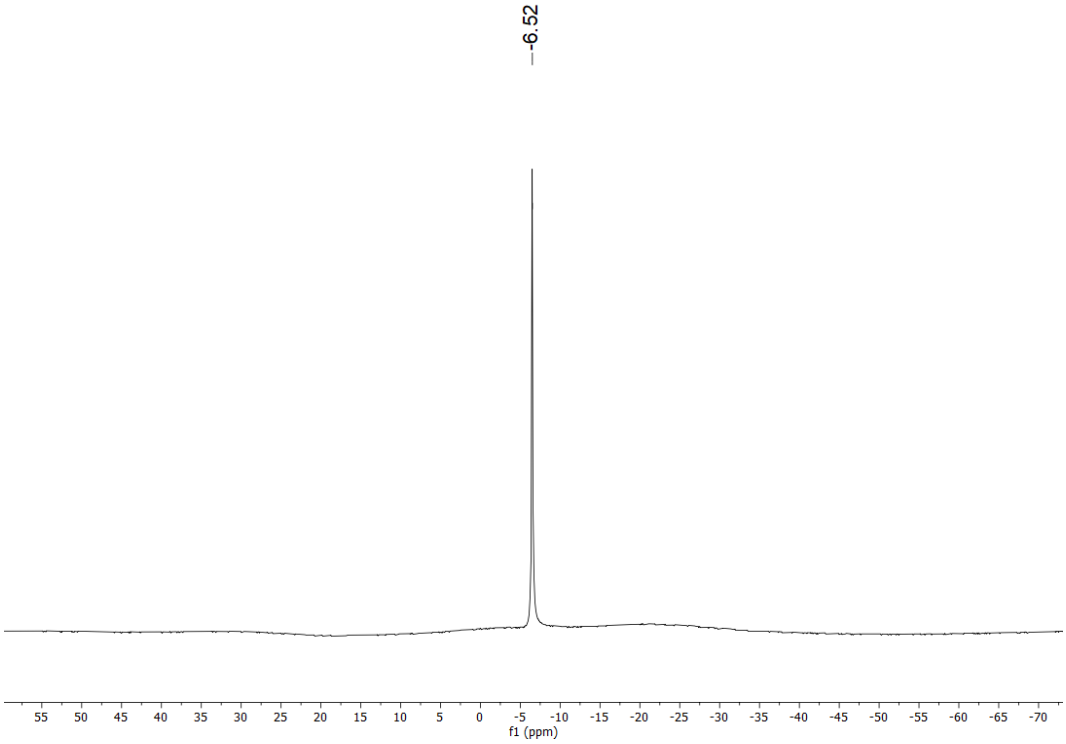


Figure S5. $^{11}B\{^{1}H\}$ NMR spectrum of [**2**][**BArF**] in THF-d_8 at 298 K.

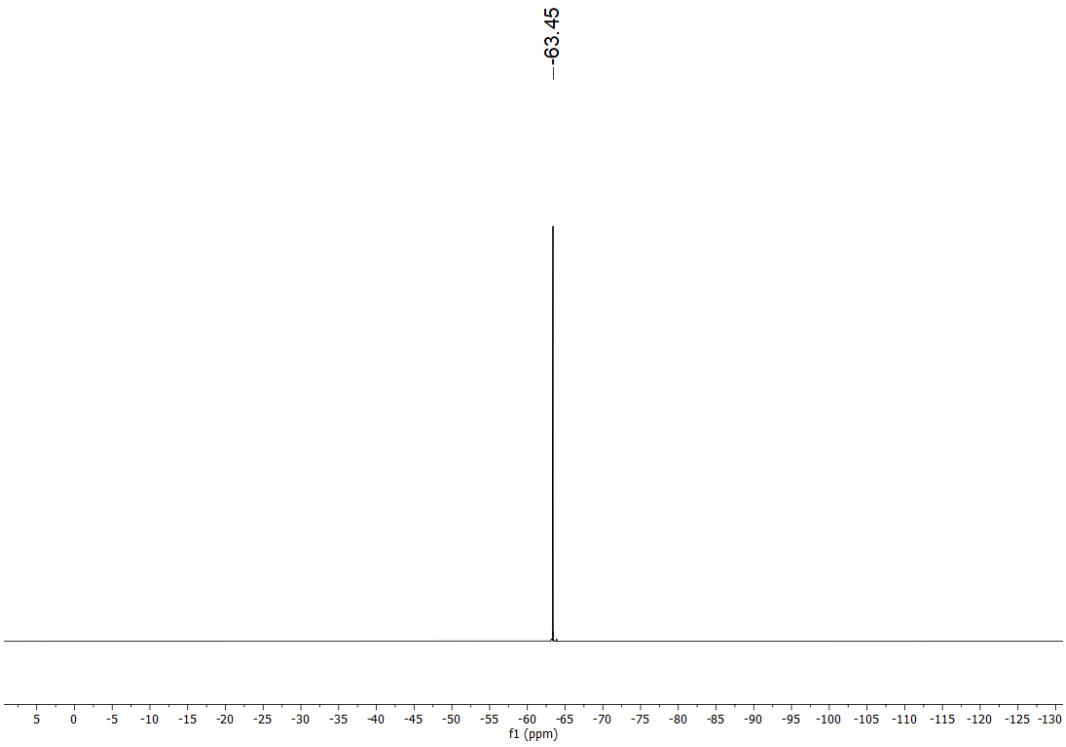


Figure S6. $^{19}F\{^{1}H\}$ NMR spectrum of [**2**][**BArF**] in THF-d_8 at 298 K.

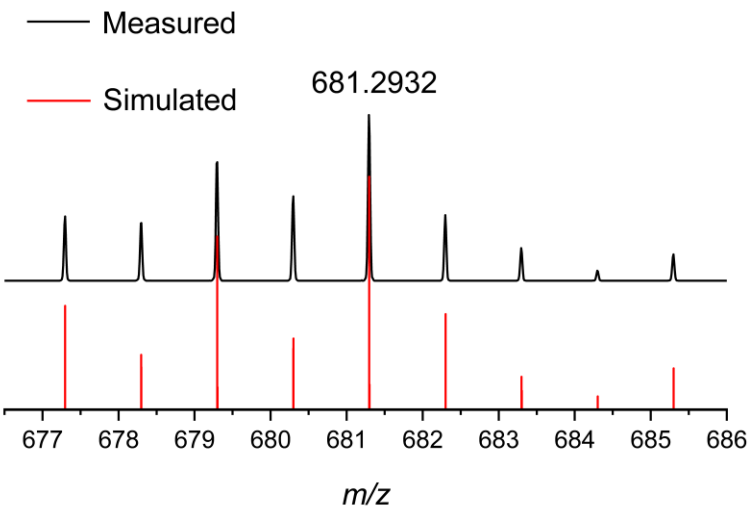
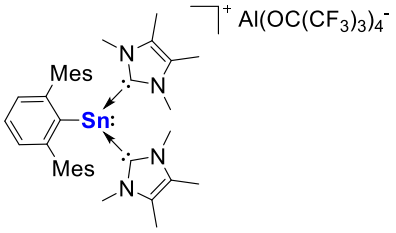


Figure S7. LIFDI-MS spectrum (detail view) of [**2**]$^+$ in [**2**][BArF] (measured spectrum: top; simulated spectrum: bottom).

1.2.2 Synthesis of [**2**][Al(OC(CF$_3$)$_3$)$_4$]



[**2**][Al(OC(CF$_3$)$_3$)$_4$]: A solution of IMe$_4$ (2.00 eq, 53.1 mg, 0.43 mmol) in toluene (2 mL) was added dropwise to [^{Mes}TerSnCl] (1.00 eq, 100.0 mg, 0.21 mmol) dissolved in toluene (3 mL) at room temperature. After stirring for 10 minutes, Li[Al(OC(CF$_3$)$_3$)$_4$] (1.00 eq, 229.9 mg, 0.21 mmol) was introduced, leading to the immediate formation of a brown precipitate. Subsequently, fluorobenzene (1 mL) was added, and the reaction was stirred overnight at room temperature, producing a colorless suspension. The mixture was filtered, and the filtrate was concentrated and stored at −35 °C. After 2 days, colorless crystals formed. Yield: 281.0 mg (0.18 mmol, 86.3%).

^{1}H NMR (400 MHz, 298 K, THF-d$_8$): δ[ppm] = 2.08 (s, 12 H, 2xC^4-C*H*$_3$, Mes), 2.09 (s, 12 H, 4xC-C*H*$_3$, NHC), 2.15 (s, 6 H, 2xC^{2,6}-C*H*$_3$, Mes), 3.41 (s, 12 H, 4xN-C*H*$_3$, NHC), 6.69 (s, 4 H, 2xC^{3,5}-*H*, Mes), 7.03 (d, $^3J_{H\text{-}H}$=8 Hz, 2 H, C^{3,5}-*H*, C$_6$H$_3$), 7.38 (t, $^3J_{H\text{-}H}$= 4 Hz, 1 H, C^4-*H*, C$_6$H$_3$).

^{13}C{^{1}H} NMR (101 MHz, 298 K, THF-d$_8$): δ[ppm] = 8.79 (2xC^{4,5}-*C*H$_3$, NHC), 21.10 (C^4-*C*H$_3$, Mes), 21.92 (C^{2,6}-*C*H$_3$, Mes), 36.49 (4xN-*C*H$_3$, NHC), 120.99, 123.90 (*C*,

Al(O*C*(*C*F$_3$)$_3$)$_4$), 128.07 (*C*^{4,5}-CH$_3$, NHC), 128.60 (*C*^{4}-H, C$_6$H$_3$), 128.68 (4x*C*^{3,5}-H, Mes), 129.72 (*C*^{3,5}-H, C$_6$H$_3$), 136.63 (2x*C*^{1}-Mes), 137.35 (2x*C*^{4}-Mes), 141.85 (2x*C*^{2,6}-Mes), 150.12 (2x*C*^{2,6}-C$_6$H$_3$),159.79 (Sn-*C*, C$_6$H$_3$), 170.30 (Sn-*C*, NHC).

^{119}Sn{^{1}H} NMR (149 MHz, 298 K, THF-d8): δ[ppm] = −235.31 (Sn).

^{19}F{^{1}H} NMR (376 MHz, 298 K, THF-d$_8$): δ[ppm] = −75.89 (C*F*$_3$, Al(OC(CF$_3$)$_3$)$_4$).

LIFDI-MS m/z C$_{38}$H$_{49}$N$_4$Sn calcd: 681.2979; m/z found: 681.2949.

m.p.: 148 °C

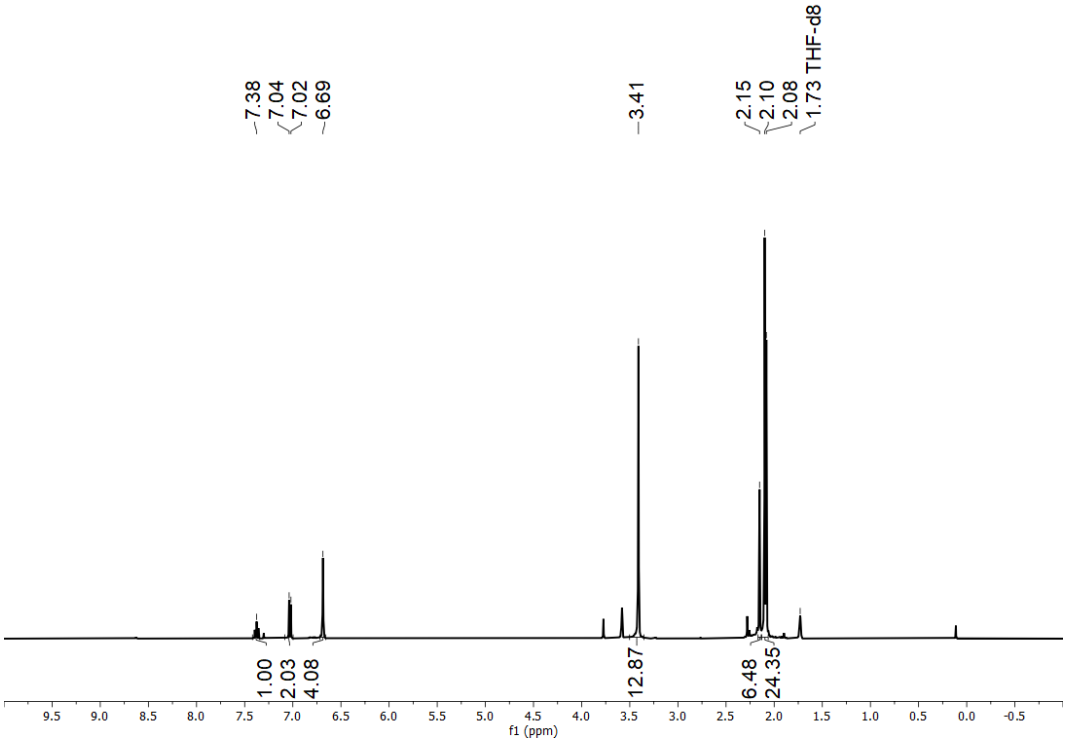


Figure S8. ^{1}H NMR spectrum of [**2**][Al(OC(CF$_3$)$_3$)$_4$] in THF-d$_8$ at 298 K.

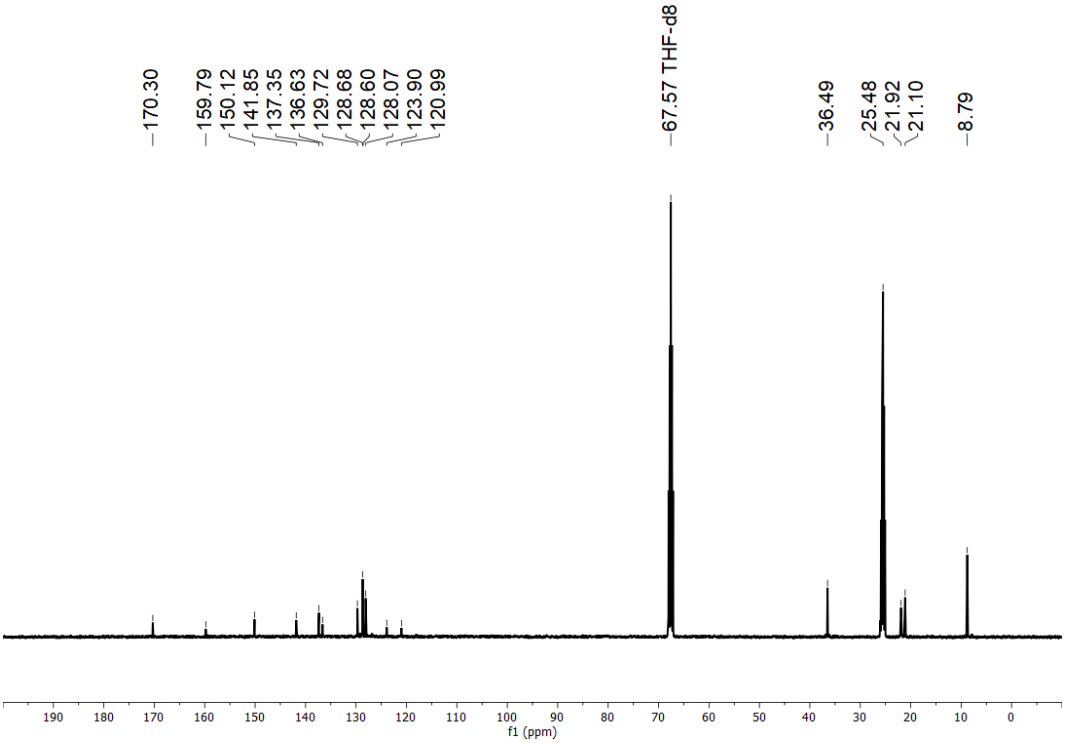


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of [**2**][Al(OC(CF_3)$_3$)$_4$] in THF-d_8 at 298 K.

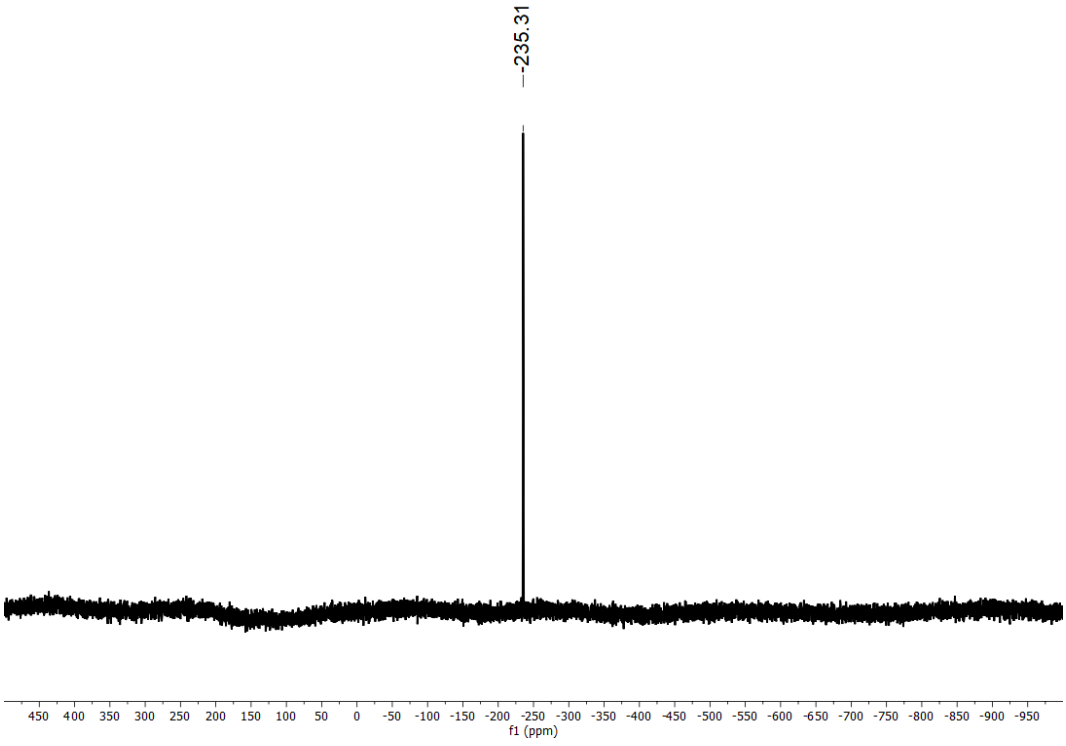


Figure S10. $^{119}Sn\{^{1}H\}$ NMR spectrum of [**2**][Al(OC(CF_3)$_3$)$_4$] in THF-d_8 at 298 K.

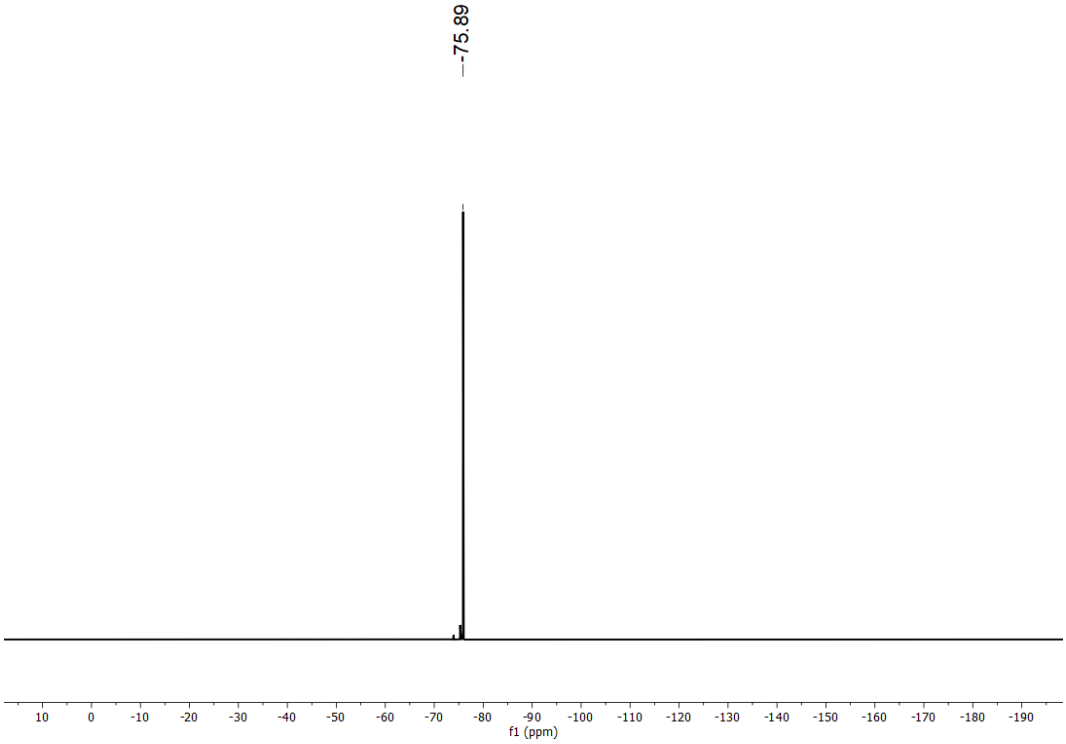


Figure S11. $^{19}F\{^{1}H\}$ NMR spectrum of [**2**][Al(OC(CF$_3$)$_3$)$_4$] in THF-d$_8$ at 298 K.

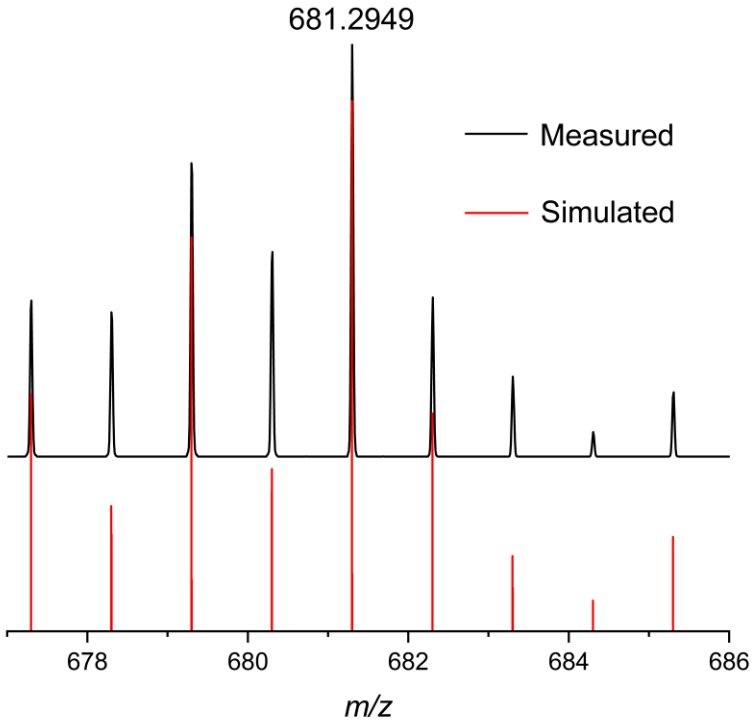
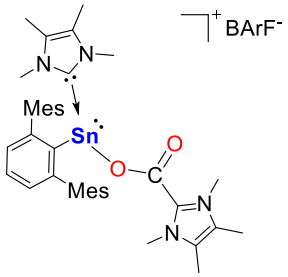


Figure S12. LIFDI-MS spectrum (detail view) of [**2**]$^+$ in [**2**][Al(OC(CF$_3$)$_3$)$_4$] (measured spectrum: top; simulated spectrum: bottom).

1.3 Synthesis of [**3**][BArF]



[**2**][BArF] (1.00 eq, 200.0 mg, 0.13 mmol) was dissolved in a mixture of toluene (3 mL) and fluorobenzene (1 mL). CO_2 (1.1 eq, 3.20 mL, 1 bar) was then added via a syringe at room temperature. After stirring for 4 hours, the solution changed from colorless to pale yellow. The mixture was filtered, and the filtrate was concentrated to 3 mL before being stored at −35 °C. After 2 days, yellow crystals suitable for XRD analysis were obtained after. Yield: 126.0 mg (0.080 mmol, 61.3%).

^{1}H NMR (400 MHz, 298 K, THF-d$_8$): δ[ppm] = 1.94, 2.21 (s, 12 H, 2xC^{2,6}-C*H*$_3$, Mes), 2.10 (s, 6 H, 2xC^4-C*H*$_3$, Mes), 2.11(s, 12 H, 2xC-C*H*$_3$, NHC), 2.28(s, 6 H, 2xC-C*H*$_3$, *NHC*-COO), 3.36 (s, 6 H, 2xN-C*H*$_3$, NHC), 3.74 (s, 6 H, 2xN-C*H*$_3$, *NHC*-COO), 6.69, 6.77 (s, 4H, 2xC^{3,5}-*H*, Mes), 6.91 (d, $^3J_{H\text{-}H}$= 7.5 Hz, 2 H, C^{3,5}-*H*, C$_6$H$_3$), 7.30 (t, $^3J_{H\text{-}H}$= 8 Hz, 1 H, C^4-*H*, C$_6$H$_3$), 7.59, 7.80 (s, 12 H, 4x*C*^{2,4,6}, 4C$_6$H$_3$(CF$_3$)$_2$).

^{13}C{^{1}H} NMR (101 MHz, 298 K, THF-d$_8$): δ[ppm] = 8.32 (C^{4,5}-*C*H$_3$, *NHC*-COO), 8.39 (*C*^{4,5}-Me, NHC), 20.96 (C^4-*C*H$_3$, Mes), 21.60, 21.03 (C^{2,6}-*C*H$_3$, Mes), 34.34 (2xN-*C*H$_3$, *NHC*-COO), 35.65 (2xN-*C*H$_3$, NHC), 118.26 (*p*-CH$_{B\text{-}Ar}$), 121.52, 124.23, 126.93, 127.11 (*C*, BArF), 128.06 (*C*^{4}-H, C$_6$H$_3$), 128.81 (*C*^{4,5}-CH$_3$, *NHC*-COO), 128.87 (*C*^{4,5}-CH$_3$, NHC), 128.95 (4x*C*^{3,5}-H, Mes), 129.64 (2x*C*^{2,6}-Mes), 129.82 (*C*^{3,5}-H, C$_6$H$_3$), 129.95-130.55 (m-C$_{B\text{-}Ar}$), 135.67 (o-CH$_{B\text{-}Ar}$), 136.64 (2x*C*^{4}-Mes), 136.69 (N$_2$*C*, NHC), 137.28 (2x*C*^{2,6}-Mes), 140.98 (2x*C*^{4}-Mes), 148.86 (2x*C*^{2,6}-C$_6$H$_3$), 157.48 (C*C*O$_2$), 162.13-163.62 (ipso-CB-Ar), 164.94 (Sn-*C*, C$_6$H$_3$), 177.70 (Sn-*C*, NHC).

^{119}Sn{^{1}H} NMR (149 MHz, 298 K, THF-d8): δ[ppm] = −10.61 (Sn).

^{11}B{^{1}H} NMR (128 MHz, 298 K, THF-d8): δ[ppm] = −6.47 (B, BArF).

^{19}F{^{1}H} NMR (376 MHz, 298 K, THF-d8): δ[ppm] = −63.36 (C*F*$_3$, BArF).

LIFDI-MS m/z C$_{39}$H$_{49}$N$_4$O$_2$Sn calcd: 725.2878; m/z found: 725.2868.

Elemental analysis (%) calcd for C$_{71}$H$_{61}$BF$_{24}$N$_4$O$_2$Sn: C 53.71, H 3.87, N 3.53, F 28.72, Sn 7.48; found: C 51.96, H 3.88, N 3.43, F 25.5, Sn 7.7.

m.p.: 128.9 °C.

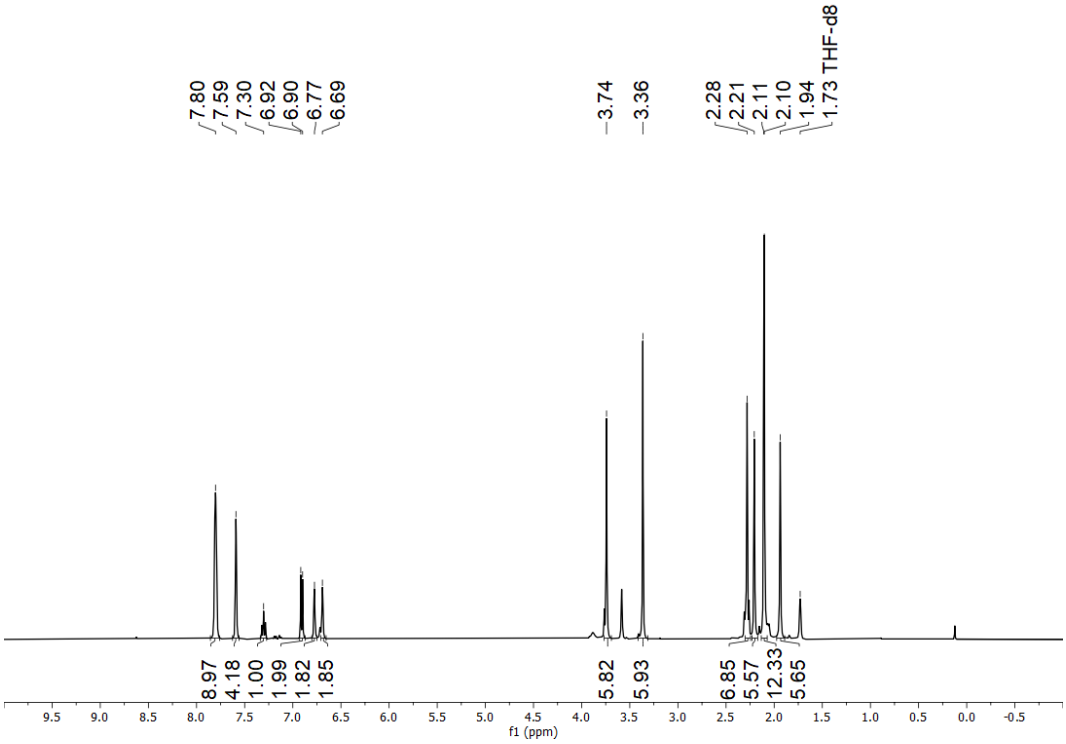


Figure S13. ^{1}H NMR spectrum of [**3**][BArF] in THF-d_8 at 298 K.

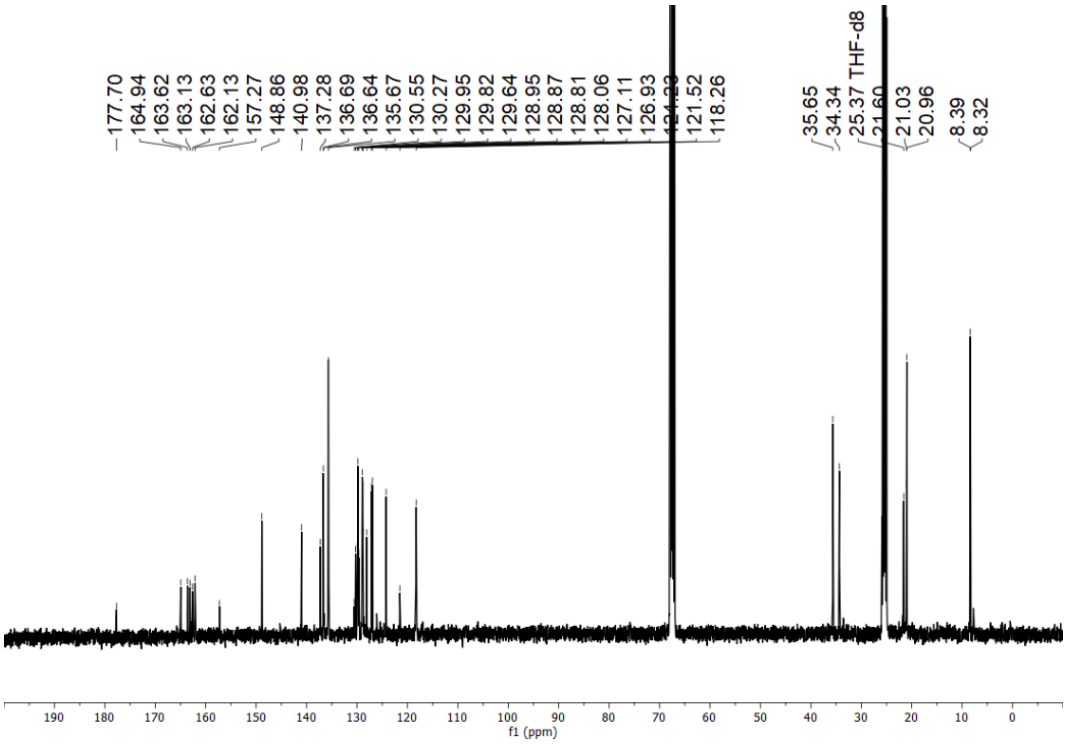


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of [**3**][BArF] in THF-d_8 at 298 K.

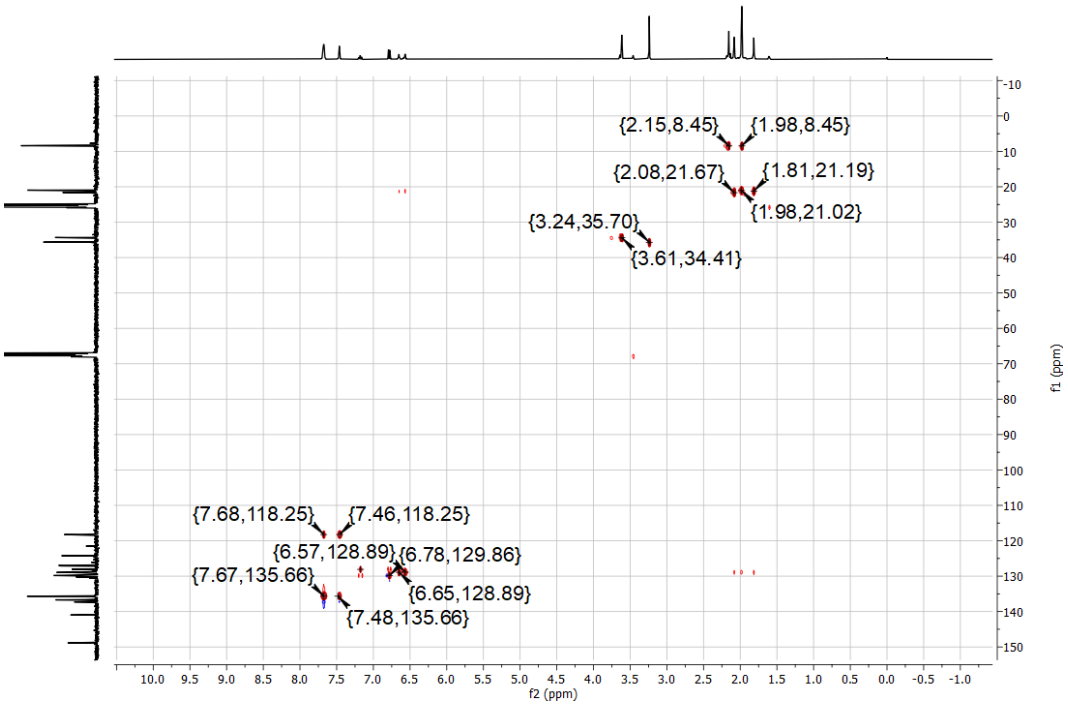


Figure S15. $^{1}H/^{13}C$ NMR HSQC spectrum of [**3**][**BArF**] in THF-d_8 at 298 K.

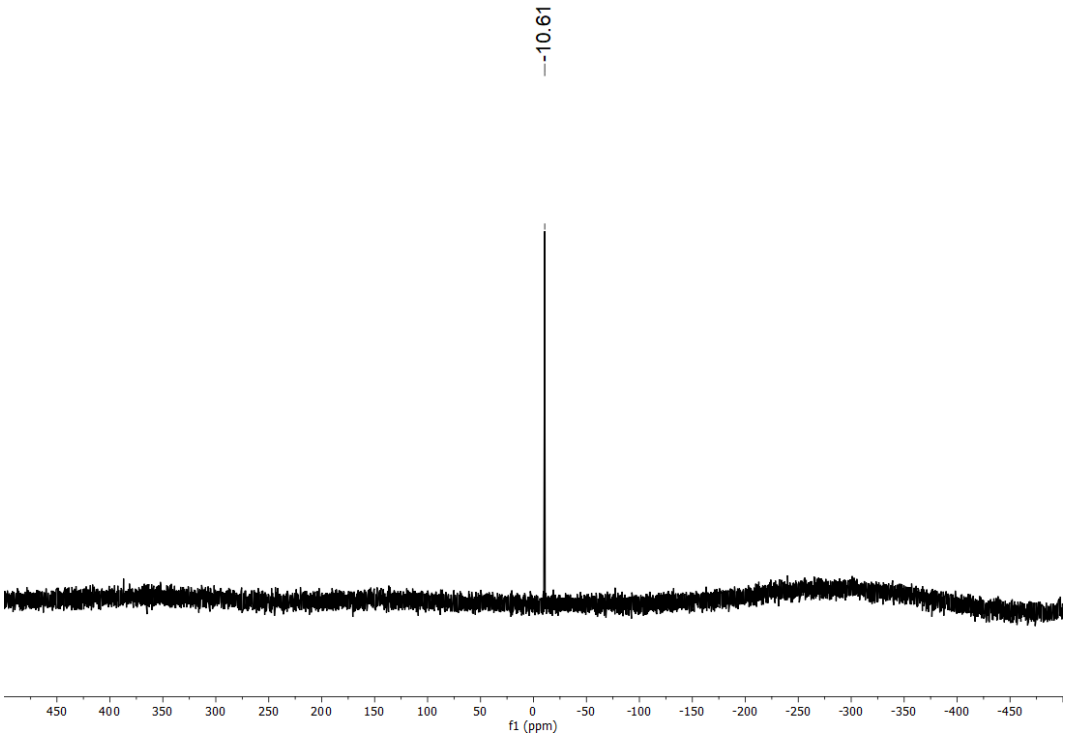


Figure S16. $^{119}Sn\{^{1}H\}$ NMR spectrum of [**3**][BArF] in THF-d_8 at 298 K.

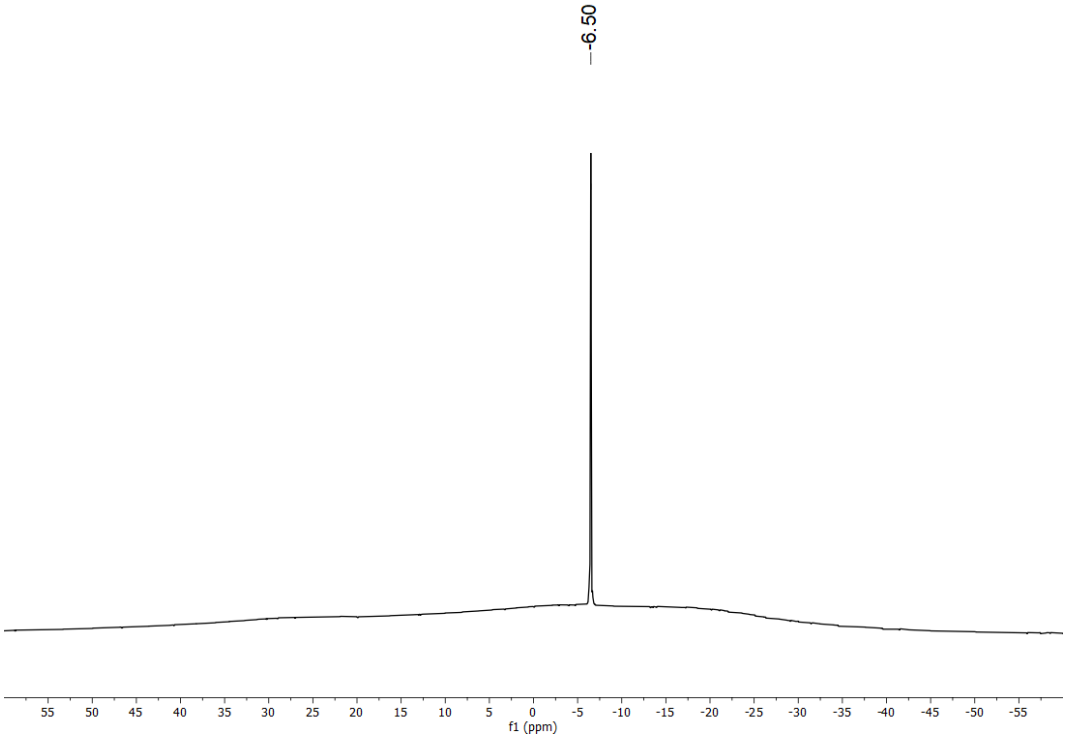


Figure S17. $^{11}B\{^{1}H\}$ NMR spectrum of [**3**][BArF] in THF-d_8 at 298 K.

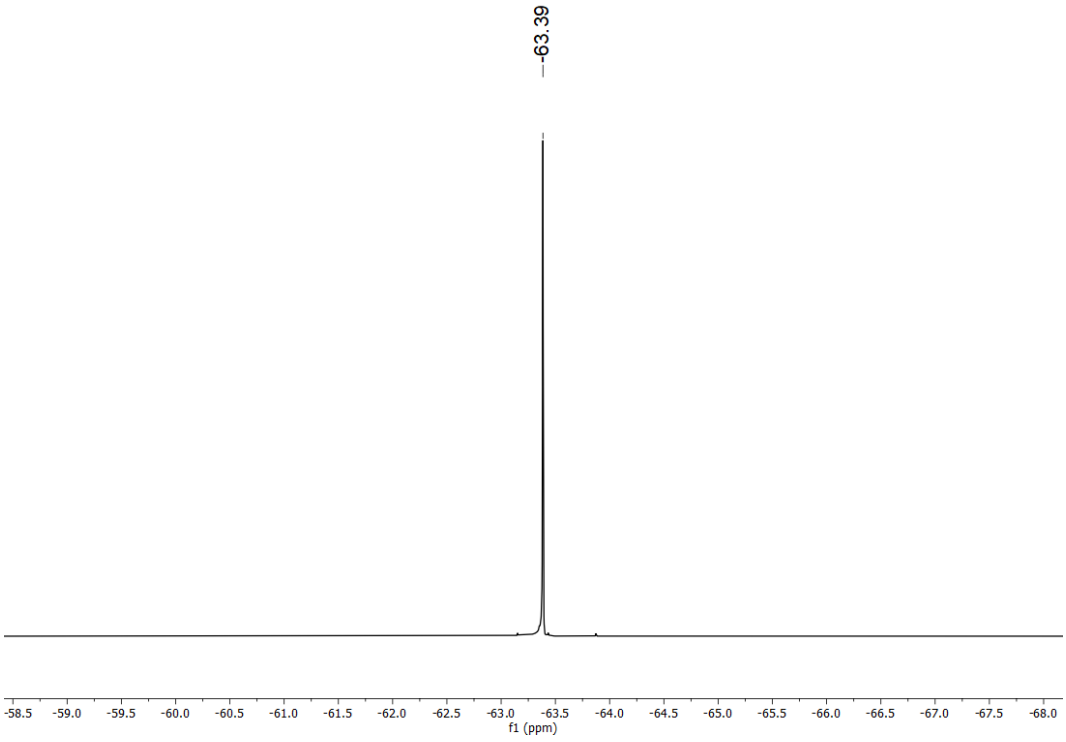


Figure S18. $^{19}F\{^{1}H\}$ NMR spectrum of [**3**][BArF] in THF-d_8 at 298 K.

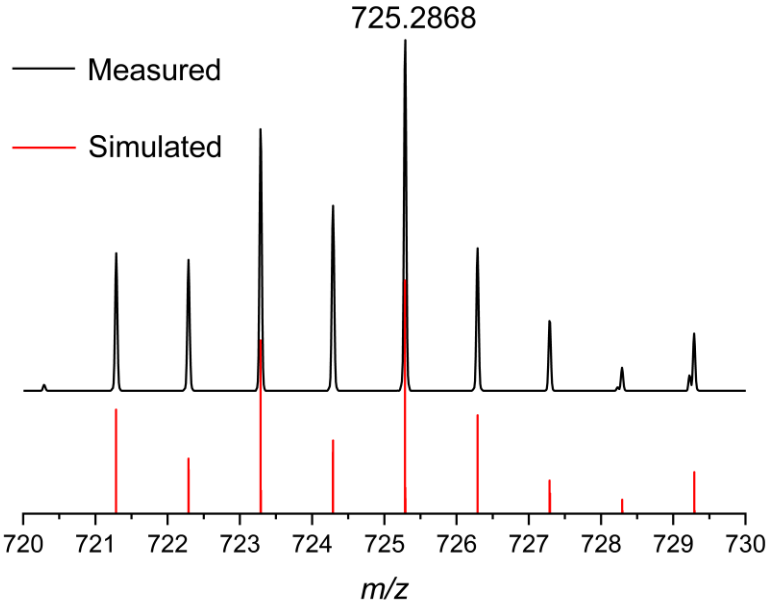
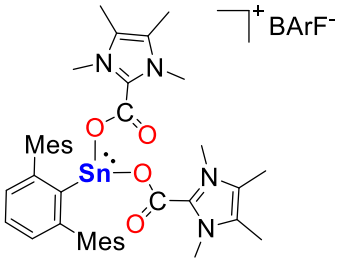


Figure S19. LIFDI-MS spectrum (detail view) of [**3**]$^+$ in [**3**][BArF] (measured spectrum: top; simulated spectrum: bottom).

1.4 Synthesis of [**4**][BArF]



1.4.1 NMR Reaction

[**2**][BArF] (16.2 µmol, 25.0 mg) was dissolved in THF-d_8 (0.4 mL) in a J-Young NMR tube. The solution was degassed using a freeze-pump-thaw cycle and then pressurized with 1 bar of CO_2 at room temperature. The reaction to form [**4**][BArF] was completed after 21 hours, as confirmed by ^{1}H, ^{13}C{^{1}H}, ^{119}Sn{^{1}H}, ^{11}B{^{1}H}, and ^{19}F{^{1}H} NMR spectroscopys.

1.4.2 Crystallisation of [**4**][BArF]

[**2**][BArF] (32.4 µmol, 50.0 mg) was dissolved in Et_2O (1 mL) and pentane (2 mL). The solution was degassed freeze-pump-thaw cycle, followed by the addition of 1 bar of CO_2 at room temperature. After stirring for 24 hours, the solution's color changed from colorless to light yellow. The reaction solution was then stored at −35 °C under the CO_2 atmosphere. After an additional 24 hours, light-yellow crystals suitable for single-crystal X-ray analysis were obtained.

*Note: It was not possible to obtain solid samples of pure [**4**][BArF] in large quantities due to decomposition when placed under vacuum.*

^{1}H NMR (400 MHz, 298 K, THF-d$_8$): δ[ppm] = 2.07 (s, 12 H, 2xC^{2,6}-C*H*$_3$, Mes), 2.11 (s, 6 H, 2xC^{4}-C*H*$_3$, Mes), 2.30 (s, 12 H, 4xC-C*H*$_3$, NHC), 3.92 (s, 12 H, 4xN-C*H*$_3$, NHC), 6.70 (s, 4 H, 2xC^{3,5}-*H*, Mes), 6.87 (d, $^{3}J_{H-H}$ = 8 Hz, 2 H, C^{3,5} -*H*, C$_6$H$_3$), 7.29 (t, $^{3}J_{H-H}$ = 8 Hz, 1 H, C^{4}-*H*, C$_6$H$_3$), 7.60, 7.81 (s, 12 H, 4x*C*^{2,4,6}, 4C$_6$H$_3$(CF$_3$)$_2$).

^{13}C{^{1}H} NMR (101 MHz, 298 K, THF-d$_8$): δ[ppm] = 8.36 (2xC^{4,5}-*C*H$_3$, NHC), 21.14 (C^{4}-*C*H$_3$, Mes), 21.88 (C^{2,6}-*C*H$_3$, Mes), 34.37 (4xN-*C*H$_3$, NHC), 118.27 (*p*-CH$_{B-Ar}$), 121.54, 124.24, 126.95 (*C*, BArF), 125.94 (*C*O$_2$ (aq)), 128.05 (4x*C*^{3,5}-H, Mes), 128.67 (*C*^{4}-H, C$_6$H$_3$), 129.04 (*C*^{3,5}-H, C$_6$H$_3$), 129.11 (*C*^{4,5}-CH$_3$, NHC), 129.65-130.59 (m-C$_{B-Ar}$), 135.68 (o-CH$_{B-Ar}$), 136.41 (2x*C*^{4}-Mes), 136.94 (N$_2$*C*, NHC), 137.77 (2x*C*^{1}-Mes), 141.74 (2xC^{2,6}-Mes), 149.45 (2x*C*^{2,6}-C$_6$H$_3$), 157.48 (C*C*O$_2$), 159.66-163.62 (ipso-CB-Ar), 172.98 (Sn-*C*, C$_6$H$_3$).

^{119}Sn{^{1}H} NMR (149 MHz, 298 K, THF-d$_8$): δ[ppm] = 46.41 (Sn).

^{11}B{^{1}H} NMR (128 MHz, 298 K, THF-d$_8$): δ[ppm] = −6.47 (B, BArF).

^{19}F{^{1}H} NMR (376 MHz, 298 K, THF-d$_8$): δ[ppm] = −63.36 (C*F*$_3$, BArF).

LIFDI-MS m/z C$_{40}$H$_{49}$N$_4$O$_4$Sn calcd: 769.2776; *m/z* found: 769.2777.

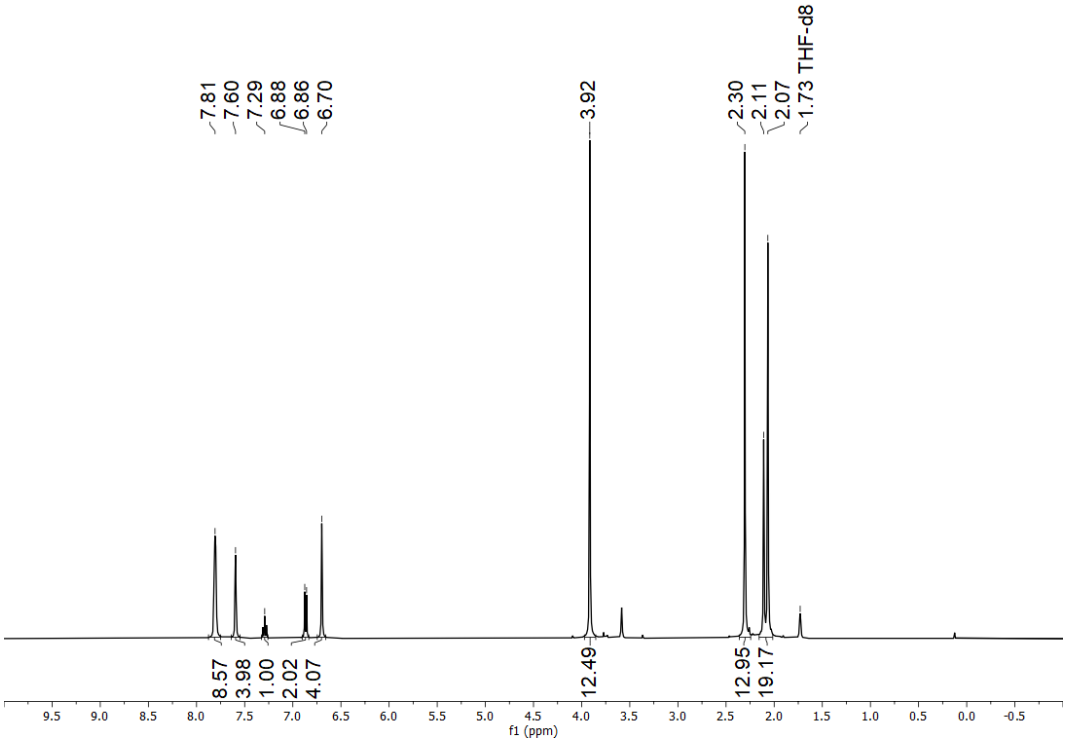


Figure S20. ^{1}H NMR spectrum of [**4**][BArF] in THF-d$_8$ at 298 K.

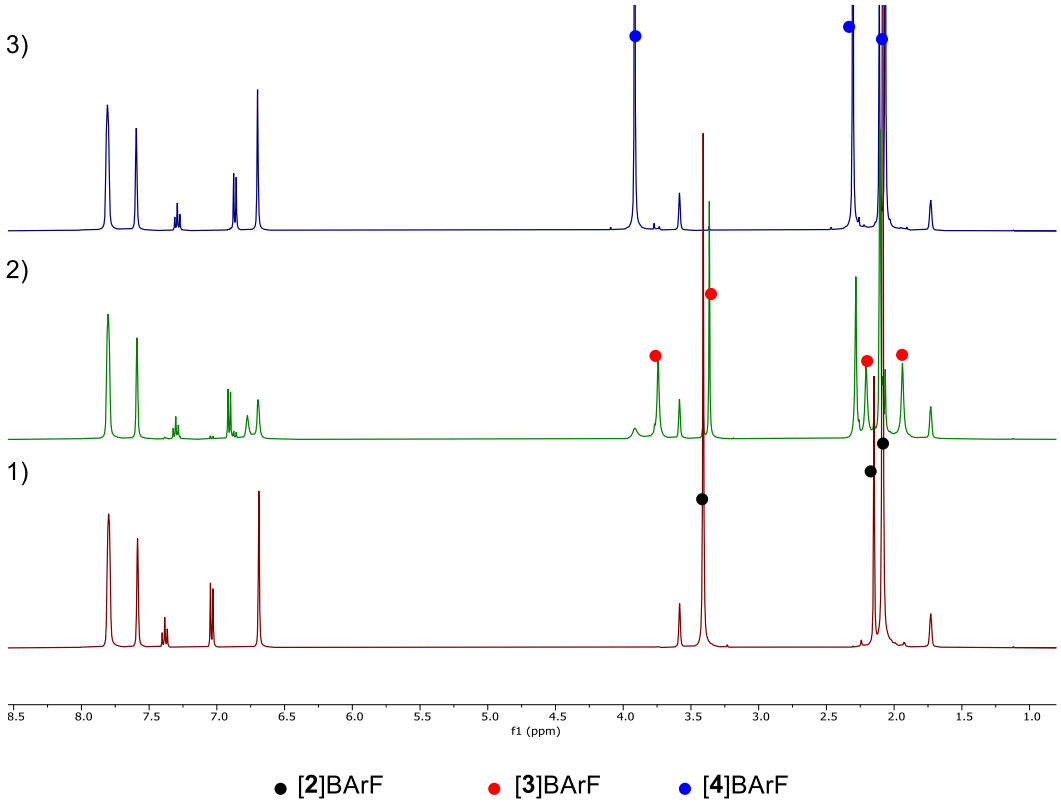


Figure S21. Stacked ^{1}H NMR spectra of the reaction of [**2**][BArF] with CO_2 (1 bar): 1) [**2**][BArF]; 2) [**2**][BArF] + CO_2, RT 6 hours; 3) [**2**][BArF] + CO_2, RT 21 hours.

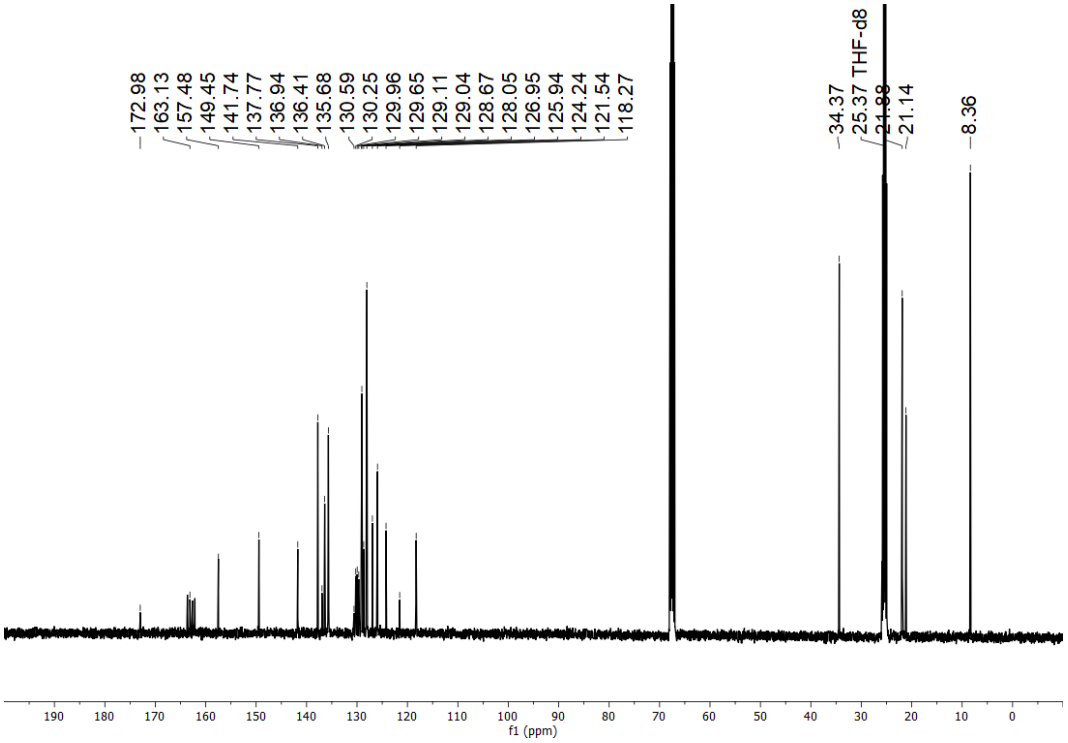


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of [**4**][BArF] in THF-d_8 at 298 K.

Figure S23. $^{1}H/^{13}C$ NMR HSQC spectrum of [**4**][BArF] in THF-d_8 at 298 K.

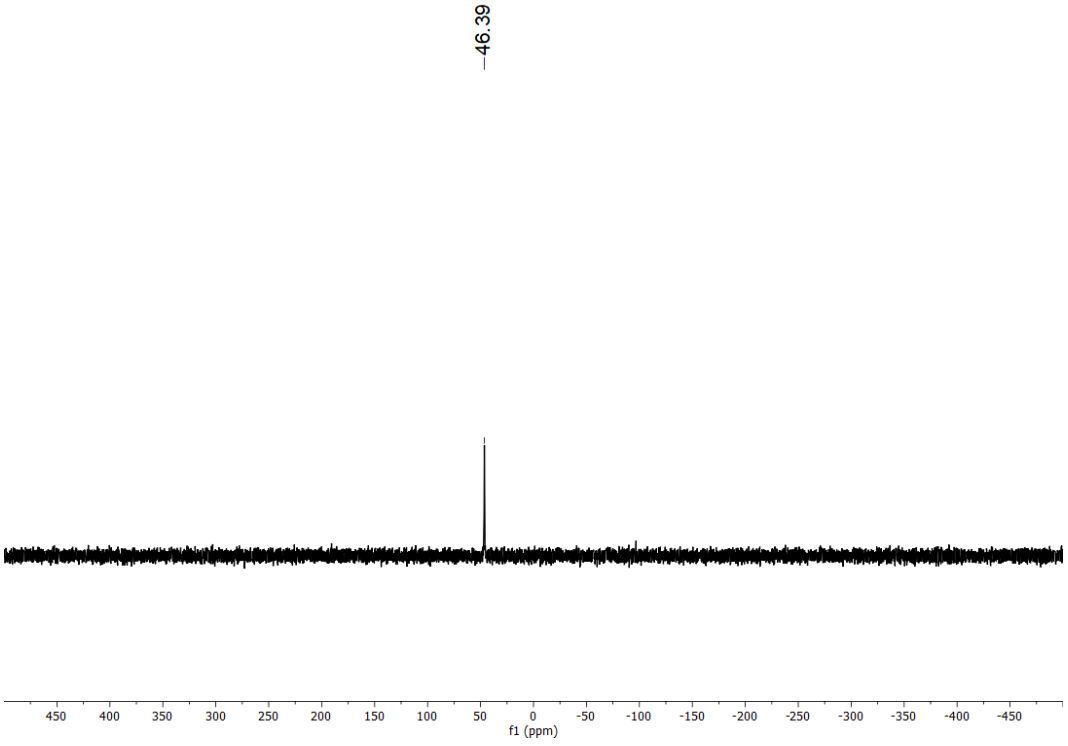


Figure S24. $^{119}Sn\{^{1}H\}$ NMR spectrum of [**4**][BArF] in THF-d_8 at 298 K.

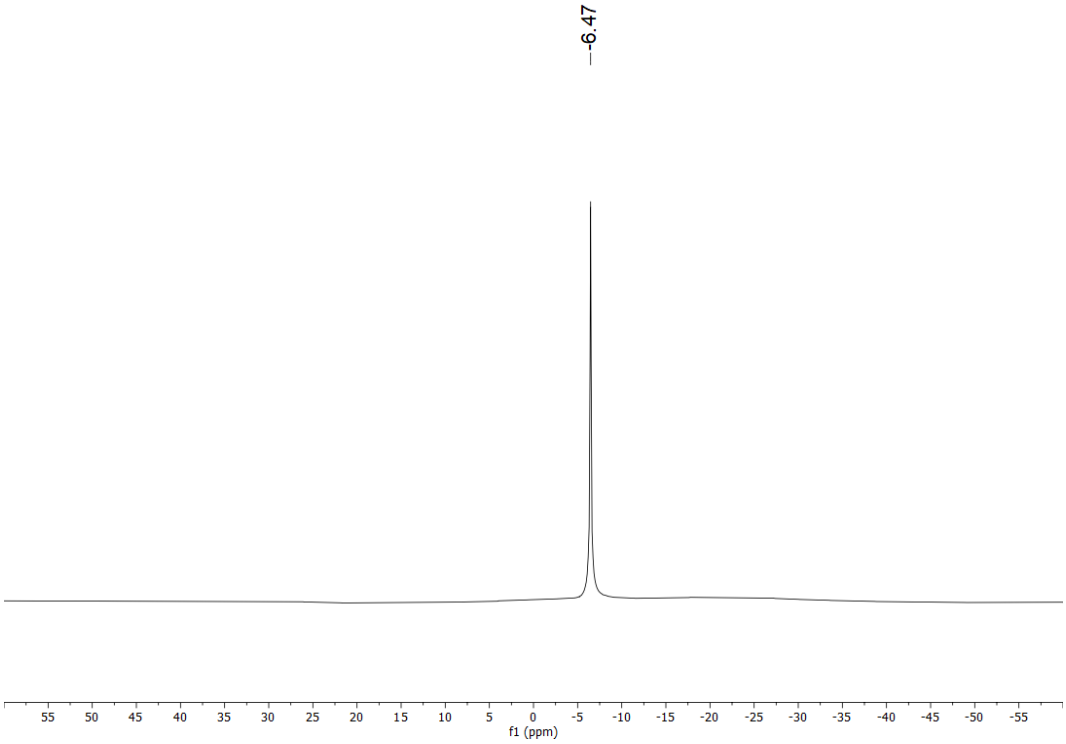


Figure S25. $^{11}B\{^{1}H\}$ NMR spectrum of [**4**][BArF] in THF-d_8 at 298 K.

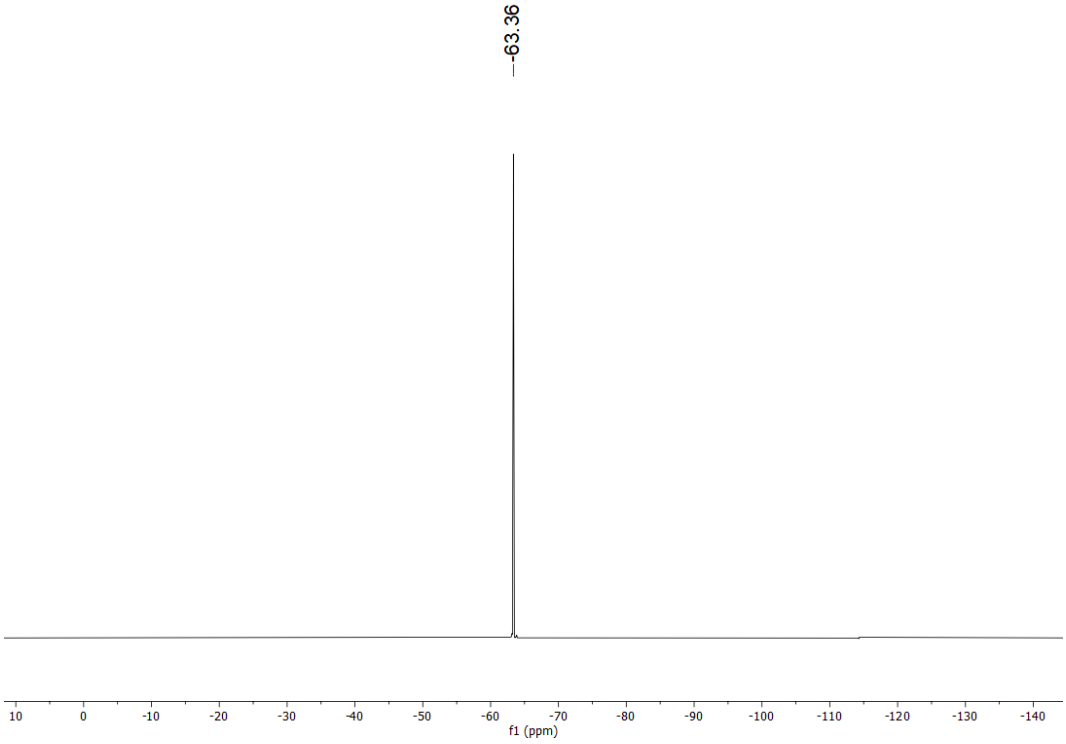


Figure S26. $^{19}F\{^{1}H\}$ NMR spectrum of [**4**][BArF] in THF-d_8 at 298 K.

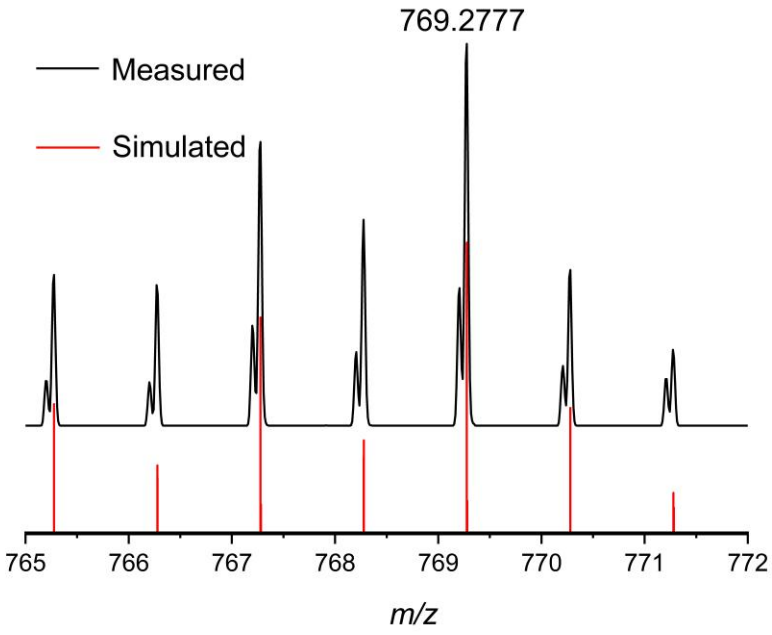


Figure S27. LIFDI-MS spectrum (detail view) of [**4**]$^+$ in [**4**][BArF] (measured spectrum: top; simulated spectrum: bottom).

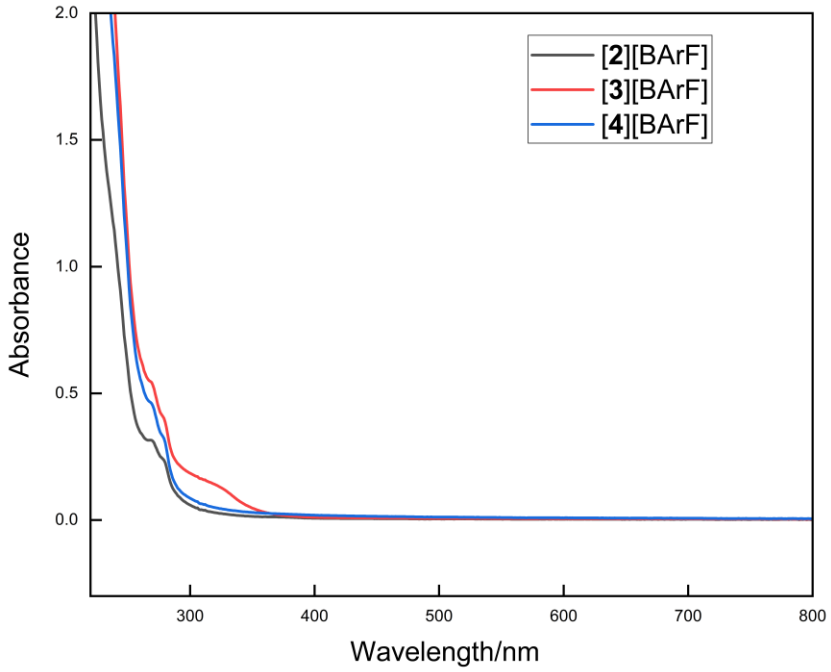
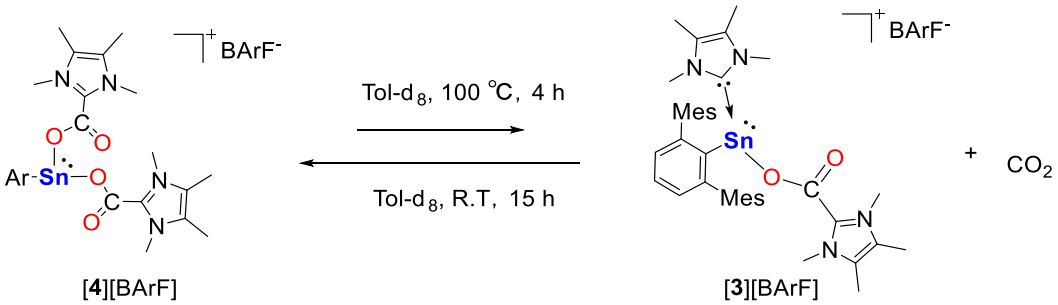


Figure S28. UV-vis spectrums of [**2**][BArF], [**3**][BArF], and [**4**][BArF] (r.t., THF, concentration: 3.125×10^{-5} M). No abstraction signal is observed in the UV spectra of [**2**][BArF], [**3**][BArF], and [**4**][BArF].

1.5 NMR Experiments

1.5.1 The thermal stability of [**4**][BArF]



To test the reversibility of [**4**][BArF], a solution of [**4**][BArF] in toluene-d_8 (0.2 mL) and fluorobenzene (0.2 mL) was heated to 100 °C under CO_2 or argon atmosphere in a J-Young NMR tube and monitored by ^{1}H NMR.

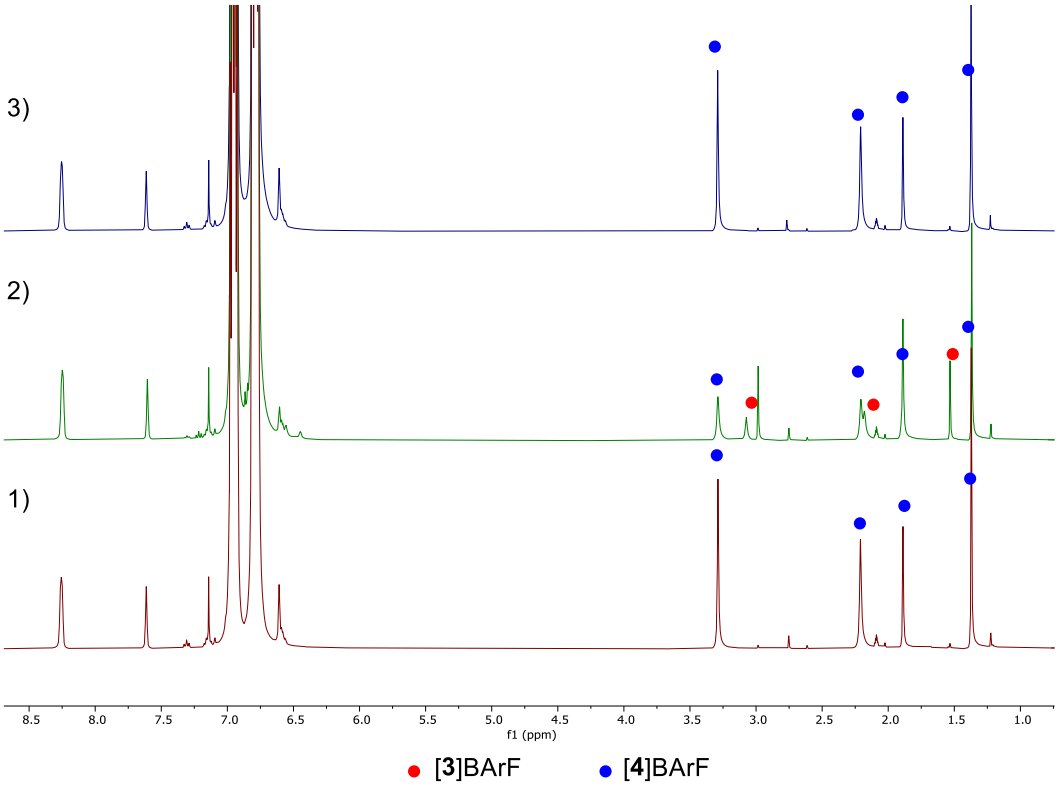


Figure S29. Stacked ^{1}H NMR spectra showing reversibility of [**4**][BArF] under CO_2 atmosphere. 1) [**4**][BArF]; 2) [**4**][BArF] heating 4 hours at 100 ^{o}C; 3) cool to rt for 15 hours.

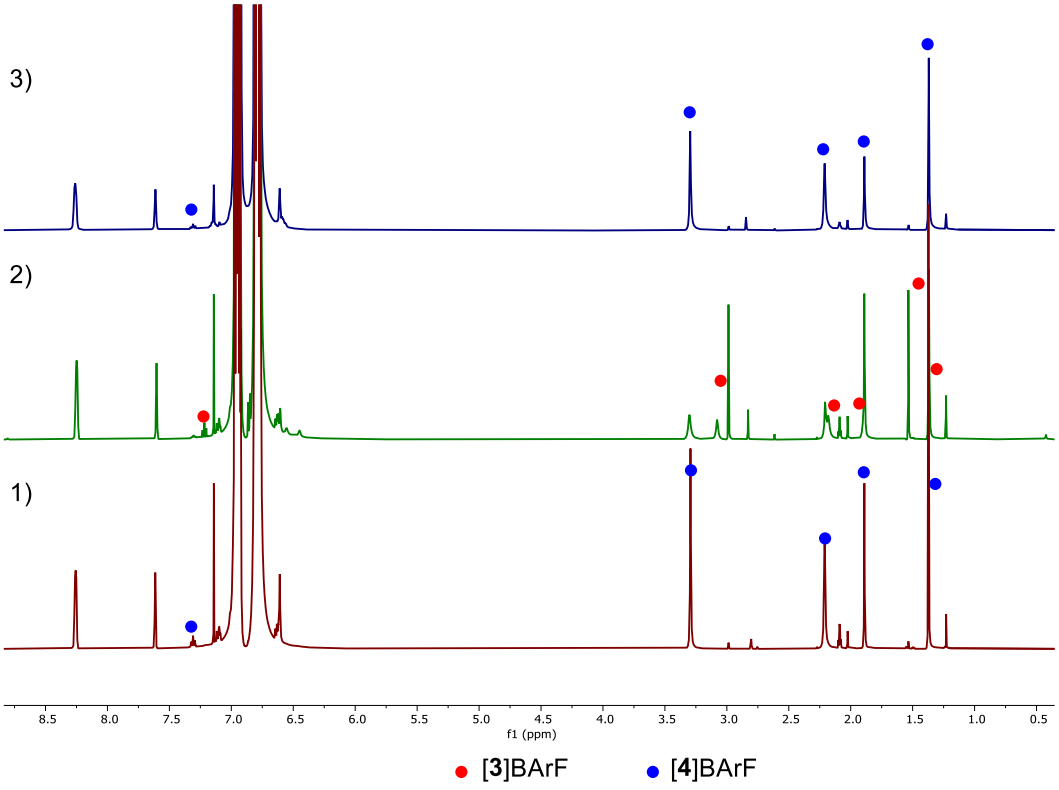


Figure S30. Stacked ^{1}H NMR spectra showing reversibility of [**4**][BArF] under argon atmosphere. 1) [**4**][BArF]; 2) [**4**][BArF] heating 4 hours at 100 °C; 3) cool to room temperature for 15 hours.

1.5.2 [**4**][BarF] reaction with Ph_2SiH_2

[**2**][BArF] (1.00 eq, 16.2 µmol, 25.0 mg) was dissolved in C_6D_6 (0.2 mL) and fluorobenzene (0.2 mL) in a J-Young NMR tube. The solution was then freeze-pump-thaw degassed and was then pressurised with 1 bar of CO_2 at room temperature. After 21 hours (when [**4**][BArF] was completely formed) the excess CO_2 was removed and H_2SiPh_2 (1.00 eq, 16.2 µmol, 2.43 µL) was added. The reaction progress was monitored by ^{1}H NMR spectroscopy.

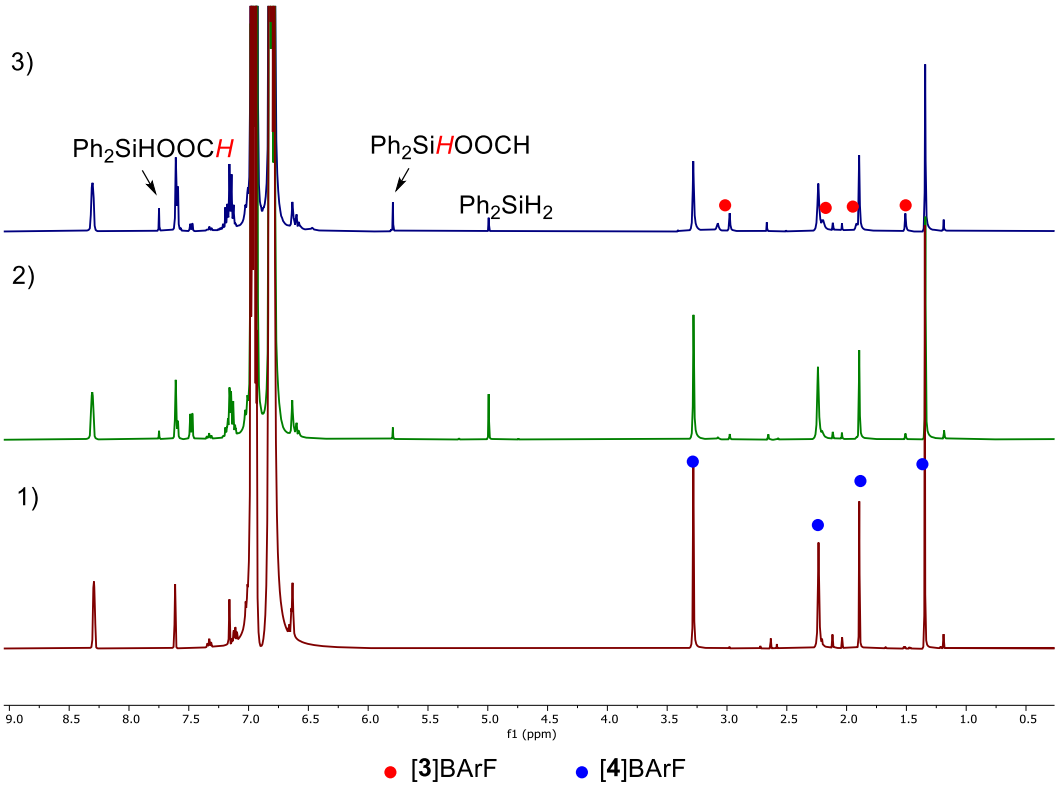


Figure S31. Stackthe^{1}H NMR spectra showing [**4**][BArF] reaction with Ph_2SiH_2: 1) the formation of [**4**][BArF]; 2) [**4**][BArF] + H_2SiPh_2, RT 1 hour; 3) [**4**][BArF] + H_2SiPh_2, RT 5 hours.

1.6 Catalytic Experiments

General Procedure for Hydrosilylation of CO_2: Silane (80.0 µmol, 14.9 µL), 1,3,5-trimethoxybenzene (0.10 eq of the silane, as an internal standard),* and catalyst were dissolved in a mixture of C_6D_6/C_6H_5F in a J-Young NMR tube under an argon atmosphere. An initial ^{1}H NMR spectrum was measured to determine the concentration of silane (by comparison to the internal standard). Subsequently, the solution was rapidly degassed using a Schlenk line and then refilled with 1 bar of CO_2. The progression of reaction was monitored via ^{1}H NMR spectroscopy by the consumption of silane alongside the

emergence of the respective hydrosilylation products resonances. After 25 hours, the conversion of silane was determined by comparing integrals of the unreacted silane resonances to the integrals of the internal standard. The yield was determined by comparing integrals of the $R_2Si\mathbf{H}(OCHO)$ or $R_3Si(OC\mathbf{H}O)$ resonances of the hydrosilylation product to the integral of the internal standard. The summary of the results was shown in **Table S1**.

* = 1,3,5-trimethoxybenzene was seleted as the internal standard, setting its concentration to 10 mol% of the added silane. This equivalent exhibits a strong signal-to-noise ratio, and the signal of internal standard is comparable to that of silane.

Mercury Test Experiment

[**2**][BArF] (5 mol%, 4.00 µmol, 80.0 µL, 0.05 M in C_6H_5F), H_2SiPh_2 (80.0 µmol, 14.9 µL), and 1,3,5-trimethoxybenzene (0.10 eq of the Ph_2SiH_2) as an internal standard were dissolved in C_6D_6 (0.32 mL) in a J-Young NMR tube. Then mercury (13.5 mg) was added to the solution. The solution was rapidly degassed using a Schlenk line and then refilled with 1 bar of CO_2 at room temperature. The progression of reaction was monitored via ^1H NMR spectroscopy. The results are shown in Table S1 (Entry 11).

Catalytic reduction of CO_2 with Ph_2SiH_2 by [4][BArF]

[**2**][BArF] (5 mol%, 4.00 µmol, 80.0 µL, 0.05 M in C_6H_5F) and 1,3,5-trimethoxybenzene (0.10 eq, 8.0 µmol) were introduced into 0.32 mL of C_6D_6 within a J-Young NMR tube. The solution was degassed and refilled with 1 bar of CO_2 at room temperature. The solution of [**4**][BArF] was obtained after 21 hours and excess CO_2 was removed, then H_2SiPh_2 (1.0 eq, 80.0 µmol, 14.9 µL) was added in gloves box. The solution was degassed again and then pressurised with 1 bar of CO_2 at room temperature. The reaction was monitored via ^1H NMR spectroscopy.

Table S1. Hydrosilylation of CO_2

Entry	Catalysis (mol%)	Solvent	T /°C	Silane	Conversion/% (time)	NMR Yield/% [$R_3Si(OCHO)$]	TOF /h^{-1}	^1H NMR Number
1	[**2**][BArF] (0.5)	C_6D_6:C_6H_5F (4:1)	25	H_2SiPh_2	4	<1	0.35	Figure S32
2	[**2**][BArF] (1)	C_6D_6:C_6H_5F (4:1)	25	H_2SiPh_2	11	4	0.45	Figure S33
3	[**2**][BArF] (2.5)	C_6D_6:C_6H_5F (4:1)	25	H_2SiPh_2	74	63	1.18	Figure S34
4	[**2**][BArF] (5)	C_6D_6:C_6H_5F (4:1)	25	H_2SiPh_2	94	81	0.75	Figure S35
5	[**2**][BArF] (5)	C_6D_6	25	H_2SiPh_2	78	71	0.62	Figure S36
6	[**2**][BArF] (5)	THF-d_8	25	H_2SiPh_2	75	54	0.60	Figure S37
7	[**2**][BArF] (5)	C_6D_6:$C_6H_4F_2$ (4:1)	25	H_2SiPh_2	97	77	0.77	Figure S38
8	[**2**][BArF] (5)	C_6D_6:$C_6H_4F_2$ (1:1)	25	H_2SiPh_2	94	81	0.75	Figure S39
9	[**2**][BArF] (5)	C_6D_6:C_6H_5F (4:1)	50	H_2SiPh_2	64 (2 hours)	64	0.79	Figure S40
10	[**2**][$Al(OC(CF_3)_3)_4$] (5)	C_6D_6:C_6H_5F (4:1)	25	H_2SiPh_2	70	60	0.56	Figure S41
11	[**2**][BArF] (5)+Hg	C_6D_6:C_6H_5F (4:1)	25	H_2SiPh_2	89	69	0.71	Figure S42
12	[**3**][BArF] (5)	C_6D_6:C_6H_5F (4:1)	25	H_2SiPh_2	92	83	0.74	Figure S43
13	[**4**][BArF] (5)	C_6D_6:C_6H_5F (4:1)	25	H_2SiPh_2	93	93	0.74	Figure S44
14	IMe_4 (10)	C_6D_6:C_6H_5F (4:1)	25	H_2SiPh_2	51	< 1	0.39	Figure S45
15	IMe_4-CO_2 (10)	C_6D_6:$C_6H_4F_2$ (1:1)	25	H_2SiPh_2	51	9	0.41	Figure S46
16	[**2**][BArF] (5)	C_6D_6:C_6H_5F (4:1)	25	Me_2PhSiH	47	46	0.37	Figure S47
17	[**2**][BArF] (5)	C_6D_6:C_6H_5F (4:1)	25	H_3SiPh	48 (2 hours) 71 (12 hours)	39 <1	4.8 1.18	Figure S48

18	[**2**][BArF] (5)	C_6D_6:C_6H_5F (4:1)	60	$HSiEt_3$	29	27	0.23	Figure S49
19	[**2**][BArF] (5)	C_6D_6:C_6H_5F (4:1)	80	$HSiPh_3$	No reaction	-	-	Figure S50

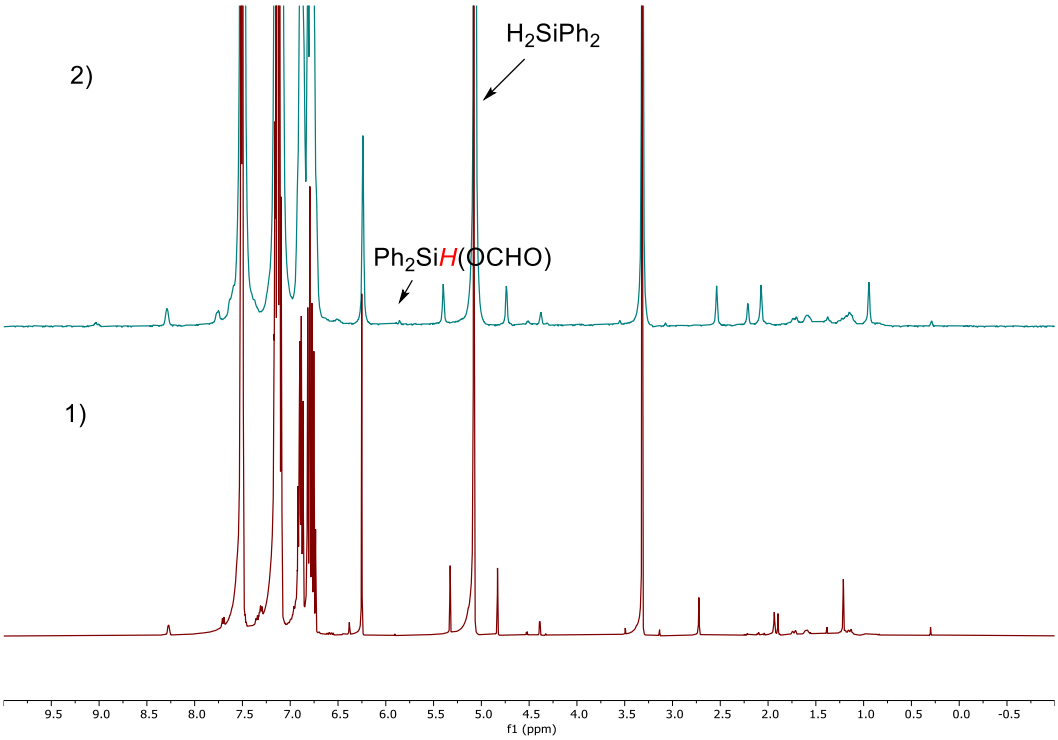


Figure S32. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by [**2**][BArF] (0.5 mol%) in C_6D_6/C_6H_5F (4:1): 1) [**2**][BArF] (0.5 mol%) + H_2SiPh_2; 2) [**2**][BArF] (0.5 mol%) + H_2SiPh_2 + CO_2, RT 25 hours.

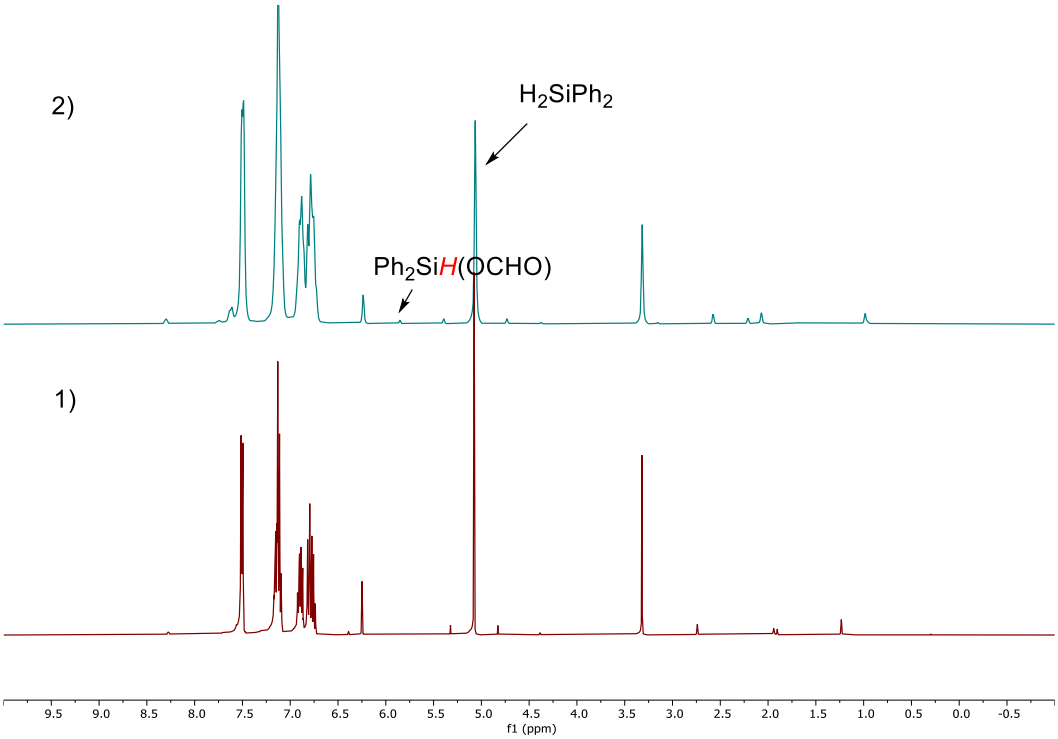


Figure S33. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by [**2**][BArF] (1 mol%) in C_6D_6/C_6H_5F (4:1): 1) [**2**][BArF] (1 mol%) + H_2SiPh_2; 2) [**2**][BArF] (1 mol%) + H_2SiPh_2 + CO_2, RT 25 hours.

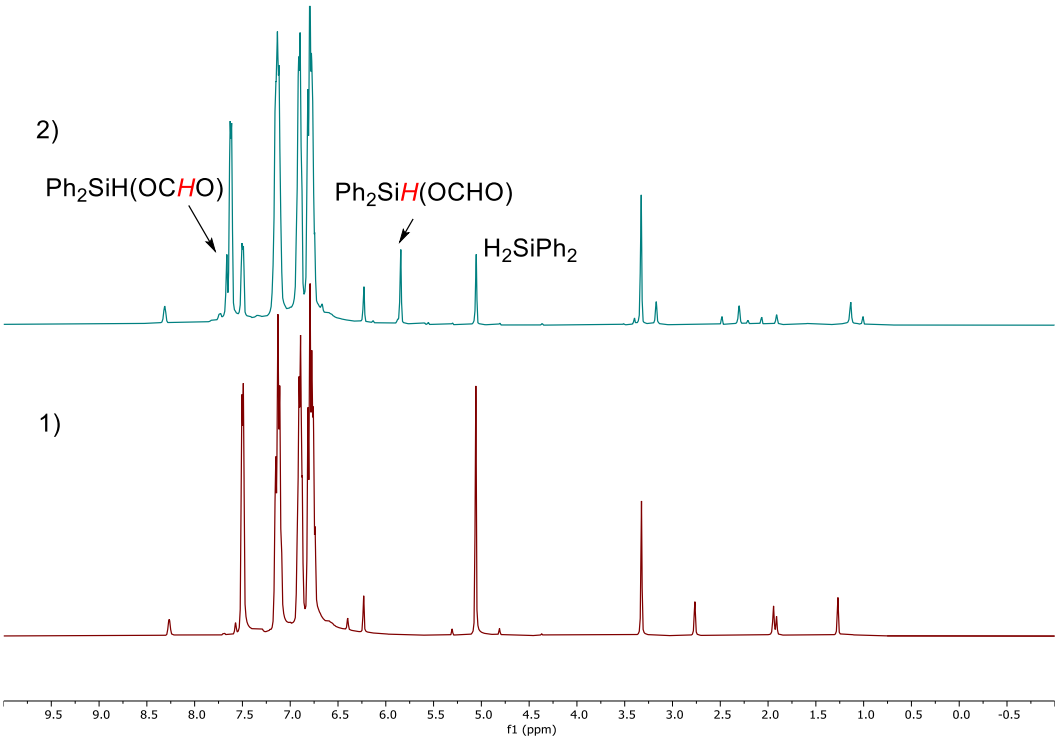


Figure S34. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by [**2**][BArF] (2.5 mol%) in C_6D_6/C_6H_5F (4:1): 1) [**2**][BArF] (2.5 mol%) + H_2SiPh_2; 2) [**2**][BArF] (2.5 mol%) + H_2SiPh_2 + CO_2, RT 25 hours.

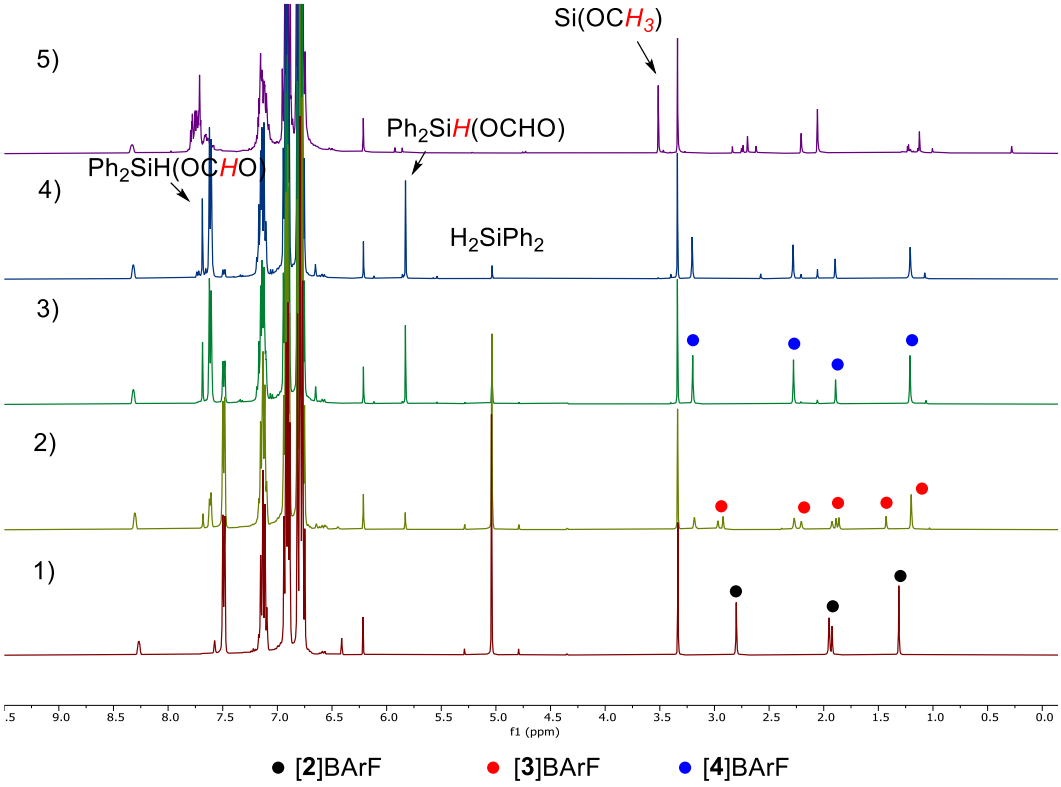


Figure S35. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by [**2**][BArF]: 1) [**2**][BArF](5 mol%) + H_2SiPh_2; 2) [**2**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, RT 2 hours; 3) [**2**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, RT 12 hours; 4) [**2**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, RT 25 hours; [**2**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, RT 72 hours.

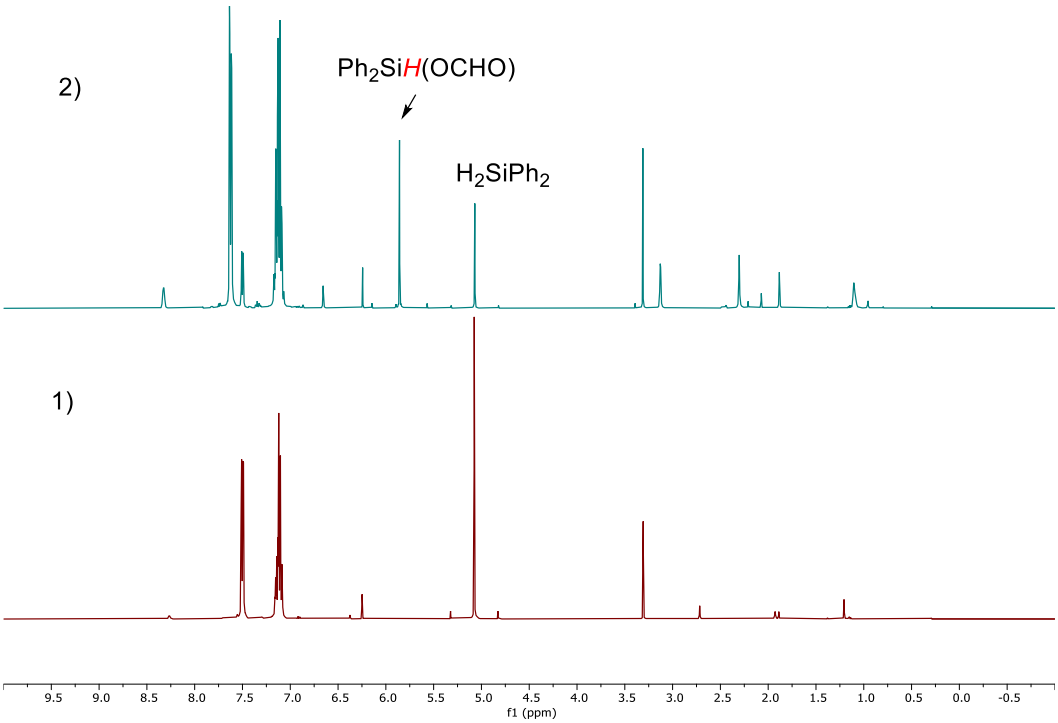


Figure S36. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by [**2**][BArF] in C_6D_6: 1) [**2**][BArF] (5 mol%) + H_2SiPh_2; 2) [**2**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, RT 25 hours.

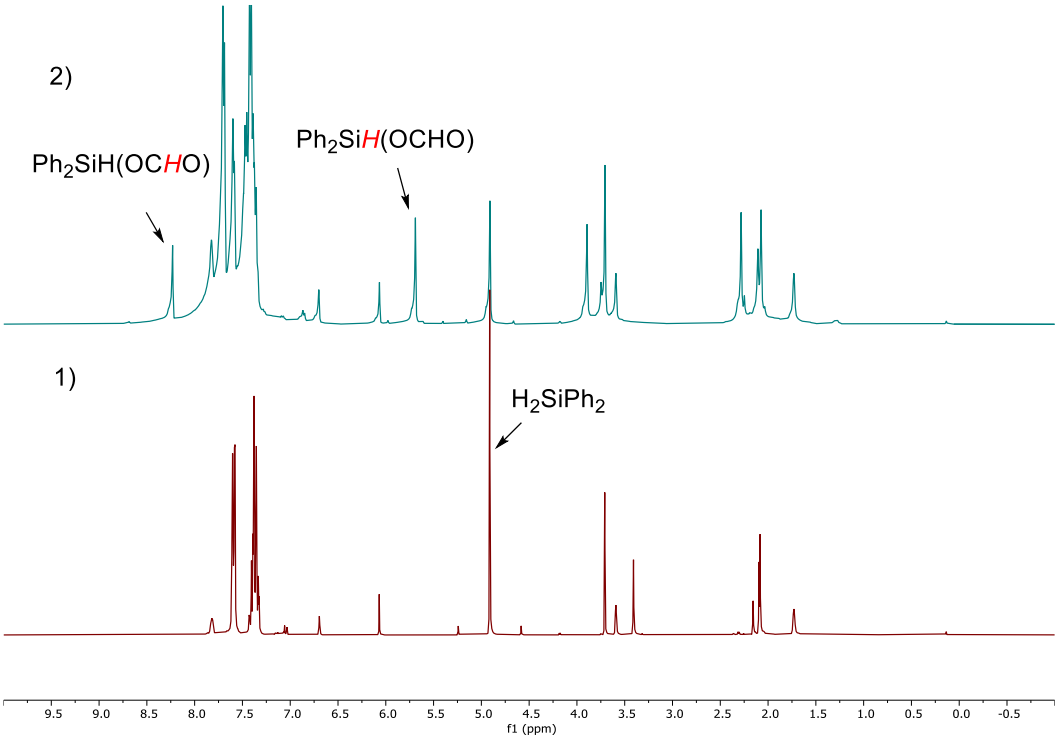


Figure S37. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by [**2**][BArF] in THF-d_8: 1) [**2**][BArF] (5 mol%) + H_2SiPh_2; 2) [**2**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, RT 25 hours.

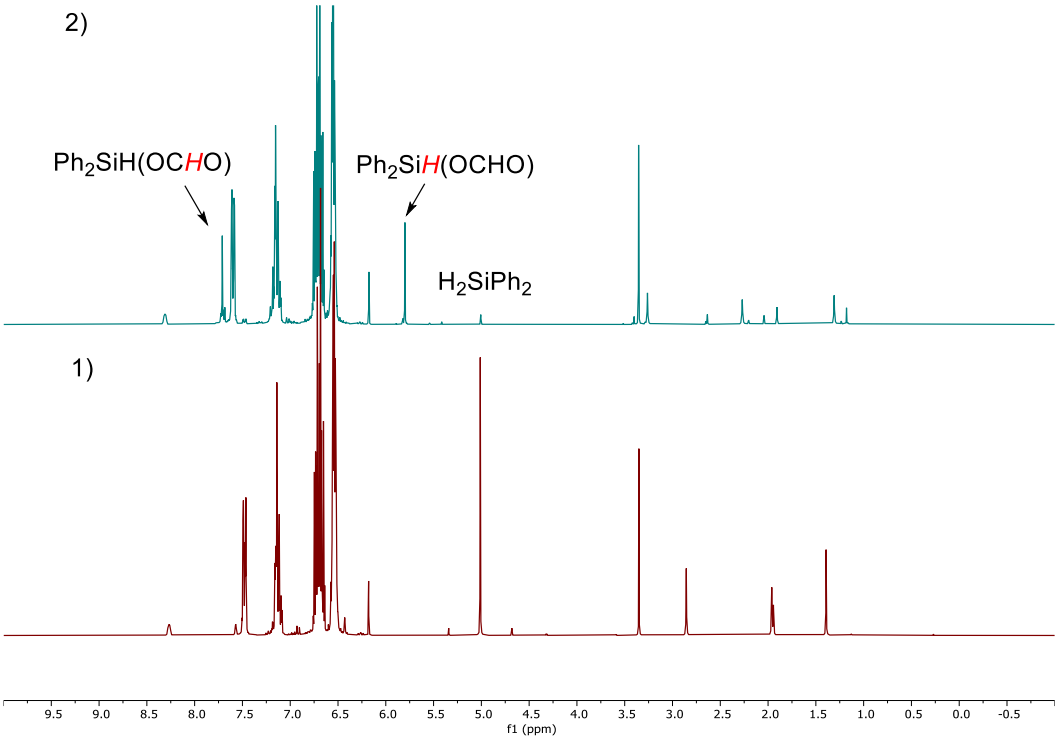


Figure S38. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by [**2**][BArF] in $C_6D_6/C_6H_4F_2$ (4:1): 1) [**2**][BArF] (5 mol%) + H_2SiPh_2; 2) [**2**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, RT 25 hours.

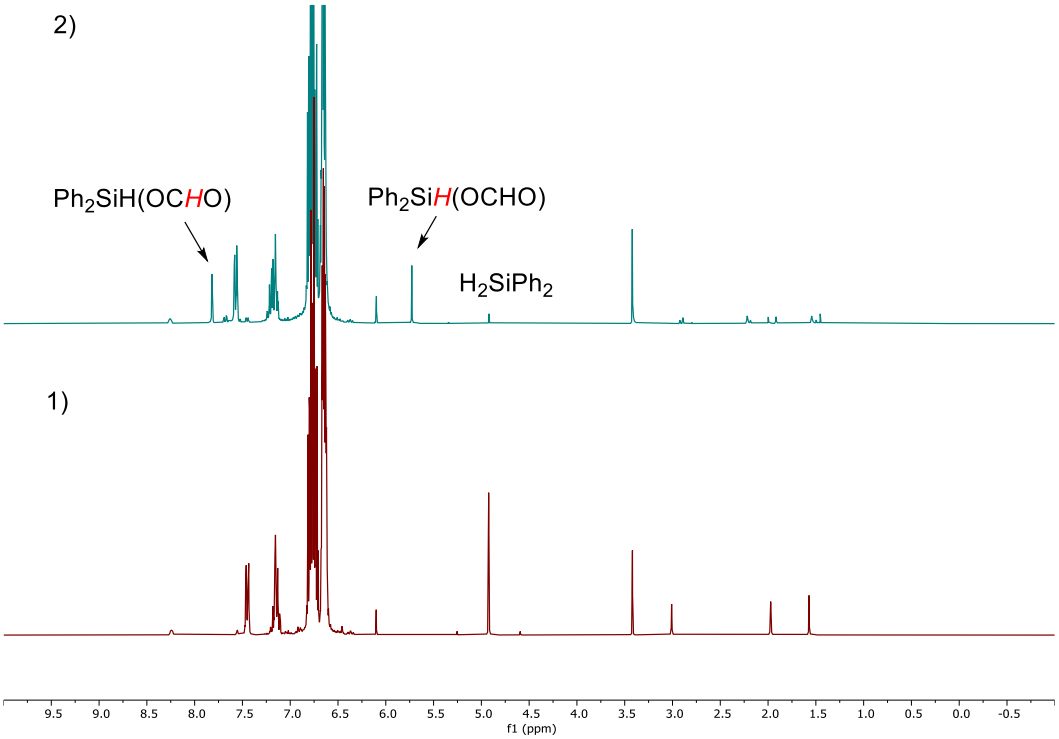


Figure S39. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by [**2**][BArF] in $C_6D_6/C_6H_4F_2$ (1:1): 1) [**2**][BArF] (5 mol%) + H_2SiPh_2; 2) [**2**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, RT 25 hours.

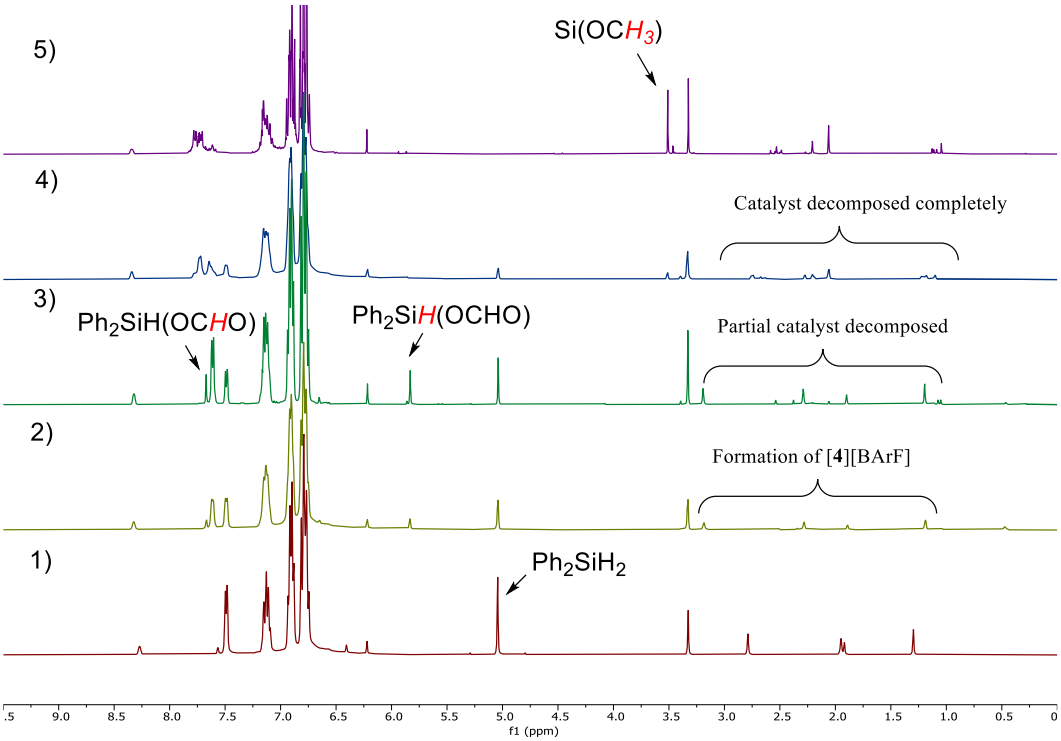


Figure S40. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by [**2**][BArF] in C_6D_6/C_6H_5F (4:1) at 50 ^{o}C: 1) [**2**][BArF] (5 mol%) + H_2SiPh_2; 2) [**2**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, 50 $^{\circ}$C 1 hour; 3) [**2**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, 50 $^{\circ}$C 2 hours; 4) [**2**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, 50 $^{\circ}$C 7 hours; 5) [**2**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, 50 $^{\circ}$C 25 hours.

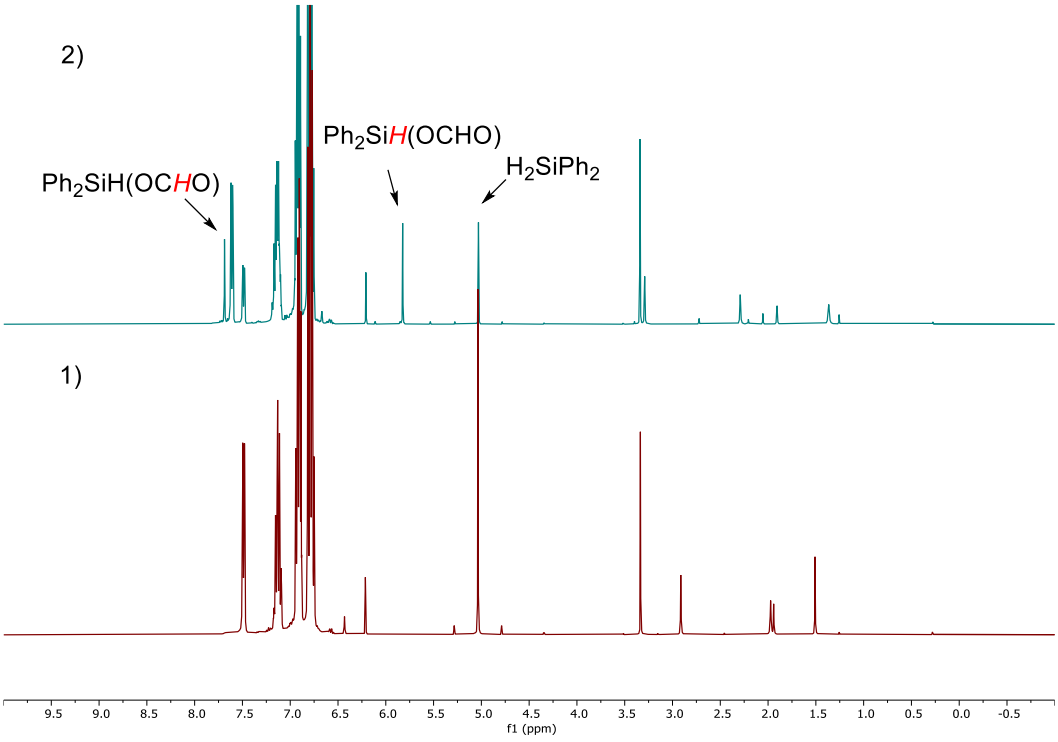


Figure S41 Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by [**2**][Al(OC(CF$_3$)$_3$)$_4$] in C_6D_6/C_6H_5F (4:1): 1) [**2**][Al(OC(CF$_3$)$_3$)$_4$] (5 mol%); 2) [**2**][Al(OC(CF$_3$)$_3$)$_4$] (5 mol%) + H_2SiPh_2 + CO_2, RT 25 hours.

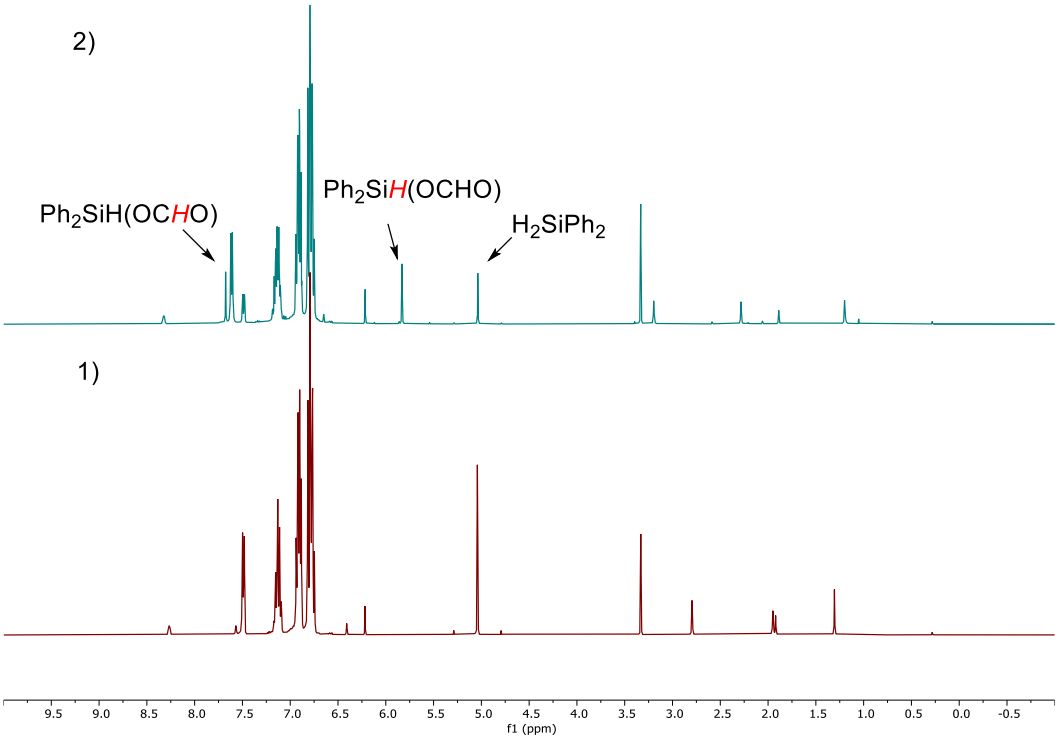


Figure S42. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by [**2**][BArF] in C_6D_6/C_6H_5F (4:1) in the presence of Hg: 1) [**2**][BArF] (5 mol%) + H_2SiPh_2; 2) [**2**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, RT 25 hours.

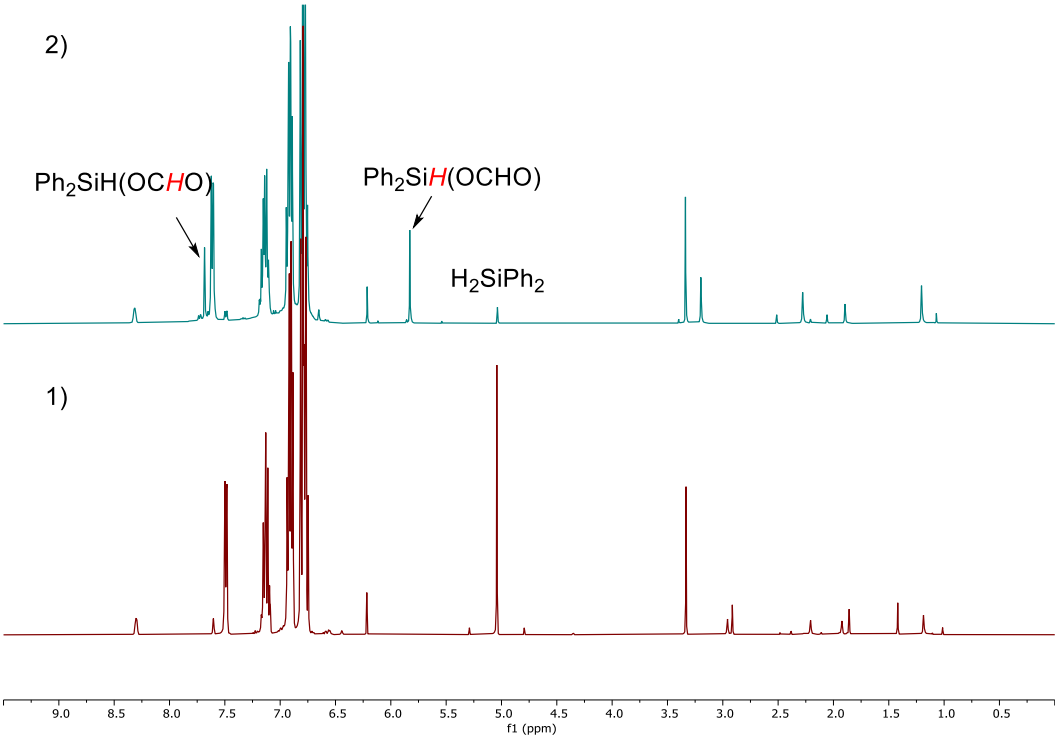


Figure S43. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by [**3**][BArF]: 1) [**3**][BArF] (5 mol%) + H_2SiPh_2; 2) [**3**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, RT 25 hours.

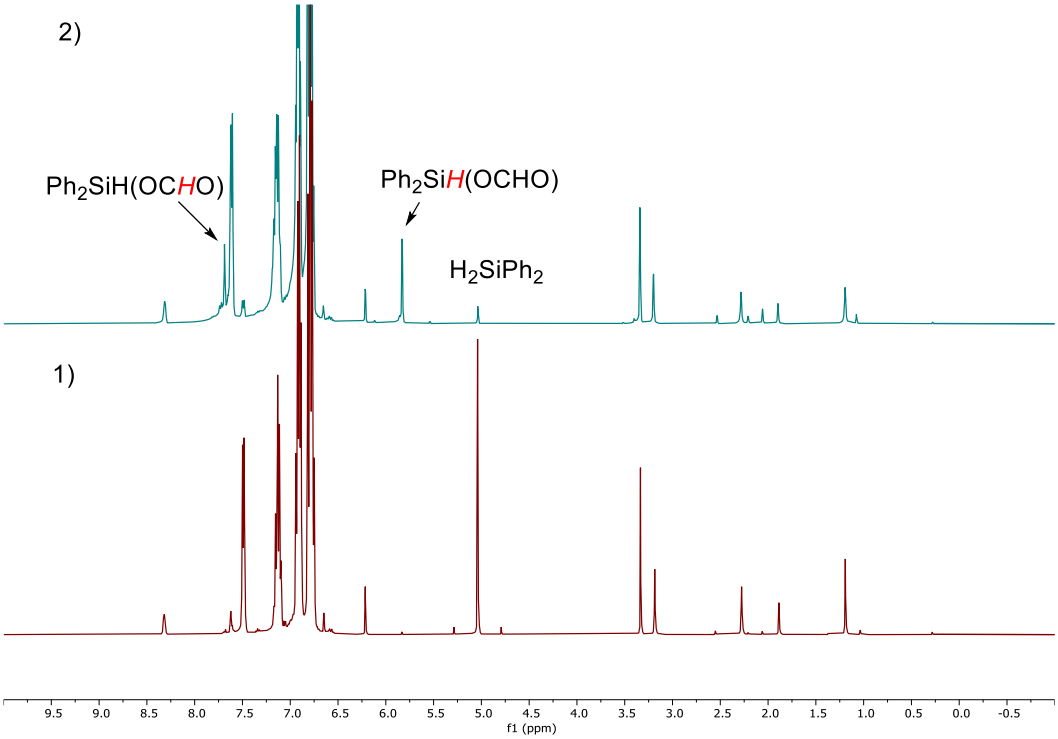


Figure S44. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by [**4**][BArF]: 1) [**4**][BArF] (5 mol%) + H_2SiPh_2; 2) [**4**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, RT 25 hours.

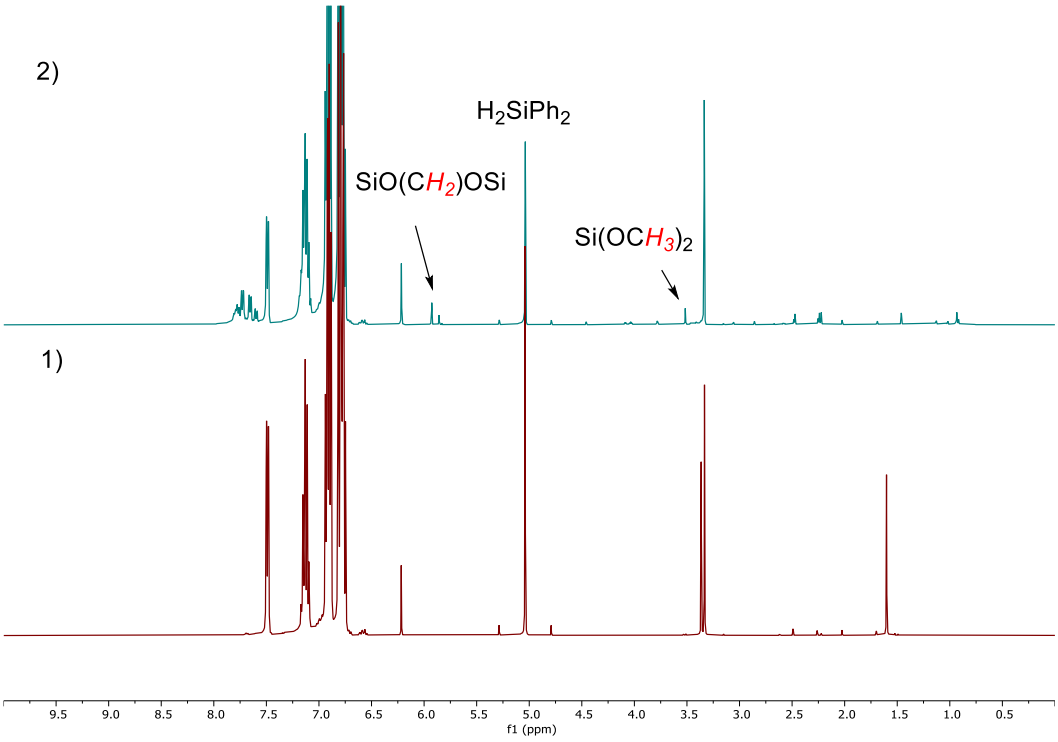


Figure S45. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by IMe_4: 1) IMe_4 (10 mol%) + H_2SiPh_2; 2) IMe_4 + H_2SiPh_2 + CO_2, after 25 hours.

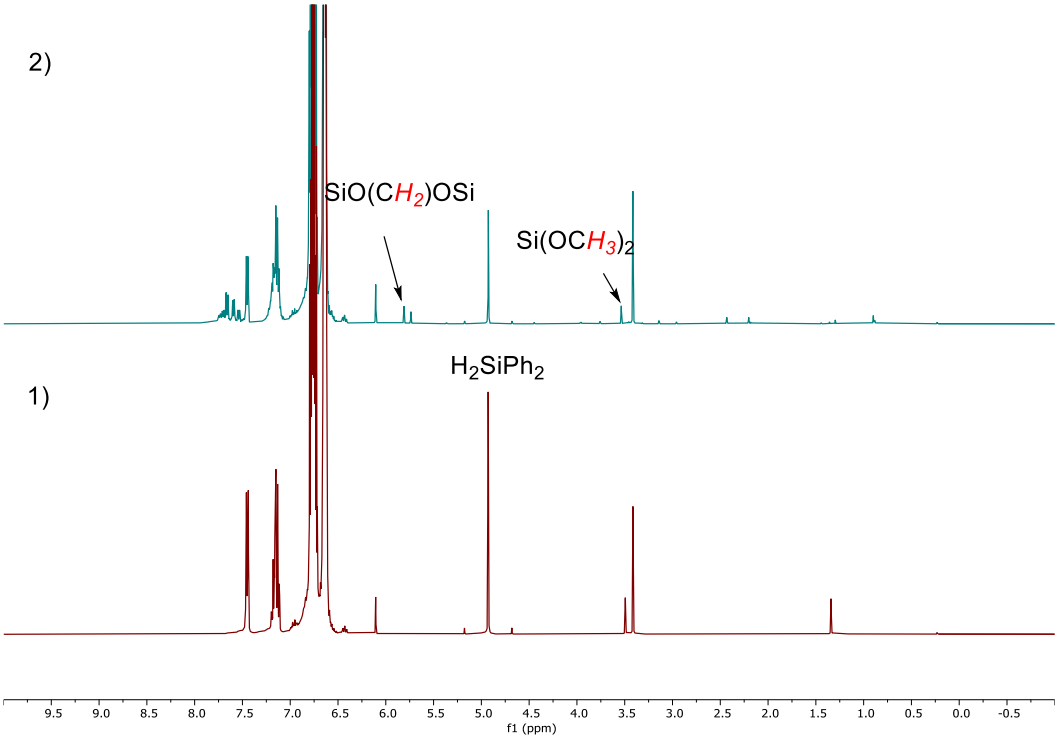


Figure S46. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_2SiPh_2 by IMe_4-CO_2: 1) IMe_4-CO_2 (10 mol%) + H_2SiPh_2; 2) IMe_4-CO_2 + H_2SiPh_2 + CO_2, RT 25 hours.

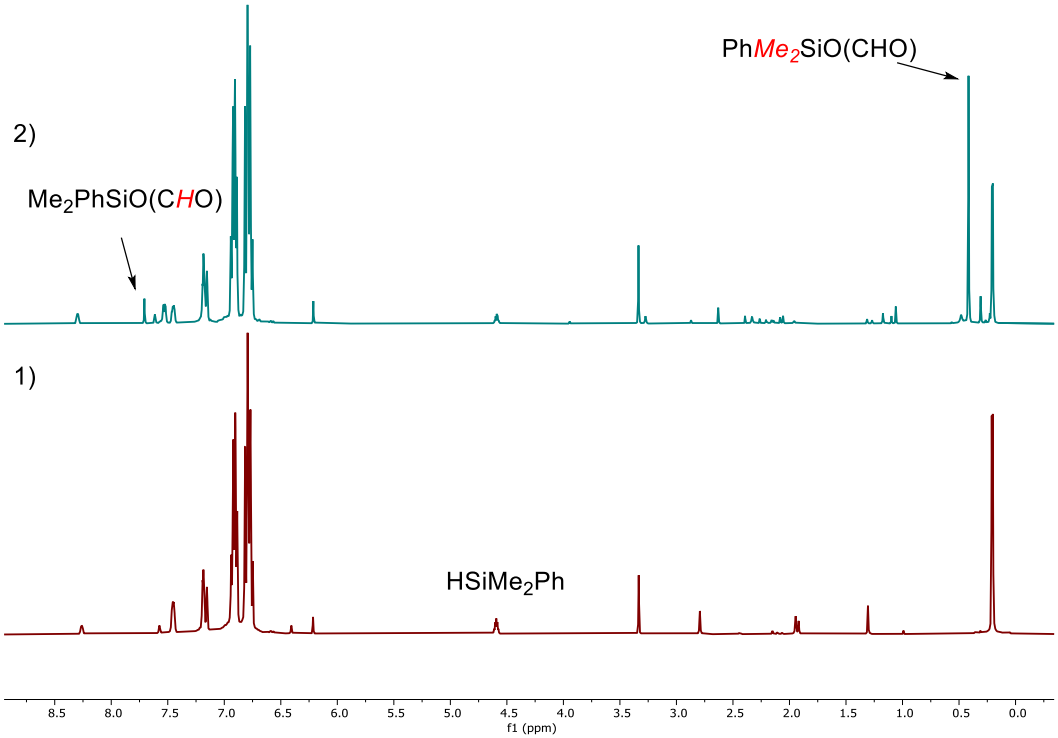


Figure S47. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with $HSiMe_2Ph$ by [**2**][BArF]: 1) [**2**][BArF] (5 mol%) + $HSiMe_2Ph$; 2) [**2**][BArF] (5 mol%) + $HSiMe_2Ph$ + CO_2, RT 25 hours.

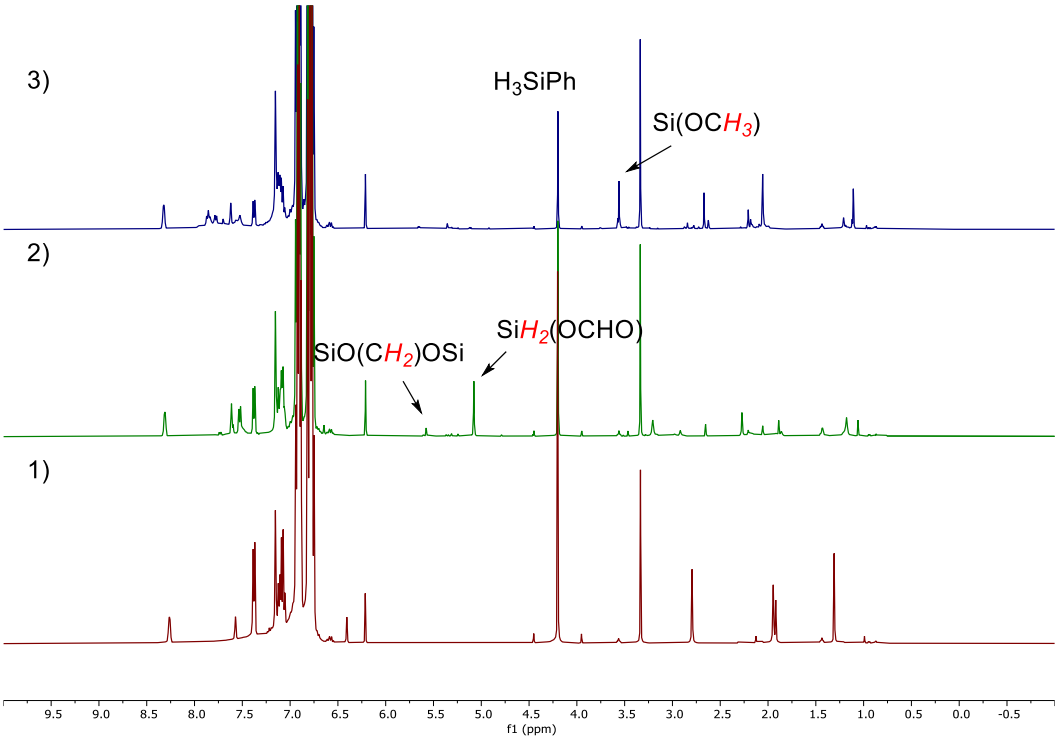


Figure S48. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with H_3SiPh by [**2**][BArF]: 1) [**2**][BArF] (5 mol%) + H_3SiPh; 2) [**2**][BArF] (5 mol%) + H_3SiPh + CO_2, RT 2 hours; [**2**][BArF] (5 mol%) + H_3SiPh + CO_2, RT 12 hours.

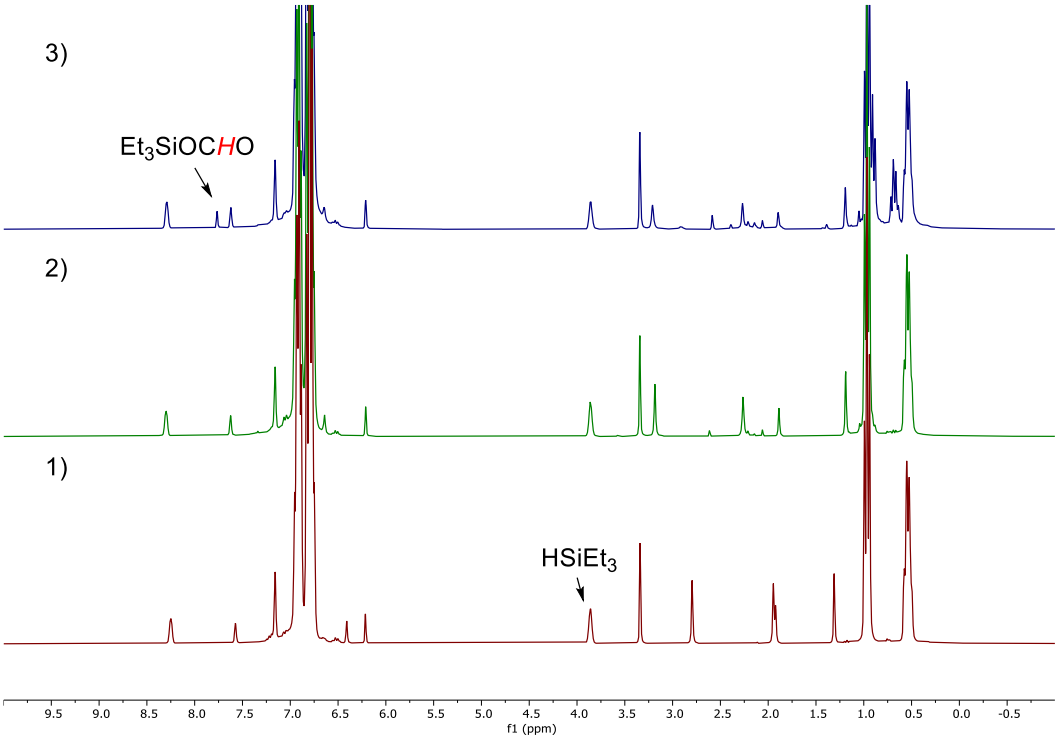


Figure S49. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with $HSiEt_3$ by [**2**][BArF]: 1) [**2**][BArF] (5 mol%) + $HSiEt_3$; 2) [**2**][BArF] (5 mol%) + $HSiEt_3$ + CO_2, RT 21 hours; [**2**][BArF] (5 mol%) + $HSiEt_3$ + CO_2, RT 21 hours + 60 ^{o}C 25 hours.

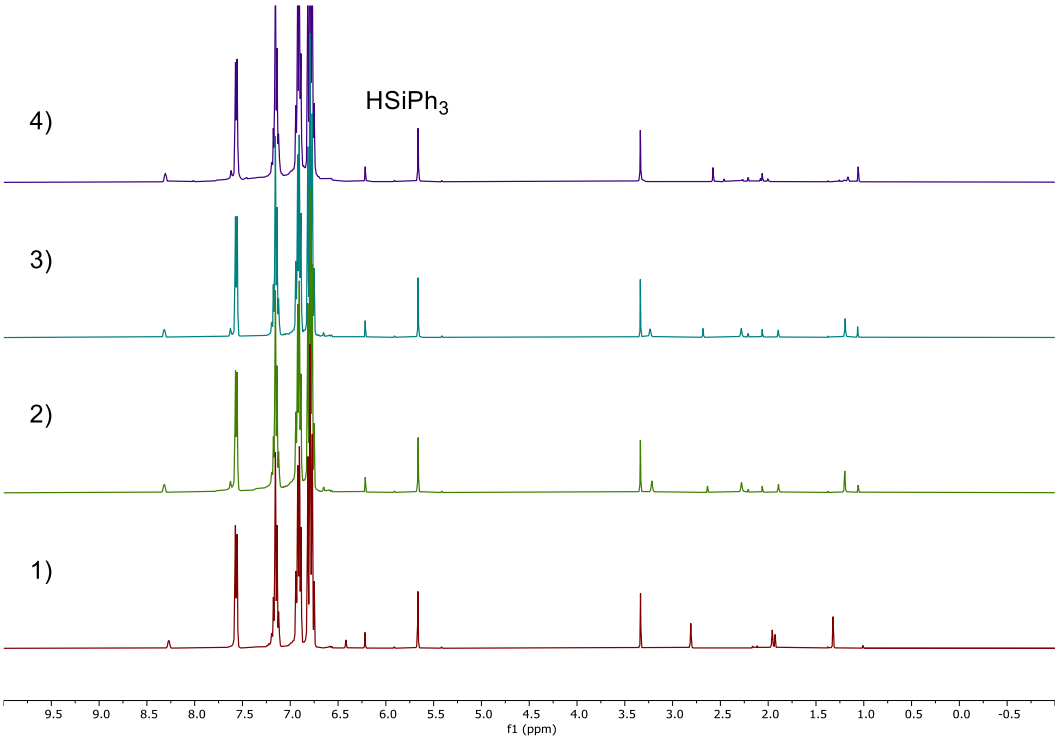
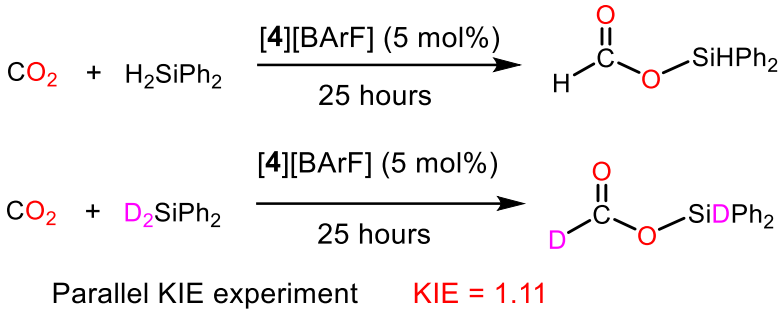


Figure S50. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with $HSiPh_3$ by [**2**][BArF]: 1) [**2**][BArF] (5 mol%) + $HSiPh_3$; 2) [**2**][BArF] (5 mol%) + $HSiPh_3$ + CO_2, RT 17 hours + 60 ^{o}C 18 hours + 80 ^{o}C 18 hours.

2. Mechanistic Studies

2.1 Kinetic Isotope Experiments



Parallel KIE experiment KIE = 1.11

[**2**][BArF] (5 mol%, 4.00 µmol, 80.0 µL, 0.05 M in C_6H_5F) and 1,3,5-trimethoxybenzene (0.10 eq, 8.0 µmol) were introduced into 0.32 mL of C_6D_6 within a J-Young NMR tube. The solution was degassed and refilled with 1 bar of CO_2 at room temperature. The solution of [**4**][BArF] was obtained after 21 hours and excess CO_2 was removed, then H_2SiPh_2 (1.0 eq, 80.0 µmol, 14.9 µL) (or D_2SiPh_2 (1.0 eq, 80.0 µmol, 14.7 µL)) was added in gloves box. The solution was degassed again and then pressurised with 1 bar of CO_2 at room temperature. The reaction progression was monitored via ^{1}H NMR spectroscopy by the consumption of silane alongside the emergence of the respective hydrosilylation products resonances. After 25 hours, the conversion of silane was determined by comparing integrals of the unreacted silane resonances to the integrals of the internal standard.

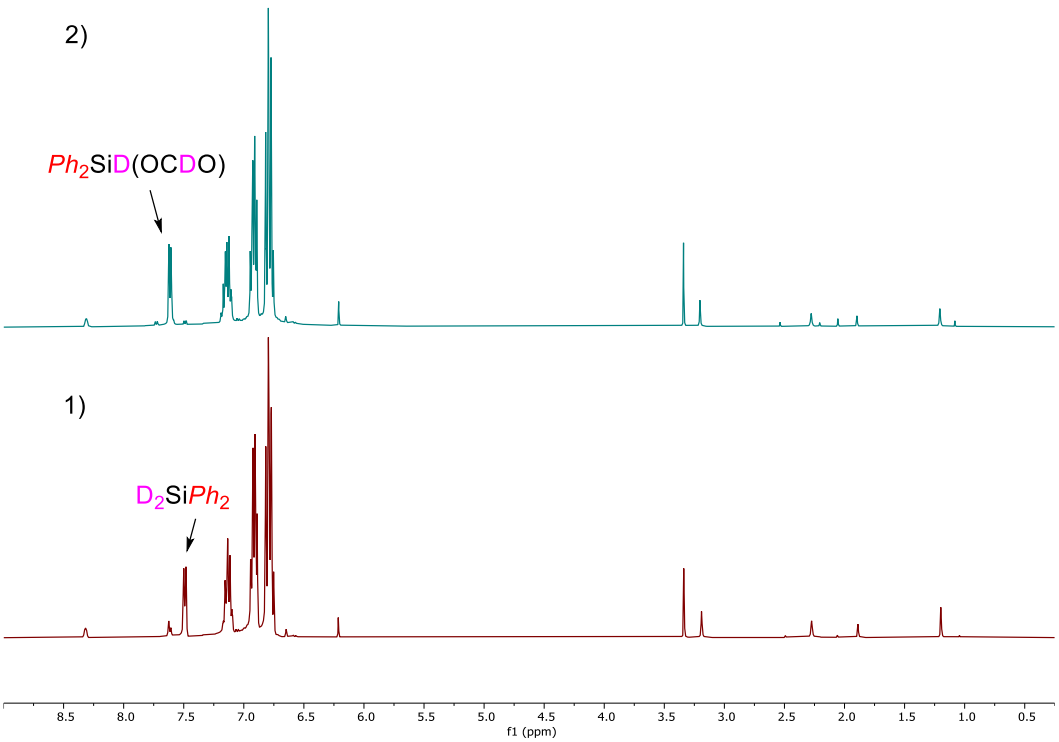


Figure S51. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with D_2SiPh_2 by [**4**][BArF]: 1) [**4**][BArF] (5 mol%) + D_2SiPh_2; 2) [**4**][BArF] (5 mol%) + H_2SiPh_2 + CO_2, RT 25 hours.

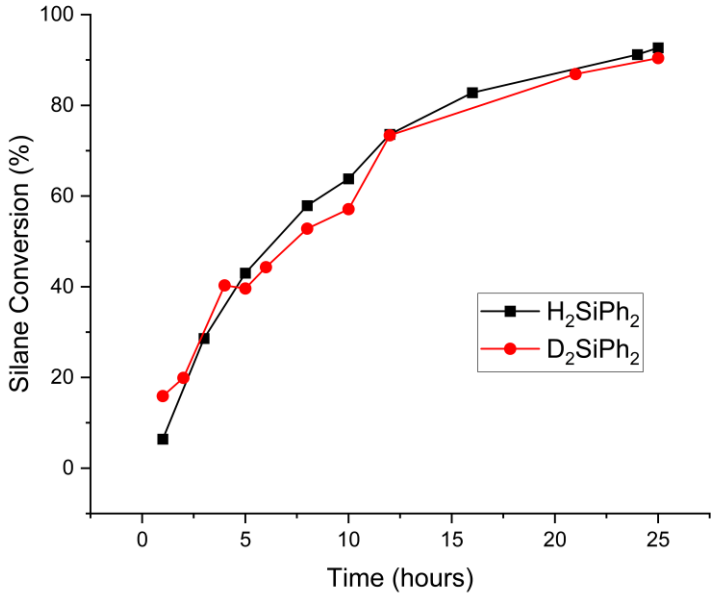


Figure S52. Kinetic isotope effect experiments.

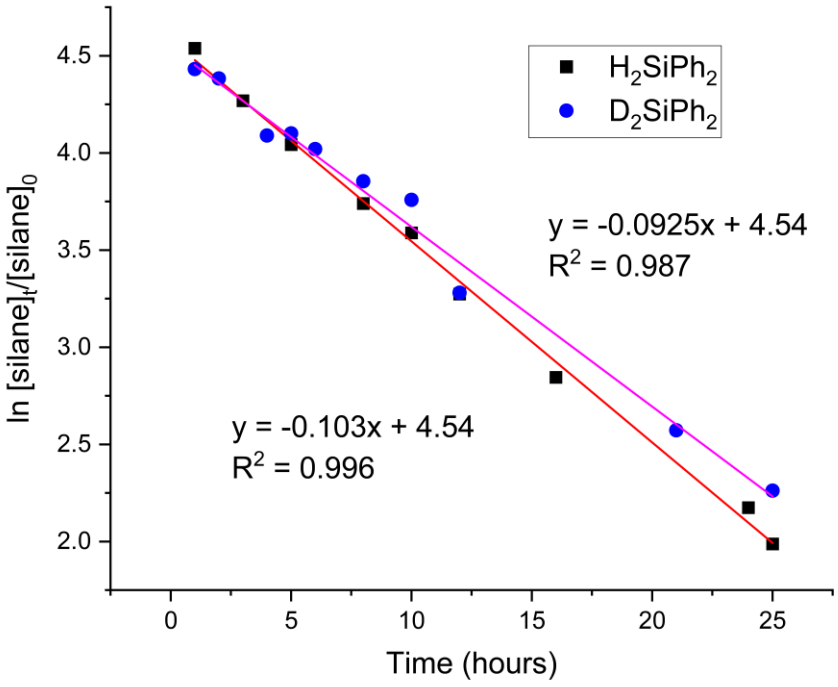
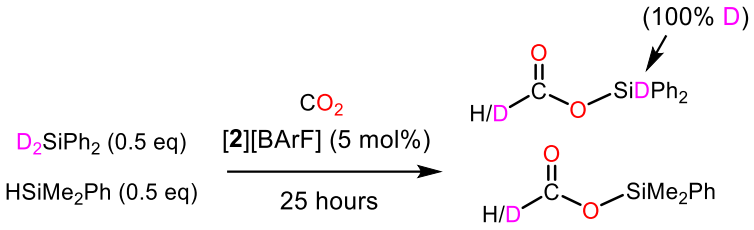


Figure S53. Kinetic isotope effect experiments.

2.2 H/D Exchange Experiments



[**2**][BArF] (5 mol%, 4.00 µmol, 80.0 µL, 0.05 M in C_6H_5F), D_2SiPh_2 (0.5 eq, 40.0 µmol, 8.35 µL)), $HSiMe_2Ph$ (0.5 eq, 40.0 µmol, 6.13 µL), and 1,3,5-trimethoxybenzene (0.10 eq of the H_2SiPh_2) as an internal standard were dissolved in C_6D_6 (0.32 mL) in a J-Young NMR tube. The solution was rapidly degassed using a Schlenk line and then refilled with 1 bar of CO_2 at room temperature. The progression of reaction was monitored via ^1H NMR spectroscopy.

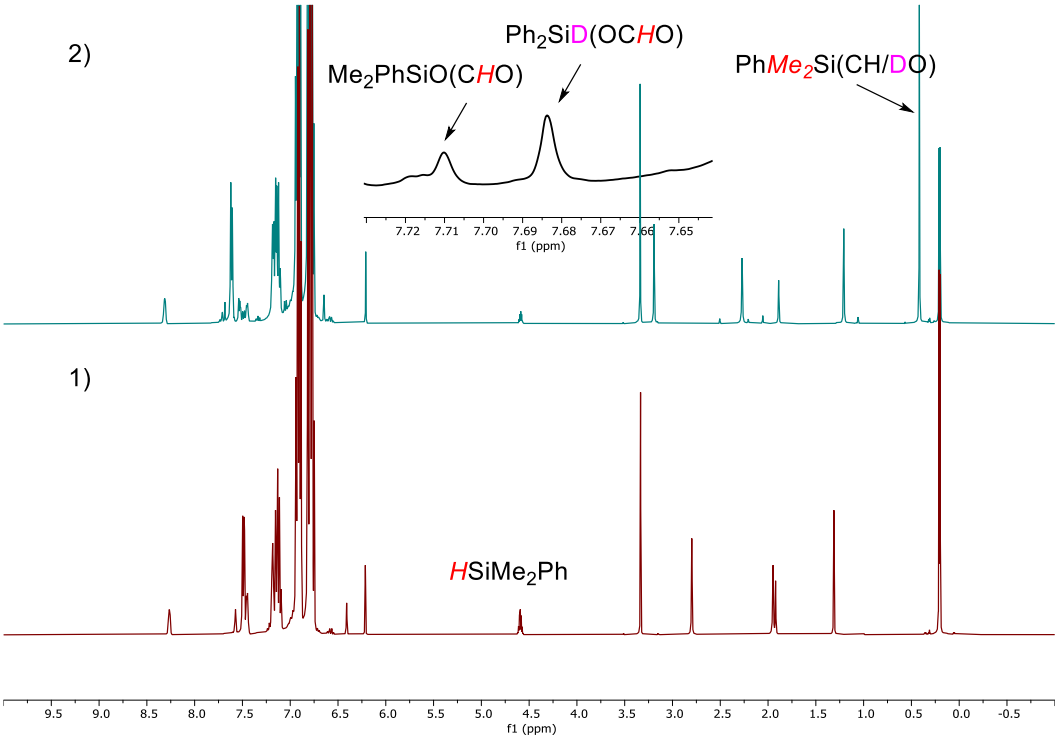


Figure S54. Stacked ^{1}H NMR spectra of hydrosilylation of CO_2 with D_2SiPh_2/$HSiMe_2Ph$ by [**2**][BArF]: 1) [**2**][BArF] (5 mol%) + D_2SiPh_2 + $HSiMe_2Ph$; 2) [**2**][BArF] (5 mol%) + D_2SiPh_2 + $HSiMe_2Ph$ + CO_2, RT 25 hours.

3. X-Ray Crystallographic Details

General considerations

Single crystals diffraction data were recorded on a Bruker Photon D8 Venture DUO IMS system equipped with a Helios optic monochromator and a Mo IMS microsource (λ = 0.71073 Å) and an Atlas SuperNova system equipped with a mirror monochromator and a Cu micro-focus sealed X-ray tube (λ = 1.54178 Å). The data collection was performed, using the APEX IV software package[S4] and CrysAlisPro[S5] on single crystals coated with Fomblin®Y as perfluorinated ether. The single crystal was picked on a micro sampler, transferred to the diffractometer, and measured frozen under a stream of cold nitrogen. A matrix scan was used to determine the initial lattice parameters. Reflections were merged and corrected for Lorenz and polarization effects, scan speed, and background using SAINT.[S6] Absorption corrections, including odd and even ordered spherical harmonics were performed using SADABS.[S6] Space group assignments were based upon systematic absences, E statistics, and successful refinement of the structures. Structures were solved by direct methods with the aid of successive difference Fourier maps and were refined against all data using the APEX IV software in conjunction with SHELXL-2014[S7] and SHELXLE.[S8] H atoms were placed in calculated positions and refined using a riding model, with methylene and aromatic C–H distances of 0.99 and 0.95 Å, respectively, and Uiso(H) = 1.2 Ueq(C). Non-hydrogen atoms were refined with anisotropic displacement parameters. Fullmatrix least-squares refinements were carried

out by minimizing Σw(Fo2-Fc2)2 with the SHELXL weighting scheme.[S9] Neutral atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from International Tables for Crystallography.[S10] The images of the crystal structures were generated by Mercury.[S11] The CCDC numbers 2255434, 2255353 and 2255355 contain the supplementary crystallographic data for the structures [**2**][BArF], [**3**][BArF] and [**4**][BArF], respectively. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/.

Table S2. Crystallographic details

Compound #	[**2**][BArF]	[**3**][BArF]	[**4**][BArF]
CCDC-Number	2255434	2255353	2255355
Empirical formula	$C_{70}H_{61}BF_{24}N_4Sn$	$C_{79}H_{80}N_5O_2B_5F_{24}Sn$	$C_{72}H_{61}N_4O_4BF_{24}Sn$
Formula weight	1543.84	1760.22	1631.74
Temperature/K	100.00	100.00	100.00
Crystal system	triclinic	triclinic	triclinic
Space group	P-1	P-1	P-1
a/Å	13.4232(4)	15.2450(13)	10.4739(5)
b/Å	17.0569(6)	17.2704(13)	16.0890(8)
c/Å	18.5469(7)	17.6243(14)	23.3384(11)
α/°	102.535(3)	92.495(3)	109.831(2)
β/°	101.839(3)	102.397(3)	92.107(2)
γ/°	109.969(3)	112.807(2)	102.860(2)
Volume/Å^3	3711.1(2)	4136.1(6)	3579.7(3)
Z	2	2	2
ρ_{calc}g/cm^3	1.382	1.413	1.514
μ/mm^{-1}	3.644	0.411	0.471
F(000)	1560.0	1792.0	1648.0
Crystal size/mm^3	0.1 × 0.07 × 0.05	0.382 × 0.287 × 0.198	0.347 × 0.26 × 0.106
Radiation	CuKα (λ = 1.54184)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θrange for data collection/°	5.124 to 147.842	4.684 to 50.7	3.864 to 50.7
Index ranges	-16 ≤ h ≤ 11, -20 ≤ k ≤ 21, -23 ≤ l ≤ 22	-18 ≤ h ≤ 18, -20 ≤ k ≤ 20, -21 ≤ l ≤ 21	-12 ≤ h ≤ 12, -19 ≤ k ≤ 19, -27 ≤ l ≤ 28
Reflections collected	26916	93421	66144
Independent reflections	14585 [R_{int} = 0.0442, R_{sigma} = 0.0593]	15133 [R_{int} = 0.0264, R_{sigma} = 0.0179]	13105 [R_{int} = 0.0252, R_{sigma} = 0.0179]
Data/restraints/parameters	14585/9/969	15133/272/1069	13105/737/1206
Goodness-of-fit on F^2	1.032	1.067	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0484, wR_2 = 0.1198	R_1 = 0.0418, wR_2 = 0.1026	R_1 = 0.0299, wR_2 = 0.0702
Final R indexes [all data]	R_1 = 0.0649, wR_2 = 0.1323	R_1 = 0.0457, wR_2 = 0.1061	R_1 = 0.0325, wR_2 = 0.0719
Largest diff. peak/hole / e Å^{-3}	0.78/-0.96	1.24/-0.81	0.75/-0.52

4. Quantum chemical calculations

Calculations were carried out using ORCA 5.0.4 software.[S12]

Geometry optimizations were carried using the r^{2}SCAN-3c composite method, utilizing the regularized and restored SCAN functional,[S13-14] geometrical counterpoise correction gCP,[S15] the atom-pairwise dispersion correction based on tight binding partial charges (D4),[S16-18] the def2-mTZVPP basis set and def2-mTZVPP/J auxiliary basis set. [S19] Effective core potential def2-ECP was used for Sn (ECP parameters for Sn have been obtained from TURBOMOLE (7.0.2)).[S20] The optimized geometries were verified as minima or transition states by analytical frequency calculations. The transition states were additionally verified by IRC calculations. Single point calculations of the optimized geometries were carried out at the r^{2}SCAN-3c level using the SMD solvation module[S21] to obtain electrostatic contribution and the cavity term in order to account for the solvent effects. To get more accurate electronic energies for the mechanistic investigations, single point calculations of the r^{2}SCAN-3c optimized geometries were carried using the PW6B95 [S22] functional, with D4 dispersion correction, the def2-QZVPP[S23] basis set and def2/J[S24] and def2-QZVPP/C[S25] auxiliary basis sets. def2-ECP was used for Sn. The method is denoted as PW6B95-D4(SMD)/def2-QZVPP//r^{2}SCAN-3c. The summary of the thermochemistry results is presented in Table S2. The NBO analysis was done using the NBO7 software,[S26] at the PBE0[S27]/def2-TZVP[S28]/r^{2}SCAN-3c level of theory.

Table S3. Calculated energies (Eh). E_{PW6B95} - electronic energy at the PW6B95-D4/def2-QZVPP//r^{2}SCAN-3c level; $G\text{-}E_{el}$ - Gibbs energy minus the electronic energy at the r^{2}SCAN-3c// r^{2}SCAN-3c level; G_{cds} (cavity term) and G_{enp} (electrostatic contribution) at r^{2}SCAN-3c (SMD=Benzene)// r^{2}SCAN-3c level; G_{conc} - concentration-induced free-energy shift (G_{conc} = RTln(24.5)); G – free energy at the PW6B95-D4(SMD)/def2-QZVPP//r^{2}SCAN-3c level, $G = E_{PW6B95} + [G\text{-}E_{el}] + G_{cds} + G_{enp} + G_{conc}$. Thermochemistry at 298.15 K.

Compound	ID	E_{PW6B95}	$G\text{-}E_{el}$	G_{cds}	G_{enp}	G_{conc}	G
[**2**]$^+$	3525538	-1913.90390	0.70795	-0.04503	-0.02061	0.00302	-1913.25857
[**2**][BArF]	3536119	-5567.93743	1.05894	-0.03668	-0.01860	0.00302	-5566.93074
[**2a**]$^+$	3531069	-1529.73254	0.53363	-0.04332	-0.01812	0.00302	-1529.25733
[**2a**][BArF]	3539097	-5183.77457	0.88298	-0.03103	-0.01624	0.00302	-5182.93584
[**3**]$^+$	3525578	-2102.82456	0.71945	-0.04727	-0.02122	0.00302	-2102.17058
[**3**][BArF]	3746351	-5756.86611	1.07621	-0.03610	-0.01667	0.00302	-5755.83965
[**3a**]$^+$	3529038	-1718.65656	0.54497	-0.04506	-0.01757	0.00302	-1718.17119
[**3a**][BArF]	3690093	-5372.69690	0.89536	-0.03274	-0.01600	0.00302	-5371.84726
[**4**]$^+$	3525581	-2291.73103	0.72772	-0.05029	-0.02500	0.00302	-2291.07558
[**4**][BArF]	3748659	-5945.78061	1.08218	-0.03854	-0.02036	0.00302	-5944.75431
TS(2_3)	3527035	-2102.76624	0.71701	-0.04662	-0.01985	0.00302	-2102.11268
TS(3_4)	3529058	-2291.69025	0.72861	-0.04819	-0.02048	0.00302	-2291.02728
TS1	4191715	-3046.84610	0.91624	-0.05369	-0.02890	0.00302	-3046.00943
INT_A	3685470	-3046.84678	0.91442	-0.05369	-0.03156	0.00302	-3046.01460

TS2	3969171	-3046.84872	0.91828	-0.05673	-0.02918	0.00302	-3046.01333
INT_B	597622	-1327.40280	0.33756	-0.04675	-0.01672	0.00302	-1327.12569
INT_C	3549415	-1719.40308	0.54938	-0.02562	-0.01758	0.00302	-1718.89388
TS3	3607573	-3046.84986	0.91654	-0.05162	-0.02707	0.00302	-3046.00898
INT_D	612540	-1328.16718	0.34679	-0.01659	-0.01457	0.00302	-1327.84852
TS4	3734923	-1328.15477	0.34547	-0.01265	-0.01423	0.00302	-1327.83316
IMe_4	592934	-384.10329	0.14625	-0.01132	-0.01048	0.00302	-383.97582
IMe_4CO_2	592935	-573.02057	0.15737	-0.01695	-0.00877	0.00302	-572.88590
H_2SiPh_2	3543195	-755.11620	0.16050	-0.00590	-0.00935	0.00302	-754.96794
HCO_2SiHPh_2	3614592	-944.04318	0.17260	-0.00777	-0.00900	0.00302	-943.88432
$[BArF]^-$	3536159	-3653.94294	0.31746	-0.03055	-0.00259	0.00302	-3653.65559
CO_2	592933	-188.89490	-0.00901	-0.00094	0.00057	0.00302	-188.90126

According to the request by one of the referees, in addition to the Lewis structure of **[2]$^+$** presented in the main text, also shown in **Figure S55 [2]^+_a**, here we additionally discuss the ionic representation, i.e. **[2]^+_b**. The dative form, **[2]^+_a** is a bis(NHC) stabilized stannyliumylidene in which the interactions between the NHC units and the Sn centre are depicted as dative bonds. In **[2]^+_b** the negative charge is located on the Sn atom to which the two positively charged NHC moieties are bound covalently **[2]^+_b**, which results a stannyl-anion-type species.

As discussed in the main text, the NBO depiction of bonding between the NHCs and the low valent Sn centre in **[2]$^+$** is that of polarized bonds between the carbons and the tin. This may hint to the stannyl anion character of **[2]$^+$**, which is why **[2]^+_b** is considered.

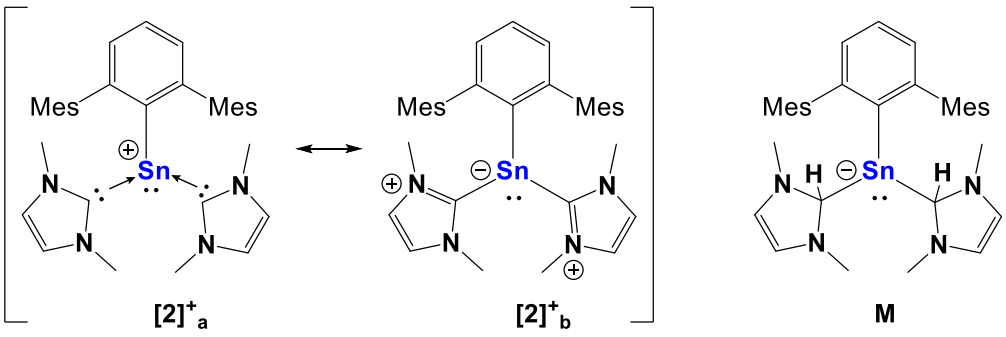


Figure S55. Resonance structures of donor stabilized stannyliumylidene [**2**]$^+$ and the related model system stannyl anion **M**.

In the main text, we depicted **[2]$^+$** as **[2]^+_a** because we accounted for the following considerations. In general, it is a common situation in the NBO analysis for a dative bond to be shown as a bonding orbital polarized toward the donor atom, reflecting that the electron pair is largely provided by the donor. Additionally, it is also worth looking at the

Wiberg bond index and Mayer bond order. In this case, the bond is strongly polarized toward carbon and the Wiberg bond index is low for each Sn-C bond (0.58 for both). The Mayer bond orders are also quite low (0.48, 0.42). In **[2]**$^{+}$ the charge distribution is such that the NPA charge on Sn centre in +0.79. Additionally, the NHC-Sn bonds are longer 2.34 and 2.33 Å in comparison to the covalent Sn-C^{Ar} bond (2.24 Å). Furthermore, the reactivity of the complex, where NHC behaves as a donor ligand, which can facilely dissociate from the metal centre, intuitively leads to the dative bond representation being more plausible.

In order to distinguish between the electronic properties of donor stabilized stannyliumylidene and stannyl anion we carried out additional calculation of compound **M**, which is obtained by substituting the carbenic carbons with H^- (**Figure S55, S56**).

As in **[2]**$^{+}$, in **M** the NPA charge on the Sn centre is positive (+0.74 el.). However, the Sn-C Wiberg bond indexes of 0.63 and 0.65 are somewhat higher than those in **[2]**$^{+}$ (0.58 and 0.58). The Mayer bond orders in the more covalent bonds Sn-C of **M** are also higher than in **[2]**$^{+}$: 0.73 and 0.75 vs 0.48 and 0.42.

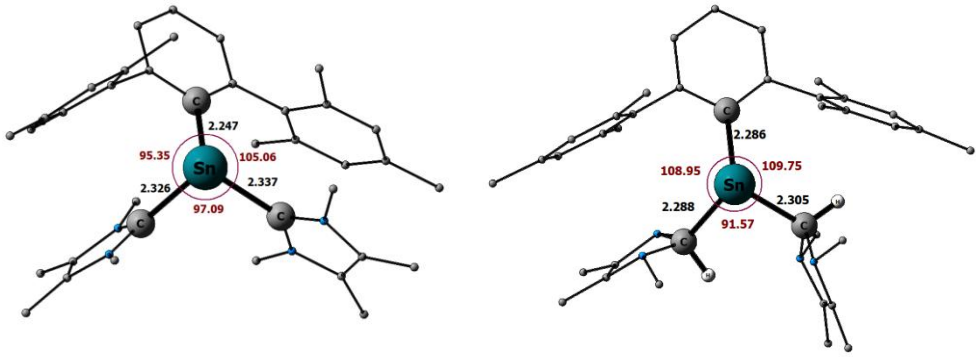


Figure S56. Optimized geometries of **[2]**$^{+}$ and **M**.

In term of geometries, the optimized structure of **M** exhibits a substantial shortening of the Sn-C bonds by 0.038 and 0.031 Å (**Figure S56**)., which would be typical for more covalent bonds. Also, the geometry of the Sn centre in **M** is less pyramidalized than in **[2]**$^{+}$ Σα=310.27° vs Σα=305.46°, respectively, which would be typical for a stannyl anion.

According to the NBO analysis in **M** the Sn-C bonds are slightly less polarized than in **[2]**$^{+}$: Sn(22.54%)-C(77.46%) and Sn(21.12%)-C(78.88%) in **M** vs Sn(18.25%)-C(81.75%) and Sn(18.72%)-C(81.28%).

The very important difference in the electronic structure between the two species is in the hybridization of the orbitals that constitute the Sn-C interaction. In **M**, in comparison to **[2]**$^{+}$, there is significant increase of the s character of the Sn hybrid orbitals and a significant increase in the p character of the C hybrid orbitals in comparison to **[2]**$^{+}$: Sn($sp^{9.11}$)-C($sp^{2.61}$) and Sn($sp^{9.91}$)-C($sp^{2.50}$) in **M** vs Sn($sp^{19.72}$)-C($sp^{1.45}$) and Sn($sp^{15.52}$)-

C($sp^{1.45}$) in **[2]$^+$**. And this is the distinction between the formal C(sp^2)→Sn(p) interaction between a donor and stannyliumylidene, and the C(sp^3)-Sn(sp^3) interaction expected in a stannyl anion.

In general, we are not strictly in favour of either dative or ionic representations. We think that both annotations could be correct, and each case should be looked at separately. In this case, when comparing **[2]^+_a** with **[2]^+_b**, we think that the representation of **[2]^+_a** with dative bonds between the Sn-centre and the NHCs is the more intuitive and reflects better the electronic properties and the reactivity of [**2**]$^+$.

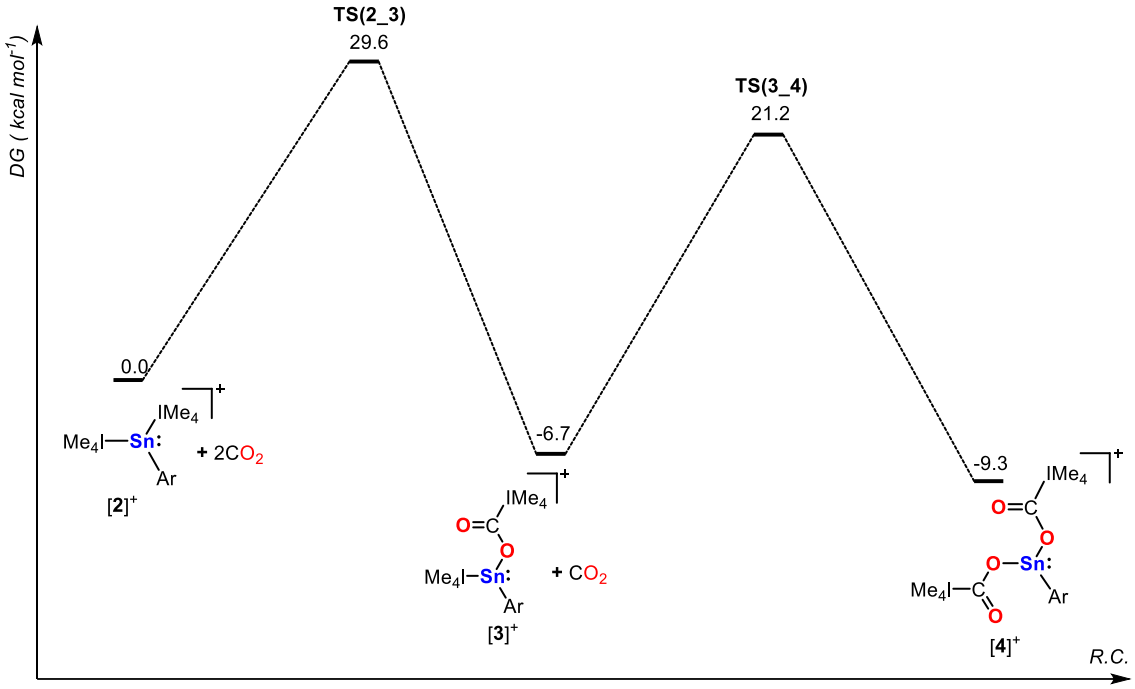


Figure S57. Calculated reaction coordinate diagram for the concerted reactions of [**2**]$^+$ with CO_2 to form [**3**]$^+$ and [**4**]$^+$.

In addition to the reaction of [**2**]$^+$ to form [**3**]$^+$ and [**4**]$^+$ via the stepwise dissociation of IMe_4 described in Scheme 4, we also considered a mechanism in which [**2**]$^+$ and [**3**]$^+$ react with CO_2 concertedly (Scheme S57). In this case, the barrier for the first reaction is 29.6 kcal mol^{-1} (**TS(2_3)**). For the second reaction the barrier (**TS(3_4)**) (at 21.2 kcal mol^{-1}) is 27.9 kcal mol^{-1} (**TS(3_4)**). This makes this mechanism kinetically less preferable to the one which involves the IMe_4 dissociation, presented in Scheme 4 in the main text.

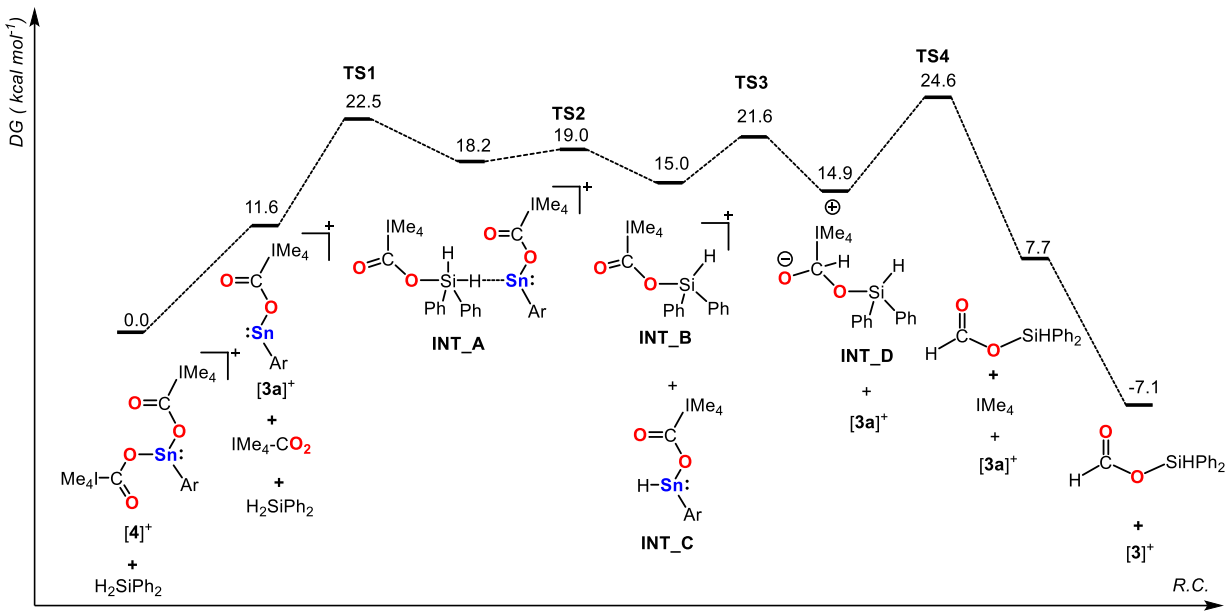


Figure S58. Calculated reaction coordinate diagram for the reaction of [**4**]$^+$ with H_2SiPh_2.

The proposed mechanism for the reaction of [**4**]$^+$ with H_2SiPh_2 to form the CO_2 hydrosilylation product $Ph_2SiH(OCHO)$ and [**3**]$^+$ as observed experimentally (Scheme 3) is presented in Figure S58. Drawings of the geometries of key intermediates and transition states are shown in Figure S59. In the first step of the proposed mechanism, compound [**4**]$^+$ dissociates to the imidazolium carboxylate and [**3a**]$^+$ at 11.6 kal mol^{-1}. The Si-H bond in Ph_2SiH_2 is activated by the stannylium center of [**3a**]$^+$ via a **TS1** at 22.5 kcal mol^{-1} to generate intermediate **INT_A** at 18.2 kcal mol^{-1}. This is followed by the hydride transfer from the hyper-coordinate silane to the stannylium center, generating ((silylcarbonyl)oxy)imidazolium intermediate (**INT_B**) and the stannyl hydride (**INT_C**) at 15.0 kcal mol^{-1}. The next step is a hydride abstraction from **INT_C** by **INT_B**, releasing [**3a**]$^+$ and forming a zwitterionic adduct **INT_D**. In the last step, **INT_D** releases diphenylformoxysilane ($Ph_2SiH(OCHO)$) and free IMe_4, which then bonds to the Sn center of [**3a**]$^+$ to generate the [**3**]$^+$.

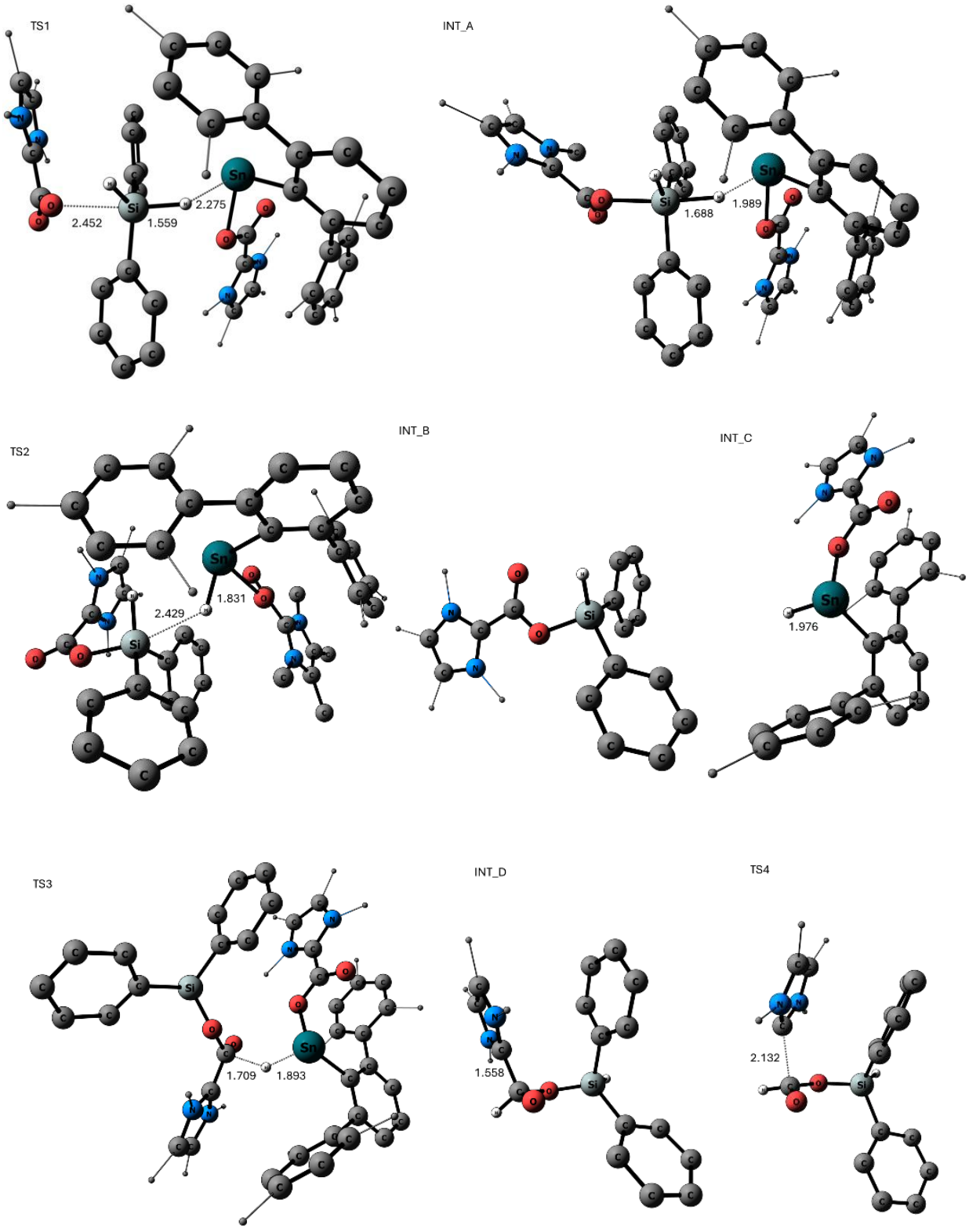


Figure S59. Geometries of key intermediates and transition states.

Cartesian coordinates and energies of the optimized geometries at the r^{2}SCAN-3c level

Calculated energies and coordinates of [**2**]$^+$
Electronic energy ... -1910.38008407 Eh
Total Enthalpy ... -1909.54907147 Eh
Final Gibbs free energy ... -1909.67212994 Eh
CARTESIAN COORDINATES (ANGSTROEM)

Sn	1.871044	9.948868	3.058533
N	-1.118512	10.207896	4.729189
N	2.696946	7.297550	4.680012
N	2.796556	8.836635	6.166870
N	-1.310525	10.271967	2.600358
C	-0.384233	10.244358	3.593601
C	-0.548118	10.140676	6.062437
H	-0.413238	9.100421	6.382225
H	-1.198793	10.660855	6.768573
H	0.411173	10.651365	6.041013
C	2.425454	8.612786	4.879415
C	3.232073	6.705182	5.816781
C	2.739055	10.115617	6.861134
H	2.601099	10.907065	6.122225
H	3.679255	10.290695	7.389561
H	1.924928	10.124815	7.594302
C	2.900219	11.791546	3.829720
C	4.303630	11.707444	3.683588
C	-2.482386	10.233915	4.465463
C	2.348401	13.004503	4.289694
C	0.874714	13.224023	4.380692
C	3.287508	7.682067	6.766564
C	0.130137	13.371672	3.189565
C	0.227812	13.360676	5.617078
C	2.552142	6.574842	3.419231
H	2.060577	7.223436	2.692108
H	1.954777	5.671254	3.570664
H	3.540606	6.305930	3.031370
C	5.123036	12.781455	4.038995
H	6.199902	12.691545	3.915606
C	-2.604482	10.285565	3.109043
C	-1.242961	13.577646	3.261829
H	-1.808148	13.713712	2.340435
C	0.972292	13.353212	6.928594
H	1.988769	12.967985	6.831960
H	0.436429	12.768424	7.684810
H	1.057134	14.373398	7.321996
C	4.928654	10.475521	3.102948
C	4.567935	13.958676	4.524832
H	5.206761	14.794804	4.794268
C	5.565462	9.524805	3.917852
C	-1.912859	13.651349	4.485738
C	-1.027668	10.399607	1.175767
H	-1.210618	11.426655	0.842614
H	-1.664271	9.716453	0.607379
H	0.018679	10.143139	0.994690
C	-1.159262	13.552326	5.648221
H	-1.652323	13.656602	6.614115
C	6.029309	8.335217	3.349510
H	6.510553	7.598706	3.991968
C	5.836833	9.780569	5.375628
H	6.877598	10.101286	5.508708
H	5.703089	8.869582	5.968459
H	5.207353	10.576310	5.775311
C	3.188471	14.070363	4.636419
H	2.743794	15.000092	4.984050
C	4.887469	10.272478	1.705446
C	0.816243	13.377877	1.849347
H	1.680276	14.050449	1.855178
H	0.130096	13.703316	1.062802
H	1.205814	12.390361	1.572060
C	3.636389	5.277056	5.860675
H	2.787864	4.607397	5.680120
H	4.050109	5.031722	6.840131
H	4.402378	5.053642	5.109411
C	4.330321	11.321519	0.782078
H	3.233513	11.270839	0.739239
H	4.704469	11.176218	-0.234479
H	4.592096	12.330119	1.113917
C	-3.806499	10.374076	2.241519
H	-3.779305	11.268632	1.608158
H	-4.708940	10.428146	2.853060
H	-3.904845	9.502593	1.584141
C	5.931691	8.089060	1.983710
C	-3.509119	10.250868	5.536790
H	-3.405656	9.399182	6.218243
H	-4.508921	10.205382	5.101284
H	-3.446553	11.171351	6.131064
C	3.765175	7.650288	8.172238
H	4.638195	8.297576	8.318838
H	4.055911	6.635387	8.448273
H	2.988380	7.976260	8.873118
C	5.381772	9.084402	1.174432
H	5.343794	8.933559	0.097146
C	-3.401484	13.856146	4.527637
H	-3.698622	14.721230	3.925488
H	-3.757103	14.018718	5.548642
H	-3.929039	12.984257	4.119616
C	6.454051	6.814186	1.379986
H	7.358050	7.004461	0.790096
H	5.720350	6.363423	0.703041
H	6.710915	6.080862	2.149543

Calculated energies and coordinates of [**2**][BArF]
Electronic energy ... -5558.27970811 Eh
Total Enthalpy ... -5556.99596624 Eh
Final Gibbs free energy ... -5557.22076880 Eh
CARTESIAN COORDINATES (ANGSTROEM)

Sn	1.831134	9.677246	3.045045
F	-1.429303	-3.143716	7.834758
F	1.661373	-2.003442	1.296276
F	-0.210833	-3.036877	6.031564
F	0.575682	-2.298085	7.919080
F	2.095163	-0.304976	0.011166
F	0.573854	-1.750208	-0.574505
F	3.970498	3.549019	1.733213
F	-3.795816	2.014004	0.517970
F	5.480192	1.058728	7.343180
F	3.568238	0.208003	7.948186
N	-1.017001	10.183730	4.881356
N	2.506524	7.158114	4.925875
F	-1.884278	7.367920	6.991424
F	-4.461092	0.545034	1.975717
N	2.826758	8.841472	6.213399
N	-1.382452	10.056532	2.777060
F	3.994614	2.306764	8.333013
C	-0.442598	1.206872	3.091818
C	-0.533924	3.527784	4.477973
C	-0.847669	1.104121	5.645884
C	1.550421	2.003177	4.740413
C	-0.557088	4.272264	5.667695
H	-0.290628	3.782607	6.602568
C	-1.096450	-1.002997	6.860135
C	0.448037	0.411652	2.365197
H	1.477052	0.306859	2.702047
C	0.056112	-0.266960	1.209662
C	2.171433	1.615059	5.930417
H	1.567897	1.232840	6.750149
C	-0.379008	10.094626	3.691309
C	-1.999615	1.543793	6.303733
H	-2.396577	2.535283	6.097401
C	-1.760012	1.259695	2.611760
H	-2.505662	1.831798	3.162139
F	5.627633	2.328914	2.447170
C	2.391537	2.517701	3.736260
H	1.951914	2.859050	2.801899

C	-0.429613	-0.203864	5.937910
H	0.436793	-0.614405	5.422051
C	-0.883911	4.217650	3.309426
H	-0.881481	3.689641	2.360086
F	-4.842615	1.665024	6.988063
C	-2.675395	0.742437	7.225922
C	-1.244241	-0.176599	0.732548
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C	-0.955044	5.608239	5.695491
C	3.558321	1.684428	6.095557
F	-1.322061	5.540404	8.035196
C	-0.549820	-2.369476	7.159343
C	-0.334377	10.258999	6.162116
H	-0.135465	9.260942	6.563290
H	-0.946540	10.823541	6.868563
H	0.597892	10.797094	6.008493
C	-1.265813	5.558189	3.332760
C	-2.151347	0.594645	1.454684
C	2.383233	8.508485	4.971737
C	1.085293	-1.083574	0.483858
F	5.285621	4.300048	3.300860
C	3.014300	6.648614	6.112130
C	2.939638	10.186352	6.754217
H	2.820259	10.902643	5.939740
H	3.928967	10.323575	7.199241
H	2.185226	10.359561	7.530086
C	-2.228322	-0.536733	7.524636
H	-2.749175	-1.158354	8.242641
C	2.932132	11.564228	3.614549
C	4.152710	1.302169	7.420095
C	4.374310	2.155965	5.079714
H	5.451683	2.201080	5.202087
F	-3.879445	-0.093987	-0.024332
C	-1.312320	6.272478	4.525286
H	-1.643876	7.306332	4.543905
B	-0.066451	1.959058	4.493464
C	3.769246	2.588108	3.898423
C	4.321477	11.427746	3.390832
F	0.216756	6.895649	7.314241
C	-2.397407	10.217507	4.726397
F	-3.601683	2.432532	8.598649
C	2.448429	12.821189	4.035581
C	0.989578	13.105546	4.179646
C	3.212959	7.717760	6.933390
C	0.182189	13.157443	3.022002
C	0.415095	13.389342	5.427982
F	-4.473190	0.441386	8.752374
C	2.229799	6.306986	3.769419
H	1.682969	6.880737	3.020558
H	1.627507	5.448268	4.078720
H	3.172532	5.957688	3.334257
C	5.196096	12.484717	3.655657
H	6.260560	12.349014	3.477037
C	-2.629008	10.147356	3.384394
C	-1.179199	13.413226	3.145776
H	-1.791574	13.466260	2.246253
C	1.229703	13.475691	6.694413
H	2.198927	12.982928	6.601825
H	0.686655	13.040999	7.540881
H	1.430869	14.523412	6.949541
C	4.870409	10.170186	2.785223
C	-3.895031	1.307394	7.892025
C	4.709479	13.702243	4.115695
H	5.390439	14.525234	4.314035
C	5.505947	9.183209	3.555312
C	-1.778008	13.626115	4.389055
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H	-0.196782	9.725174	1.091386
C	-0.995208	6.336925	7.003714
C	-1.611605	6.259303	2.055467
C	-0.962244	13.625271	5.513517
H	-1.399263	13.831641	6.489890
C	5.920774	7.995890	2.943747
H	6.396010	7.228504	3.553148
C	5.818745	9.386511	5.013723
H	6.897654	9.533571	5.146898
H	5.536513	8.508923	5.606049
H	5.319358	10.269550	5.413805
C	-3.566528	0.753856	0.980522
C	3.341566	13.871831	4.284044
H	2.947569	14.835571	4.599223
C	4.649751	3.174993	2.837654
C	4.762126	9.992946	1.387272
C	0.783374	12.994521	1.651898
H	1.724239	13.546468	1.564177
H	0.093722	13.351471	0.881658
H	1.022190	11.947540	1.426677
C	3.238303	5.201281	6.329781
H	2.317772	4.621940	6.190289
H	3.598545	5.015362	7.342828
H	3.979251	4.802102	5.629851
C	4.165954	11.062913	0.514362
H	3.071437	11.077470	0.603657
H	4.410049	10.884115	-0.535911
H	4.521383	12.058882	0.795870
C	-3.896801	10.188935	2.612684
H	-3.918507	11.043345	1.925207
H	-4.746121	10.286113	3.291569
H	-4.045379	9.278672	2.022175
C	5.770438	7.783778	1.577624
C	-3.334784	10.355671	5.868999
H	-3.177945	9.576125	6.621402
H	-4.366120	10.276690	5.519753
H	-3.221471	11.331315	6.359328
C	3.715533	7.790815	8.328214
H	4.659947	8.344881	8.395538
H	3.893387	6.784848	8.712074
H	2.993032	8.277650	8.993565
C	5.211561	8.809407	0.812386
H	5.123390	8.680303	-0.264760
C	-3.260041	13.856490	4.491553
H	-3.591329	14.628053	3.788519
H	-3.550331	14.167708	5.498851
H	-3.812986	12.939715	4.249030
C	6.204042	6.498001	0.930451
H	6.713405	6.688327	-0.019636
H	5.339306	5.859361	0.714413
H	6.876437	5.929493	1.577521
F	-2.637165	7.142325	2.221190
F	-1.966568	5.420241	1.069681
F	-0.559219	6.996253	1.586277

Calculated energies and coordinates of [**2a**]$^+$

Electronic energy ... -1526.98783236 Eh

Total Enthalpy ... -1526.35173142 Eh

Final Gibbs free energy ... -1526.45419801 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Sn	-1.475789	9.810765	2.693709
N	-0.793559	12.664716	4.335156
N	-2.512344	11.669422	5.145700
C	-0.720087	10.999834	0.995815
C	-1.650132	11.882307	0.433843
C	-1.324536	12.606490	-0.712650
H	-2.045262	13.290540	-1.153874
C	-0.074173	12.427506	-1.300126
H	0.180427	12.977653	-2.201315
C	0.848728	11.539175	-0.752048
H	1.817336	11.400704	-1.226236
C	0.533179	10.814882	0.401394
C	-2.958553	11.966623	1.140832
C	-3.319249	13.120010	1.865953
C	-4.474042	13.099966	2.643220
H	-4.744082	13.994269	3.202804
C	-5.290212	11.969235	2.735513
C	-4.930750	10.840088	2.010300
H	-5.572820	9.961200	2.033601
C	-3.792341	10.820053	1.187797
C	-2.478869	14.366912	1.820695
H	-1.417729	14.132948	1.706942
H	-2.624232	14.965530	2.724474
H	-2.755870	14.993332	0.964424

C	-6.552435	11.996877	3.552803
H	-6.461929	12.666805	4.413662
H	-6.825989	10.999611	3.909478
H	-7.390091	12.365790	2.949142
C	-3.639446	9.674797	0.210004
H	-3.939156	8.721924	0.655953
H	-2.627553	9.582890	-0.187782
H	-4.303446	9.856781	-0.643971
C	1.477062	9.854596	1.041961
C	2.623381	10.307261	1.724475
C	3.402537	9.386076	2.423088
H	4.285469	9.740396	2.952694
C	3.098531	8.025284	2.444580
C	2.000890	7.586494	1.708157
H	1.783706	6.521455	1.659525
C	1.189183	8.473000	0.998274
C	3.079476	11.743521	1.667009
H	3.535693	12.049640	2.613581
H	2.273088	12.436137	1.416869
H	3.845699	11.863030	0.891261
C	3.947179	7.062468	3.226975
H	3.736512	7.141612	4.300183
H	5.012510	7.271498	3.089729
H	3.759148	6.028607	2.927125
C	0.086857	7.924137	0.125941
H	-0.884607	7.885093	0.638616
H	0.320903	6.899772	-0.175385
H	-0.047155	8.528706	-0.775130
C	-1.560832	11.559915	4.187226
C	-1.259981	13.470276	5.364610
C	-2.360229	12.839930	5.875692
C	0.440758	12.921909	3.602119
H	1.308091	12.728682	4.242219
H	0.469797	13.960283	3.262043
H	0.473187	12.261925	2.734553
C	-0.601038	14.745729	5.742290
H	0.447761	14.590890	6.019304
H	-1.107040	15.195137	6.598215
H	-0.625327	15.471691	4.921238
C	-3.282650	13.223684	6.973860
H	-2.983272	14.182371	7.399851
H	-3.281394	12.484739	7.782963
H	-4.314037	13.325688	6.616790
C	-3.553526	10.686212	5.430619
H	-3.419248	10.282830	6.439218
H	-3.488561	9.871222	4.708178
H	-4.540775	11.147280	5.349780

Calculated energies and coordinates of [**2a**][BArF]
Electronic energy ... -5174.89548763 Eh
Total Enthalpy ... -5173.80705990 Eh
Final Gibbs free energy ... -5174.01250912 Eh
CARTESIAN COORDINATES (ANGSTROEM)

Sn	-2.758607	1.755398	0.310386
F	5.986825	1.860066	-2.036746
F	1.316993	-7.187328	-0.720350
F	7.623358	0.504508	-2.518411
F	5.723919	0.344825	-3.572538
F	2.872156	-5.928611	-1.582083
F	0.805252	-5.695846	-2.222838
F	1.688890	-1.367739	-4.993973
F	-1.583282	-5.352068	2.813323
F	-1.423522	3.002643	-1.774686
F	0.326231	3.711825	-2.855300
N	-2.389849	-1.171813	-0.998717
F	4.152290	1.628982	5.813774
F	-1.218474	-3.334380	3.555063
N	-3.198825	0.064530	-2.551610
F	0.364365	3.634461	-0.681874
C	1.711991	-2.608813	0.714484
C	2.195264	-0.208633	1.813764
C	3.863231	-1.199125	-0.035854
C	1.449278	-0.393504	-0.781102
C	3.302754	0.119504	2.601803
H	4.297982	-0.169279	2.272739
C	5.772734	-0.386259	-1.322460
C	1.971225	-3.654871	-0.186644
H	2.682038	-3.500902	-0.995154
C	1.364161	-4.904085	-0.068507
C	1.054608	0.954733	-0.753001
H	1.236032	1.545676	0.139591
C	-2.823906	0.081904	-1.252278
C	4.732348	-2.137485	0.537308
H	4.349440	-2.839291	1.276391
C	0.877720	-2.929870	1.793915
H	0.677434	-2.182557	2.555639
F	-0.339784	-0.624837	-5.254271
C	1.203169	-1.075537	-1.980843
H	1.490624	-2.118719	-2.075820
C	4.424421	-0.324702	-0.972556
H	3.799869	0.428622	-1.447899
C	0.947523	0.208384	2.306717
H	0.050583	-0.001140	1.729114
F	6.463998	-4.490592	0.644244
C	6.080184	-2.201090	0.190629
C	0.495168	-5.180983	0.981231
H	0.020840	-6.151677	1.073069
C	3.173241	0.803882	3.812116
C	0.454547	1.566776	-1.851827
F	5.204947	0.042640	4.754379
C	6.284248	0.574920	-2.355889
C	-1.839759	-1.645515	0.266593
H	-2.306235	-2.593469	0.545015
H	-2.051051	-0.921363	1.055667
H	-0.759797	-1.788203	0.172351
C	0.810278	0.874081	3.521029
C	0.275025	-4.180230	1.921082
C	1.599870	-5.933463	-1.136218
F	0.017243	-2.482274	-4.168783
C	6.618631	-1.326910	-0.747314
H	7.665399	-1.378122	-1.020694
C	-4.733469	2.635061	-0.234039
C	-0.027133	2.979096	-1.781786
C	0.240641	0.873695	-3.039767
H	-0.195238	1.365461	-3.902808
F	0.088988	-4.967904	4.151002
C	1.928052	1.184754	4.291698
H	1.827959	1.699405	5.240150
B	2.304454	-1.096618	0.444863
C	0.625261	-0.457708	-3.089664
C	-5.800018	1.828893	0.189886
F	5.173629	2.057424	3.938359
C	-2.491882	-1.979284	-2.121164
F	6.974175	-3.064119	2.203168
C	-4.998355	3.912620	-0.751493
C	-3.875973	4.809035	-1.147953
C	-3.040579	5.358322	-0.152821
C	-3.635031	5.106622	-2.500489
F	8.216904	-3.216146	0.420379
C	-7.119256	2.262421	0.056712
H	-7.935319	1.626230	0.391773
C	-3.006724	-1.191823	-3.113292
C	-1.946807	6.131219	-0.535432
H	-1.304832	6.552673	0.236288
C	-4.549672	4.638509	-3.605200
H	-5.171819	3.792610	-3.305160
H	-3.974489	4.360522	-4.494628
H	-5.233311	5.442704	-3.904578
C	-5.469448	0.513408	0.813267
C	6.938734	-3.237077	0.858014
C	-7.377748	3.517948	-0.484235
H	-8.401897	3.867070	-0.581590
C	-5.691970	-0.687554	0.104107
C	-1.657737	6.385503	-1.875484
C	-3.674770	1.226295	-3.289320
H	-2.899443	1.592548	-3.970807
H	-3.926353	2.011288	-2.574920
H	-4.567547	0.966400	-3.865611
C	4.420239	1.131986	4.584446
C	-0.550349	1.286500	3.992281
C	-2.524664	5.880968	-2.839842
H	-2.331233	6.091011	-3.890451
C	-5.355018	-1.898167	0.696237

H	-5.531132	-2.821455	0.145472
C	-6.296942	-0.671791	-1.273899
H	-5.988121	0.213057	-1.836154
H	-7.392062	-0.644584	-1.220713
H	-6.013217	-1.568920	-1.832165
C	-0.602214	-4.458673	3.105779
C	-6.325449	4.338372	-0.878086
H	-6.527452	5.329485	-1.277644
C	0.498996	-1.228551	-4.371329
C	-4.913203	0.466323	2.111918
C	-3.331029	5.182317	1.317757
H	-2.984627	6.056176	1.876736
H	-2.812735	4.313140	1.746075
H	-4.400183	5.052876	1.505366
C	-4.828080	1.685544	2.999366
H	-5.682245	1.686459	3.687872
H	-4.867289	2.622176	2.440072
H	-3.918001	1.669385	3.606010
C	-3.368640	-1.505098	-4.518368
H	-2.987544	-2.490823	-4.791078
H	-2.937378	-0.781803	-5.217049
H	-4.456492	-1.509695	-4.661925
C	-4.797724	-1.966742	1.978320
C	-2.085012	-3.406227	-2.104075
H	-2.164996	-3.836851	-3.103011
H	-2.715535	-3.996076	-1.427654
H	-1.045568	-3.521786	-1.775964
C	-4.568563	-0.779082	2.659914
H	-4.140888	-0.808698	3.659870
C	-0.436344	7.173121	-2.259544
H	-0.504096	7.541276	-3.286755
H	0.462300	6.548368	-2.188422
H	-0.290427	8.029926	-1.594360
C	-4.485619	-3.297962	2.601492
H	-5.411600	-3.814974	2.880272
H	-3.875293	-3.190085	3.500081
H	-3.950725	-3.955161	1.907378
F	-0.916680	2.508103	3.513023
F	-0.634635	1.361976	5.337589
F	-1.518474	0.416526	3.584352

Calculated energies and coordinates of [**3**]$^+$
Electronic energy ... -2098.97915889 Eh
Total Enthalpy ... -2098.13057677 Eh
Final Gibbs free energy ... -2098.25970783 Eh
CARTESIAN COORDINATES (ANGSTROEM)

Sn	-1.421963	9.642426	3.138694
O	0.638493	9.427200	4.079652
C	0.986204	8.193509	4.174196
O	0.344996	7.196885	3.851221
N	-0.770639	12.619960	4.605180
N	-2.651882	11.819946	5.237642
N	3.213466	8.903305	5.222179
N	2.953730	6.774601	4.882305
C	-0.681758	10.808159	1.348066
C	-1.658530	11.655387	0.781464
C	-1.420342	12.334429	-0.415504
H	-2.197323	12.973869	-0.828372
C	-0.213104	12.176151	-1.082956
H	-0.032260	12.692365	-2.021346
C	0.750640	11.330218	-0.553223
H	1.687210	11.174848	-1.084080
C	0.528659	10.641112	0.646863
C	-2.992247	11.833645	1.435469
C	-3.303596	13.043598	2.086343
C	-4.549417	13.196250	2.692185
H	-4.780255	14.135895	3.192591
C	-5.511471	12.187042	2.656676
C	-5.200501	11.006939	1.987828
H	-5.946585	10.216311	1.925321
C	-3.967136	10.818119	1.358241
C	-2.336183	14.197224	2.104544
H	-1.298930	13.856426	2.091419
H	-2.502416	14.828652	2.982564
H	-2.469882	14.826510	1.216117
C	-6.862866	12.382129	3.289172
H	-6.837283	13.153625	4.064828
H	-7.237320	11.454202	3.732880
H	-7.597979	12.700227	2.540348
C	-3.770199	9.577847	0.523109
H	-4.195031	8.698467	1.015968
H	-2.720087	9.382461	0.299765
H	-4.287518	9.699936	-0.436788
C	1.615632	9.712444	1.083350
C	2.853889	10.224164	1.515306
C	3.882329	9.343218	1.854388
H	4.838427	9.749721	2.184269
C	3.735620	7.962962	1.725690
C	2.514779	7.474972	1.267530
H	2.388478	6.403187	1.122017
C	1.450979	8.321407	0.949574
C	3.126541	11.706729	1.567421
H	3.860244	11.947972	2.344367
H	2.219301	12.291420	1.731685
H	3.548420	12.053683	0.616348
C	4.889609	7.033390	1.990710
H	4.546139	6.052397	2.336666
H	5.577485	7.445642	2.736069
H	5.466766	6.863131	1.073889
C	0.171416	7.718769	0.435773
H	-0.526853	7.508748	1.257527
H	0.370023	6.765543	-0.062210
H	-0.332143	8.384187	-0.269810
C	-1.574876	11.540412	4.468320
C	-1.340906	13.580500	5.433793
C	-2.542586	13.071789	5.832374
C	0.535434	12.758573	3.980947
H	1.317938	12.816390	4.745795
H	0.575642	13.664825	3.368379
H	0.704373	11.888046	3.347441
C	-0.678999	14.876847	5.725857
H	0.299137	14.737782	6.200538
H	-1.293828	15.471845	6.403454
H	-0.524692	15.464580	4.812875
C	-3.606504	13.638512	6.698927
H	-3.322322	14.633083	7.046912
H	-3.789191	13.015484	7.581823
H	-4.554289	13.731626	6.155748
C	-3.798846	10.940188	5.440460
H	-3.872540	10.657052	6.495516
H	-3.669034	10.042324	4.833581
H	-4.716368	11.444098	5.126112
C	2.353452	7.975868	4.755008
C	4.379901	8.287622	5.637665
C	4.213636	6.942061	5.425996
C	2.979172	10.348676	5.255140
H	2.086136	10.566068	5.843185
H	2.832327	10.711599	4.236744
H	3.849405	10.825745	5.705831
C	5.540032	9.030079	6.194113
H	6.339380	8.332778	6.447475
H	5.276606	9.574138	7.107861
H	5.946065	9.747852	5.472677
C	5.145165	5.814963	5.685037
H	4.711407	5.077718	6.369012
H	6.062222	6.188275	6.142186
H	5.423809	5.300954	4.758227
C	2.387697	5.479160	4.483315
H	1.505265	5.253652	5.083910
H	3.151789	4.716591	4.632537
H	2.086816	5.520183	3.436308

Calculated energies and coordinates of [**3**][BArF]
Electronic energy ... -5746.88680094 Eh
Total Enthalpy ... -5745.58602844 Eh
Final Gibbs free energy ... -5745.81592677 Eh
CARTESIAN COORDINATES (ANGSTROEM)

Sn	-2.865784	-0.624782	-0.004643
O	-1.415617	-2.256964	-0.671147
C	-0.687717	-2.561844	0.341950
O	-0.800680	-2.121438	1.485101
N	-3.192692	-0.941812	-3.357695

N	-2.716948	1.064572	-2.786159
N	0.569378	-4.415602	-0.924000
N	1.315941	-3.906454	1.049099
C	-4.728598	-1.921435	-0.117229
C	-5.896263	-1.160525	-0.334105
C	-7.154620	-1.764155	-0.401020
H	-8.033402	-1.144834	-0.567833
C	-7.281310	-3.136817	-0.233767
H	-8.259128	-3.608573	-0.276398
C	-6.148562	-3.897207	0.023000
H	-6.239277	-4.967477	0.197239
C	-4.878663	-3.307328	0.090429
C	-5.815127	0.328016	-0.454941
C	-5.966206	0.958847	-1.701512
C	-5.854067	2.348221	-1.782672
H	-5.962160	2.828922	-2.754493
C	-5.621686	3.131625	-0.654828
C	-5.536188	2.495878	0.583336
H	-5.390994	3.095050	1.479270
C	-5.635940	1.111380	0.706484
C	-6.291285	0.173834	-2.944504
H	-5.918695	-0.850627	-2.883042
H	-5.870681	0.655384	-3.832960
H	-7.377779	0.110102	-3.084615
C	-5.454073	4.622346	-0.759030
H	-5.744975	4.991496	-1.746667
H	-4.410361	4.910378	-0.580271
H	-6.055855	5.142692	-0.006922
C	-5.594467	0.482719	2.074757
H	-4.619737	0.024455	2.284978
H	-6.345297	-0.307499	2.170582
H	-5.771270	1.235824	2.846703
C	-3.747366	-4.207556	0.471142
C	-3.296633	-5.225310	-0.387812
C	-2.280957	-6.084923	0.040384
H	-1.947738	-6.880015	-0.627473
C	-1.715115	-5.978839	1.307740
C	-2.197404	-4.986849	2.158996
H	-1.787445	-4.896589	3.163539
C	-3.206233	-4.107858	1.769160
C	-3.888537	-5.451582	-1.757539
H	-4.371985	-6.434345	-1.808867
H	-3.111415	-5.439556	-2.532060
H	-4.640604	-4.703331	-2.010440
C	-0.662723	-6.948211	1.776498
H	0.031720	-6.472084	2.476610
H	-0.084360	-7.352874	0.939552
H	-1.119110	-7.796381	2.301493
C	-3.714090	-3.092282	2.754149
H	-3.238952	-2.117952	2.594591
H	-3.475949	-3.395430	3.776711
H	-4.795034	-2.952643	2.664578
C	-2.930665	-0.170577	-2.278552
C	-3.150815	-0.203242	-4.533128
C	-2.851609	1.076666	-4.168200
C	-3.456171	-2.369700	-3.304143
H	-4.460675	-2.591465	-3.681858
H	-3.389441	-2.692630	-2.265940
H	-2.719973	-2.910869	-3.907987
C	-3.382222	-0.812566	-5.866196
H	-3.325715	-0.049220	-6.644460
H	-4.369485	-1.285709	-5.930482
H	-2.628833	-1.576493	-6.093895
C	-2.632341	2.300475	-4.978340
H	-1.596379	2.649972	-4.901681
H	-3.281834	3.121753	-4.654230
H	-2.842542	2.100155	-6.030665
C	-2.355799	2.247215	-2.010975
H	-1.397606	2.641844	-2.359129
H	-2.271132	1.975662	-0.956536
H	-3.128465	3.015160	-2.112300
C	0.392827	-3.578042	0.118523
C	1.599757	-5.290929	-0.647708
C	2.071901	-4.970345	0.598507
C	-0.195892	-4.463645	-2.167199
H	-0.585764	-5.475793	-2.303715
H	0.458141	-4.201393	-3.003999
H	-1.010256	-3.747092	-2.099732
C	2.022039	-6.341897	-1.605113
H	2.284294	-5.911646	-2.577489
H	1.231446	-7.084828	-1.765537
H	2.903058	-6.861960	-1.227367
C	3.140587	-5.611773	1.404350
H	3.581891	-6.435364	0.841095
H	2.740233	-6.020089	2.339336
H	3.944448	-4.912838	1.651616
C	1.547819	-3.215101	2.325498
H	1.602932	-2.139908	2.153466
H	2.492553	-3.569886	2.737284
H	0.725149	-3.412077	3.015743
B	2.126787	1.327969	0.665634
F	-2.775187	3.818338	1.572214
F	-1.310868	4.844404	2.811311
F	-2.241310	5.884516	1.137946
F	-0.088939	4.446043	-3.674403
F	2.040294	4.619189	-3.252376
F	0.688456	6.243775	-2.726873
F	4.702486	-3.155413	0.080794
F	5.545443	-2.320991	-1.739832
F	4.173103	-4.002253	-1.860490
F	-0.339672	-1.760731	-3.815732
F	1.417459	-1.138225	-4.925984
F	0.111698	0.358713	-4.035059
F	7.171226	0.988062	-1.382782
F	6.256979	2.512636	-2.633513
F	7.895364	3.041232	-1.297980
C	5.315360	4.779615	2.695817
F	6.630428	4.915633	2.990982
F	4.671724	4.503349	3.852069
F	4.880872	6.001616	2.288656
F	4.977481	0.023598	4.865431
F	4.342872	-2.030308	4.523917
F	3.653393	-0.957569	6.289580
C	-1.001536	-0.527445	4.380510
F	-1.202916	-1.865824	4.543022
F	-1.983974	-0.067059	3.581653
F	-1.192374	0.027715	5.605815
C	1.105229	2.535910	0.235833
C	0.111681	3.094098	1.043317
H	-0.078494	2.686894	2.032165
C	-0.642926	4.198522	0.631731
C	-0.421380	4.802598	-0.595287
H	-0.993627	5.669959	-0.905467
C	0.583975	4.277047	-1.408406
C	1.321735	3.173115	-1.002638
H	2.118252	2.812518	-1.649135
C	-1.731240	4.695553	1.536528
C	0.822689	4.899129	-2.752201
C	2.125767	0.108010	-0.432413
C	3.082677	-0.912983	-0.314883
H	3.740610	-0.923136	0.551719
C	3.265397	-1.874444	-1.305495
C	2.486775	-1.864027	-2.459344
H	2.673333	-2.569017	-3.263133
C	1.500184	-0.891124	-2.573175
C	1.310580	0.060807	-1.569878
H	0.542645	0.816750	-1.704735
C	4.415026	-2.831392	-1.204973
C	0.680019	-0.848032	-3.827250
C	3.598154	2.061816	0.649643
C	4.576650	1.865647	-0.325630
H	4.415165	1.141081	-1.120900
C	5.779990	2.577398	-0.317109
C	6.047469	3.514630	0.667706
H	6.983391	4.060785	0.681716
C	5.077300	3.731143	1.646781
C	3.879821	3.028282	1.630759
H	3.141881	3.227726	2.404939
C	6.778269	2.288791	-1.399461
C	1.854976	0.667747	2.137019
C	0.569212	0.347118	2.606843
H	-0.299296	0.533370	1.981896
C	0.372932	-0.234771	3.856141
C	1.451433	-0.587582	4.663356

H	1.292730	-1.045986	5.634257
C	2.731610	-0.335060	4.191595
C	2.925608	0.299491	2.964201
H	3.942616	0.520511	2.650340
C	3.921088	-0.807084	4.973460

Calculated energies and coordinates of [**3a**]$^+$
Electronic energy ... -1715.59126734 Eh
Total Enthalpy ... -1714.93782488 Eh
Final Gibbs free energy ... -1715.04629365 Eh
CARTESIAN COORDINATES (ANGSTROEM)

Sn	-1.358324	9.548407	3.279070
O	0.772151	9.531429	4.314947
C	0.941687	8.327618	3.967919
O	0.111723	7.690510	3.258428
N	3.144948	8.156018	5.180262
N	2.496821	6.352110	4.146399
C	-0.596171	10.369707	1.363533
C	-1.643965	11.094498	0.752705
C	-1.472481	11.726212	-0.476205
H	-2.298878	12.276335	-0.919561
C	-0.244905	11.646710	-1.122435
H	-0.098347	12.135266	-2.081554
C	0.798421	10.939781	-0.537399
H	1.760824	10.877333	-1.040932
C	0.642163	10.298658	0.698041
C	-2.953767	11.168649	1.467513
C	-3.183346	12.196137	2.403593
C	-4.370064	12.188541	3.136145
H	-4.546700	12.979135	3.862592
C	-5.336708	11.198560	2.957596
C	-5.101723	10.206369	2.006562
H	-5.853366	9.436726	1.844230
C	-3.928517	10.175881	1.251655
C	-2.178678	13.301203	2.598058
H	-1.159319	12.916659	2.715494
H	-2.427235	13.907824	3.471974
H	-2.155562	13.961012	1.722750
C	-6.590963	11.192561	3.785698
H	-6.921418	12.209723	4.014075
H	-6.420337	10.681351	4.740901
H	-7.404570	10.671784	3.274065
C	-3.725276	9.107997	0.209294
H	-4.477911	8.321535	0.301770
H	-2.730735	8.652482	0.273414
H	-3.801040	9.532329	-0.798839
C	1.853088	9.579924	1.203458
C	2.819060	10.277820	1.947514
C	4.023468	9.645063	2.264124
H	4.784871	10.202678	2.808533
C	4.298820	8.341918	1.851175
C	3.318709	7.659902	1.130876
H	3.522961	6.648686	0.780466
C	2.102686	8.259252	0.794510
C	2.573199	11.697581	2.378975
H	3.436399	12.104682	2.912836
H	1.695530	11.761688	3.032339
H	2.371463	12.343253	1.517711
C	5.644653	7.718300	2.106512
H	5.578770	6.628370	2.182266
H	6.103144	8.104079	3.022455
H	6.334096	7.941906	1.283495
C	1.085034	7.504832	-0.016455
H	0.141298	7.407075	0.532216
H	1.445303	6.504805	-0.273457
H	0.853240	8.031185	-0.948476
C	2.157444	7.627147	4.428297
C	4.132313	7.212240	5.364598
C	3.722511	6.071649	4.710867
C	3.185580	9.525843	5.708524
H	2.340098	9.691973	6.377988
H	3.129333	10.234879	4.881549
H	4.121054	9.653450	6.251560
C	5.371798	7.471596	6.139835
H	6.009390	6.587066	6.129954
H	5.153388	7.710381	7.186478
H	5.949050	8.299122	5.713259
C	4.395859	4.754564	4.582358
H	3.802647	3.949946	5.030520
H	5.359069	4.777218	5.092983
H	4.584120	4.497968	3.534150
C	1.705390	5.406461	3.348490
H	0.737932	5.236945	3.823749
H	2.257768	4.469961	3.284225
H	1.544636	5.819062	2.351641

Calculated energies and coordinates of [**3a**][BArF]
Electronic energy ... -5363.49812873 Eh
Total Enthalpy ... -5362.39235147 Eh
Final Gibbs free energy ... -5362.60276821 Eh
CARTESIAN COORDINATES (ANGSTROEM)

Sn	-2.312789	2.433152	0.026458
F	6.074535	1.260299	-2.779122
F	1.278923	-6.749500	1.013093
F	7.629941	-0.264075	-2.846080
F	5.715696	-0.610758	-3.825564
F	2.668723	-5.754605	-0.336008
F	0.551081	-5.860423	-0.836596
F	1.351962	-1.789122	-5.006630
F	-2.162863	-3.874963	3.284502
F	-0.854358	3.329856	-3.053725
F	1.188502	3.488528	-3.777192
N	-2.401209	-2.362755	-1.638139
F	4.540105	2.942507	5.144741
F	-1.653347	-1.791089	3.667808
N	-3.322766	-1.315617	-3.307106
F	0.745179	3.909008	-1.688429
C	1.557976	-1.966675	1.044173
C	2.291327	0.553958	1.615043
C	3.814869	-0.955340	0.011923
C	1.468958	-0.111513	-0.884156
C	3.444615	0.897495	2.328536
H	4.389642	0.421198	2.080823
C	5.743836	-0.677453	-1.460424
C	1.838607	-3.225936	0.487336
H	2.608801	-3.312013	-0.274995
C	1.176432	-4.381677	0.897573
C	1.235709	1.239934	-1.185474
H	1.518048	2.002545	-0.466049
C	-2.764340	-1.144455	-2.088897
C	4.625031	-1.781260	0.804498
H	4.211248	-2.228700	1.706954
C	0.588356	-1.946927	2.056876
H	0.337502	-1.009094	2.541729
F	-0.771079	-1.328823	-4.943365
C	1.112114	-1.032918	-1.878165
H	1.292940	-2.091689	-1.713262
C	4.416089	-0.409875	-1.127218
H	3.840685	0.243612	-1.779099
C	1.115638	1.228629	1.986723
H	0.190729	1.015525	1.453476
F	6.175563	-4.180543	1.478193
C	5.951311	-2.050254	0.475397
C	0.205202	-4.334412	1.891429
H	-0.312043	-5.233386	2.210918
C	3.427600	1.836903	3.360062
C	0.669207	1.638514	-2.395924
F	5.345151	1.028463	4.484433
C	6.297893	-0.075888	-2.719305
C	-1.725590	-2.649072	-0.367566
H	-1.396037	-3.686937	-0.382972
H	-2.414247	-2.473356	0.461652
H	-0.861039	-1.995065	-0.256311
C	1.093776	2.163667	3.018844
C	-0.081389	-3.099735	2.463647
C	1.437554	-5.683184	0.199481
F	0.051235	-2.890135	-3.658794
C	6.528904	-1.503551	-0.665574
H	7.559174	-1.714393	-0.924846
C	-4.488299	2.694916	0.464460
C	0.446610	3.089693	-2.714923
C	0.325430	0.705573	-3.368581

H	-0.099665	1.021621	-4.316168
F	-0.636704	-3.378750	4.754481
C	2.253756	2.481031	3.721218
H	2.238507	3.205361	4.527216
B	2.280483	-0.606202	0.461740
C	0.558291	-0.637626	-3.095403
C	-5.533532	1.792519	0.717984
F	5.586064	2.794627	3.240015
C	-2.739408	-3.318446	-2.570083
F	6.801072	-2.456326	2.645130
C	-4.768859	4.075064	0.493697
C	-3.645511	5.002200	0.162470
C	-2.890004	5.589731	1.197092
C	-3.274890	5.199326	-1.183843
F	8.012599	-3.128108	0.963599
C	-6.807976	2.280638	1.030492
H	-7.606707	1.571102	1.236443
C	-3.321744	-2.657179	-3.623880
C	-1.759512	6.332469	0.867918
H	-1.160850	6.762473	1.668422
C	-4.111979	4.651900	-2.312451
H	-4.369148	3.598138	-2.165821
H	-3.587247	4.752470	-3.265685
H	-5.061152	5.196960	-2.382382
C	-5.362614	0.312436	0.629838
C	6.740716	-2.949169	1.382946
C	-7.061165	3.646804	1.079856
H	-8.056534	4.005322	1.327467
C	-5.792423	-0.356251	-0.528287
C	-1.356751	6.512841	-0.456514
C	-3.810143	-0.285845	-4.227557
H	-3.191770	-0.298405	-5.129853
H	-3.739329	0.685321	-3.744919
H	-4.848566	-0.502385	-4.491694
C	4.718653	2.151462	4.061770
C	-0.171112	2.891892	3.348263
C	-2.132186	5.952045	-1.466989
H	-1.835905	6.088507	-2.504449
C	-5.669422	-1.745134	-0.600060
H	-6.006293	-2.261535	-1.498764
C	-6.378788	0.408266	-1.685758
H	-5.714659	1.221217	-2.000668
H	-7.332819	0.873831	-1.415122
H	-6.560475	-0.254394	-2.537340
C	-1.123399	-3.029236	3.541766
C	-6.042487	4.550638	0.799037
H	-6.231802	5.621594	0.810796
C	0.305953	-1.655703	-4.165230
C	-4.823493	-0.416601	1.700797
C	-3.276753	5.385261	2.636655
H	-4.247411	5.844546	2.854812
H	-2.530321	5.817841	3.306379
H	-3.376402	4.320048	2.875995
C	-4.318666	0.275770	2.935614
H	-4.289538	-0.409939	3.786094
H	-4.933315	1.142113	3.195499
H	-3.294975	0.638642	2.782132
C	-3.826363	-3.162551	-4.923433
H	-3.741681	-4.249032	-4.962091
H	-3.245388	-2.751552	-5.757230
H	-4.878334	-2.900333	-5.081792
C	-5.154796	-2.487642	0.461968
C	-2.426038	-4.759080	-2.406047
H	-2.840290	-5.326203	-3.240830
H	-2.847880	-5.163943	-1.480635
H	-1.344071	-4.928714	-2.388061
C	-4.735663	-1.805687	1.602857
H	-4.328378	-2.367287	2.441939
C	-0.095321	7.265841	-0.773184
H	-0.035902	7.518629	-1.834880
H	0.784066	6.659763	-0.525555
H	-0.028936	8.190978	-0.191783
C	-5.084231	-3.989749	0.396854
H	-5.917639	-4.443100	0.946795
H	-4.161601	-4.368823	0.850839
H	-5.142044	-4.347049	-0.636413
F	-0.314324	4.025199	2.607125
F	-0.239687	3.266920	4.642201
F	-1.283919	2.138158	3.099001
O	-2.896221	1.219068	-1.899861
C	-2.642625	0.117600	-1.322580
O	-2.295717	0.047782	-0.114246

Calculated energies and coordinates of [**4**]$^+$

Electronic energy ... -2287.56604510 Eh

Total Enthalpy ... -2286.70013232 Eh

Final Gibbs free energy ... -2286.83832856 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Sn	3.390065	11.977764	8.063714
O	1.687531	13.180963	8.932262
O	3.036134	12.827292	10.687914
O	2.367100	12.437654	6.064367
O	0.381805	11.460423	6.567078
C	4.669595	13.767370	7.589197
C	4.521501	15.138350	7.867123
C	5.420372	16.066954	7.322798
H	5.286239	17.122409	7.551976
C	6.475505	15.660444	6.516820
H	7.163299	16.394599	6.106449
C	6.656454	14.307369	6.261881
H	7.494134	13.964630	5.658513
C	5.766921	13.373189	6.795319
C	3.479049	15.720228	8.771915
C	3.799358	15.958436	10.119061
C	2.879369	16.624735	10.932807
H	3.145978	16.833078	11.968406
C	1.651365	17.066716	10.444230
C	1.345791	16.808116	9.108775
H	0.399150	17.161406	8.700772
C	2.241127	16.146457	8.267314
C	5.116660	15.503730	10.684400
H	5.207671	14.413761	10.617267
H	5.220519	15.800971	11.731958
H	5.957095	15.926890	10.124566
C	0.712094	17.861061	11.311891
H	-0.335375	17.657653	11.065994
H	0.873056	18.937194	11.174209
H	0.865992	17.644517	12.373648
C	1.867332	15.871914	6.838569
H	0.953024	16.404715	6.559586
H	1.707630	14.795907	6.699606
H	2.669987	16.170567	6.155402
C	6.005755	11.918377	6.538455
C	5.669028	11.339597	5.303240
C	5.868076	9.971349	5.113275
H	5.598013	9.526492	4.156956
C	6.417979	9.166834	6.107392
C	6.782670	9.764419	7.314142
H	7.234233	9.154525	8.094353
C	6.585978	11.122644	7.548695
C	5.126885	12.177602	4.176450
H	5.944240	12.584267	3.567448
H	4.552950	13.022324	4.561005
H	4.488274	11.578281	3.518438
C	6.607470	7.689769	5.898361
H	6.553161	7.424886	4.838995
H	5.833003	7.120012	6.425872
H	7.574959	7.355841	6.285875
C	6.986266	11.720517	8.871545
H	7.480884	12.687748	8.741084
H	7.658464	11.048201	9.410548
H	6.113301	11.898351	9.515051
C	1.980334	13.224330	10.172318
C	1.224620	11.928924	5.804815
N	-0.336533	14.121186	10.687547
H	-0.484774	14.678290	8.666282
H	-1.999119	14.100927	9.432190
H	-0.707012	12.948963	8.973513
H	-1.763198	10.178856	1.804325
N	1.062407	14.105082	12.352313
H	3.135185	14.312393	12.602308
H	2.446351	12.853297	13.333330
H	2.154998	14.446934	14.093681
H	2.396401	14.038746	4.572468

C	0.921016	13.796409	11.048599
H	-1.433032	9.992702	4.749620
C	-0.998040	14.663477	11.773139
H	-2.532504	15.916538	10.948933
H	-2.690226	15.572935	12.672034
H	-3.101951	14.326942	11.493454
H	0.543397	14.208997	1.025549
C	-0.114758	14.652516	12.824659
H	0.395442	15.935863	14.468324
H	-0.117471	14.305576	14.943025
H	-1.305684	15.479352	14.374360
C	-0.922930	13.948469	9.351438
C	-0.742394	10.356818	1.450103
H	-0.807351	10.827628	0.468170
H	-0.255064	9.383885	1.318331
C	0.900644	13.179459	0.912992
H	1.958209	13.221379	0.628734
H	0.352825	12.724967	0.086516
C	1.994072	14.024045	3.561809
H	2.816568	14.066013	2.843342
H	1.327260	14.877698	3.404256
C	-2.402659	15.141637	11.712395
H	-0.461888	8.949875	3.666050
C	-0.288618	15.114988	14.225177
H	0.189508	9.485668	5.242257
C	2.280201	13.916938	13.149585
N	0.148837	10.945456	3.733036
N	1.246855	12.778519	3.370664
C	0.898104	11.894602	4.325971
C	0.014598	11.229793	2.382391
C	0.701273	12.392335	2.155398
C	-0.425821	9.765993	4.389533

Calculated energies and coordinates of [**4**][BArF]
Electronic energy ... -5935.48159210 Eh
Total Enthalpy ... -5934.16336500 Eh
Final Gibbs free energy ... -5934.39940847 Eh
CARTESIAN COORDINATES (ANGSTROEM)

Sn	-4.367022	1.282271	0.664131
F	3.098727	-2.519958	4.977083
F	3.781768	-3.778354	3.334340
F	5.098295	-2.255087	4.160881
F	0.970859	2.159259	-5.352165
F	1.848459	0.273678	-5.998057
F	2.918803	2.142381	-6.324397
F	-1.494899	-5.792929	-0.745920
F	0.288733	-6.104515	-1.952200
F	0.476496	-5.789486	0.188495
F	-1.939046	0.146122	-2.830841
F	-2.708419	-1.749712	-3.567523
F	-3.248159	-1.071486	-1.577269
F	3.859541	-5.844031	-3.734189
F	5.848273	-5.470630	-4.541463
F	4.153153	-4.277432	-5.212334
O	-3.078969	-0.270524	1.580766
O	-4.789394	-1.619662	1.043502
O	-2.578556	2.648982	1.069414
O	-1.190994	1.367117	-0.182506
C	-5.255619	1.983057	2.618928
C	-5.194053	1.433388	3.912151
C	-5.814449	2.083990	4.987337
H	-5.750973	1.637745	5.978010
C	-6.507395	3.273372	4.802208
H	-6.983542	3.765469	5.646110
C	-6.599885	3.818076	3.527564
H	-7.156183	4.737700	3.357679
C	-5.987482	3.176592	2.449269
C	-4.513808	0.141157	4.235750
C	-3.168453	0.130138	4.635084
C	-2.579278	-1.071834	5.026429
H	-1.538896	-1.071828	5.350239
C	-3.297950	-2.267289	5.034792
C	-4.626874	-2.239729	4.617041
H	-5.205884	-3.162358	4.617072
C	-5.248651	-1.053633	4.219757
C	-2.361504	1.396966	4.600008
H	-1.357272	1.241075	5.004159
H	-2.849559	2.196636	5.168154
H	-2.269781	1.748823	3.565316
C	-2.671425	-3.540997	5.536988
H	-3.174903	-4.422320	5.126518
H	-2.744180	-3.605825	6.629698
H	-1.609255	-3.599394	5.277910
C	-6.683105	-1.066756	3.768017
H	-6.755351	-0.774123	2.714644
H	-7.288965	-0.357379	4.341697
H	-7.118549	-2.064008	3.875875
C	-6.137516	3.765219	1.081349
C	-7.113201	3.248969	0.205542
C	-7.227161	3.782190	-1.076234
H	-7.979494	3.377925	-1.751032
C	-6.397733	4.812683	-1.517756
C	-5.455029	5.326890	-0.631239
H	-4.810494	6.143364	-0.953190
C	-5.319055	4.827829	0.664899
C	-8.011867	2.120641	0.634149
H	-8.396969	2.277302	1.646431
H	-7.469977	1.164822	0.650395
H	-8.853310	2.010630	-0.054769
C	-6.507305	5.335539	-2.924112
H	-7.549867	5.370762	-3.254909
H	-5.965805	4.685916	-3.622669
H	-6.085117	6.340783	-3.010838
C	-4.321147	5.446474	1.605948
H	-4.800733	6.203293	2.239734
H	-3.516888	5.936438	1.047038
H	-3.887704	4.694008	2.267986
N	-1.395887	-2.477431	1.979643
N	-3.065944	-3.857382	1.840927
C	-2.715045	-2.560067	1.711923
C	-0.908746	-3.728244	2.302183
C	-1.962075	-4.600969	2.208444
C	-0.561543	-1.270687	1.932438
H	0.480526	-1.587185	1.922704
H	-0.766556	-0.648770	2.807504
H	-0.782164	-0.694046	1.034400
C	0.499758	-3.968415	2.699017
H	1.195346	-3.728354	1.888194
H	0.642725	-5.018147	2.957924
H	0.775701	-3.362462	3.569510
C	-2.030397	-6.062312	2.452096
H	-2.482709	-6.586977	1.604759
H	-2.615301	-6.295387	3.350270
H	-1.025647	-6.463731	2.588911
C	-4.397182	-4.436260	1.654052
H	-4.413327	-5.019620	0.727513
H	-5.122881	-3.627879	1.588443
H	-4.618321	-5.091722	2.500529
N	-0.328629	4.562766	1.125436
N	0.193417	3.800034	-0.836155
C	-0.585108	3.579143	0.241346
C	0.643208	5.406257	0.612604
C	0.962634	4.933169	-0.631457
C	-0.868395	4.687552	2.479592
H	-1.611133	3.908572	2.636240
H	-1.340763	5.667282	2.592172
H	-0.054980	4.584198	3.203712
C	1.185706	6.551139	1.384138
H	0.401942	7.267215	1.655574
H	1.932952	7.080222	0.791056
H	1.668590	6.212696	2.308223
C	1.893394	5.458634	-1.660693
H	2.582136	6.179009	-1.216580
H	1.352682	5.960116	-2.472802
H	2.491514	4.656357	-2.099943
C	0.239213	3.000449	-2.067067
H	-0.685191	2.437252	-2.174226
H	1.079383	2.299957	-2.020500
H	0.374716	3.672225	-2.916554
C	-3.627334	-1.412679	1.412693
C	-1.523015	2.406131	0.386886
C	2.833889	-0.865066	0.523848
C	2.300614	0.326486	1.028942

H	1.876098	1.054436	0.340413
C	2.294311	0.610368	2.393849
C	2.779677	-0.305295	3.319620
H	2.769816	-0.088704	4.382022
C	3.275562	-1.514763	2.839872
C	3.312879	-1.781283	1.472869
H	3.727247	-2.727852	1.134419
C	1.694860	1.900358	2.852398
F	1.994236	2.205432	4.132549
F	2.092976	2.954825	2.089383
F	0.330916	1.875924	2.769417
C	3.815136	-2.516385	3.820849
C	3.002647	0.125976	-1.982692
C	2.508488	0.234755	-3.292877
H	1.888344	-0.560480	-3.698395
C	2.792647	1.335304	-4.097145
C	3.607322	2.369315	-3.639948
H	3.836706	3.218911	-4.273451
C	4.129063	2.266262	-2.356536
C	3.830674	1.168887	-1.548687
H	4.266539	1.127672	-0.552823
C	2.146089	1.464603	-5.445603
C	5.038793	3.325430	-1.806274
F	4.592041	3.786148	-0.602430
F	6.291273	2.866292	-1.598977
F	5.136351	4.404116	-2.621168
C	1.325256	-1.928323	-1.296903
C	1.140662	-3.285740	-1.001124
H	1.991236	-3.880447	-0.672251
C	-0.097953	-3.912716	-1.151234
C	-1.199185	-3.206384	-1.616918
H	-2.153960	-3.696620	-1.777197
C	-1.038830	-1.853607	-1.905288
C	0.189005	-1.225005	-1.725873
H	0.260507	-0.163325	-1.936214
C	-0.206982	-5.389875	-0.917869
C	-2.223901	-1.119691	-2.464623
C	4.011227	-2.189520	-1.528900
C	3.878392	-3.115855	-2.569852
H	2.909405	-3.256133	-3.044885
C	4.956816	-3.873437	-3.023582
C	6.219210	-3.730665	-2.460101
H	7.057103	-4.321225	-2.809715
C	6.375139	-2.799005	-1.439321
C	5.295292	-2.043624	-0.988777
H	5.465490	-1.318512	-0.194831
C	4.714860	-4.863716	-4.125940
C	7.708539	-2.601771	-0.778263
F	7.692383	-3.029817	0.511880
F	8.704528	-3.267994	-1.402154
F	8.062522	-1.293168	-0.742003
B	2.781131	-1.214606	-1.071541

Calculated energies and coordinates of **TS(2_3)**

Electronic energy ... -2098.92836904 Eh
Total Enthalpy ... -2098.08225296 Eh
Final Gibbs free energy ... -2098.21135727 Eh
CARTESIAN COORDINATES (ANGSTROEM)

Sn	-0.956589	-0.755452	-0.022301
O	0.485229	-0.105657	3.701418
C	-0.095057	-0.985842	3.119054
O	-1.099869	-1.657148	3.128254
N	-0.700064	2.299405	1.366265
N	-2.365575	1.188691	2.136757
N	2.298955	-1.139440	1.729774
N	1.130081	-2.938469	1.559218
C	-0.248032	0.379242	-1.833361
C	-1.301484	1.097408	-2.440084
C	-1.120305	1.748631	-3.660182
H	-1.950874	2.290987	-4.106211
C	0.105974	1.679022	-4.309801
H	0.248399	2.174878	-5.265527
C	1.137543	0.940006	-3.747819
H	2.083394	0.843030	-4.275349
C	0.973969	0.280138	-2.520937
C	-2.647032	1.112685	-1.787445
C	-3.142369	2.279593	-1.172561
C	-4.369696	2.237988	-0.514259
H	-4.739117	3.143522	-0.034832
C	-5.139170	1.075883	-0.460089
C	-4.659376	-0.059334	-1.105701
H	-5.262300	-0.965778	-1.111329
C	-3.439414	-0.059308	-1.789819
C	-2.400116	3.587471	-1.236346
H	-1.344479	3.447312	-1.472250
H	-2.495204	4.135196	-0.293051
H	-2.820912	4.224599	-2.023847
C	-6.474371	1.063444	0.231978
H	-6.530819	1.827864	1.012749
H	-6.686020	0.088125	0.680701
H	-7.279729	1.271855	-0.482426
C	-3.092646	-1.261877	-2.634344
H	-3.400569	-2.191242	-2.146463
H	-2.029901	-1.321810	-2.874928
H	-3.632942	-1.196970	-3.587186
C	2.124024	-0.557142	-2.065493
C	3.349149	0.046053	-1.726627
C	4.466814	-0.755599	-1.486488
H	5.417312	-0.276015	-1.255059
C	4.409729	-2.143519	-1.583469
C	3.184734	-2.726982	-1.900184
H	3.125765	-3.808904	-2.008402
C	2.046602	-1.962274	-2.156318
C	3.509515	1.545022	-1.677278
H	4.314408	1.829511	-0.992240
H	2.588635	2.049282	-1.373885
H	3.771912	1.945873	-2.663387
C	5.644445	-2.987059	-1.422002
H	5.415914	-3.953730	-0.961687
H	6.405052	-2.483673	-0.818448
H	6.093677	-3.197396	-2.399978
C	0.795087	-2.655384	-2.627704
H	0.017545	-2.691098	-1.852424
H	1.012197	-3.686201	-2.919588
H	0.357258	-2.137468	-3.486843
C	-1.339028	1.108926	1.260214
C	-1.315192	3.118527	2.303858
C	-2.376411	2.411654	2.791133
C	0.479447	2.701903	0.613683
H	1.326330	2.869195	1.286860
H	0.281812	3.628617	0.067724
H	0.717153	1.916312	-0.105518
C	-0.813508	4.477154	2.629094
H	0.209724	4.446414	3.020618
H	-1.444197	4.938673	3.390516
H	-0.816214	5.134224	1.751368
C	-3.397957	2.761732	3.808907
H	-3.210217	3.761121	4.204426
H	-3.382542	2.060096	4.650204
H	-4.408775	2.753992	3.384753
C	-3.364331	0.153726	2.389982
H	-3.276989	-0.205057	3.418613
H	-3.192336	-0.683530	1.712923
H	-4.363294	0.558983	2.209359
C	1.003552	-1.575911	1.690344
C	3.194713	-2.175036	1.652231
C	2.448192	-3.323302	1.524306
C	2.693162	0.251813	1.891501
H	3.340389	0.359038	2.766872
H	1.794368	0.838501	2.056425
H	3.219472	0.589156	0.992417
C	4.657876	-1.982798	1.790732
H	5.188009	-2.911003	1.573248
H	4.916064	-1.679560	2.812761
H	5.024429	-1.215107	1.103027
C	2.878003	-4.734482	1.370655
H	2.586815	-5.346742	2.232133
H	3.963973	-4.787925	1.278007
H	2.440820	-5.188336	0.474119
C	0.018181	-3.875959	1.428739
H	-0.884496	-3.405116	1.811781
H	0.234645	-4.777331	2.007135

H	-0.120931	-4.144507	0.374632

Calculated energies and coordinates of **TS(3_4)**

Electronic energy ... -2287.52986583 Eh
Total Enthalpy ... -2286.66645624 Eh
Final Gibbs free energy ... -2286.80125225 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Sn	0.658985	-1.257593	0.201077
O	-1.075959	0.156470	0.739824
O	-0.005579	-0.533203	2.563227
O	-3.396481	-1.245895	-0.922361
O	-2.156917	-2.576732	0.481773
C	1.991910	0.479271	-0.337772
C	2.069562	1.794436	0.167137
C	3.114713	2.639315	-0.225070
H	3.149405	3.649788	0.176784
C	4.103161	2.205230	-1.098705
H	4.910448	2.872886	-1.386020
C	4.054414	0.909063	-1.591175
H	4.825346	0.544372	-2.266480
C	3.014635	0.056398	-1.213827
C	1.102834	2.390950	1.141197
C	1.356290	2.303465	2.520361
C	0.512033	2.971335	3.410165
H	0.727997	2.926740	4.476823
C	-0.572817	3.727477	2.968041
C	-0.805334	3.804189	1.595710
H	-1.630808	4.412821	1.227297
C	0.025026	3.160015	0.677111
C	2.530253	1.518870	3.037292
H	2.428729	0.455486	2.794157
H	2.621659	1.615426	4.122559
H	3.465284	1.861847	2.582198
C	-1.425535	4.498354	3.939935
H	-1.049915	5.522081	4.056970
H	-1.420954	4.037911	4.932900
H	-2.462516	4.572412	3.596799
C	-0.208583	3.333711	-0.798384
H	0.428859	4.132295	-1.198014
H	-1.247112	3.607961	-1.010526
H	0.047087	2.424771	-1.348013
C	3.018101	-1.331185	-1.774371
C	2.538444	-1.554849	-3.075739
C	2.590086	-2.843123	-3.609848
H	2.242391	-3.005086	-4.628567
C	3.112706	-3.914735	-2.888230
C	3.606685	-3.669901	-1.605917
H	4.046531	-4.488986	-1.040148
C	3.582279	-2.395501	-1.041499
C	2.038506	-0.411274	-3.915397
H	2.869379	0.224439	-4.242919
H	1.359391	0.235823	-3.349983
H	1.527389	-0.781763	-4.807306
C	3.155291	-5.300284	-3.473392
H	2.976355	-5.285178	-4.552111
H	2.398541	-5.949839	-3.014639
H	4.126391	-5.773655	-3.298540
C	4.183522	-2.161305	0.317677
H	4.886330	-1.322050	0.297554
H	4.708288	-3.051860	0.670946
H	3.420677	-1.908214	1.067188
C	-0.950960	0.059032	2.002268
C	-2.494030	-1.880838	-0.439578
N	-3.115483	1.308242	2.416067
H	-3.612952	0.552558	0.508412
H	-2.743991	2.109035	0.514340
H	-4.461131	2.043728	1.006817
H	-1.440123	-4.803181	-4.505886
N	-2.015743	0.694134	4.191193
H	-0.013510	0.514034	4.798400
H	-0.970686	-0.970739	4.950768
H	-1.237373	0.375475	6.097190
H	-1.612970	0.708985	-1.597239
C	-2.005722	0.671870	2.842083
H	-0.860097	-5.071491	-2.044404
C	-3.832368	1.754568	3.506914
H	-4.975235	3.437091	2.824550
H	-5.472563	2.775709	4.381905
H	-5.885240	1.915172	2.897979
H	-2.414244	-0.627394	-5.414676
C	-3.138617	1.365048	4.628560
H	-2.677879	2.159602	6.569516
H	-3.567237	0.624039	6.597056
H	-4.392912	2.120786	6.162769
C	-3.509350	1.513833	1.016223
C	-0.615317	-4.083935	-4.578518
H	-0.545496	-3.764513	-5.620038
H	0.311731	-4.607630	-4.322974
C	-1.369439	-0.940343	-5.301387
H	-0.742246	-0.048861	-5.410807
H	-1.134339	-1.619373	-6.122932
C	-1.685906	0.434543	-2.649037
H	-1.042019	1.089987	-3.244095
H	-2.724788	0.541063	-2.977380
C	-5.106568	2.508138	3.390126
H	0.685941	-4.289586	-1.587278
C	-3.454303	1.574477	6.064344
H	-0.760046	-4.098092	-0.553279
C	-0.991424	0.114190	5.068510
N	-0.791196	-2.994363	-2.320017
N	-1.256905	-0.948779	-2.791846
C	-1.055232	-1.785757	-1.733881
C	-0.836487	-2.913498	-3.693436
C	-1.145842	-1.608037	-3.995175
C	-0.407104	-4.192328	-1.579876

Calculated energies and coordinates of **TS1**

Electronic energy ... -3041.42260597 Eh
Total Enthalpy ... -3040.34613708 Eh
Final Gibbs free energy ... -3040.50636656 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Sn	1.670829	-0.103240	0.307410
O	-0.123629	0.881114	1.353828
O	1.268136	-0.003426	2.850411
C	2.909428	1.756179	0.119703
C	3.119995	2.827005	1.005703
C	4.056846	3.820736	0.695533
H	4.202569	4.641514	1.394857
C	4.797960	3.766611	-0.477790
H	5.523017	4.544283	-0.701018
C	4.607596	2.711513	-1.360432
H	5.181660	2.651068	-2.282411
C	3.676302	1.716130	-1.064059
C	2.395806	2.985650	2.303153
C	2.967126	2.501650	3.489914
C	2.330200	2.759028	4.704752
H	2.796992	2.414217	5.626250
C	1.134065	3.471579	4.770051
C	0.574191	3.932463	3.577682
H	-0.350662	4.508027	3.609246
C	1.197036	3.714378	2.346849
C	4.240332	1.703641	3.460373
H	4.080874	0.743831	2.952168
H	4.600285	1.496450	4.471422
H	5.027967	2.225786	2.909994
C	0.502098	3.786855	6.099529
H	-0.585065	3.886297	6.017536
H	0.886270	4.733586	6.498067
H	0.727215	3.014173	6.842564
C	0.594196	4.249602	1.077448
H	-0.287189	4.865135	1.280825
H	0.301628	3.422315	0.420651
H	1.316372	4.857183	0.521272
C	3.474715	0.597640	-2.035676
C	2.623180	0.781924	-3.138108
C	2.409537	-0.283651	-4.013572
H	1.744350	-0.136821	-4.862863
C	3.029103	-1.518307	-3.829597
C	3.895945	-1.673328	-2.748630
H	4.401807	-2.625115	-2.600982

C	4.140406	-0.631745	-1.855101
C	1.965236	2.110452	-3.387069
H	2.695373	2.845271	-3.748087
H	1.540727	2.522620	-2.465830
H	1.173941	2.020198	-4.136069
C	2.785639	-2.653718	-4.787667
H	2.613675	-3.596930	-4.256899
H	3.649164	-2.804962	-5.446449
H	1.918763	-2.445786	-5.421568
C	5.104363	-0.823528	-0.715139
H	5.803230	0.016301	-0.642588
H	5.673490	-1.747971	-0.837084
H	4.589628	-0.880304	0.253623
C	0.200536	0.566148	2.543067
N	-1.925802	1.577398	3.472577
H	-1.676180	2.846911	1.816226
H	-3.337761	2.728257	2.455155
H	-2.640933	1.402579	1.487021
N	-0.658902	0.548976	4.913770
H	1.383210	0.335526	5.349531
H	0.529211	-1.187633	5.029616
H	0.250059	-0.327305	6.571196
C	-0.777022	0.885534	3.612463
C	-2.538702	1.697225	4.703163
H	-3.740639	3.476009	4.641715
H	-4.123838	2.357129	5.950845
H	-4.628539	1.979425	4.302742
C	-1.739778	1.046028	5.613698
H	-1.092980	1.317538	7.639237
H	-1.978843	-0.194660	7.352470
H	-2.839510	1.344751	7.401661
C	-2.427763	2.175406	2.227661
C	-3.823562	2.415758	4.903926
C	-1.915946	0.864485	7.076754
C	0.449499	-0.209409	5.506566
H	0.268976	0.690370	-1.298555
Si	-0.985018	0.076500	-1.991628
H	-0.520913	0.173022	-3.391142
O	-2.755507	-0.946848	-3.345143
C	-3.429336	-1.961391	-3.027353
O	-4.460753	-2.059880	-2.347499
C	-0.953515	-1.665861	-1.297886
C	-1.722347	-2.059641	-0.197311
C	-0.088350	-2.607124	-1.875083
C	-1.626487	-3.352334	0.313693
H	-2.409288	-1.352856	0.262805
C	0.005112	-3.900030	-1.371524
H	0.543584	-2.316452	-2.713566
C	-0.763594	-4.274785	-0.271025
H	-2.230049	-3.641179	1.170395
H	0.691412	-4.610457	-1.825074
H	-0.680583	-5.279395	0.135641
C	-2.280381	1.307556	-1.427217
C	-1.878318	2.642633	-1.289235
C	-3.619216	0.985609	-1.160470
C	-2.777422	3.632823	-0.904802
H	-0.849130	2.920893	-1.502749
C	-4.514816	1.972420	-0.754295
H	-3.979814	-0.027782	-1.311760
C	-4.099879	3.296094	-0.628292
H	-2.447840	4.666337	-0.830841
H	-5.550761	1.706036	-0.563598
H	-4.810007	4.066406	-0.337606
C	-2.843700	-3.271376	-3.546626
C	-1.558466	-4.730658	-4.655312
C	-2.223221	-5.416905	-3.676262
N	-1.960820	-3.409127	-4.557752
N	-3.018465	-4.496917	-3.013957
C	-1.474248	-2.337005	-5.430997
H	-2.249306	-1.583676	-5.556790
H	-0.601120	-1.856039	-4.981546
H	-1.206968	-2.774402	-6.394814
C	-3.905945	-4.851059	-1.904023
H	-4.251387	-3.931580	-1.434459
H	-4.767053	-5.405209	-2.290292
H	-3.353287	-5.471169	-1.194185
C	-0.584441	-5.205098	-5.670141
H	0.352482	-4.639375	-5.625335
H	-0.349582	-6.257234	-5.497198
H	-0.978915	-5.118689	-6.688674
C	-2.168437	-6.846522	-3.281806
H	-1.743436	-6.965836	-2.277266
H	-3.163251	-7.304447	-3.280118
H	-1.544724	-7.408009	-3.978508

Calculated energies and coordinates of **INT_A**

Electronic energy ... -3041.42447827 Eh

Total Enthalpy ... -3040.34726393 Eh

Final Gibbs free energy ... -3040.51006015 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Sn	1.937681	-0.088136	0.465927
O	0.247046	0.763463	1.700263
O	1.191804	-0.384622	3.396922
C	2.915831	1.919460	0.160174
C	2.960801	3.047651	0.998234
C	3.737952	4.157653	0.641630
H	3.769703	5.015764	1.309926
C	4.484346	4.163477	-0.529694
H	5.087526	5.029460	-0.787610
C	4.472969	3.045320	-1.354615
H	5.070431	3.022867	-2.263537
C	3.704038	1.933647	-1.008243
C	2.260579	3.124848	2.316082
C	2.795575	2.469660	3.436567
C	2.188262	2.646015	4.682534
H	2.632608	2.165309	5.552972
C	1.056886	3.440953	4.844121
C	0.528259	4.070257	3.716127
H	-0.351734	4.704472	3.821580
C	1.122837	3.938131	2.461484
C	4.009069	1.587577	3.323531
H	3.724560	0.579893	2.992368
H	4.503731	1.480624	4.292905
H	4.728598	1.982033	2.600847
C	0.460705	3.666981	6.208029
H	-0.614274	3.867314	6.149593
H	0.927140	4.529894	6.698707
H	0.619683	2.803069	6.862791
C	0.547721	4.663357	1.274500
H	-0.437864	5.079633	1.505020
H	0.459976	3.993670	0.412620
H	1.194363	5.490521	0.961110
C	3.736019	0.718150	-1.879512
C	2.928978	0.645543	-3.026522
C	2.936240	-0.522588	-3.790760
H	2.300960	-0.578081	-4.672910
C	3.736914	-1.610945	-3.454958
C	4.562025	-1.507510	-2.335006
H	5.210054	-2.341197	-2.071037
C	4.584377	-0.358635	-1.546825
C	2.088895	1.819418	-3.446304
H	2.707732	2.585597	-3.929047
H	1.617304	2.298601	-2.583768
H	1.311982	1.518169	-4.153934
C	3.743340	-2.859667	-4.294809
H	2.884952	-2.888077	-4.972287
H	3.721080	-3.758514	-3.669647
H	4.651050	-2.914734	-4.907517
C	5.517440	-0.267937	-0.369103
H	6.130755	0.637732	-0.423937
H	6.178032	-1.137258	-0.328314
H	4.972342	-0.214943	0.582058
C	0.328527	0.346694	2.908229
N	-1.829993	1.594042	3.470743
H	-1.277111	2.753139	1.810540
H	-3.020768	2.743188	2.201753
H	-2.260599	1.336632	1.415785
N	-0.860391	0.572836	5.126543
H	1.099488	0.216605	5.789567
H	0.119934	-1.239627	5.578447
H	-0.202615	-0.153245	6.964294
C	-0.772581	0.827749	3.803876
C	-2.593152	1.839933	4.596011

H	-3.613894	3.699919	4.271912
H	-4.266063	2.704383	5.574435
H	-4.579884	2.261003	3.895429
C	-1.982725	1.192742	5.641521
H	-1.608912	1.584399	7.718773
H	-2.515897	0.090596	7.407127
H	-3.302802	1.659446	7.234460
C	-2.115852	2.140814	2.138470
C	-3.825833	2.669120	4.577107
C	-2.366388	1.123515	7.074702
C	0.101253	-0.203136	5.918715
H	0.559527	0.272872	-0.922382
Si	-0.699003	-0.459054	-1.776066
H	0.153594	-0.368752	-2.979905
O	-1.985335	-1.372158	-2.995898
C	-2.797875	-2.315300	-2.670741
O	-3.507468	-2.429227	-1.679964
C	-0.565991	-2.030398	-0.751847
C	-1.171788	-2.166463	0.501210
C	0.183292	-3.105545	-1.249077
C	-1.030118	-3.337538	1.240267
H	-1.767910	-1.349289	0.901719
C	0.332580	-4.276366	-0.509845
H	0.679912	-3.017218	-2.214743
C	-0.275450	-4.394407	0.737859
H	-1.508271	-3.426924	2.211934
H	0.936708	-5.091338	-0.900097
H	-0.153291	-5.303201	1.320661
C	-1.861449	0.962797	-1.352193
C	-1.343937	2.262009	-1.258230
C	-3.243354	0.791014	-1.182233
C	-2.175203	3.356591	-1.040963
H	-0.272403	2.419512	-1.356405
C	-4.073440	1.881271	-0.930549
H	-3.674555	-0.203554	-1.245330
C	-3.544699	3.167885	-0.872688
H	-1.753550	4.357344	-1.001030
H	-5.140906	1.725067	-0.798077
H	-4.196823	4.021069	-0.704605
C	-2.826832	-3.452456	-3.658194
C	-2.827150	-4.692440	-5.514165
C	-2.999719	-5.533497	-4.446167
N	-2.711192	-3.410204	-4.998095
N	-3.000007	-4.740088	-3.309035
C	-2.556424	-2.208202	-5.821066
H	-2.481470	-1.341394	-5.167225
H	-1.641495	-2.290614	-6.414339
H	-3.416684	-2.110780	-6.489438
C	-3.118174	-5.239274	-1.932309
H	-2.467529	-4.661076	-1.274903
H	-4.150138	-5.141280	-1.586938
H	-2.812397	-6.286171	-1.920947
C	-2.766518	-4.965442	-6.971901
H	-1.811049	-4.645550	-7.402335
H	-2.874503	-6.034289	-7.160452
H	-3.567229	-4.448306	-7.512548
C	-3.155560	-7.009347	-4.398256
H	-2.303467	-7.492202	-3.906317
H	-4.066038	-7.300393	-3.863937
H	-3.221457	-7.409813	-5.410870

Calculated energies and coordinates of **TS2**

Electronic energy ... -3041.42230439 Eh
Total Enthalpy ... -3040.34637604 Eh
Final Gibbs free energy ... -3040.50402540 Eh
CARTESIAN COORDINATES (ANGSTROEM)

Sn	1.439176	-0.063164	-0.463597
O	0.414277	0.263946	1.499414
O	0.813342	-1.777153	2.416558
C	2.708083	1.760509	-0.315306
C	3.097182	2.491251	0.818285
C	3.993549	3.560038	0.692743
H	4.289265	4.108719	1.584709
C	4.511787	3.915958	-0.545890
H	5.210400	4.743512	-0.627841
C	4.131228	3.204732	-1.677467
H	4.525132	3.472247	-2.655697
C	3.243377	2.134632	-1.561272
C	2.583388	2.189435	2.187143
C	3.149071	1.159795	2.951190
C	2.691525	0.948918	4.254603
H	3.164362	0.175200	4.858191
C	1.681107	1.729456	4.811371
C	1.106033	2.727283	4.022818
H	0.315204	3.348629	4.442990
C	1.547204	2.972722	2.723449
C	4.222275	0.273867	2.381367
H	3.783031	-0.492700	1.727115
H	4.768073	-0.243387	3.175242
H	4.932460	0.842762	1.775472
C	1.263895	1.550761	6.247342
H	0.195189	1.751528	6.382425
H	1.808319	2.244625	6.899309
H	1.480005	0.538717	6.605084
C	0.904476	4.051498	1.893514
H	0.069614	4.516807	2.426027
H	0.542488	3.645802	0.940035
H	1.620501	4.839277	1.636268
C	2.843543	1.379632	-2.788385
C	1.746979	1.821364	-3.550155
C	1.379969	1.107741	-4.690258
H	0.533272	1.461929	-5.274799
C	2.088060	-0.018415	-5.106889
C	3.174891	-0.441789	-4.342018
H	3.750283	-1.308892	-4.664018
C	3.568408	0.241880	-3.189553
C	1.006128	3.070134	-3.163481
H	1.633354	3.955458	-3.321892
H	0.739653	3.054194	-2.101830
H	0.090441	3.185406	-3.748752
C	1.721478	-0.726713	-6.382829
H	2.097234	-1.754015	-6.397176
H	2.157088	-0.216709	-7.250581
H	0.637564	-0.744384	-6.535475
C	4.764831	-0.218324	-2.403134
H	5.540588	0.553829	-2.385963
H	5.193034	-1.127631	-2.832817
H	4.501550	-0.418220	-1.356625
C	0.302870	-0.657512	2.372343
N	-1.633949	0.629604	3.417461
H	-1.253042	2.284356	2.173033
H	-2.978750	1.846971	2.393471
H	-1.918227	0.865464	1.344355
N	-0.665225	-0.819862	4.709206
H	1.270410	-1.612261	4.810390
H	-0.019275	-2.822445	4.873925
H	0.289345	-1.777818	6.295466
C	-0.638878	-0.272560	3.480425
C	-2.296861	0.669564	4.632957
H	-3.165703	2.627564	4.738930
H	-3.761216	1.476707	5.938616
H	-4.301649	1.349451	4.264134
C	-1.683938	-0.246080	5.449821
H	-1.119389	-0.323192	7.518925
H	-2.127682	-1.680206	6.984298
H	-2.842795	-0.084563	7.221200
C	-1.967595	1.461622	2.256615
C	-3.440133	1.578231	4.900889
C	-1.952943	-0.606250	6.865082
C	0.278425	-1.825272	5.206117
H	-0.022670	0.829358	-1.109634
Si	-1.621449	-0.310268	-2.539814
H	-0.233746	-0.711066	-2.778093
O	-2.440106	-1.264173	-3.777970
C	-2.597034	-2.571490	-3.841638
O	-3.371626	-3.135493	-4.576681
C	-2.405168	-0.869539	-0.934916
C	-3.733554	-0.496812	-0.674048
C	-1.750280	-1.679278	0.004652
C	-4.384189	-0.909978	0.485396
H	-4.263740	0.136174	-1.383247
C	-2.397797	-2.095373	1.165971

H	-0.714595	-1.973690	-0.159352
C	-3.715754	-1.710215	1.408877
H	-5.413039	-0.609848	0.665034
H	-1.860652	-2.705838	1.887590
H	-4.220982	-2.034830	2.315385
C	-2.181400	1.380404	-3.047317
C	-2.350105	2.395334	-2.096763
C	-2.405184	1.678181	-4.397616
C	-2.721464	3.677256	-2.485591
H	-2.178225	2.178562	-1.045505
C	-2.770011	2.961474	-4.788200
H	-2.303038	0.900661	-5.151369
C	-2.925651	3.963352	-3.833990
H	-2.847443	4.456244	-1.739459
H	-2.939251	3.179647	-5.838640
H	-3.209101	4.966132	-4.140166
C	-1.761245	-3.395201	-2.895400
C	-0.055955	-4.352313	-1.827117
C	-1.217951	-4.776163	-1.237221
N	-0.422320	-3.499167	-2.859361
N	-2.260977	-4.188378	-1.935886
C	0.518963	-2.949908	-3.840352
H	-0.022124	-2.332249	-4.558550
H	1.267991	-2.329206	-3.335453
H	1.005443	-3.776002	-4.367769
C	-3.673380	-4.285008	-1.564782
H	-4.280827	-3.855851	-2.360005
H	-3.942505	-5.337118	-1.440705
H	-3.839807	-3.740285	-0.630006
C	1.364604	-4.627818	-1.507789
H	1.881890	-3.701190	-1.227687
H	1.433050	-5.319526	-0.668924
H	1.892584	-5.077126	-2.358625
C	-1.450630	-5.666628	-0.073713
H	-2.059699	-5.170925	0.687147
H	-1.962177	-6.589222	-0.368431
H	-0.497257	-5.941157	0.383906

Calculated energies and coordinates of **INT_B**

Electronic energy ... -1325.04745581 Eh
Total Enthalpy ... -1324.63125306 Eh
Final Gibbs free energy ... -1324.70989275 Eh
CARTESIAN COORDINATES (ANGSTROEM)

O	-0.049662	-0.314659	0.571652
O	-0.958281	1.548539	1.479133
C	-1.039511	0.516550	0.847425
H	-4.286104	-2.993418	-1.547206
H	-4.816142	1.792242	1.750204
H	-0.780887	-1.134571	-1.709116
H	-6.340921	0.149383	1.048389
C	-4.524030	-1.959354	-1.817960
H	-5.609771	-1.859948	-1.812296
H	-4.182454	-1.784291	-2.844198
C	-5.964918	0.331660	0.035625
H	-6.138542	1.384234	-0.211426
H	-6.561227	-0.270731	-0.650070
C	-3.745278	1.703711	1.572831
H	-3.228133	1.485591	2.507175
H	-3.350664	2.636626	1.165635
H	-1.096128	-2.433809	-0.541533
H	-2.049543	-2.338448	-2.047133
N	-2.568860	-0.917987	-0.611365
N	-3.528775	0.607874	0.614241
C	-2.337206	0.060352	0.293230
C	-3.923557	-0.991214	-0.865550
C	-4.529643	-0.027678	-0.088944
C	-1.556229	-1.760816	-1.267184
Si	1.605244	0.087067	0.993462
H	1.582022	0.343236	2.449586
C	2.103451	1.587615	0.032020
C	2.480326	-1.472026	0.499352
C	3.737297	-1.424481	-0.119825
C	1.924228	-2.728121	0.789761
C	2.597673	-3.898264	0.460565
C	3.842521	-3.832261	-0.161315
C	4.412660	-2.596226	-0.447774
H	4.195257	-0.464686	-0.347112
H	4.371057	-4.746346	-0.415498
H	5.386299	-2.543610	-0.925598
H	0.961682	-2.795289	1.293721
H	2.159090	-4.863474	0.696696
C	2.333026	1.514103	-1.351347
H	2.249991	0.559751	-1.868511
C	2.686855	2.648653	-2.071851
C	2.820166	3.872081	-1.419186
H	2.868206	2.579696	-3.140429
C	2.595437	3.961631	-0.048550
H	3.104361	4.757250	-1.980853
C	2.235918	2.828034	0.672058
H	2.702240	4.915611	0.459011
H	2.054104	2.908391	1.741054

Calculated energies and coordinates of **INT_C**

Electronic energy ... -1716.33206638 Eh
Total Enthalpy ... -1715.67322741 Eh
Final Gibbs free energy ... -1715.78268516 Eh
CARTESIAN COORDINATES (ANGSTROEM)

Sn	3.829209	11.931927	8.576658
O	2.220643	13.128437	9.652846
O	3.104913	13.121067	11.748449
C	4.887783	13.734116	7.710236
C	4.773188	15.104639	7.996605
C	5.615824	16.038953	7.377439
H	5.498381	17.094159	7.618986
C	6.579862	15.637335	6.462553
H	7.225022	16.371424	5.987303
C	6.703485	14.286674	6.158508
H	7.445238	13.948066	5.437303
C	5.872245	13.351768	6.776432
C	3.754783	15.673470	8.931050
C	4.101457	15.966101	10.257928
C	3.177552	16.619933	11.076160
H	3.465940	16.874853	12.095326
C	1.912435	16.975721	10.613688
C	1.571082	16.641461	9.302921
H	0.585269	16.909957	8.922267
C	2.474443	15.998578	8.455058
C	5.439737	15.552500	10.803014
H	5.533700	14.460564	10.780021
H	5.563542	15.884695	11.837601
H	6.260066	15.957944	10.201676
C	0.963165	17.749837	11.490091
H	-0.082031	17.528746	11.248496
H	1.106439	18.830385	11.364331
H	1.127854	17.525733	12.550169
C	2.075951	15.626374	7.054256
H	1.080570	16.010562	6.809369
H	2.078731	14.534316	6.935543
H	2.790405	16.016859	6.321812
C	6.017394	11.907310	6.417725
C	5.272509	11.372359	5.352698
C	5.405685	10.017782	5.044017
H	4.821275	9.603669	4.224313
C	6.266112	9.187035	5.757285
C	7.014887	9.740198	6.795550
H	7.696110	9.104888	7.358946
C	6.905271	11.085952	7.137819
C	4.361854	12.252006	4.539800
H	4.940763	12.954847	3.928247
H	3.713308	12.846928	5.190034
H	3.734280	11.653587	3.873725
C	6.368015	7.719647	5.437964
H	6.022049	7.507807	4.422112
H	5.753468	7.128105	6.127770
H	7.398696	7.362989	5.532146
C	7.716684	11.653092	8.269736
H	8.347922	12.481815	7.930242
H	8.355505	10.886317	8.715881
H	7.062136	12.055253	9.052734
C	2.229983	13.325854	10.909616

N	-0.230318	14.010254	10.700241
H	0.154037	14.238759	8.645854
H	-1.499249	13.693150	9.079017
H	-0.108403	12.570523	9.164416
N	0.696246	14.413393	12.620991
H	2.623349	14.897736	13.286050
H	1.886425	13.525710	14.119092
H	1.298221	15.184719	14.460078
C	0.920887	13.904186	11.394155
C	-1.195003	14.608478	11.494015
H	-2.572684	15.558283	10.149834
H	-3.143301	15.386235	11.810856
H	-3.111042	13.977995	10.747786
C	-0.611227	14.860066	12.707105
H	-0.675519	16.453469	14.144035
H	-1.069750	14.854566	14.805101
H	-2.232170	15.704161	13.784468
C	-0.436642	13.600174	9.305467
C	-2.574360	14.893459	11.020980
C	-1.169875	15.499499	13.925454
C	1.689691	14.512764	13.694938
H	2.631239	11.961092	7.238805

Calculated energies and coordinates of **TS3**

Electronic energy ... -3041.42997837 Eh
Total Enthalpy ... -3040.35489622 Eh
Final Gibbs free energy ... -3040.51343766 Eh
CARTESIAN COORDINATES (ANGSTROEM)

Sn	0.649834	1.221211	0.581754
O	-1.034665	-0.047720	1.298486
O	-2.083215	0.859373	-0.463813
C	1.568246	-0.315825	-0.754138
C	1.027355	-1.461615	-1.365736
C	1.777570	-2.170326	-2.314489
H	1.342638	-3.059819	-2.765636
C	3.055781	-1.765294	-2.673837
H	3.619778	-2.326821	-3.413255
C	3.608763	-0.643298	-2.070274
H	4.614516	-0.315760	-2.325595
C	2.872934	0.069942	-1.123374
C	-0.312623	-2.046461	-1.050813
C	-1.376636	-1.889053	-1.954337
C	-2.570943	-2.576628	-1.728560
H	-3.384541	-2.470524	-2.445240
C	-2.731203	-3.428139	-0.636630
C	-1.671457	-3.553130	0.260326
H	-1.770337	-4.226001	1.111060
C	-0.467294	-2.872163	0.074705
C	-1.241073	-0.982821	-3.147079
H	-0.471634	-1.341748	-3.838835
H	-0.945803	0.024113	-2.833120
H	-2.184019	-0.913344	-3.696772
C	-3.990918	-4.234188	-0.463825
H	-4.194901	-4.443882	0.591305
H	-3.907085	-5.200542	-0.975998
H	-4.859058	-3.718758	-0.887266
C	0.644184	-3.018908	1.076665
H	0.753445	-2.093903	1.657126
H	1.602376	-3.210185	0.581916
H	0.437878	-3.835446	1.775044
C	3.521464	1.241483	-0.457706
C	4.290194	1.032512	0.700450
C	4.934306	2.117355	1.295430
H	5.564738	1.938694	2.165182
C	4.828452	3.406580	0.774510
C	4.061292	3.594882	-0.374485
H	3.981362	4.591584	-0.803813
C	3.417399	2.532506	-1.008461
C	4.456716	-0.354044	1.261392
H	5.024394	-0.327422	2.196374
H	4.987933	-1.002864	0.555890
H	3.482686	-0.824203	1.442020
C	5.527683	4.568937	1.427200
H	5.875531	5.290819	0.682675
H	6.396355	4.239529	2.005818
H	4.855849	5.112048	2.105098
C	2.642717	2.759636	-2.276803
H	3.072472	2.185113	-3.104800
H	2.639913	3.816888	-2.551927
H	1.602410	2.427505	-2.175570
C	-2.051440	0.153658	0.548424
N	-3.534750	-1.301105	2.056319
H	-1.616470	-1.237333	2.915990
H	-2.461880	-2.799491	3.047056
H	-2.968648	-1.422252	4.066745
N	-4.477883	-0.454311	0.292284
H	-4.571488	1.347240	-0.794167
H	-5.718688	0.067683	-1.294571
H	-3.979669	-0.048093	-1.707598
C	-3.313742	-0.528353	0.973436
C	-4.849191	-1.721022	2.061392
H	-5.361661	-2.078462	4.110228
H	-4.840006	-3.519810	3.227417
H	-6.439915	-2.832141	2.928395
C	-5.446172	-1.187034	0.949231
H	-7.420730	-1.927357	1.160695
H	-6.898078	-1.786417	-0.517573
H	-7.340649	-0.335913	0.402447
C	-2.578355	-1.712637	3.087613
C	-5.399056	-2.581874	3.137015
C	-6.845529	-1.311133	0.468335
C	-4.702818	0.276427	-0.958980
H	1.398333	0.559841	2.189446
C	0.978669	0.286197	3.823654
O	0.508585	-0.843384	3.946180
O	0.228000	1.427700	3.987748
C	2.403708	0.551620	4.178619
Si	-1.194349	1.552992	4.888065
N	3.024947	1.742607	4.297228
N	3.284917	-0.403387	4.536225
H	-1.365704	0.329436	5.707785
C	-2.677670	1.821271	3.790853
C	-0.877575	3.041706	5.967527
C	4.315250	1.542804	4.764179
C	2.484514	3.050526	3.905288
C	3.048716	-1.851986	4.507523
C	4.482373	0.191910	4.909654
C	-2.586271	2.545445	2.595118
C	-3.939723	1.369454	4.201928
C	-1.556100	4.253574	5.791032
C	0.108547	2.967948	6.964622
C	5.243341	2.664248	5.056022
H	3.324634	3.728908	3.757672
H	1.939099	2.948863	2.966432
H	1.815602	3.437948	4.678928
H	2.375343	-2.145208	5.315462
H	2.592014	-2.131174	3.558050
H	4.010377	-2.352675	4.620773
C	5.662622	-0.584769	5.367022
H	-1.618015	2.897752	2.243595
C	-3.719261	2.804878	1.829979
C	-5.075146	1.624351	3.438202
H	-4.041506	0.819054	5.136421
C	-1.255008	5.360782	6.580616
H	-2.329936	4.332829	5.030709
C	0.410634	4.071043	7.754663
H	0.641874	2.032434	7.133179
H	4.810867	3.358838	5.784793
H	6.175238	2.280044	5.473118
H	5.492597	3.234851	4.154648
H	6.461977	0.096269	5.662000
H	5.426388	-1.214258	6.231817
H	6.057780	-1.230319	4.573946
C	-4.964456	2.344187	2.250886
H	-3.623868	3.364412	0.903813
H	-6.047299	1.273835	3.774509
C	-0.271578	5.271048	7.560402
H	-1.791197	6.293764	6.433071
H	1.168310	3.995954	8.529702
H	-5.852060	2.556955	1.660251
H	-0.040968	6.132999	8.179914

Calculated energies and coordinates of **INT_D**

Electronic energy ... -1325.80488896 Eh
Total Enthalpy ... -1325.38013281 Eh
Final Gibbs free energy ... -1325.45809480 Eh
CARTESIAN COORDINATES (ANGSTROEM)

O	-0.348945	-1.388986	1.128033
O	-0.615975	-1.355306	-1.191575
C	0.132839	-1.796623	-0.233560
H	5.315963	0.845862	-1.094996
H	1.314599	-2.577635	1.989112
H	2.062531	-0.046619	-3.198011
H	5.272229	-2.073875	1.267576
C	4.335495	0.752412	-1.565521
H	4.486288	0.405295	-2.594088
H	3.884375	1.750606	-1.613347
C	4.958862	-1.028289	1.168064
H	5.780372	-0.477621	0.706378
H	4.814489	-0.626215	2.177981
C	2.379695	-2.468470	1.786231
H	2.831463	-3.441045	1.561596
H	2.864136	-2.041543	2.668180
H	0.481581	-0.194467	-2.327451
H	1.482995	1.282997	-2.143277
N	2.157958	-0.428576	-1.139921
N	2.547990	-1.558691	0.655665
C	1.593297	-1.255291	-0.246945
C	3.480138	-0.177838	-0.787796
C	3.731394	-0.899312	0.342123
C	1.500821	0.199209	-2.291362
H	0.227779	-2.909380	-0.138563
Si	-1.326980	-0.041046	1.101890
H	-1.426252	0.275479	2.557643
C	-3.108093	-0.147084	0.516001
C	-0.445575	1.434877	0.320923
C	-1.008955	2.189890	-0.715058
C	0.814769	1.819998	0.800275
C	1.495333	2.908159	0.259776
C	0.914545	3.648617	-0.768464
C	-0.341646	3.287891	-1.251940
H	-1.983885	1.907888	-1.106837
H	1.433963	4.508317	-1.184058
H	-0.800507	3.864006	-2.051299
H	1.273151	1.257962	1.614127
H	2.469796	3.190322	0.652007
C	-3.537290	-0.783297	-0.657848
H	-2.799613	-1.298139	-1.266590
C	-4.878819	-0.757225	-1.028932
C	-5.816110	-0.090419	-0.244002
H	-5.195125	-1.261057	-1.938844
C	-5.408081	0.548196	0.923128
H	-6.862351	-0.072138	-0.538343
C	-4.068271	0.512991	1.298821
H	-6.133696	1.066380	1.544593
H	-3.765132	1.005100	2.221465

Calculated energies and coordinates of **TS4**
Electronic energy ... -1325.79283035 Eh
Total Enthalpy ... -1325.36937631 Eh
Final Gibbs free energy ... -1325.44736048 Eh
CARTESIAN COORDINATES (ANGSTROEM)

O	-0.622189	-1.959877	0.565532
O	-0.829826	-1.448482	-1.638875
C	-0.328814	-2.182739	-0.777433
H	4.722426	1.565709	-1.110927
H	1.484087	-2.916572	1.511433
H	2.592682	-0.839122	-3.633664
H	4.939933	-0.758992	1.735414
C	3.974965	1.088881	-1.748858
H	4.491986	0.685500	-2.628045
H	3.284369	1.868364	-2.091285
C	4.277860	0.043587	1.387951
H	4.905797	0.871125	1.050684
H	3.701261	0.396335	2.251829
C	2.243707	-2.155688	1.684507
H	3.178854	-2.629060	2.003469
H	1.891645	-1.488413	2.480076
H	0.935843	-1.260975	-3.084551
H	1.452859	0.435661	-3.114218
N	2.241109	-0.737736	-1.561435
N	2.444483	-1.419224	0.446624
C	1.728690	-1.631947	-0.685115
C	3.256878	0.029774	-0.996457
C	3.386351	-0.404519	0.288461
C	1.783964	-0.593243	-2.936090
H	-0.128321	-3.247795	-0.936268
Si	-1.228550	-0.451686	0.999448
H	-1.118868	-0.485546	2.483407
C	-3.034688	-0.167754	0.594471
C	-0.146051	0.983171	0.445744
C	-0.261625	1.568161	-0.824072
C	0.762911	1.549223	1.349165
C	1.536443	2.655241	1.002609
C	1.403594	3.223356	-0.259388
C	0.502504	2.676519	-1.172226
H	-0.957566	1.142396	-1.541752
H	1.992799	4.096061	-0.529691
H	0.386918	3.126258	-2.155528
H	0.857508	1.128973	2.349476
H	2.231517	3.080739	1.722083
C	-3.650371	-0.524740	-0.614074
H	-3.066675	-1.028061	-1.378751
C	-4.994245	-0.239097	-0.837097
C	-5.746905	0.413085	0.135699
H	-5.456477	-0.527437	-1.777501
C	-5.152052	0.775999	1.340337
H	-6.795846	0.634489	-0.042606
C	-3.810568	0.483575	1.565736
H	-5.734379	1.280438	2.106656
H	-3.362375	0.762348	2.518053

Calculated energies and coordinates of IMe_4
Electronic energy ... -383.32167062 Eh
Total Enthalpy ... -383.12957541 Eh
Final Gibbs free energy ... -383.17542336 Eh
CARTESIAN COORDINATES (ANGSTROEM)

N	-1.058056	-0.708079	0.000141
N	1.058061	-0.708052	0.000183
C	-2.436046	-1.163330	0.000211
H	-2.969552	-0.811088	-0.890945
H	-2.969696	-0.810324	0.890977
H	-2.417824	-2.254157	0.000669
C	-0.680794	0.636085	-0.000149
C	0.680765	0.636102	-0.000130
C	2.436062	-1.163268	0.000169
H	2.969862	-0.809906	0.890702
H	2.969400	-0.811355	-0.891220
H	2.417868	-2.254096	0.001036
C	1.659771	1.754891	-0.000212
H	2.308634	1.729860	0.884111
H	1.140485	2.716391	-0.001491
H	2.310166	1.728347	-0.883353
C	-1.659828	1.754850	-0.000281
H	-2.309997	1.728454	-0.883595
H	-1.140566	2.716363	-0.001244
H	-2.308916	1.729638	0.883870
C	0.000013	-1.571661	0.000375

Calculated energies and coordinates of IMe_4CO_2
Electronic energy ... -571.91928470 Eh
Total Enthalpy ... -571.70945168 Eh
Final Gibbs free energy ... -571.76191821 Eh
CARTESIAN COORDINATES (ANGSTROEM)

O	0.816022	9.338188	3.651725
C	0.954329	8.242167	4.219692
O	0.166653	7.314350	4.467501
N	3.303293	8.900886	5.122384
N	3.016385	6.780601	4.833655
C	2.405154	7.978151	4.718984
C	4.489562	8.284340	5.501059

C	4.312213	6.945027	5.307064
C	3.067951	10.342673	5.209336
H	3.080303	10.656068	6.258187
H	2.100108	10.545475	4.746631
H	3.853593	10.871922	4.662015
C	5.653529	9.051886	6.011723
H	6.467334	8.372963	6.272720
H	5.395554	9.625764	6.909222
H	6.032654	9.758594	5.264541
C	5.232370	5.797484	5.509878
H	4.847069	5.095549	6.258536
H	6.206268	6.150982	5.853122
H	5.388099	5.237642	4.580575
C	2.439033	5.487130	4.465849
H	2.521790	4.798675	5.312149
H	2.976623	5.073964	3.606336
H	1.385617	5.652868	4.232144

Calculated energies and coordinates of H_2SiPh_2
Electronic energy ... -753.85890538 Eh
Total Enthalpy ... -753.64849461 Eh
Final Gibbs free energy ... -753.69840992 Eh
CARTESIAN COORDINATES (ANGSTROEM)

H	-1.106527	-0.496432	-1.322883
Si	-2.487240	0.033120	-1.149112
H	-2.424945	1.516897	-1.255968
C	-3.099338	-0.510000	0.538980
C	-3.637311	-0.587169	-2.495194
C	-4.166881	-1.884640	-2.441172
C	-3.979906	0.222875	-3.585777
C	-4.817272	-0.248071	-4.593424
C	-5.329714	-1.539948	-4.524639
C	-5.004228	-2.358218	-3.445629
H	-3.929165	-2.530029	-1.597634
H	-5.985505	-1.908306	-5.308709
H	-5.405963	-3.366001	-3.386457
H	-3.591552	1.237277	-3.647751
H	-5.073740	0.395218	-5.430624
C	-4.464947	-0.459228	0.854152
H	-5.180053	-0.125575	0.104551
C	-4.924203	-0.841284	2.110100
C	-4.023833	-1.284231	3.076017
H	-5.985977	-0.796153	2.336175
C	-2.665520	-1.345531	2.780335
H	-4.381866	-1.584998	4.056765
C	-2.209443	-0.962839	1.521783
H	-1.960746	-1.696087	3.529269
H	-1.145775	-1.021992	1.300936

Calculated energies and coordinates of HCO_2SiHPh_2
Electronic energy ... -942.45802637 Eh
Total Enthalpy ... -942.22813805 Eh
Final Gibbs free energy ... -942.28542377 Eh
CARTESIAN COORDINATES (ANGSTROEM)

H	1.018553	-3.616374	-1.699797
C	1.127897	-2.897388	-0.870504
O	0.071791	-2.076395	-0.805280
O	2.076233	-2.862401	-0.125856
Si	0.019559	-0.864238	0.409367
H	0.198580	-1.530019	1.720426
C	-1.687323	-0.142756	0.206464
C	1.335124	0.427517	0.144071
C	-2.035685	0.997364	0.946054
C	-2.647541	-0.701218	-0.646732
C	2.601259	0.293130	0.731763
C	1.081660	1.553957	-0.651713
H	-1.305352	1.459126	1.608797
C	-3.302929	1.559110	0.840411
C	-3.916101	-0.138161	-0.756029
H	-2.400299	-1.581477	-1.233405
C	3.583419	1.256380	0.530019
H	2.821195	-0.580656	1.339714
C	2.065101	2.516055	-0.857117
H	0.102647	1.683773	-1.108228
C	-4.245616	0.990658	-0.012599
H	-3.555321	2.441967	1.420874
H	-4.648861	-0.581814	-1.424283
C	3.316171	2.367893	-0.265118
H	4.560005	1.139288	0.991147
H	1.854892	3.383399	-1.476596
H	-5.235957	1.429163	-0.098293
H	4.084136	3.120331	-0.422633

Calculated energies and coordinates of $[BArF]^-$
Electronic energy ... -3647.80715843 Eh
Total Enthalpy ... -3647.35676866 Eh
Final Gibbs free energy ... -3647.48969397 Eh
CARTESIAN COORDINATES (ANGSTROEM)

F	-1.545305	-2.882373	8.060532
F	2.296378	-1.423679	0.829475
F	-2.358456	-3.056745	6.050870
F	-0.211089	-2.860052	6.337852
F	2.457838	0.552458	-0.060054
F	1.198431	-0.960557	-0.993260
F	4.077953	4.211132	2.484189
F	-3.834863	1.023600	0.374767
F	5.297659	0.611899	7.509212
F	3.628913	-0.772215	7.296910
F	-1.134221	7.715542	6.558850
F	-4.154713	-0.246824	2.110469
F	3.426082	0.985080	8.558907
C	-0.325027	1.144843	3.065756
C	-0.560775	3.514561	4.329508
C	-0.963181	1.179548	5.617332
C	1.502361	1.974455	4.866879
C	-0.258899	4.417377	5.364372
H	0.295684	4.061134	6.230187
C	-1.542259	-0.930768	6.711423
C	0.696099	0.698234	2.223735
H	1.733926	0.873948	2.497046
C	0.426453	0.017011	1.033538
C	2.063959	1.267468	5.930380
H	1.428108	0.655457	6.565960
C	-1.851505	1.805413	6.494084
H	-2.001407	2.880814	6.431805
C	-1.638419	0.854485	2.656766
H	-2.468262	1.156431	3.292689
F	5.740898	2.949611	3.108053
C	2.387114	2.761555	4.104302
H	1.992178	3.348094	3.278474
C	-0.839886	-0.215631	5.748382
H	-0.174390	-0.751798	5.075269
C	-1.252442	4.039543	3.235439
H	-1.501417	3.394546	2.395966
F	-4.516986	2.418949	7.650238
C	-2.567559	1.087673	7.456968
C	-0.877147	-0.245451	0.638621
H	-1.086891	-0.775366	-0.282851
C	-0.647708	5.751654	5.316929
C	3.432914	1.325209	6.215011
F	-0.223169	6.051869	7.631344
C	-1.407199	-2.422518	6.790027
C	-1.636115	5.382487	3.179903
C	-1.910600	0.181002	1.470853
C	1.583429	-0.451039	0.202129
F	5.194361	4.688530	4.291811
C	-2.421645	-0.285460	7.580289
H	-2.971090	-0.842069	8.330466
C	3.949903	0.543332	7.385523
C	4.289667	2.093644	5.444717
H	5.351447	2.137925	5.660957
F	-3.468595	-1.116652	0.234251
C	-1.341665	6.254388	4.217579
H	-1.644914	7.293898	4.178414
B	-0.086557	1.952956	4.470256
C	3.746938	2.814464	4.379554
F	0.961790	7.228840	6.238354
F	-2.880229	2.844176	9.014755
F	-4.085410	1.050445	9.288848
C	-3.507264	1.839918	8.351340
C	-0.267566	6.678303	6.433555

C	-2.359058	5.867375	1.958657
C	-3.334041	-0.043994	1.054866
C	4.674959	3.663026	3.562452
F	-2.815405	7.136950	2.088850
F	-3.430889	5.091203	1.661849
F	-1.559875	5.850989	0.859034

Calculated energies and coordinates of CO_2

Electronic energy ... -188.57006287 Eh
Total Enthalpy ... -188.55480755 Eh
Final Gibbs free energy ... -188.57907474 Eh

CARTESIAN COORDINATES (ANGSTROEM)

C	-3.264744	-2.136338	-0.259115
O	-4.428170	-2.136338	-0.259115
O	-2.101318	-2.136338	-0.259115

Calculated energies and coordinates of **M**

Electronic energy ... -1911.69641591 Eh
Total Enthalpy ... -1910.85136300 Eh
Final Gibbs free energy ... -1910.97358793 Eh

CARTESIAN COORDINATES (ANGSTROEM)

Sn	1.543211	10.468882	3.114231
N	-0.861915	10.094645	5.328656
N	2.498200	7.497353	3.449037
N	2.709940	8.455998	5.520237
N	-1.416580	9.960257	3.086467
C	-0.557349	10.733572	4.026461
C	-0.746674	11.007259	6.446001
H	-0.848506	10.471812	7.397806
H	-1.495807	11.824670	6.404200
H	0.243941	11.469559	6.421097
C	1.884838	8.543233	4.301141
C	3.050445	6.554756	4.351160
C	2.078893	9.008161	6.696754
H	1.907267	10.077883	6.533914
H	2.734950	8.897625	7.568016
H	1.097859	8.541106	6.917976
C	2.941988	12.090720	3.912440
C	4.341779	11.872344	3.873003
C	-2.103492	9.428061	5.175357
C	2.535605	13.437787	4.079961
C	1.098223	13.843848	4.064396
C	3.168490	7.113650	5.572368
C	0.431705	14.047587	2.843036
C	0.430356	14.108070	5.269280
C	1.588694	6.993608	2.437262
H	1.280457	7.825655	1.793162
H	0.672278	6.548322	2.879921
H	2.086700	6.241544	1.815092
C	5.255876	12.916855	4.047040
H	6.320878	12.690784	4.012770
C	-2.433099	9.359757	3.871360
C	-0.906554	14.439799	2.854348
H	-1.423890	14.571818	1.904955
C	1.152053	13.991958	6.586689
H	1.857856	13.155860	6.580630
H	0.443772	13.859924	7.411136
H	1.742960	14.894523	6.788363
C	4.940447	10.524856	3.620899
C	4.824227	14.222768	4.243204
H	5.539747	15.031591	4.370514
C	5.404510	9.758474	4.701385
C	-1.598377	14.657235	4.044534
C	-1.826042	10.742254	1.936083
H	-2.410436	11.642173	2.226626
H	-2.422478	10.132246	1.248128
H	-0.926132	11.075656	1.403921
C	-0.907873	14.504161	5.243000
H	-1.426377	14.679665	6.184975
C	6.023913	8.534108	4.457048
H	6.363645	7.934364	5.300734
C	5.288080	10.280346	6.107593
H	6.035449	11.062641	6.297721
H	5.442353	9.477456	6.834384
H	4.305848	10.725599	6.282253
C	3.458867	14.475209	4.251661
H	3.089441	15.491917	4.381533
C	5.142656	10.071835	2.307111
C	1.151282	13.862129	1.535486
H	2.091063	14.425346	1.521928
H	0.526966	14.190272	0.698704
H	1.412114	12.805131	1.380855
C	3.586309	5.266997	3.836496
H	2.790540	4.586111	3.504297
H	4.170297	4.746736	4.600986
H	4.239635	5.447853	2.970346
C	4.724052	10.908035	1.128933
H	3.627913	10.971154	1.072831
H	5.093266	10.473606	0.194567
H	5.102783	11.932605	1.216822
C	-3.513165	8.582704	3.204651
H	-4.210663	9.227611	2.653350
H	-4.096258	8.015023	3.934819
H	-3.085769	7.873824	2.480063
C	6.198365	8.052190	3.163499
C	-2.717527	8.746684	6.347559
H	-1.976466	8.107216	6.849604
H	-3.558016	8.118207	6.041111
H	-3.091415	9.458375	7.096052
C	3.867314	6.599229	6.780088
H	4.669740	7.281593	7.097461
H	4.317010	5.622480	6.580387
H	3.189714	6.482417	7.637152
C	5.752823	8.833544	2.101155
H	5.885203	8.475226	1.081074
C	-3.068765	14.975254	4.034749
H	-3.358011	15.504458	3.120886
H	-3.353278	15.590194	4.895106
H	-3.658618	14.049927	4.080280
C	6.890181	6.735798	2.922299
H	7.980993	6.858721	2.888207
H	6.579244	6.292850	1.970510
H	6.664221	6.021146	3.720693
H	0.843013	8.207319	4.564413
H	-0.921865	11.789807	4.053993

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