Electronic Supplementary Information

The Synthesis, Properties, and Reactivity of Lewis Acidic Aminoboranes

Jordan N. Bentley, Selvyn A. Simoes, Ekadashi Pradhan, Tao Zeng, and Christopher B. Caputo *

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General Considerations & Procedures

All manipulations were performed using an MBraun LABstar Glove Box Workstation under N_2 atmosphere or by employing Schlenk techniques. All glassware was oven-dried at 110 °C before being transferred into the glove box. Solvents were prepared from an MBraun MB-SPS 800 solvent drying system under N_2 atmosphere. Commercially available reagents were purchased from either Sigma-Aldrich, TCI Chemicals, or Oakwood Chemicals and employed without further purification; unless otherwise stated. Chloroform-*d* and benzene-d_6 were transferred to Strauss flasks and dried over activated molecular sieves, then degassed using freeze-pump-thaw techniques, followed by immediate transfer to a glovebox. Where "wet" solvent is stated to be used, it will imply undried solvent saturated with moisture relative to ambient conditions. Experiments monitored by NMR were conducted in NMR tubes (8" x 5 mm) sealed with standard plastic caps and wrapped with Parafilm or J-young screw cap. ^1H, ^{11}B, $^{13}C\{^1H\}$, $^{19}F\{^1H\}$, and $^{119}Sn\{^1H\}$ NMR spectra were acquired at 25 °C on either a Bruker 700 MHz, Bruker DRX 600 MHz , Bruker ARX 400 MHz, or Bruker ARX 300 MHz Spectrometers. Chemical shifts are reported relative to $SiMe_4$ and referenced to the residual solvent signal (^1H, $^{13}C\{^1H\}$) to $CDCl_3$ (δ 7.26, 77.16 ppm) or C_6D_6 (δ 7.16, 128.06 ppm). ^{11}B and $^{19}F\{^1H\}$ NMR spectra were referenced relative to 15% BF_3-Et_2O. NMR spectra were analyzed using either TopSpin 4.0.1 or MestReNova 6.0.2-5475 software. Chemical shifts are reported in ppm and coupling constants as scalar values in Hz. The conventional abbreviations were used as follows: s (singlet), d (doublet), dt (doublet of triplets), t (triplet), q (quartet), dd (doublet of doublets), m (multiplet), br (broad).

General Procedure

To a 20 mL vial of corresponding amine in THF (5 mL), NaH was added while stirring. Once the effervescence of H_2 gas had stopped, the solvent was removed *in vacuo* to give a solid residue. Dichloromethane (10 mL) was added to the residue, resulting in a suspension that was then filtered into a 20 mL vial. To a sodium amide mixture, $ClB(C_6F_5)_2$ in DCM (5 mL) was added dropwise. The mixture was stirred for 16 hrs, then the respective product was isolated following the procedures outlined below.

Synthesis

(1) 10-(bis(perfluorophenyl)boraneyl)-phenothiazine:

Sodium hydride (0.1 g, 4.17 mmol) was added to a 20 mL vial of phenothiazine (0.5733 g, 2.88 mmol) in THF (10 mL). The mixture was stirred until the evolution of gas stopped. The solvent was removed *in vacuo* to yield a yellow precipitate. The yellow precipitate was dissolved in DCM (10 mL) and filtered into a 20 mL, to which $ClB(C_6F_5)_2$ (1.0955 g, 2.88 mmol) in DCM (5 mL) was added dropwise and stirred for 16 hrs. The solvent was removed *in vacuo*, resulting in an amorphous residue that was dissolved in DCM and filtered. The solution was concentrated then triturated with MeCN to afford a white precipitate. The precipitate was vacuum filtered and rinsed with pentane to afford the title compound as a fine white powder. Crystals suitable for x-ray diffraction were obtained by the slow evaporation of dichloromethane at -35 ^oC. Yield 1.0259 g (65.7 %). **^{1}H NMR** (300 MHz, C_6D_6) δ 6.97 – 7.06 (m, 4H), 6.51 – 6.63 (m, 4H). **^{11}B NMR** (128 MHz, C_6D6_6) δ 38.50. **^{13}C NMR** (101 MHz, C_6D_6) δ 146.31 (d, *J* = 243.8 Hz), 142.16, 142.15 (d, *J* = 254.6 Hz), 137.60 (d, *J* = 252.6 Hz), 132.88, 128.21, 127.22, 127.13, 124.04, 111.25. **^{19}F NMR** (282 MHz, C_6D6_6) δ -130.41 (m, 2F), -151.57 (t, *J* = 20.6 Hz, 1F), -161.12 (m, 2F).

(2) 10-(bis(perfluorophenyl)boraneyl)-phenoxazine:

Sodium hydride (35.9 mg, 1.5 mmol) was added to a 20 mL vial of phenoxazine (238.8 mg, 1.3034 mmol) in THF (10 mL). The mixture was stirred until the evolution of gas stopped. The solvent was removed *in vacuo* to yield a yellow precipitate. The yellow precipitate was dissolved in DCM (10 mL) and filtered into a 20 mL vial, to which $ClB(C_6F_5)_2$ (495.9 g, 1.3034 mmol) in DCM (5 mL) was added dropwise and stirred for 16 hrs. The solvent was removed *in vacuo*, resulting in an amorphous residue that was dissolved in DCM and filtered. The solution was concentrated then triturated with MeCN to afford a white precipitate. The precipitate was vacuum filtered and rinsed with pentane to afford the title compound as a fine white powder. Crystals suitable for x-ray diffraction were obtained by the slow evaporation of dichloromethane at -35 ^oC. Yield 219.1 g (31.9 %). $C_{24}H_8BF_{10}NO$ (527.13 g/mol): calcd %. C 54.69; H 1.53; N 2.66%; found C 54.67, H 1.64, N 3.01%. **^{1}H NMR** (400 MHz, C_6D6_6) δ 6.83 (dd, *J* = 8.0, 53.0 Hz, 4H), 6.54 (dt, *J* = 8.0, 99.7 Hz, 4H). **^{11}B NMR** (128 MHz, C_6D6_6) δ 38.50. **^{13}C NMR** (101 MHz, C_6D_6) δ 151.33, 146.44 (d, $J_{C\text{-}F}$ = 245.8 Hz), 142.38 (d, $J_{C\text{-}F}$ = 255.5 Hz), 137.70 (d, $J_{C\text{-}F}$ = 251.8 Hz), 132.61, 127.92, 123.68, 122.23, 117.43, 111.57. **^{19}F NMR** (377 MHz, C_6D_6) δ -131.17 (m, 2F), -151.15 (t, *J* = 20.6 Hz, 1F), -160.72 (m, 2F).

(3) 1,1-bis(perfluorophenyl)-N,N-diphenylboranamine:

Sodium hydride (51.9 mg, 2.16 mmol) was added to diphenylamine (182.9 mg, 1.08 mmol) in THF (10 mL) and stirred until the evolution of gas stopped. The solvent was removed *in vacuo* and the residue was suspended in dichloromethane (10 mL), followed by the dropwise addition of $ClB(C_6F_5)_2$ (411.2 mg, 1.08 mmol); the reaction mixture was stirred for 12 h. The mixture was then filtered, concentrated, and then triturated with pentane and left to crystallize at -35 ^oC. The resulting precipitate was vacuum filtered to afford the product as a beige powder. Yield 505.6 g (91.3 %). $C_{24}H_{10}BF_{10}N$ (513.08 g/mol): calcd %. C 56.18; H 1.96; N 2.73%; found C 56.24, H 2.66, N 3.08%. **^{1}H NMR** (400 MHz, Benzene-d_6) δ: 6.96 (d, *J* = 5.4 Hz, 2H), 6.80 (t, 1H), 6.78 – 6.71 (m, 2H). ^{11}B NMR (128 MHz, Benzene-d_6) δ: 37.12. **^{13}C NMR** (101 MHz, Benzene-d_6) δ: 146.94, 146.08 (d, *J* = 251.8 Hz), 142.26 (d, *J* = 254.9 Hz), 137.55 (d, *J* = 251.5 Hz), 129.32, 127.42, 126.71. **^{19}F NMR** (377 MHz, Benzene-d_6) δ: -132.36 (dd, *J* = 9.4, 23.3 Hz, 2F), -151.24 (t, *J* = 20.5 Hz, 1F), -161.45(m, 2F).

(4) N-(bis(perfluorophenyl)boraneyl)-1,1,1-trimethyl-N-(trimethylsilyl)silanamine:

To a solution of $LiN(SiMe_3)_2$ (138.3 mg, 0.8235 mmol) in Et_2O (5 mL), in a 20 mL vial, $ClB(C_6F_5)_2$ (313.2 mg, 0.8235 mmol) in Et_2O (2 mL) was added dropwise and stirred for 1 h. The solvent was then removed *in vacuo* and the residue was dissolved in pentane. The mixture was then filtered into a 20 mL vial and left to crystallize at -35 ^oC to yield single crystals suitable for x-ray diffraction. The crystalls were vacuum filtered and rinsed with cold pentane to afford the product as clear single crystals. Yield 0.4033 g

(96.6 %). $C_{18}H_{18}BF_{10}NSi_2$ (505.31 g/mol): calcd %. C 42.78; H 3.59; N 2.77%; found C 42.86, H 3.15, N 2.85%. **^{1}H NMR** (400 MHz, C_6D_6) δ -0.00 (s, 9H). **^{11}B NMR** (96 MHz, C_6D_6) δ 44.08. **^{13}C NMR** (101 MHz, C_6D_6) δ 146.17 (d, J_{CF} = 242.2 Hz), 142.38 (d, J_{CF} = 255.7 Hz), 137.69 (d, J_{CF} = 253.9 Hz), 3.47. **^{19}F NMR** (377 MHz, C_6D_6) δ -132.02 (dd, J = 24.3, 9.6 Hz, 2F), -150.78 (t, J = 20.5 Hz, 1F), -161.27 (m, 2F).

(5) 9-(bis(perfluorophenyl)boraneyl)-9H-carbazole:

Sodium hydride (28.3 mg, 1.2 mmol) was added to a 20 mL vial of carbazole (131.5 mg, 0.7865 mmol) in THF (5 mL). The mixture was stirred until the evolution of gas stopped. The solvent was removed *in vacuo* to yield a yellow precipitate. The yellow precipitate was dissolved in DCM (10 mL) and filtered into a 20 mL vial, to which $ClB(C_6F_5)_2$ (299.2 g, 0.7865 mmol) in DCM (5 mL) was added dropwise and stirred for 16 hrs. The solvent was removed *in vacuo*, resulting in an amorphous residue that was dissolved in DCM and filtered. The solution was concentrated then triturated with pentane to afford a white precipitate. The precipitate was vacuum filtered and rinsed with pentane to afford the title compound as a fine white powder. Yield 0.2919 g (72.6 %).

Alternate Procedure: Carbazole (272.3 mg, 1.6285 mmol) and $HB(C_6F_5)_2$ (563.4 mg, 1.6285 mmol) were combine in a 20 mL vial. The mixture was dissolved in dichloromethane (5 mL) and stirred with loosened vial cap for 24 hrs. The respective product was isolated following the same procedures specific to each product as by metathesis. Yield 0.6693 g (80.4 %). Crystals suitable for x-ray diffraction were obtained by the slow evaporation of dichloromethane at -35 °C. $C_{24}H_8BF_{10}N$ (511.13 g/mol): calcd %. C 56.40; H 1.58; N 2.74%; found C 56.21, H 2.11, N 3.32%. **^{1}H NMR** (400 MHz, C_6D_6) δ 7.99 (d, J = 7.8, 1.0 Hz, 1H), 7.40 (t, J = 7.5 Hz, 0H), 7.27 – 7.21 (m, 1H), 7.00 (d, J = 8.4 Hz, 1H). **^{11}B NMR** (128 MHz, C_6D_6) δ 40.55. **^{13}C NMR** (101 MHz, C_6D_6) δ 147.88 – 144.95 (m), 143.27 (d, J = 257.6 Hz), 138.00 (dt, J = 254.4, 15.5 Hz), 111.99. **^{19}F NMR** (377 MHz, C_6D_6) δ -130.64 – -130.78 (m, 2F), -148.68 (tt, J = 20.2, 3.6 Hz, 1F), -159.23 – -159.41 (m, 2F).

(6) 10-(bis(perfluorophenyl)boraneyl)-9,10-dihydroacridine:

Sodium hydride (28.3 mg, 1.2 mmol) was added to a 20 mL vial of acridan (135.0 mg, 0.7449 mmol) in THF (5 mL). The mixture was stirred until the evolution of gas stopped. The solvent was removed *in vacuo* to yield a yellow precipitate. The yellow precipitate was dissolved in DCM (10 mL) and filtered into a 20 mL vial, to which $ClB(C_6F_5)_2$ (283.4 g, 0.7449 mmol) in DCM (5 mL) was added dropwise and stirred for 16 hrs. The solvent was removed *in vacuo*, resulting in an amorphous residue that was dissolved in DCM and filtered. The solution was concentrated then triturated with MeCN to afford a white precipitate. The precipitate was vacuum filtered and rinsed with pentane to afford the title compound as a fine white powder. Yield 0.1020 g (26.1 %).

Alternate Procedure: Acridine (308.3 mg, 1.7208 mmol) and $HB(C_6F_5)_2$ (595.3 g, 1.7208 mmol) were combine in a 20 mL vial, and dissolved in dichloromethane (5 mL), then capped and stirred for 24 hrs. The respective product was isolated following the same procedures specific to each product as by metathesis. Yield 0.7419 g (82.1 %). $C_{25}H_{10}BF_{10}N$ (525.16 g/mol): calcd %. C 57.18; H 1.92; N 2.67%; found C 57.53, H 1.71, N 2.87%. **^{1}H NMR** (400 MHz, C_6D_6) δ 7.33 (d, J = 7.5 Hz, 2H), 7.21 – 6.98 (m, 6H), 3.92 (d, J = 57.6 Hz, 2H). **^{11}B NMR** (128 MHz, C_6D_6) δ 37.68. **^{13}C NMR** (101 MHz, C_6D_6) δ 147.10 (d, J_{CF} = 162.3 Hz), 144.67 (d, J_{CF} = 162.5 Hz), 143.04, 141.88 (d, J_{CF} = 254.6 Hz), 137.39 (d, J_{CF} = 252.1 Hz), 134.17, 127.55, 126.67, 126.47, 122.31, 111.71, 34.14. **^{19}F NMR** (377 MHz, C_6D_6) δ -130.08 (s, 2F), -132.06 (s, 2F), -152.20 (t, J = 20.0 Hz, 2F), -161.04 (d, J = 67.8 Hz, 4F).

(7) 9-(bis(perfluorophenyl)boraneyl)-9H-carbazole adduct with 4-dimethylaminopyridine:

In separate 5 mL vials, 4-dimethylaminepyridine (19.7 mg, 0.161 mmol) and **5** (82.3 mg, 0.161 mmol) were each dissolved in DCM (0.5 mL) then mixed. To the mixture, toluene (1 mL) was carefully layered on top of the solution and left to crystallize in a glovebox freezer at -35 °C. Once sufficiently crystallized, the solvent was decanted and the crystals were carefully rinsed and again decanted with pentane, yielding clear crystals suitable for x-ray diffraction. Yield 79.6 mg (78.1 %). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.02 (d, J = 6.7 Hz, 2H), 7.90 (d, J = 7.1 Hz, 2H), 7.15 – 7.02 (m, 4H), 6.86 (d, J = 7.6 Hz, 2H), 6.35 (d, J = 7.0 Hz, 2H), 3.00 (s, 6H). **^{11}B NMR** (96 MHz, $CDCl_3$) δ -0.60. **^{13}C NMR** (101 MHz, $CDCl_3$) The low solubility of **7** precluded ^{13}C NMR acquisition, conversely more solvent dissociated **7** to **5** and DMAP. **^{19}F NMR** (282 MHz, $CDCl_3$) δ -130.38 (dd, J = 24.6, 8.3 Hz), -156.62 (t, J = 20.6 Hz), -162.95 (ddd, J = 24.4, 20.1, 8.7 Hz).

NMR Spectra of Synthesized Compounds

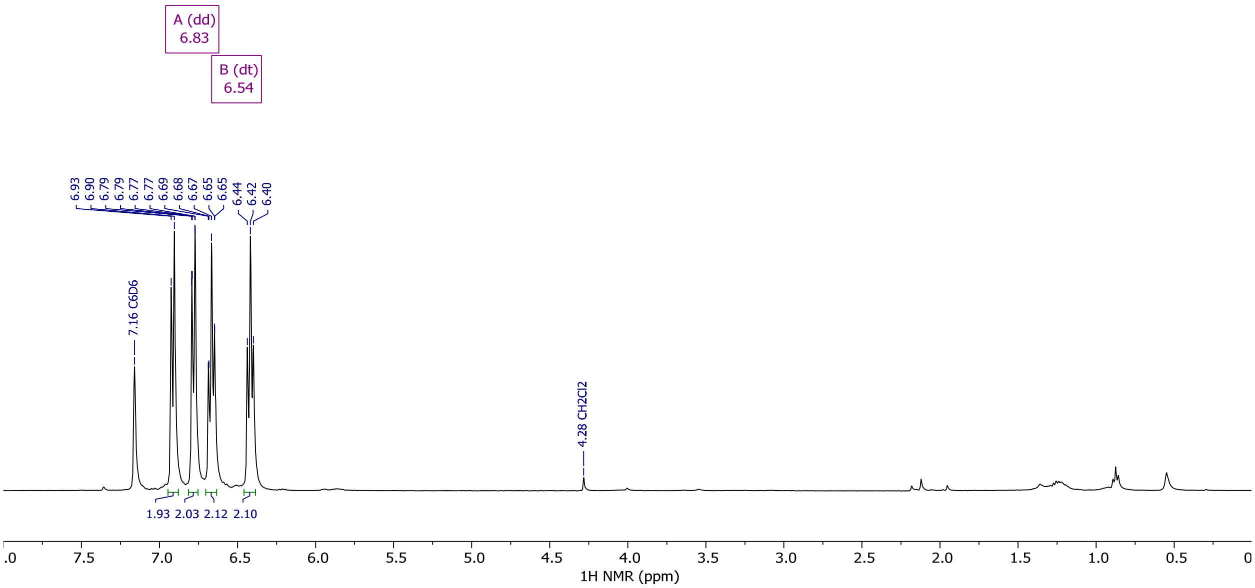


*Figure S1. [1]H NMR spectrum of **2** in C_6D_6.*

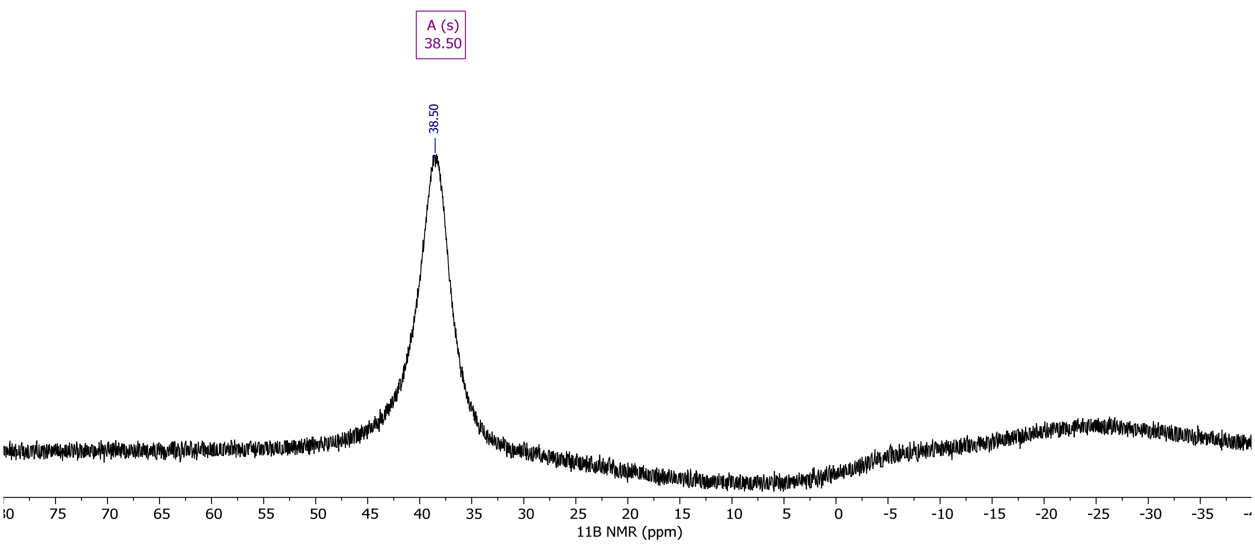


*Figure S2. [11]B NMR spectrum of **2** in C_6D_6.*

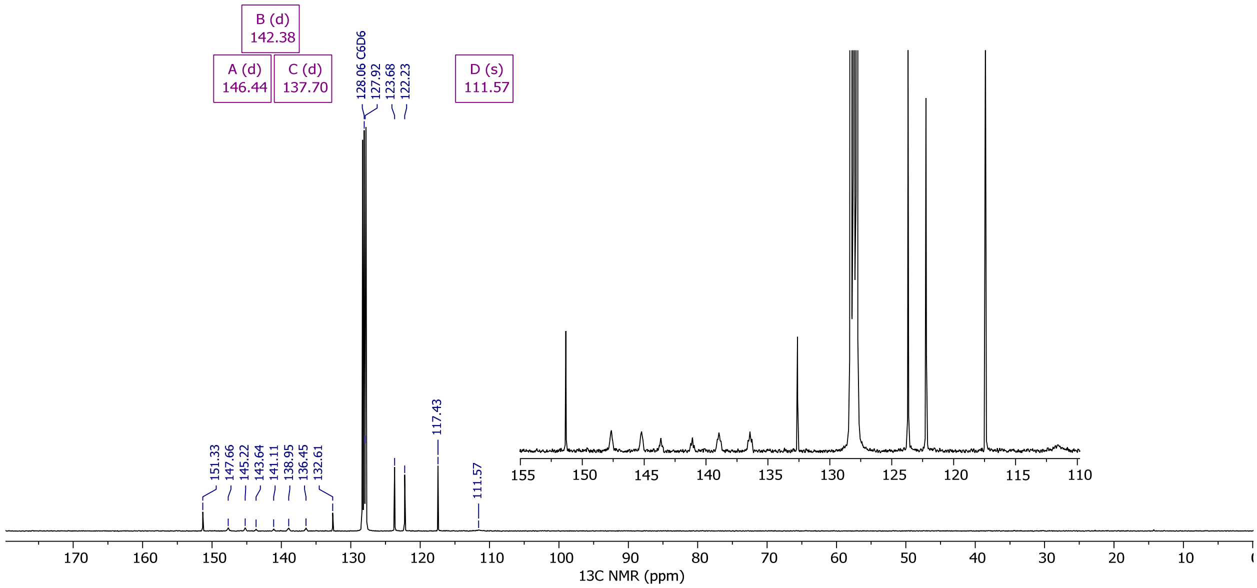


*Figure S3. ^{13}C NMR spectrum of **2** in C_6D_6.*

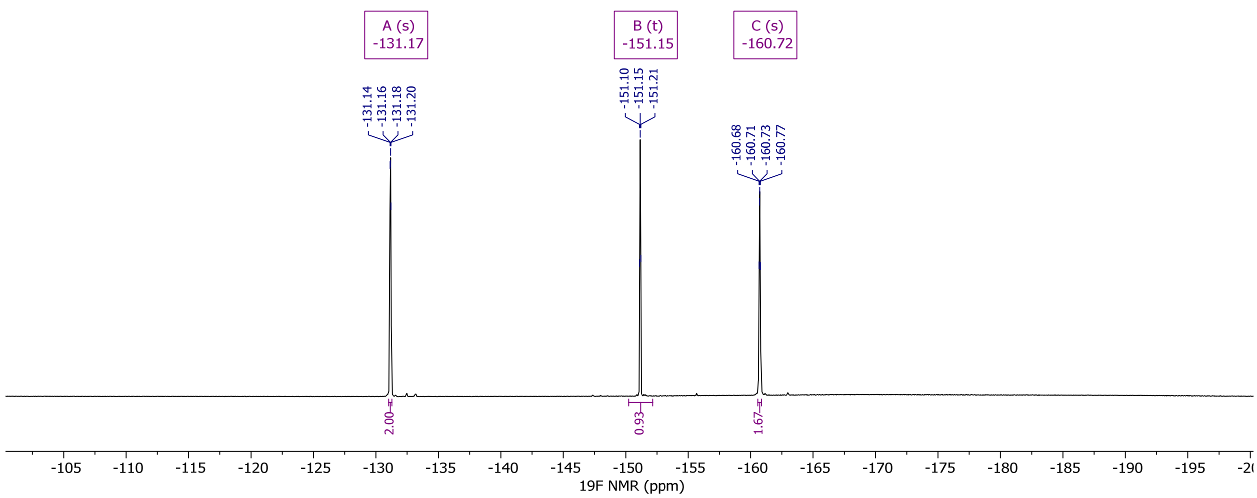


*Figure S4. ^{19}F NMR spectrum of **2** in C_6D_6.*

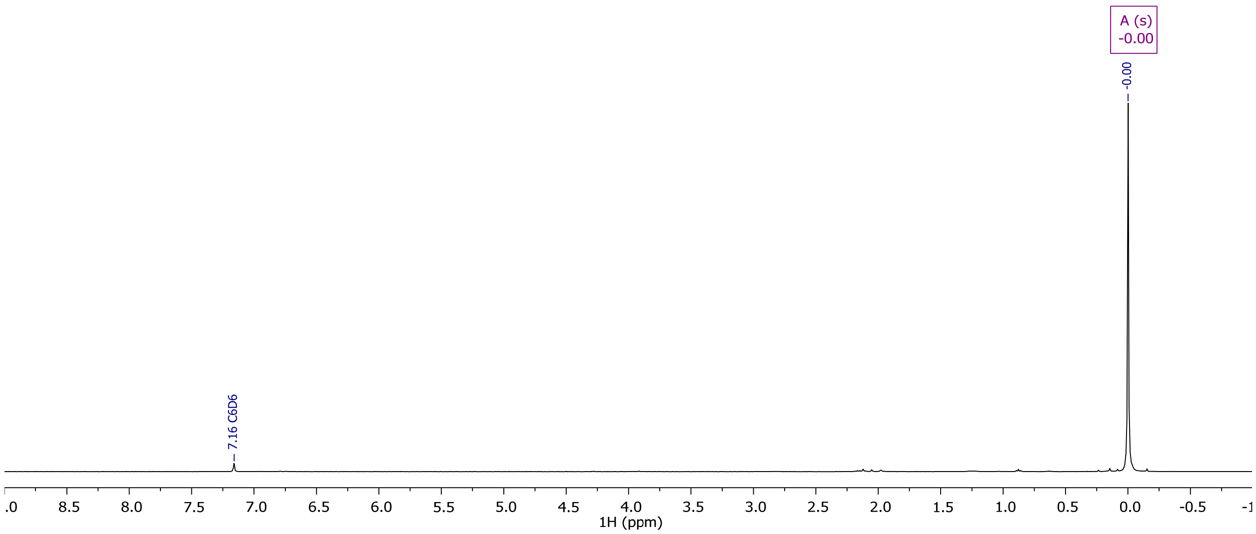


*Figure S5. ¹H NMR spectrum of **4** in C₆D₆.*

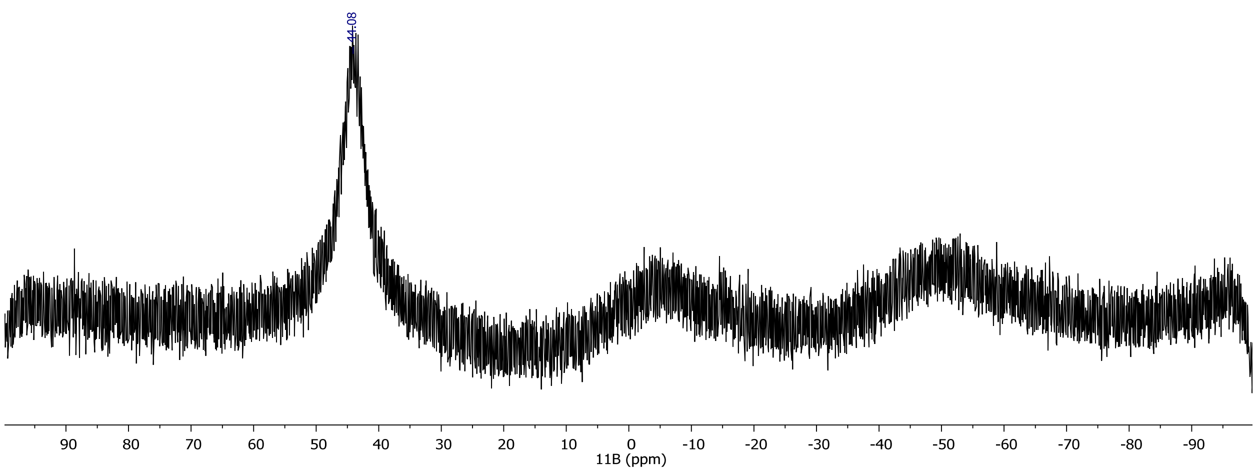


*Figure S6. ¹¹B NMR spectrum of **4** in C₆D₆.*

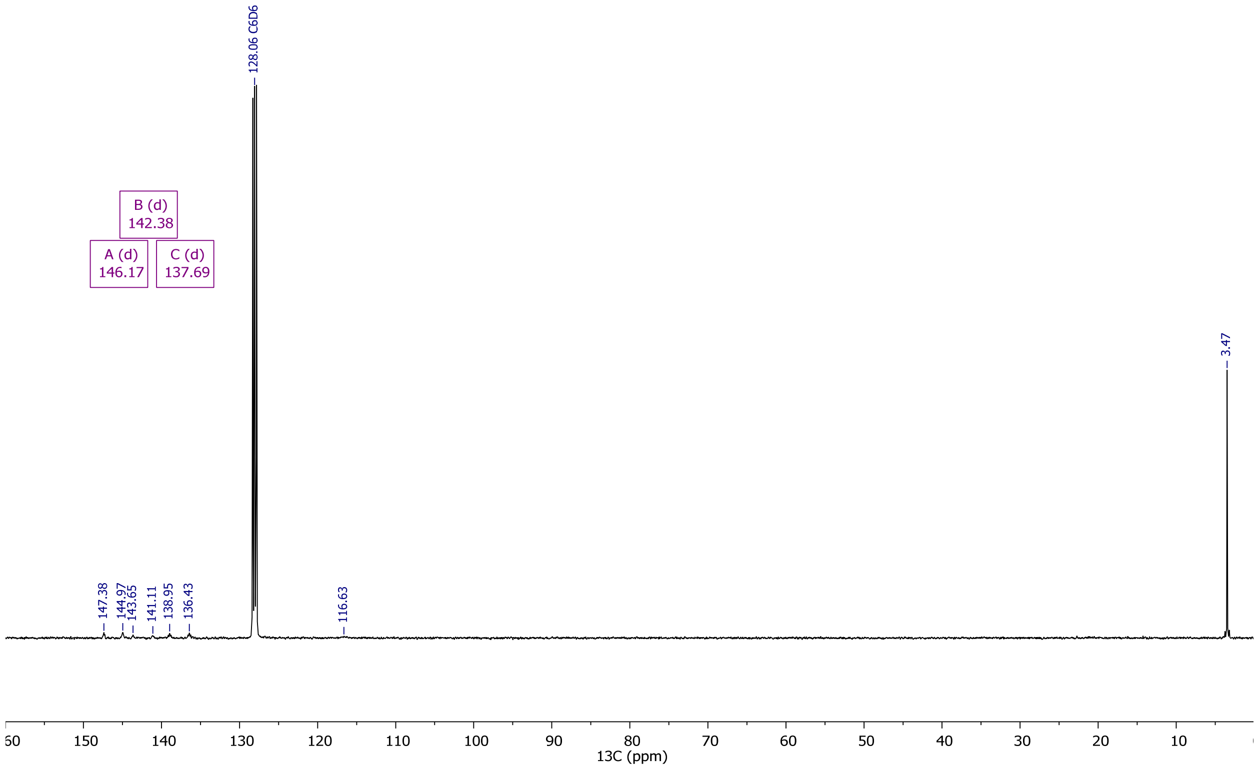


*Figure S7. ¹³C NMR spectrum of **4** in C₆D₆.*

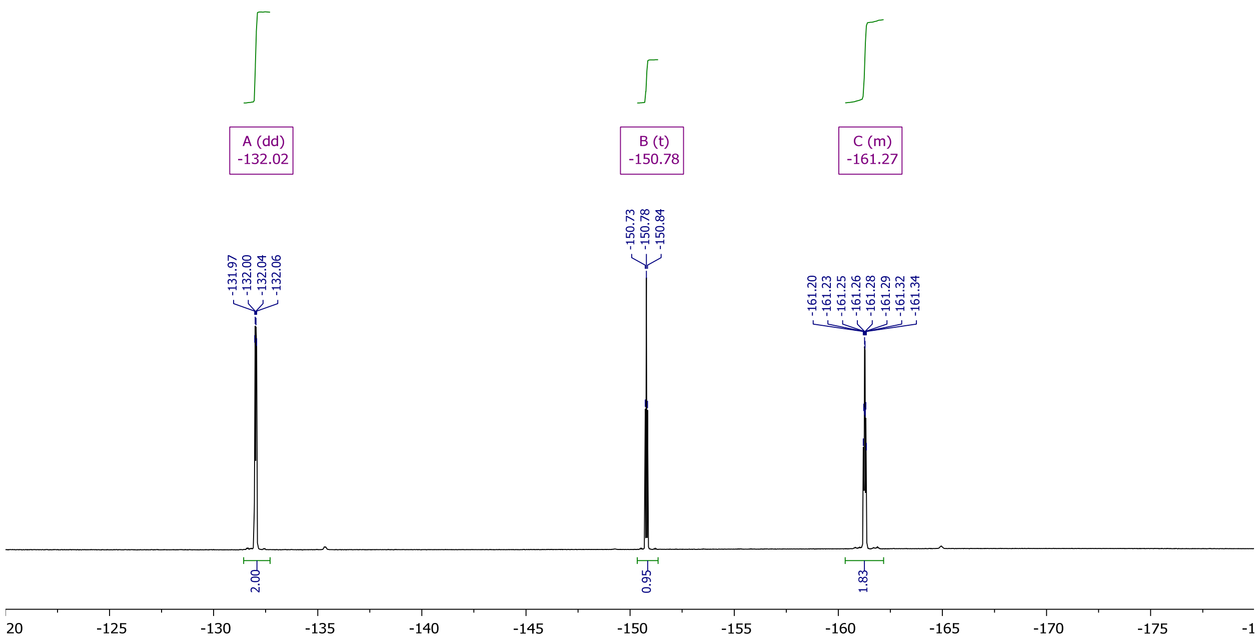


*Figure S8. ¹⁹F NMR spectrum of **4** in C₆D₆.*

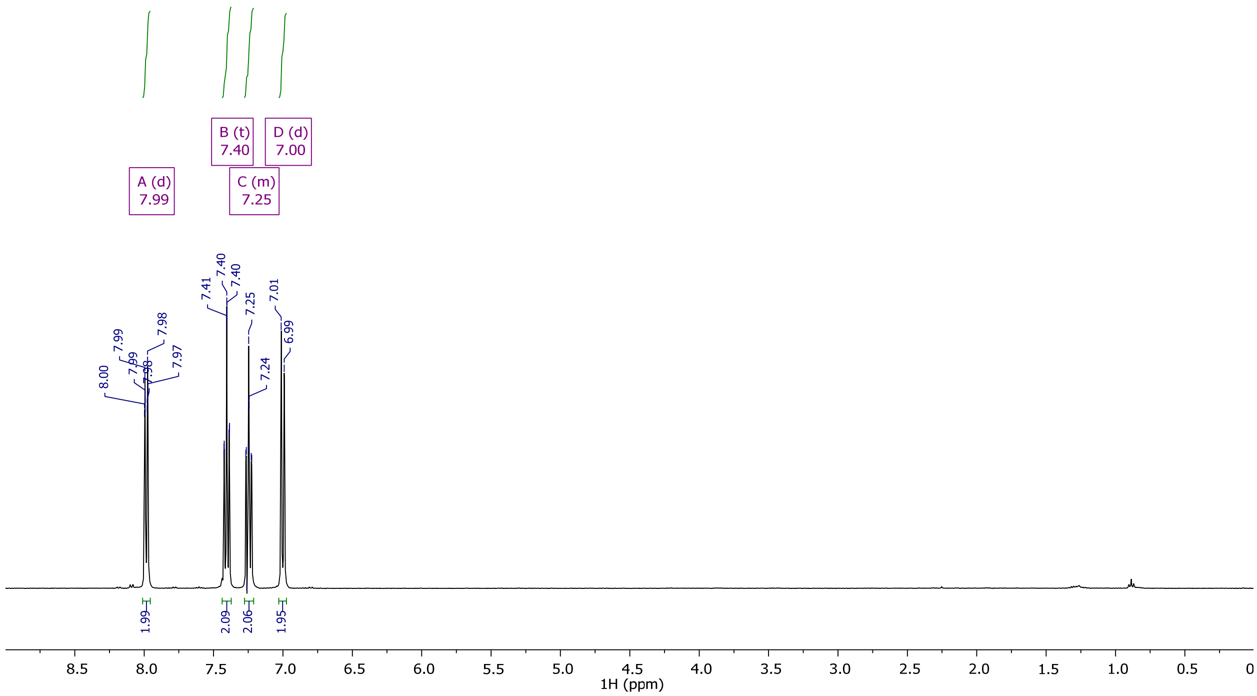


*Figure S9. [1]H NMR spectrum of **5** in C_6D_6.*

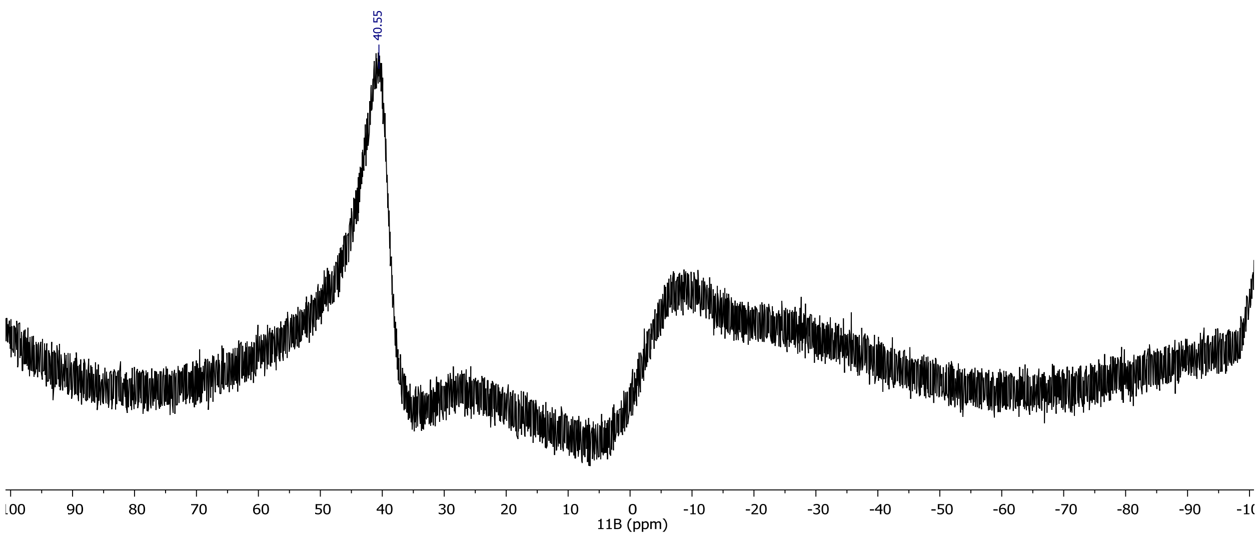


*Figure S10. [11]B NMR spectrum of **5** in C_6D_6.*

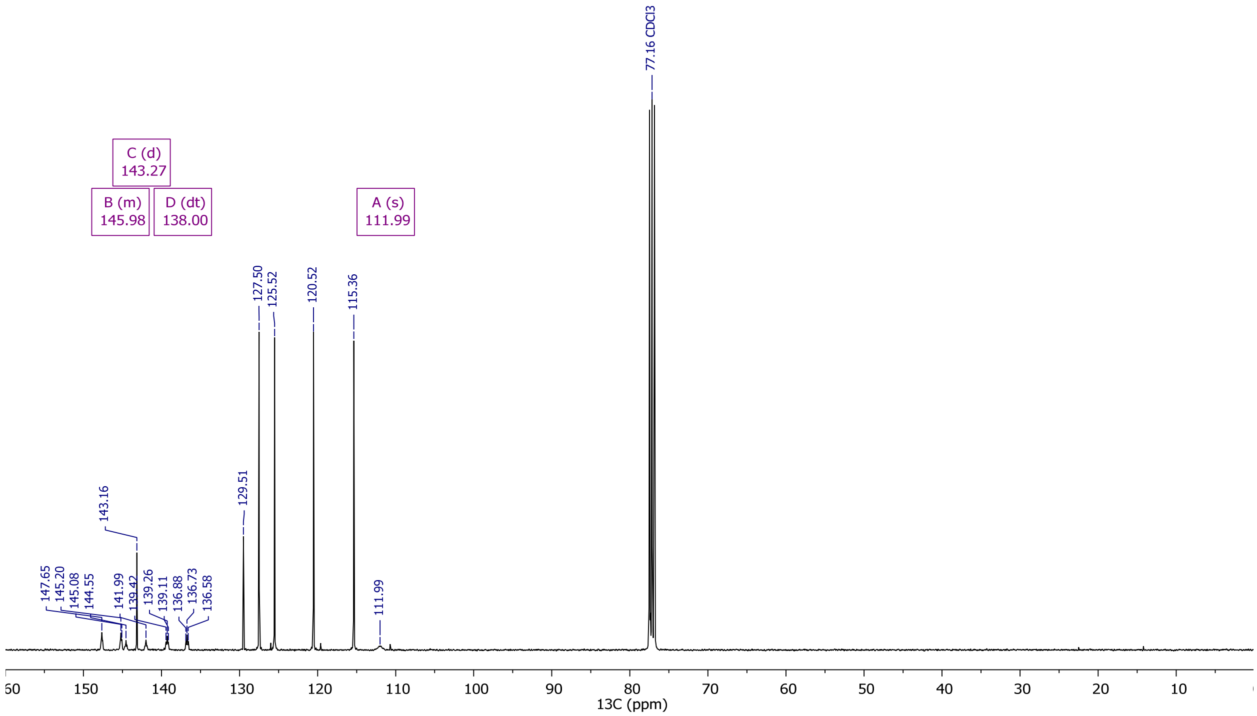


*Figure S11. [13]C NMR spectrum of **5** in C_6D_6.*

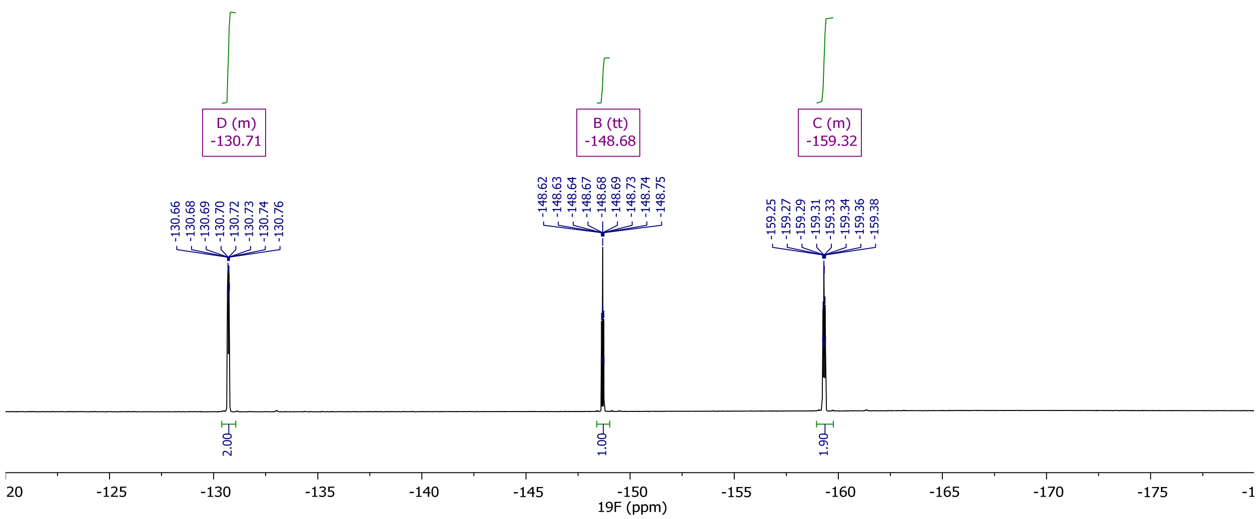


*Figure S12. [19]F NMR spectrum of **5** in C_6D_6.*

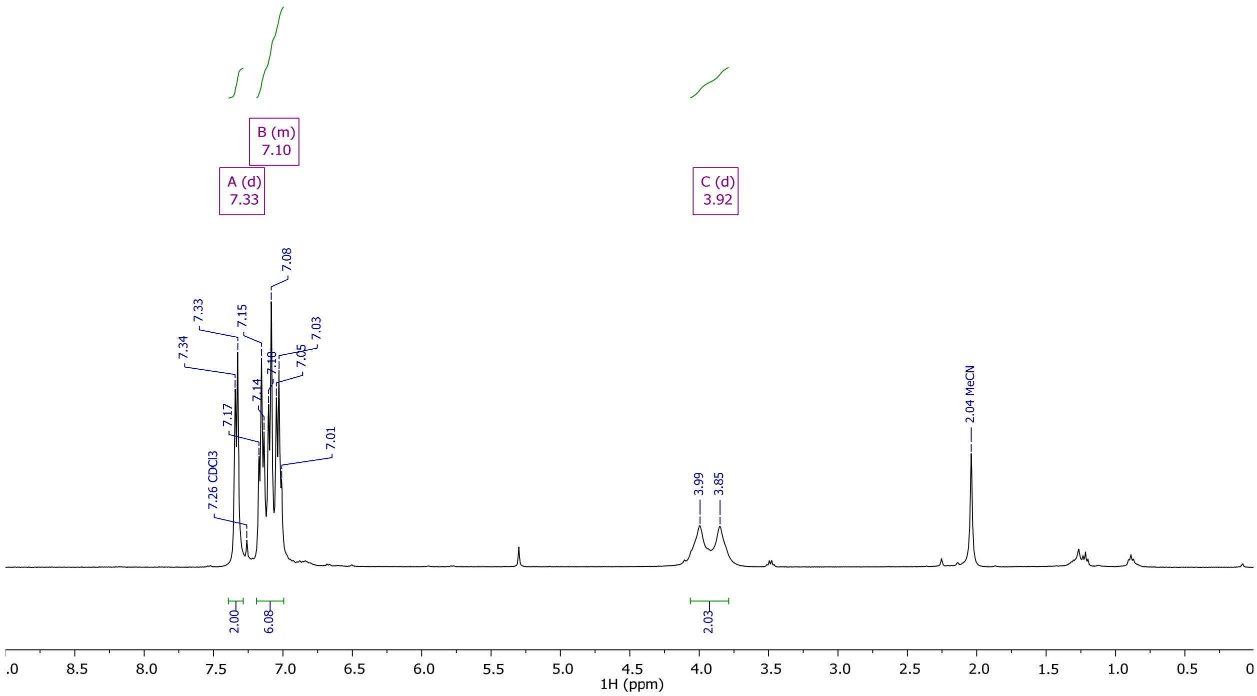


*Figure S13. [1]H NMR spectrum of **6** in C_6D_6.*

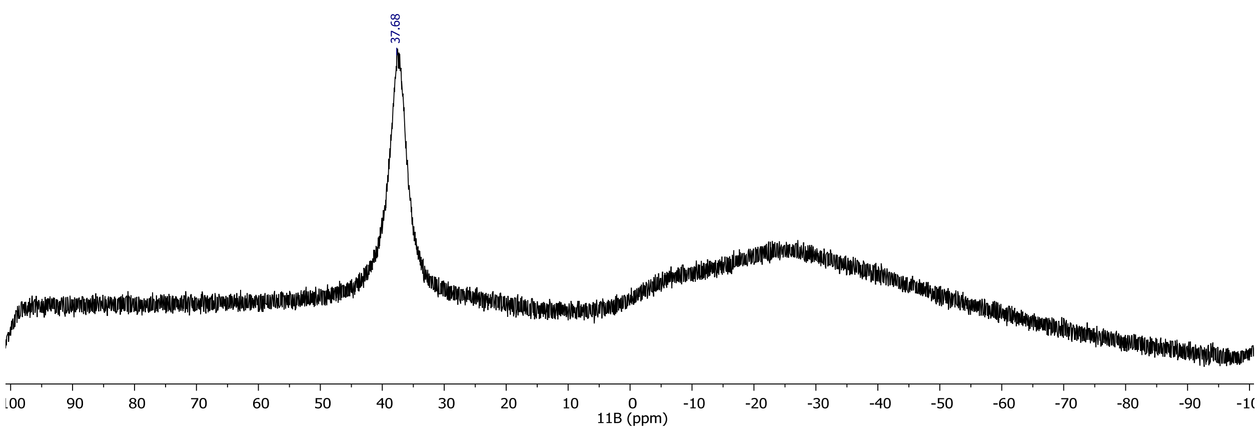


*Figure S14. [11]B NMR spectrum of **6** in C_6D_6.*

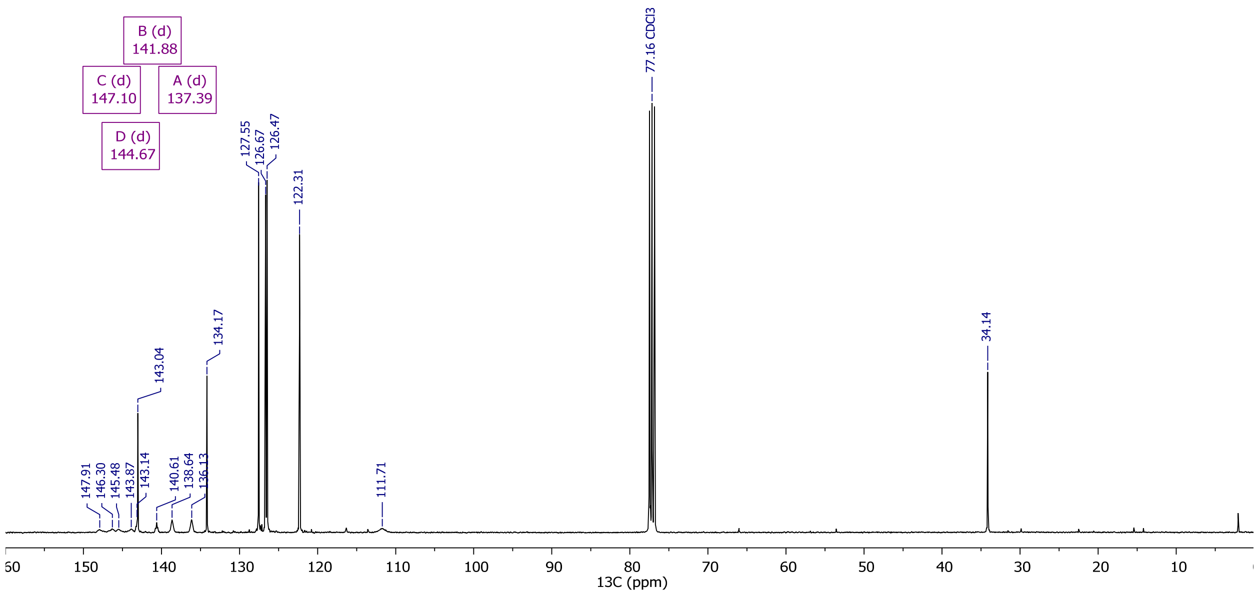


*Figure S15. [13]C NMR spectrum of **6** in C_6D_6.*

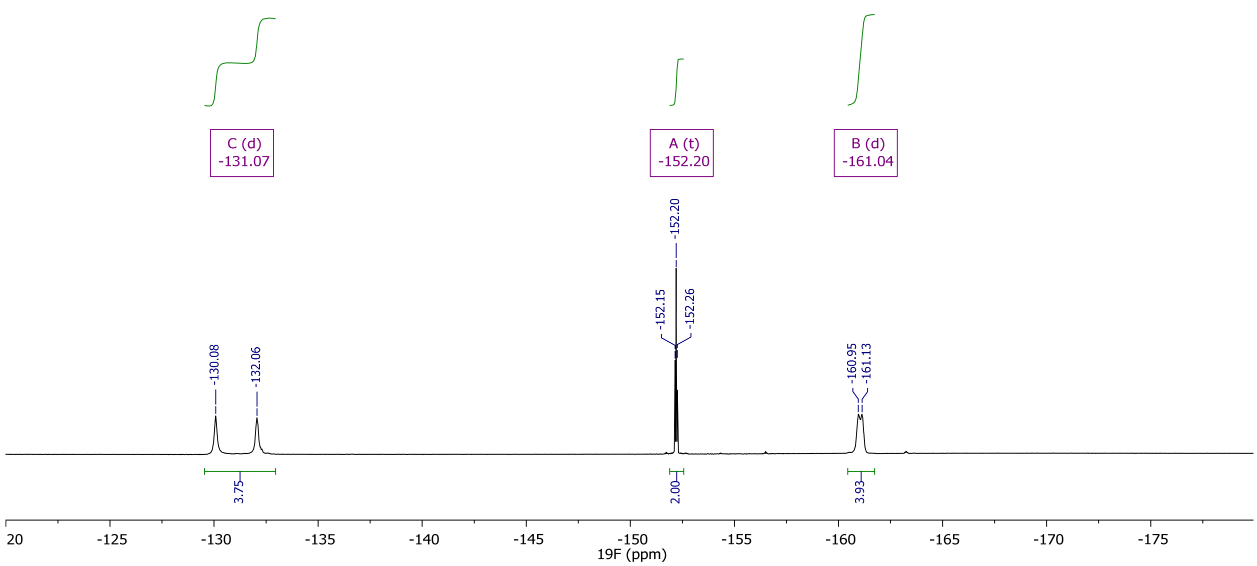


*Figure S16. [19]F NMR spectrum of **6** in C_6D_6.*

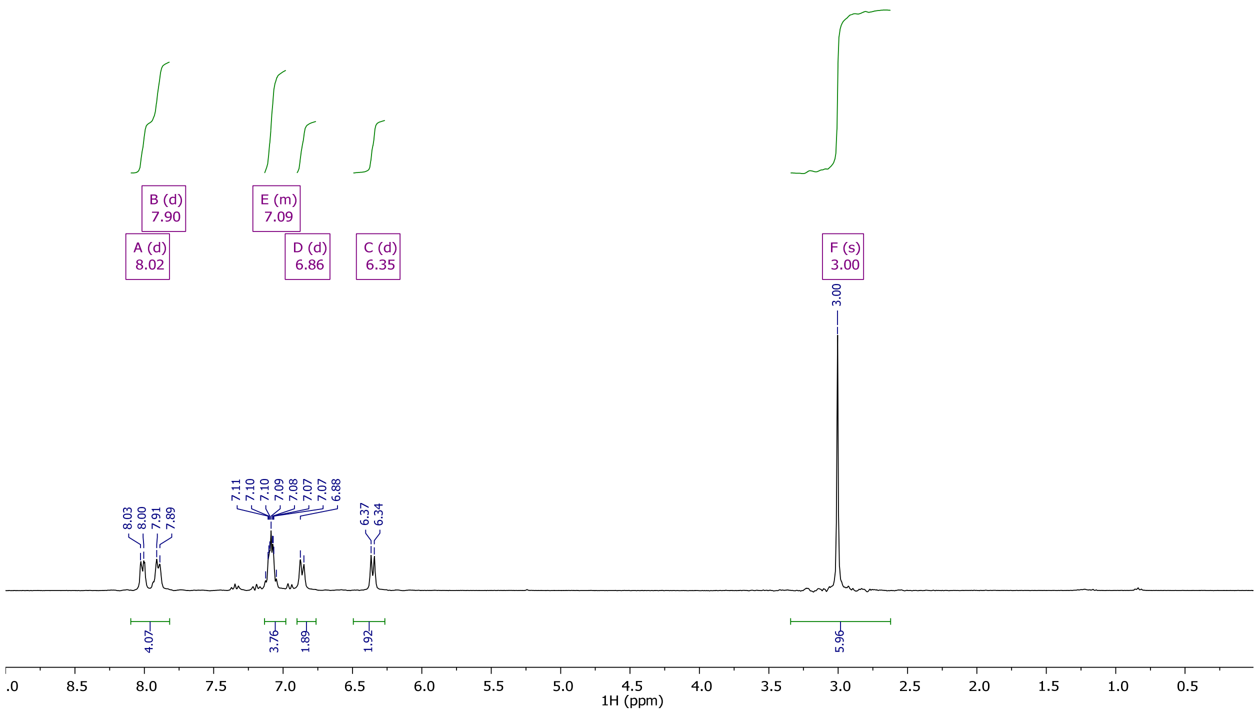


*Figure S17. ^{1}H NMR spectrum of **7** in $CDCl_3$.*

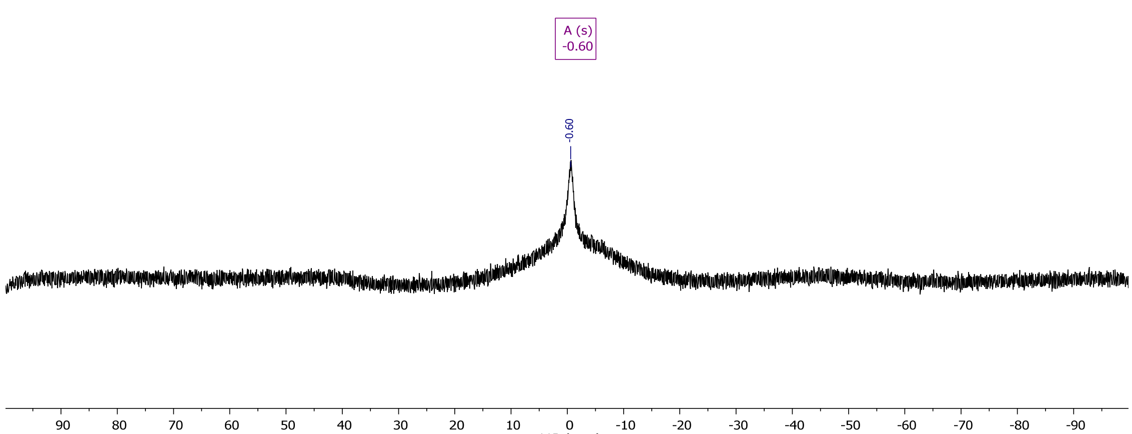


*Figure S18. ^{11}B NMR spectrum of **7** in $CDCl_3$.*

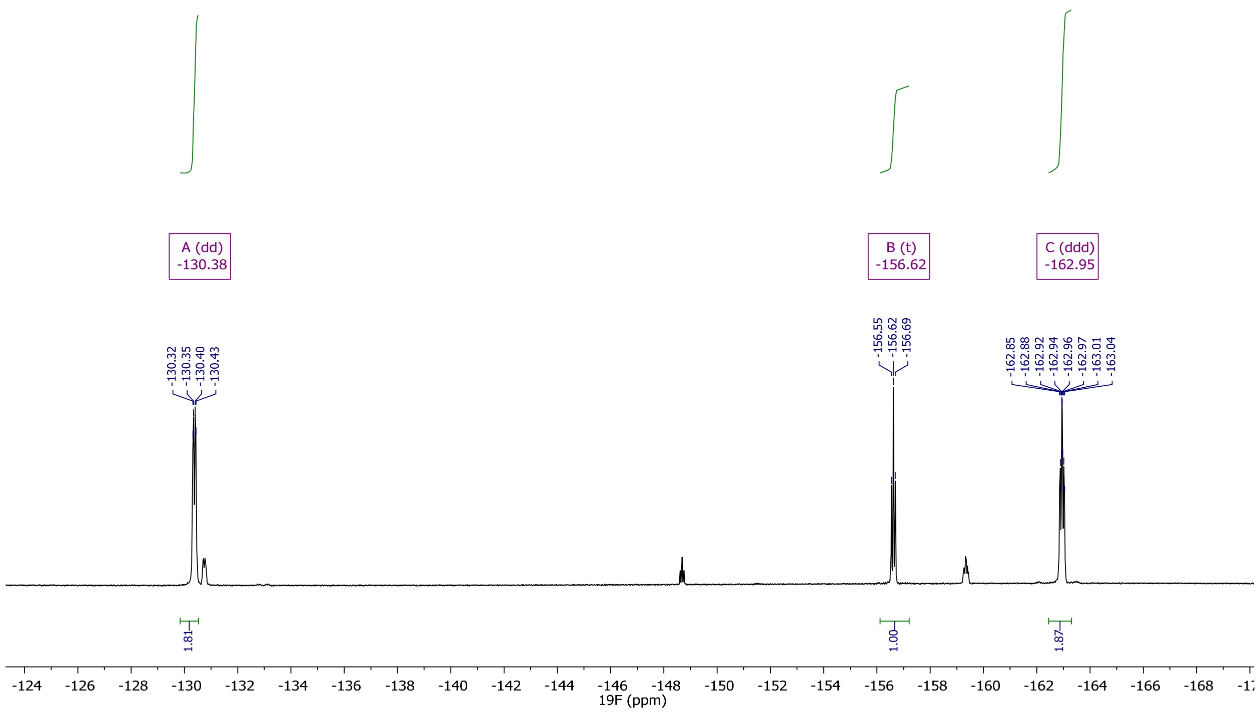
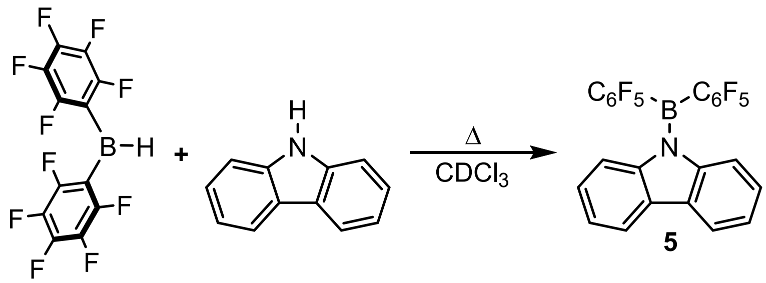


*Figure S19. ^{19}F NMR spectrum of **7** in $CDCl_3$.*

NMR Experiment – Alternate Synthesis of 5 and 6 with $HB(C_6F_5)_2$



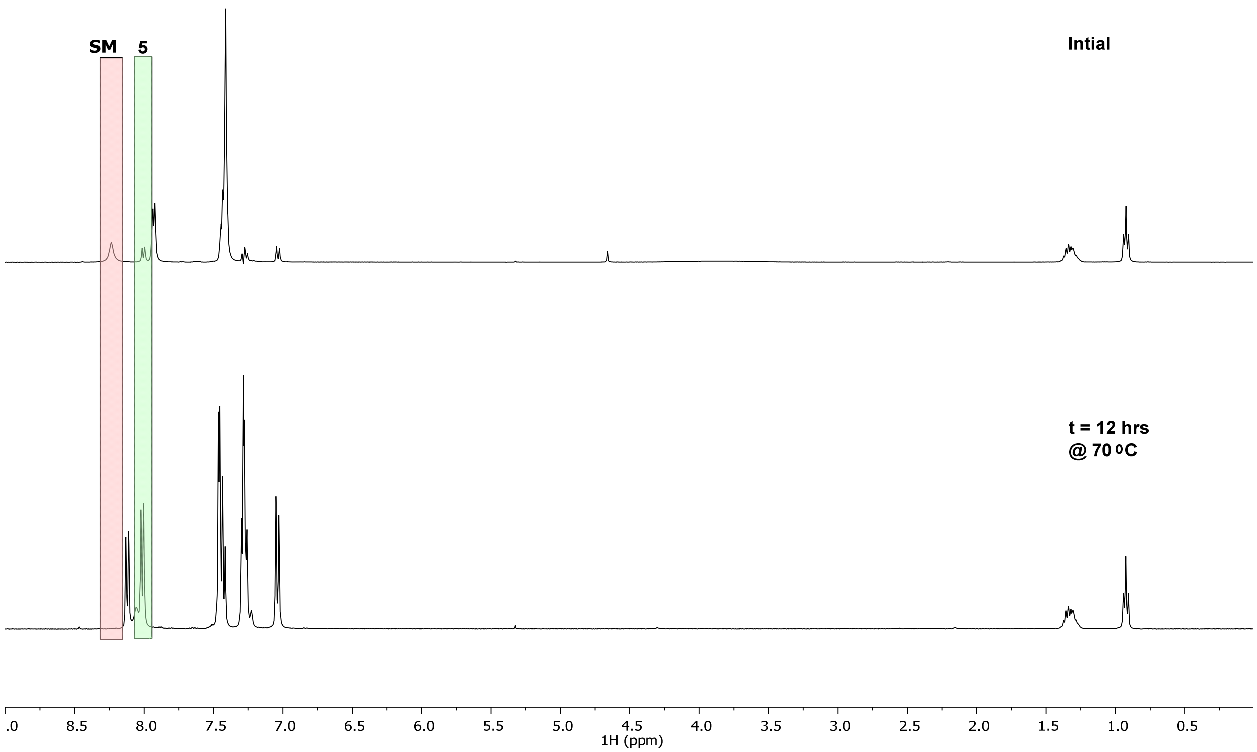


Figure S20. Stacked ^{1}H NMR spectra of the reaction of $HB(C_6F_5)_2$ with carbazole in $CDCl_3$.

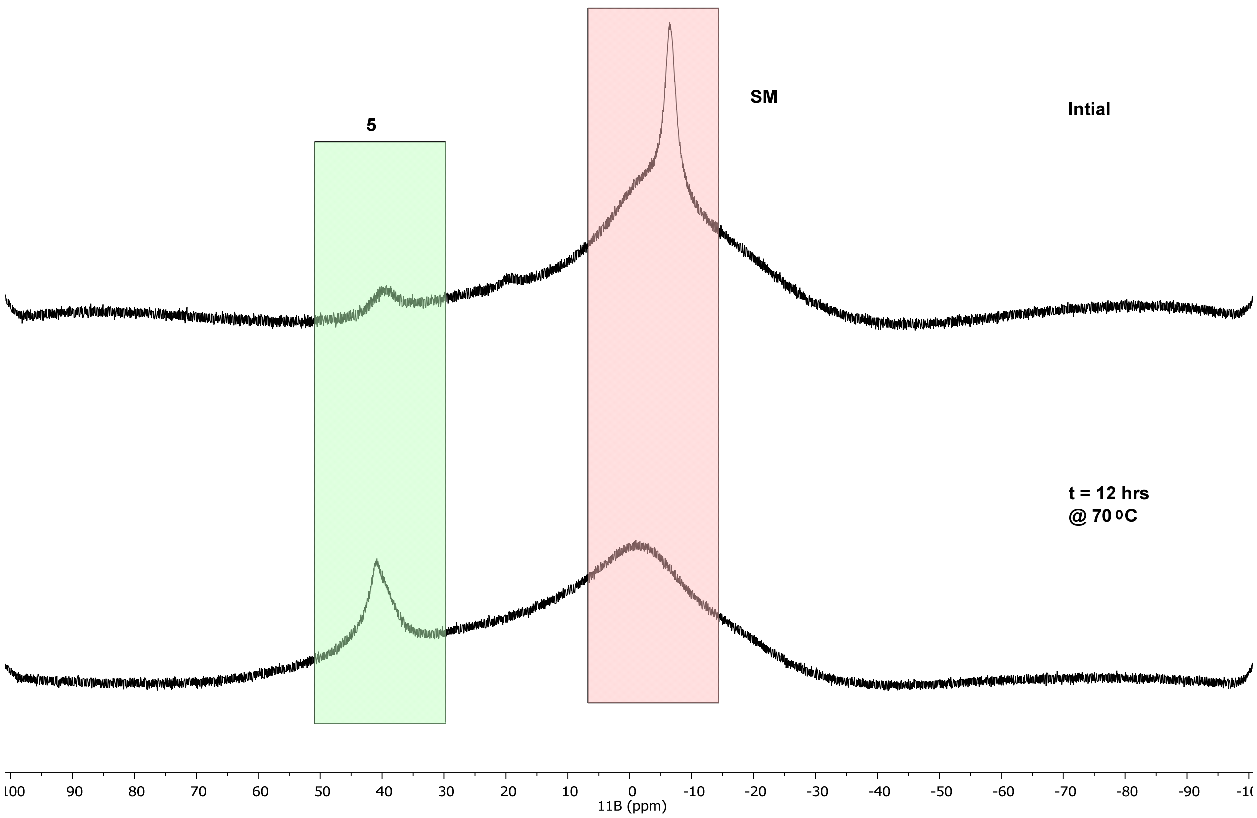


Figure S21. Stacked ^{11}B NMR spectra of the reaction of $HB(C_6F_5)_2$ with carbazole in $CDCl_3$.

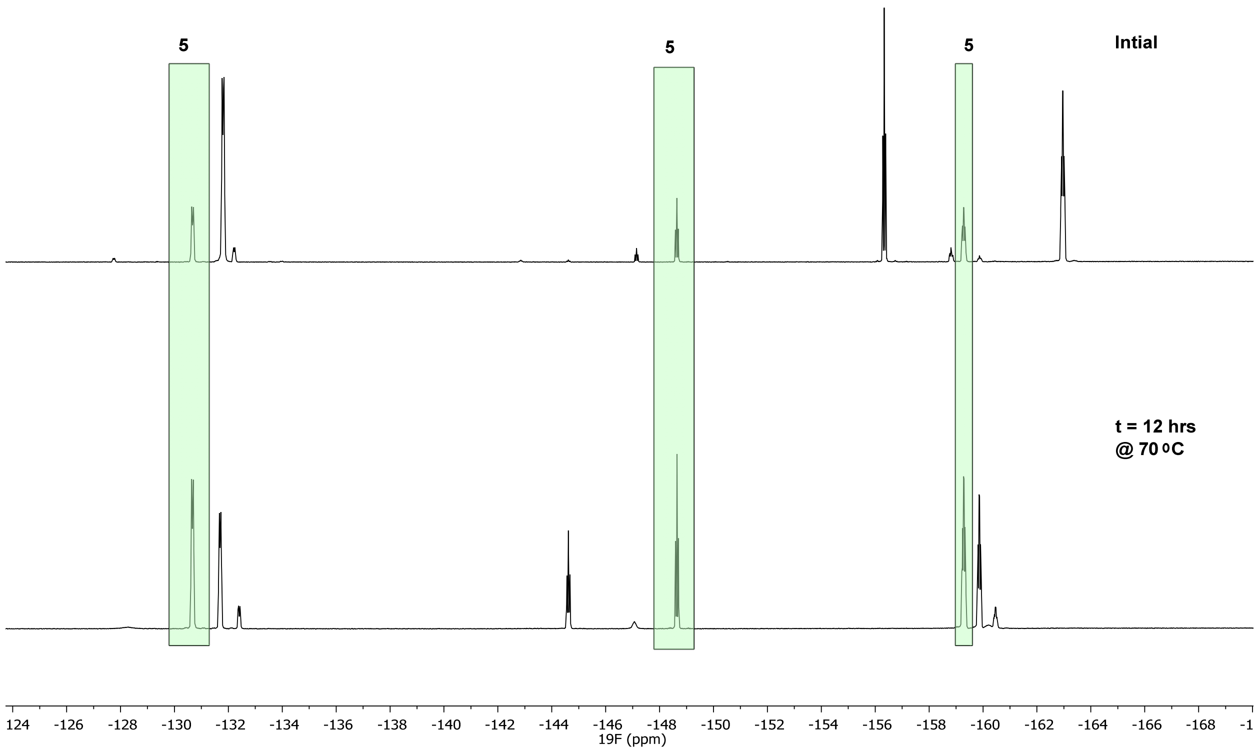
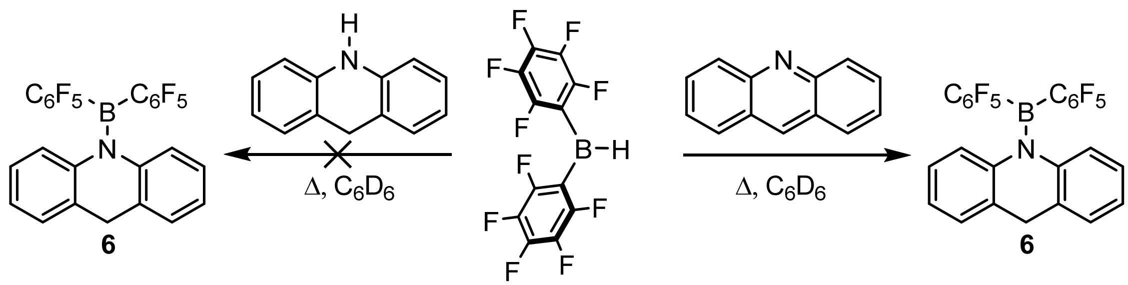


Figure S22. Stacked ^{19}F NMR spectra of the reaction of $HB(C_6F_5)_2$ with carbazole in $CDCl_3$.



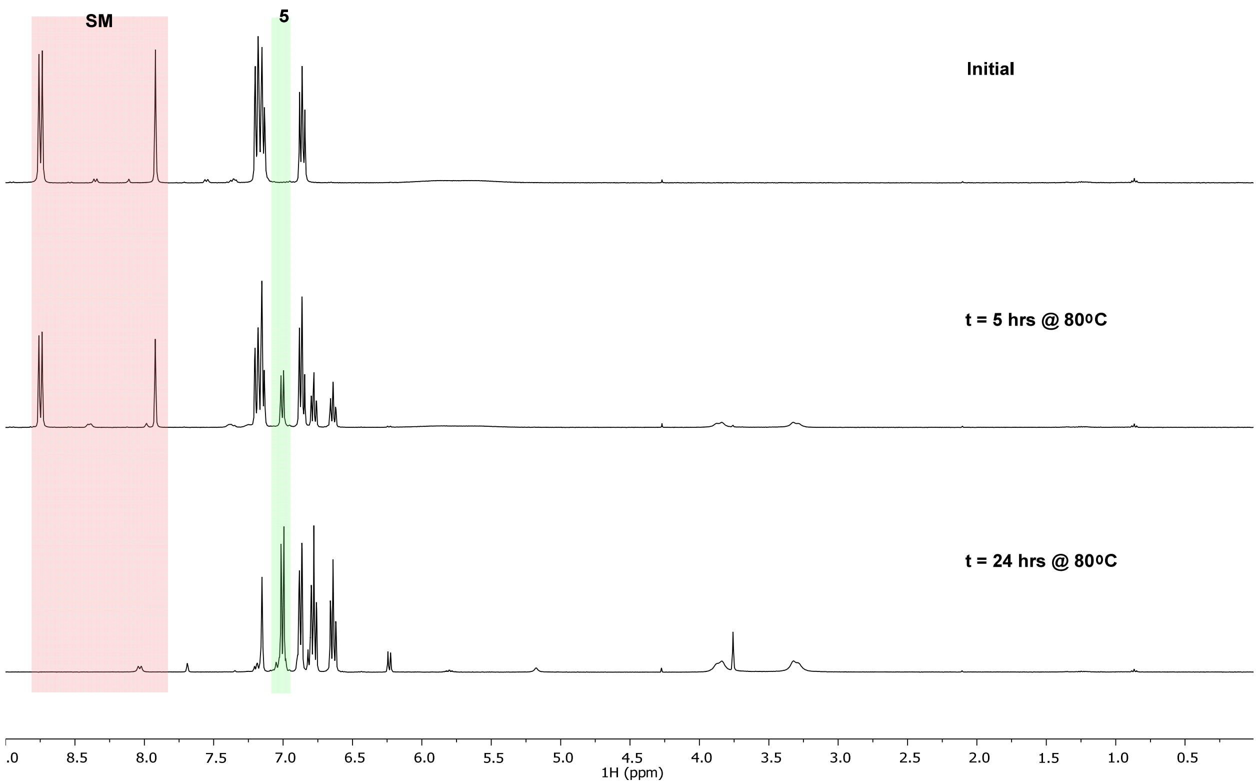


Figure S23. Stacked [1]H NMR spectra of the reaction of $HB(C_6F_5)_2$ with acridine in C_6D_6.

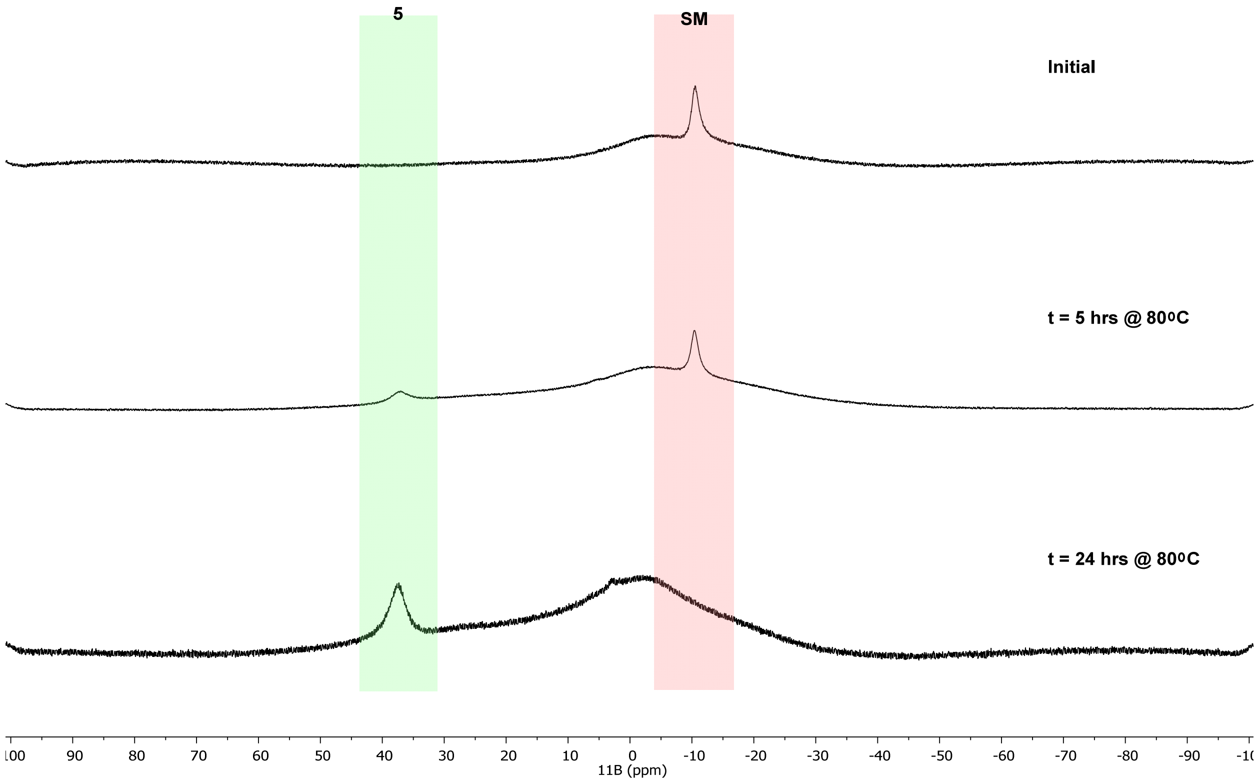


Figure S24. Stacked ^{11}B NMR spectra of the reaction of $HB(C_6F_5)_2$ with acridine in C_6D_6.

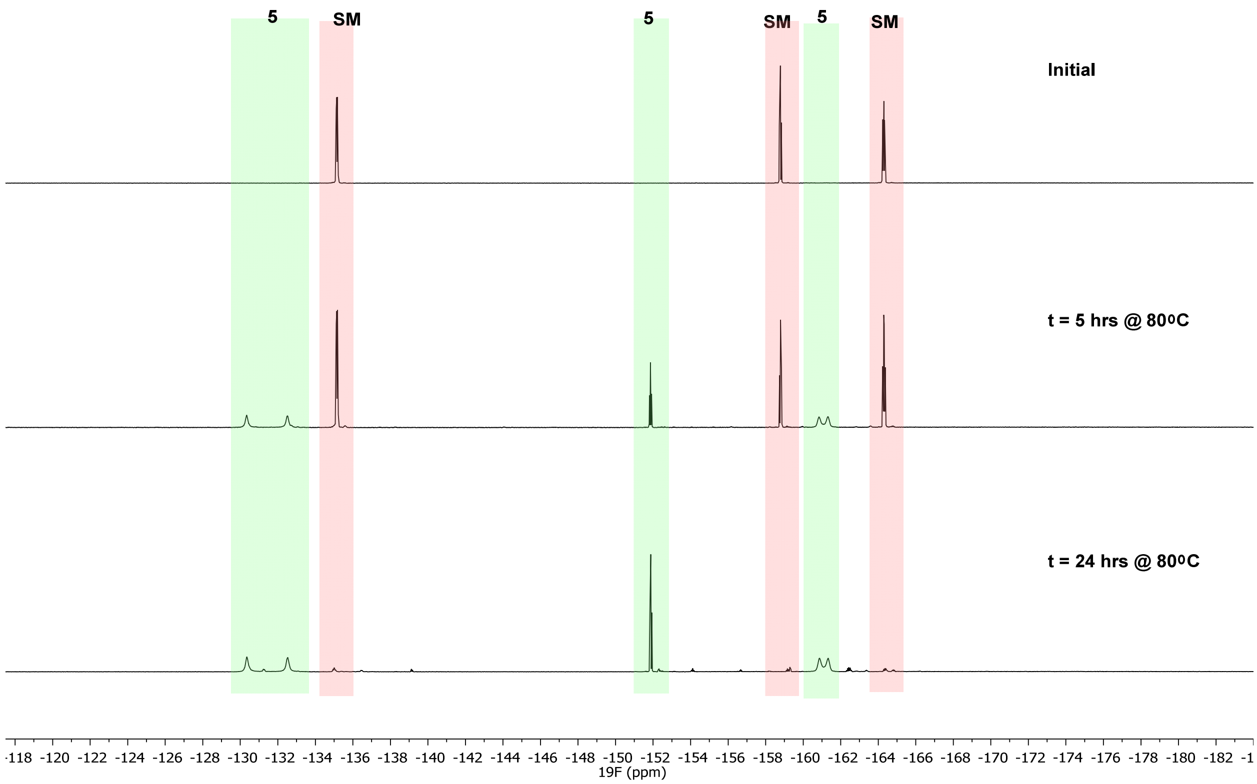
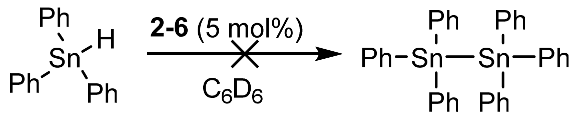


Figure S25. Stacked ${}^{19}F$ *NMR spectra of the reaction of* $HB(C_6F_5)_2$ *with acridine in* C_6D_6*.*

NMR Experiment - Reaction of Aminoboranes 2-6 with Ph_3SnH



General Catalytic Procedure: In a glovebox, Ph_3SnH (0.1 mmol) was massed out into a 5 mL scintillation vial and dissolved in C_6D_6 (0.4 mL). The respective aminoborane (**2**-**6**) (5 mol%) was massed out into a separate vial and dissolved in C_6D_6 (0.2 mL). The solution of Ph_3SnH was transferred to a J-young tap NMR spectrum tube, followed by the careful addition of the solution of aminoborane catalyst. The NMR spectrum tube was promptly sealed. The reaction was monitored by ^1H and ^{119}Sn NMR spectrum overtime at specific time intervals (ie. 0 hour, 3 hours 6 hours, etc); and heated to 50°C for comparison to **1**. The reaction was deemed complete upon either no observable progression or complete conversion.

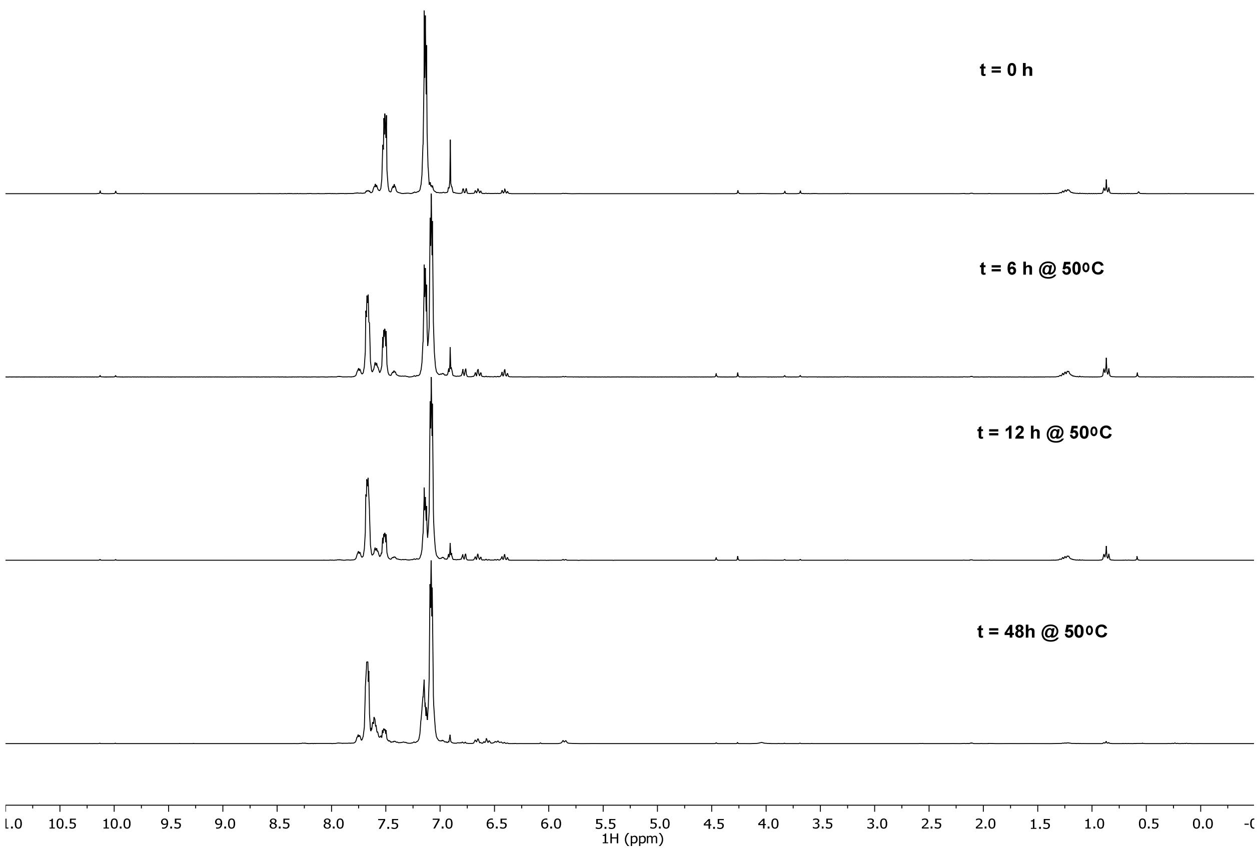


*Figure S26. Stacked ^1H NMR spectra of Ph_3SnH with **2** (5 mol%) in C_6D_6.*

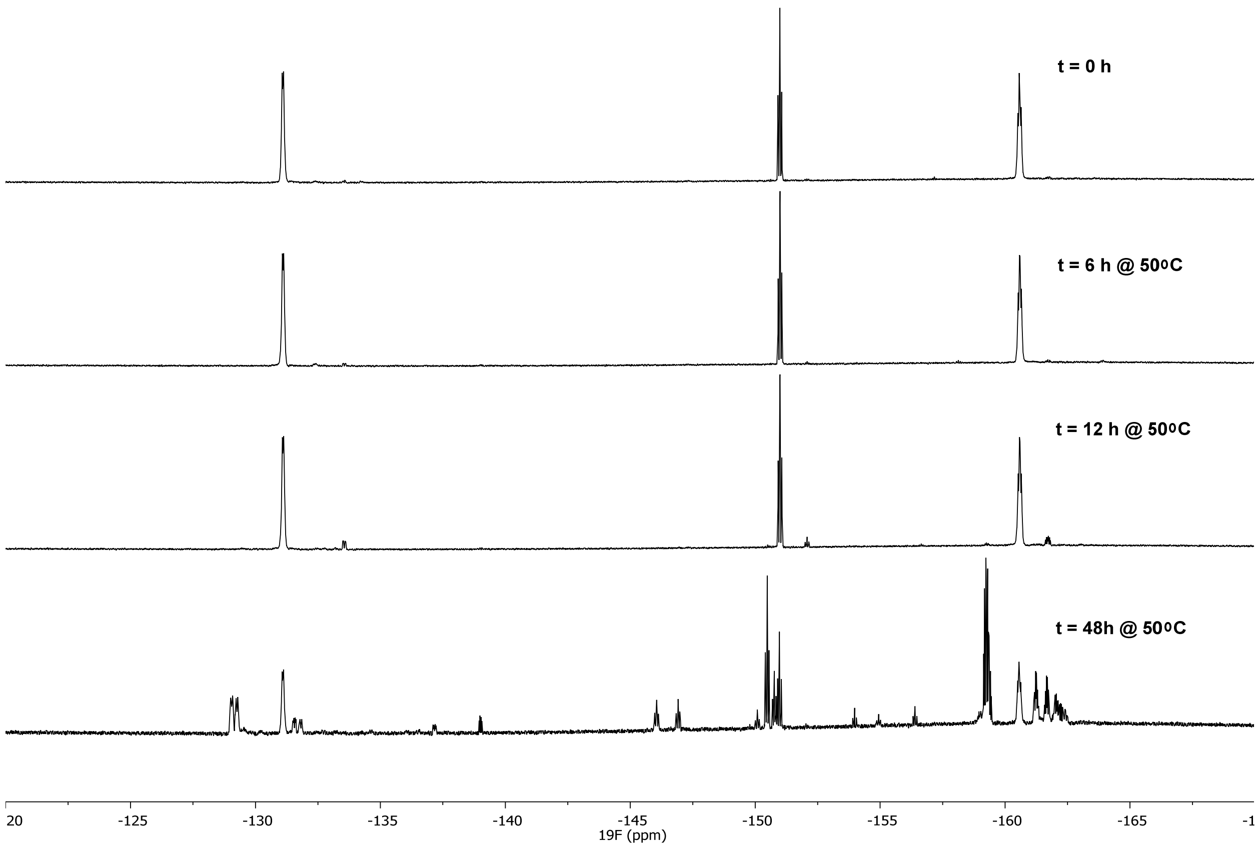


*Figure S27. Stacked ^{19}F NMR spectra of Ph_3SnH with **2** (5 mol%) in C_6D_6.*

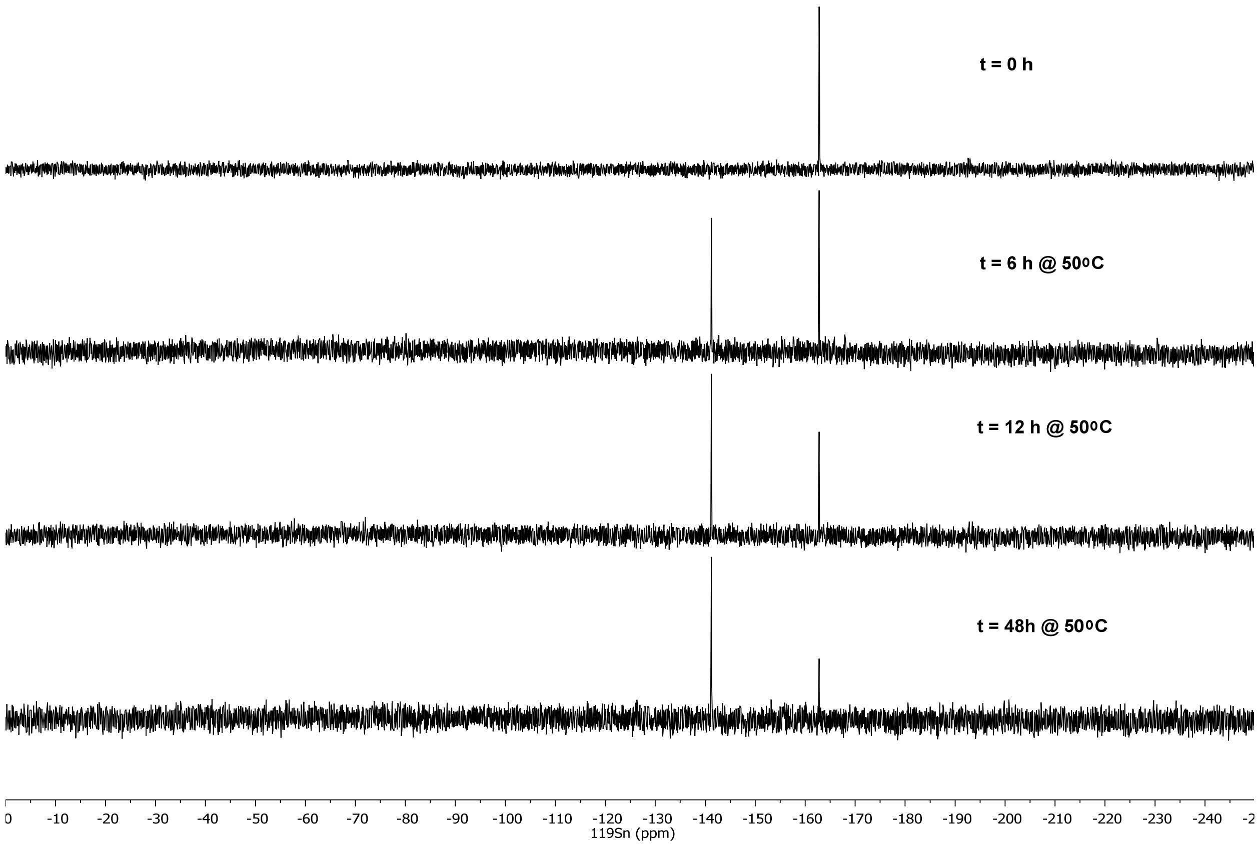


*Figure S28. Stacked ^{119}Sn NMR spectra of Ph_3SnH with **2** (5 mol%) in C_6D_6.*

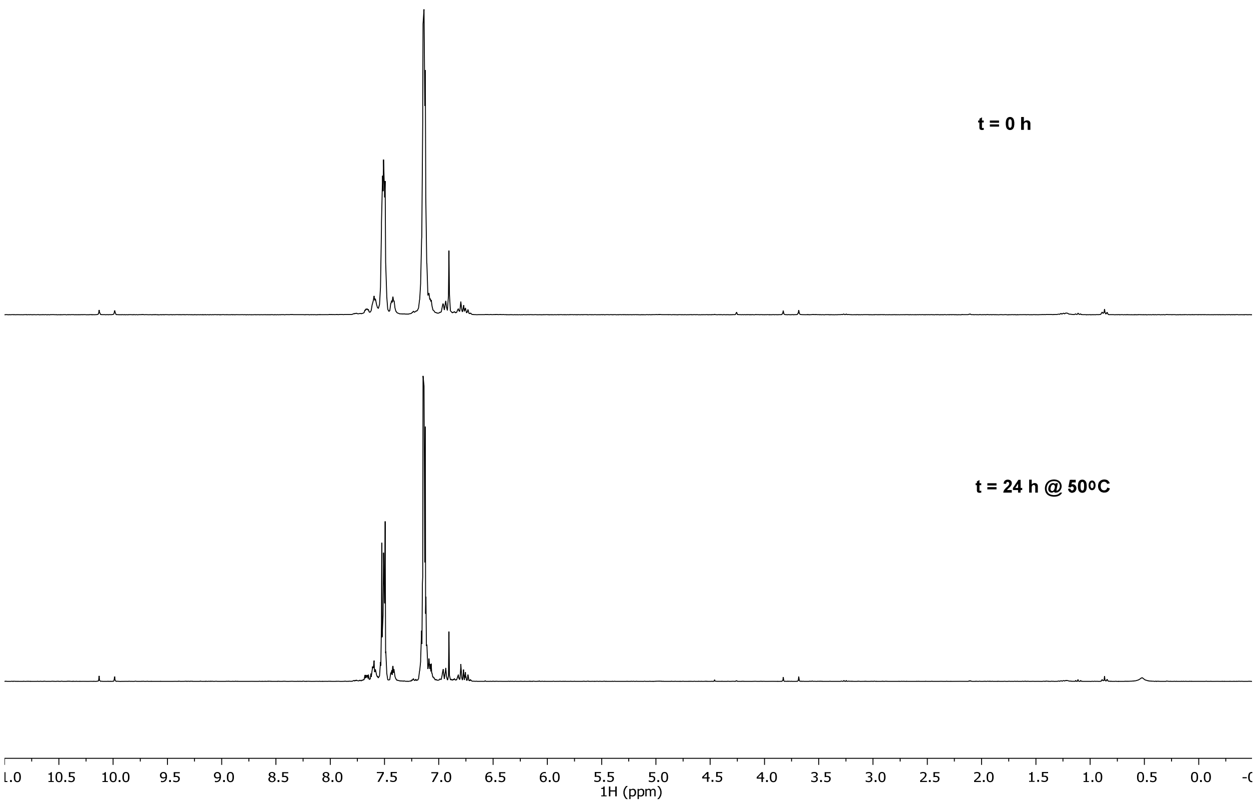


*Figure S29. Stacked [1]H NMR spectra of Ph_3SnH with **3** (5 mol%) in C_6D_6.*

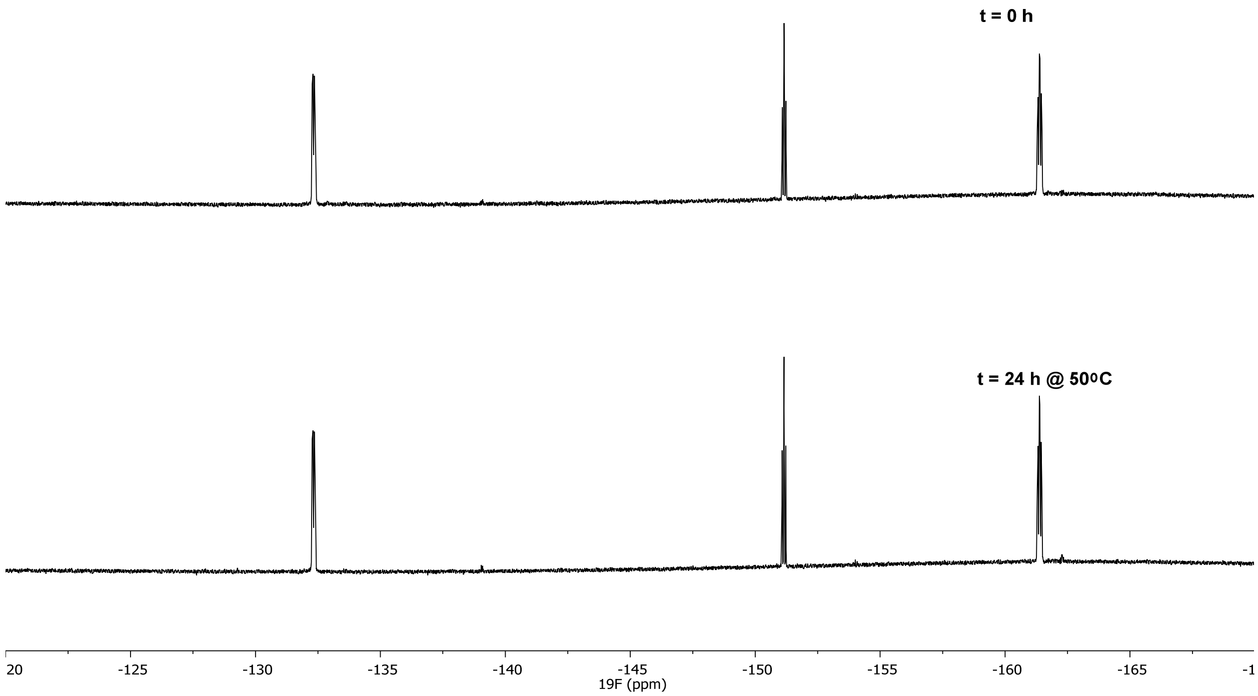


*Figure S30. Stacked ^{19}F NMR spectra of Ph_3SnH with **3** (5 mol%) in C_6D_6.*

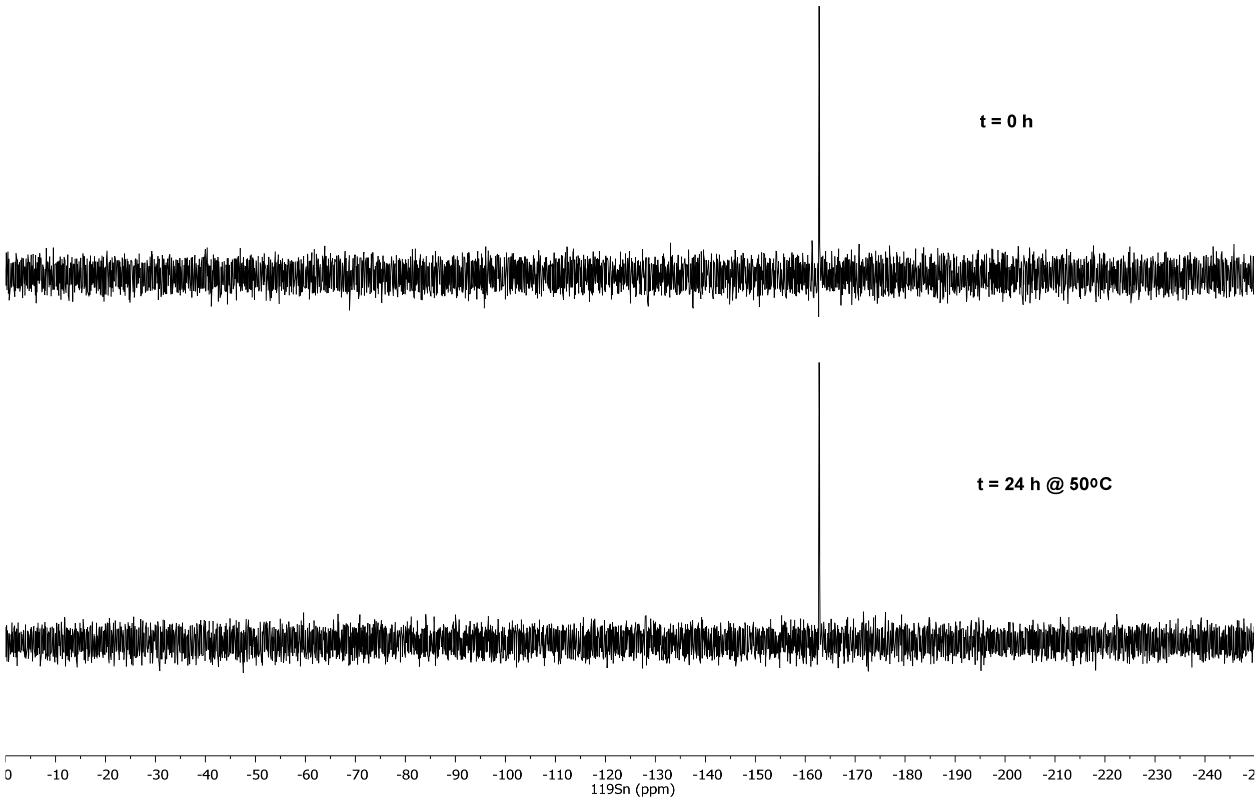


*Figure S31. Stacked ^{119}Sn NMR spectra of Ph_3SnH with **3** (5 mol%) in C_6D_6.*

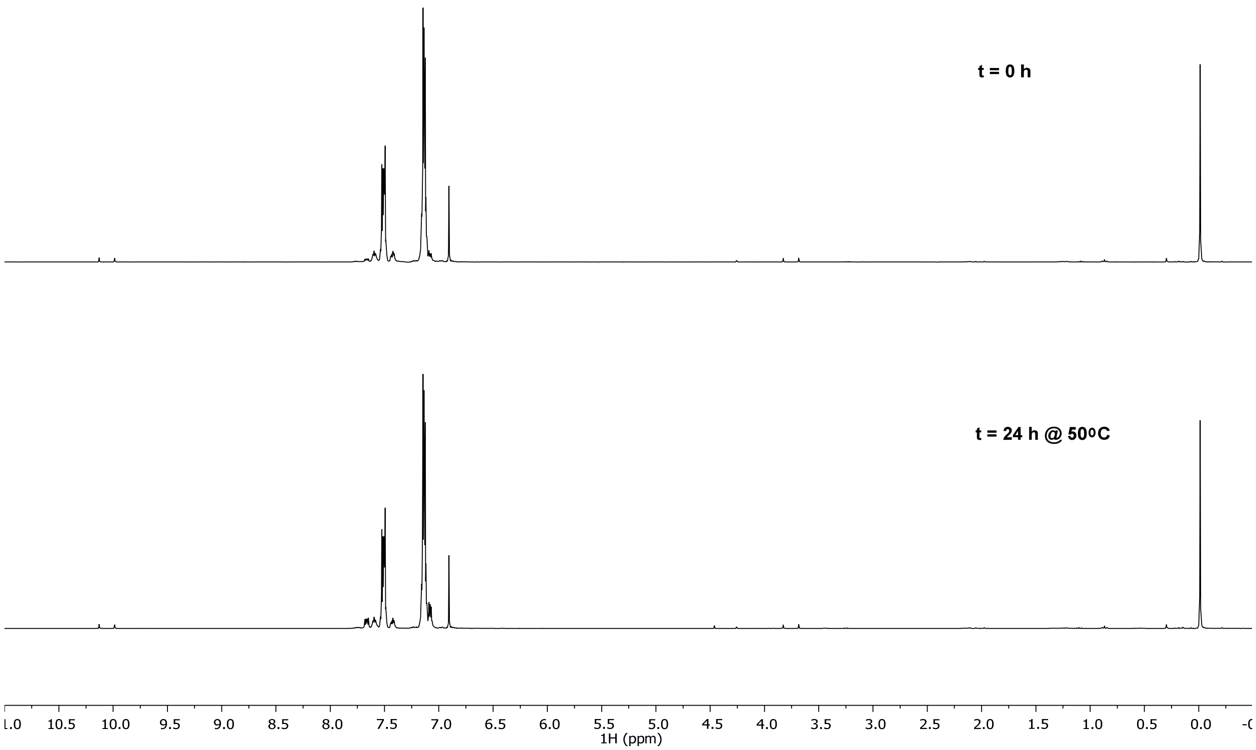


*Figure S32. Stacked ^{1}H NMR spectra of Ph_3SnH with **4** (5 mol%) in C_6D_6.*

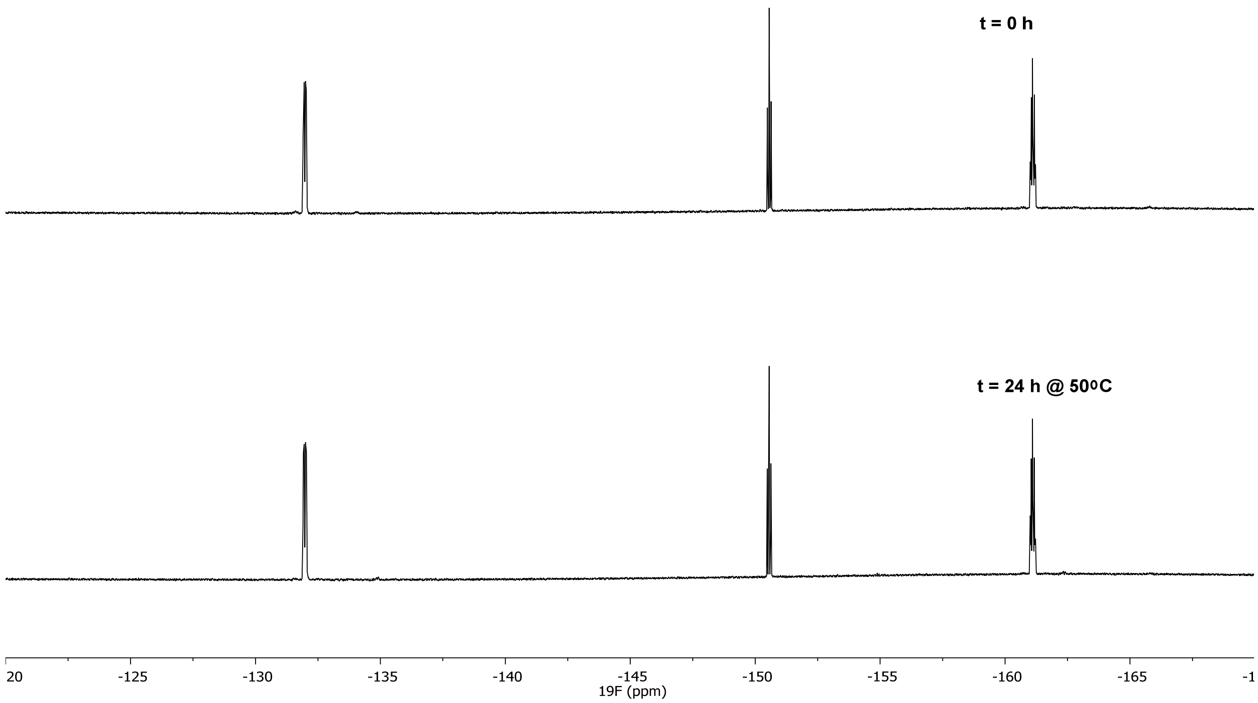


*Figure S33. Stacked ^{19}F NMR spectra of Ph_3SnH with **4** (5 mol%) in C_6D_6.*

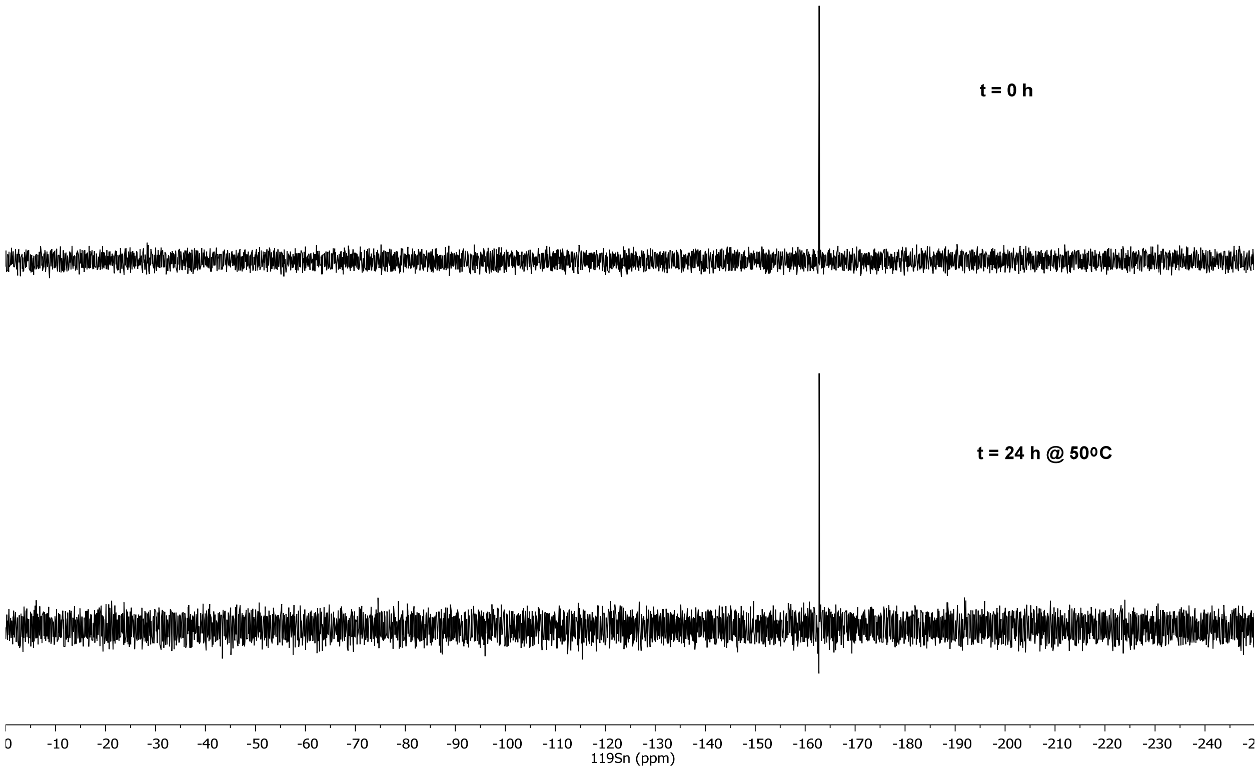


Figure S34. Stacked ^{119}Sn NMR spectra of Ph_3SnH with ***4*** *(5 mol%) in C_6D_6.*

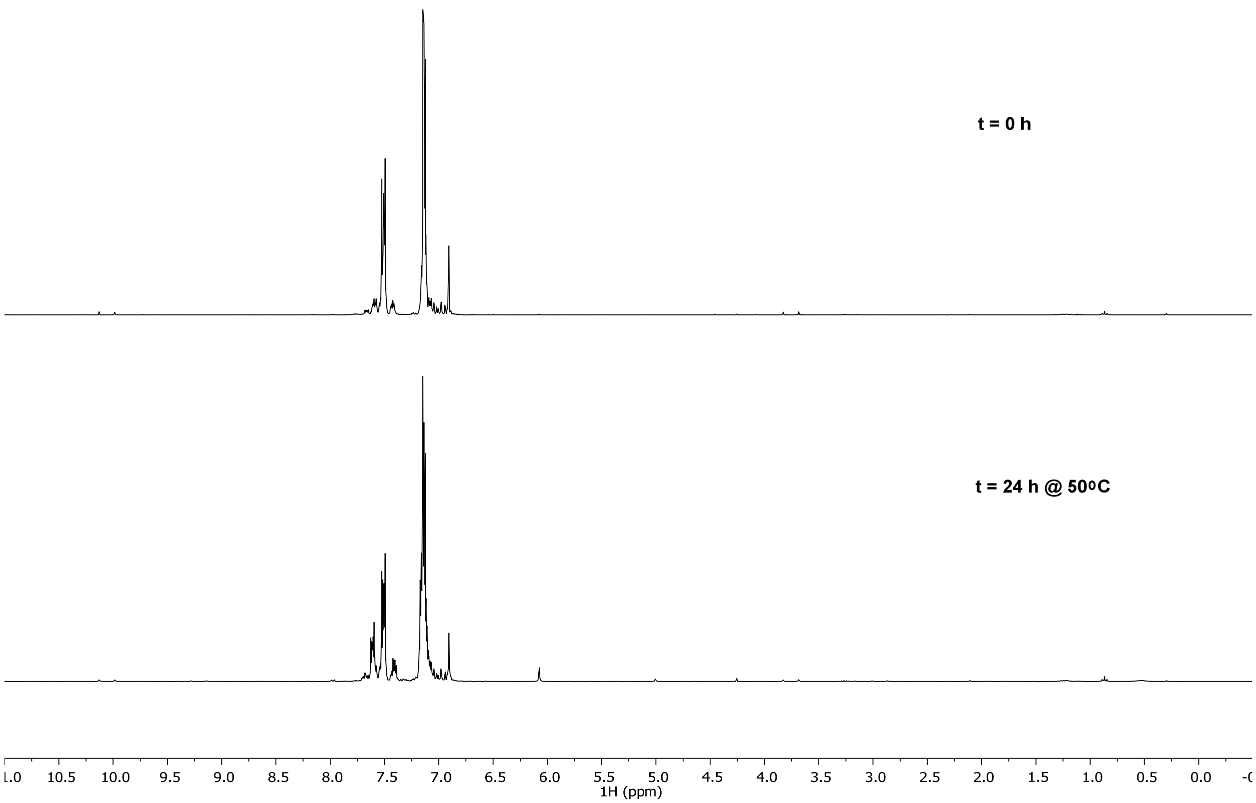


*Figure S35. Stacked [1]H NMR spectra of Ph_3SnH with **5** (5 mol%) in C_6D_6.*

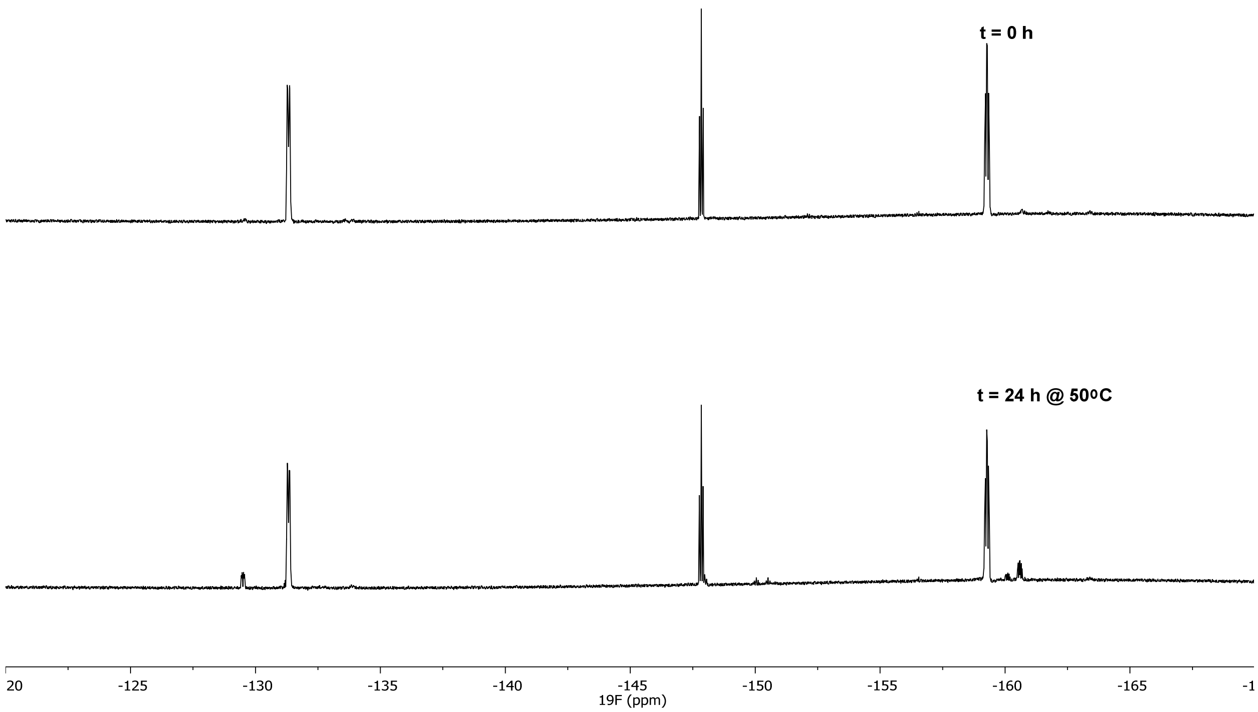


*Figure S36. Stacked ^{19}F NMR spectra of Ph_3SnH with **5** (5 mol%) in C_6D_6.*

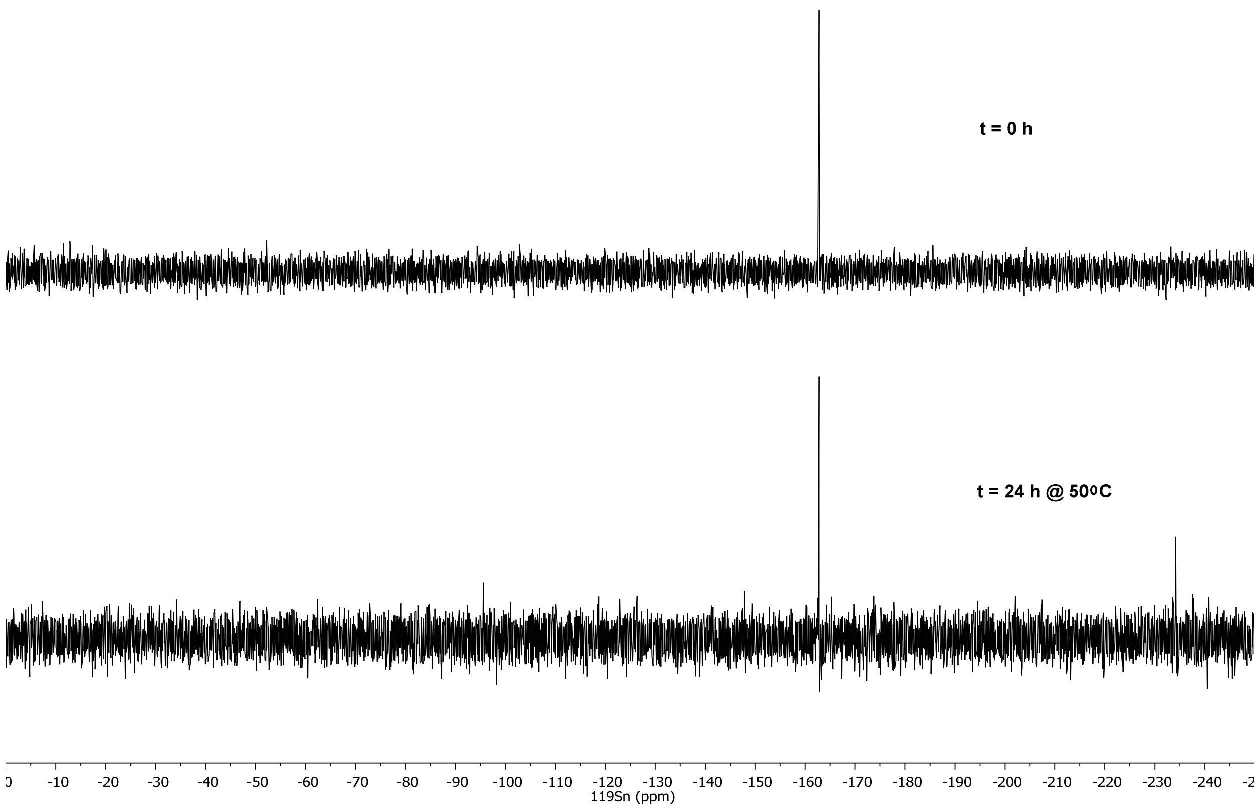


*Figure S37. Stacked ^{119}Sn NMR spectra of Ph_3SnH with **5** (5 mol%) in C_6D_6.*

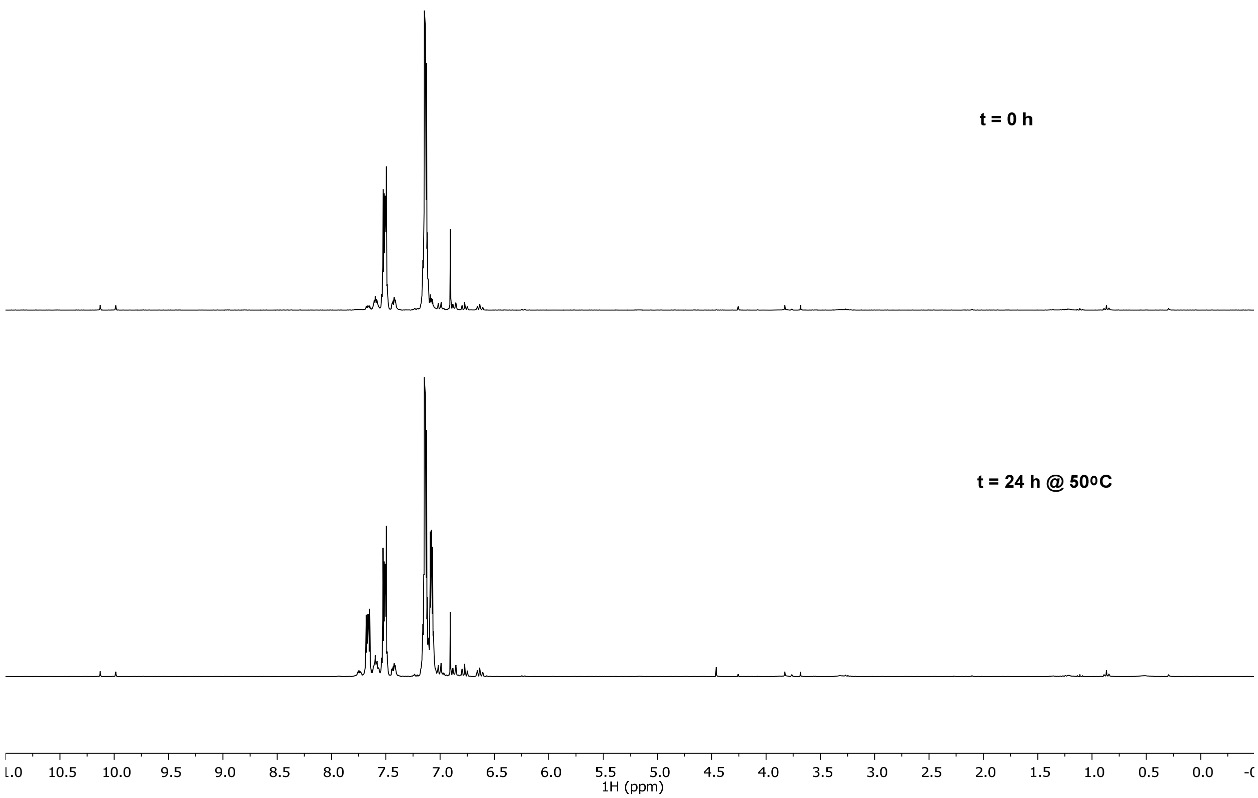


*Figure S38. Stacked ^{1}H NMR spectra of Ph_3SnH with **6** (5 mol%) in C_6D_6.*

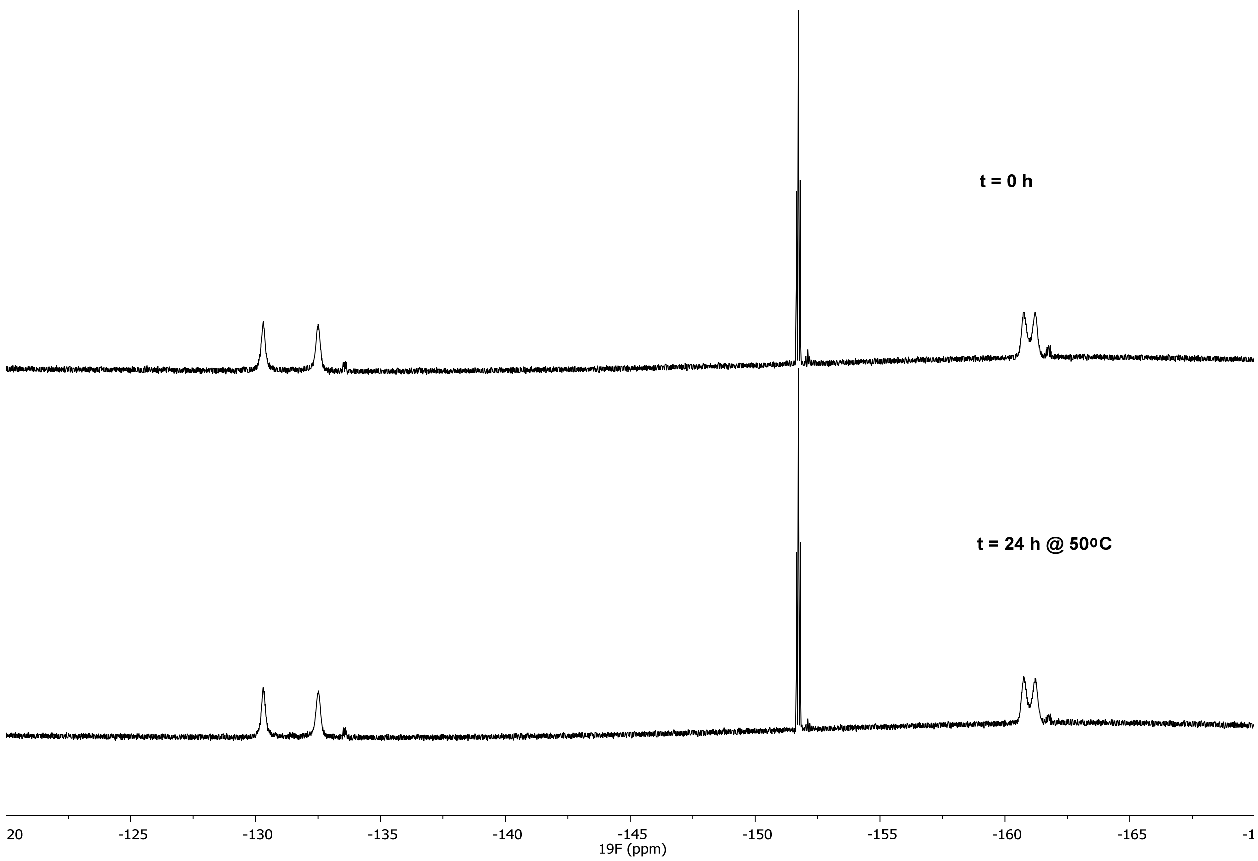


*Figure S39. Stacked ^{19}F NMR spectra of Ph_3SnH with **6** (5 mol%) in C_6D_6.*

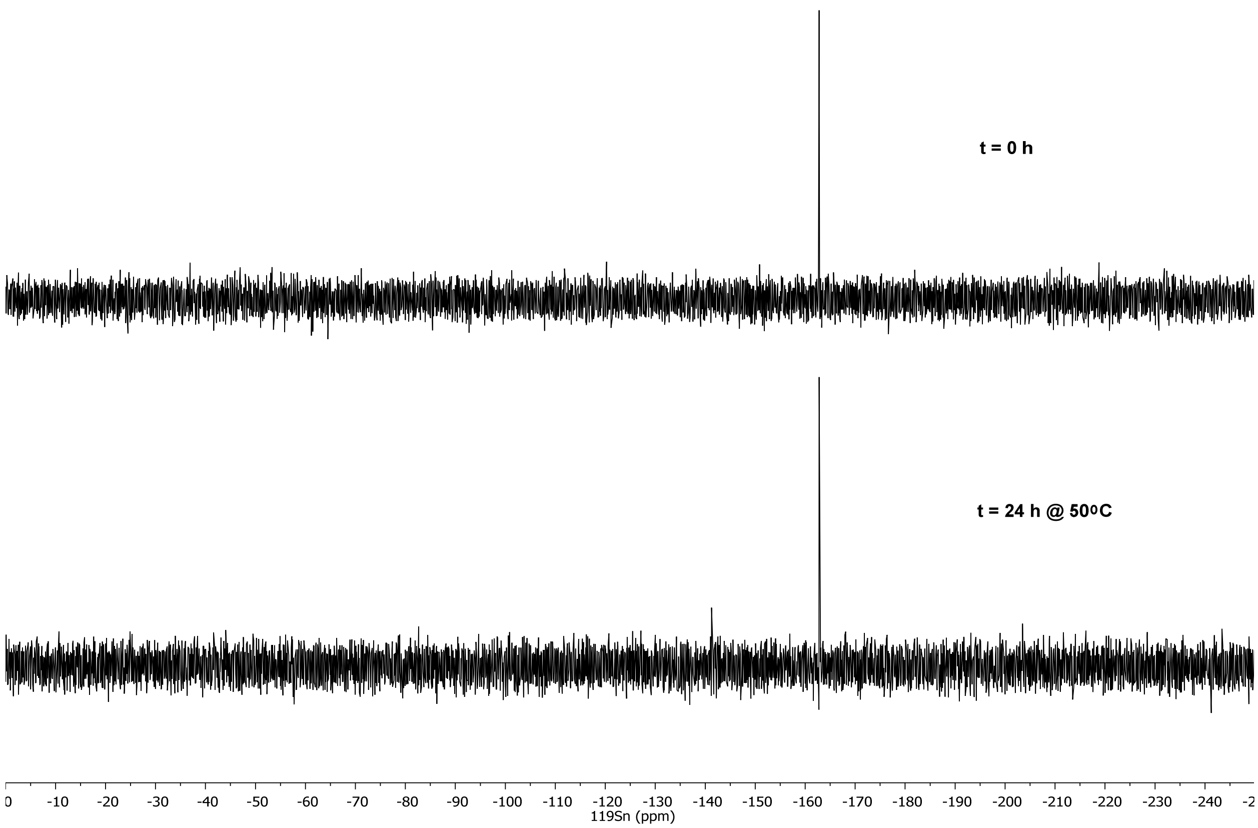
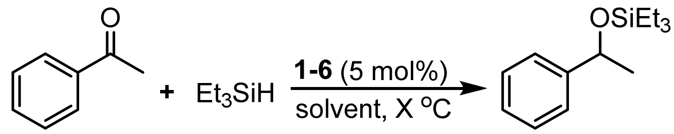


*Figure S40. Stacked ^{119}Sn NMR spectra of Ph_3SnH with **6** (5 mol%) in C_6D_6.*

NMR Experiment - Catalytic Hydrosilylation by Aminoboranes 1-6



In a glovebox, acetophenone (0.1 mmol) and triethylsilane (1 eq) were massed out into a 5 mL scintillation vial and dissolved in C_6D_6 (0.5 mL). The respective aminoborane (**1-6**) (5 mol%) was massed out into a separate vial and dissolved in $CDCl_3$ (0.2 mL). The solution of substrates was transferred to a J-young tap NMR spectrum tube, followed by the careful addition of the solution of respective catalyst. The NMR tube was promptly sealed. The reaction was monitored by the ^1H nuclei at specific time intervals (ie. 0 hour, 3 hours 6 hours, etc); at room temperature unless otherwise specificed. The reaction was deemed complete upon either no observable progression or complete conversion. * "time (h)" is relative to the start of aquisition; approximately 5 minutes from preparation in a glovebox to bringing the sample to an NMR spectrometer and setting up the experiment.

*Table 1. Consolidated percent conversions of acetophenone to product by **1-6** overtime at room temperature in $CDCl_3$.*

time (h)*	1	2	3	4	5	6
0	71.8	99.8	13.8	0	56.5	20.0
1	90.0		99.9	0	82.4	99.9
2	90.3			0	90.8	
3	90.6			0	91.2	
4	90.6			0	91.6	

*Table S2. Consolidated percent conversions of acetophenone to product by **5•H_2O** overtime at 60 ^oC in $CDCl_3$.*

time (h)*	5•H_2O
0	9.9
24	48.2
48	88.5

*Table S3. Consolidated percent conversions of acetophenone to product by **5** overtime at room temperature in CD_3CN .*

time (h)*	5 in CD_3CN
0	35.5
1	60.6
6	98.3

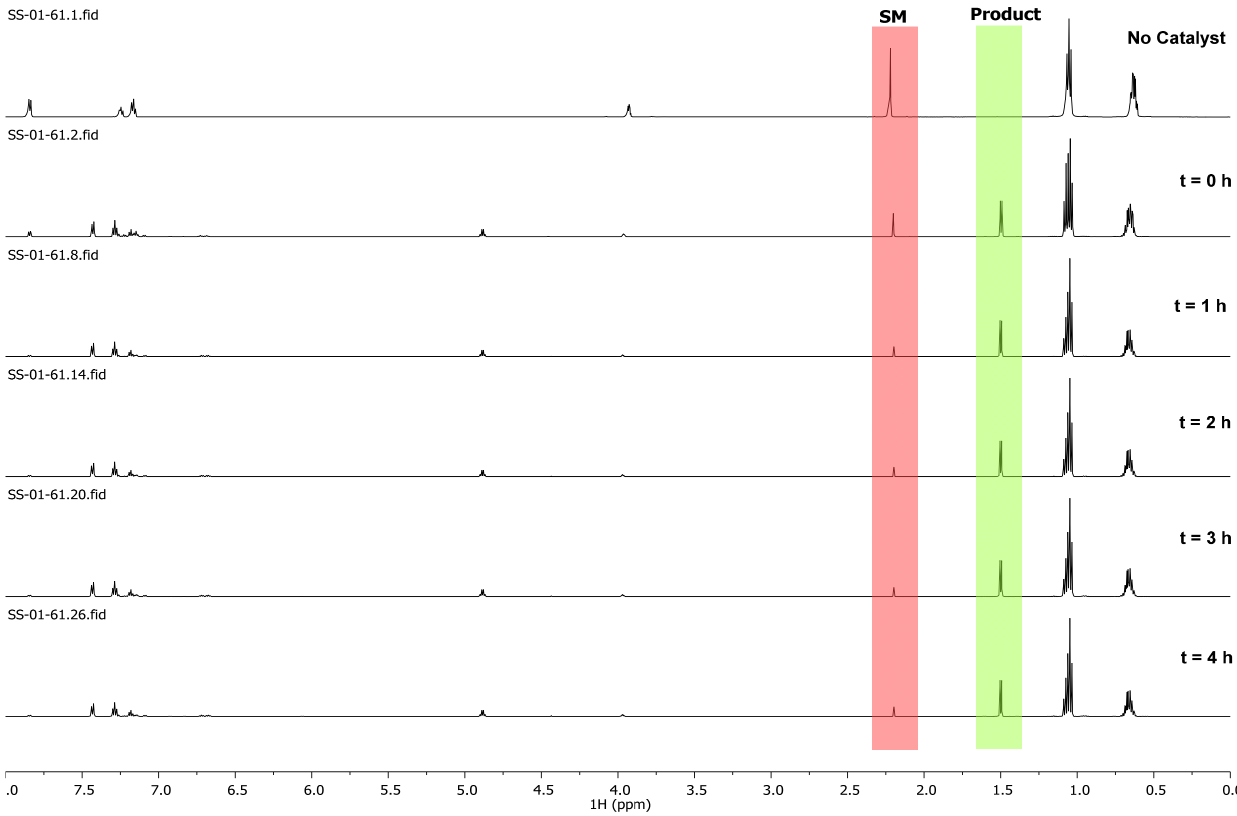


*Figure S41. Stacked ¹H NMR spectra of the hydrosilylation of acetophenone with Et_3SiH (1.1 eq.), with **1** (5 mol%) in $CDCl_3$.*

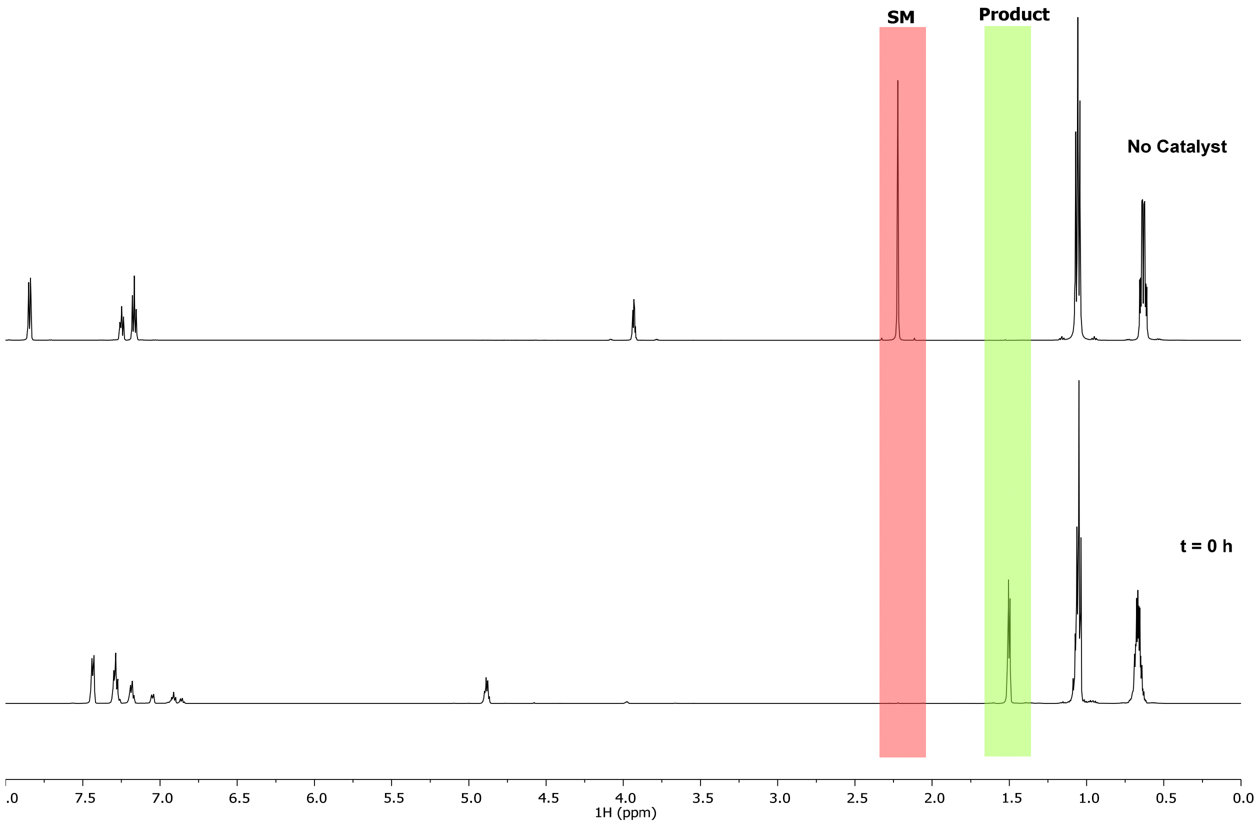


*Figure S42. Stacked [1]H NMR spectra of the hydrosilylation of acetophenone with Et_3SiH (1.1 eq.), with **2** (5 mol%) in $CDCl_3$.*

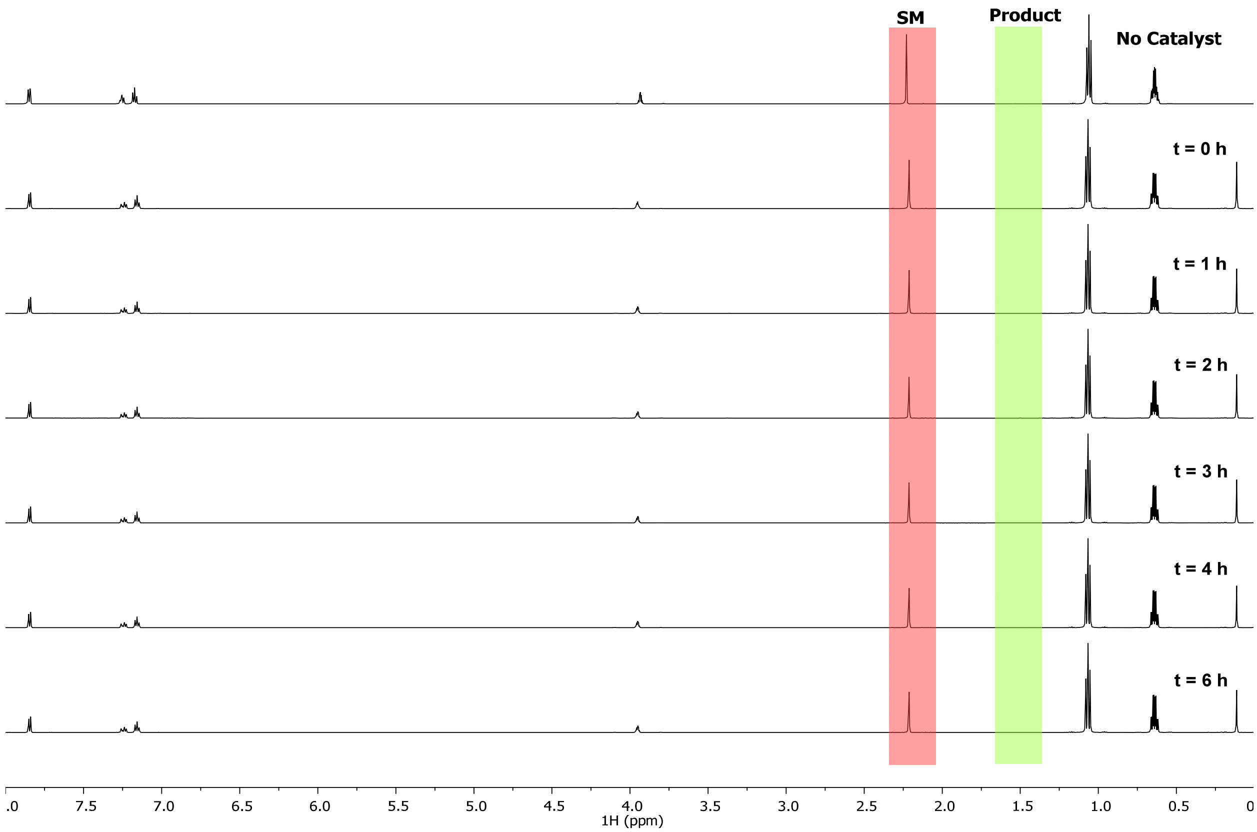


*Figure S43. Stacked ^{1}H NMR spectra of the hydrosilylation of acetophenone with Et_3SiH (1.1 eq.), with **3** (5 mol%) in $CDCl_3$.*

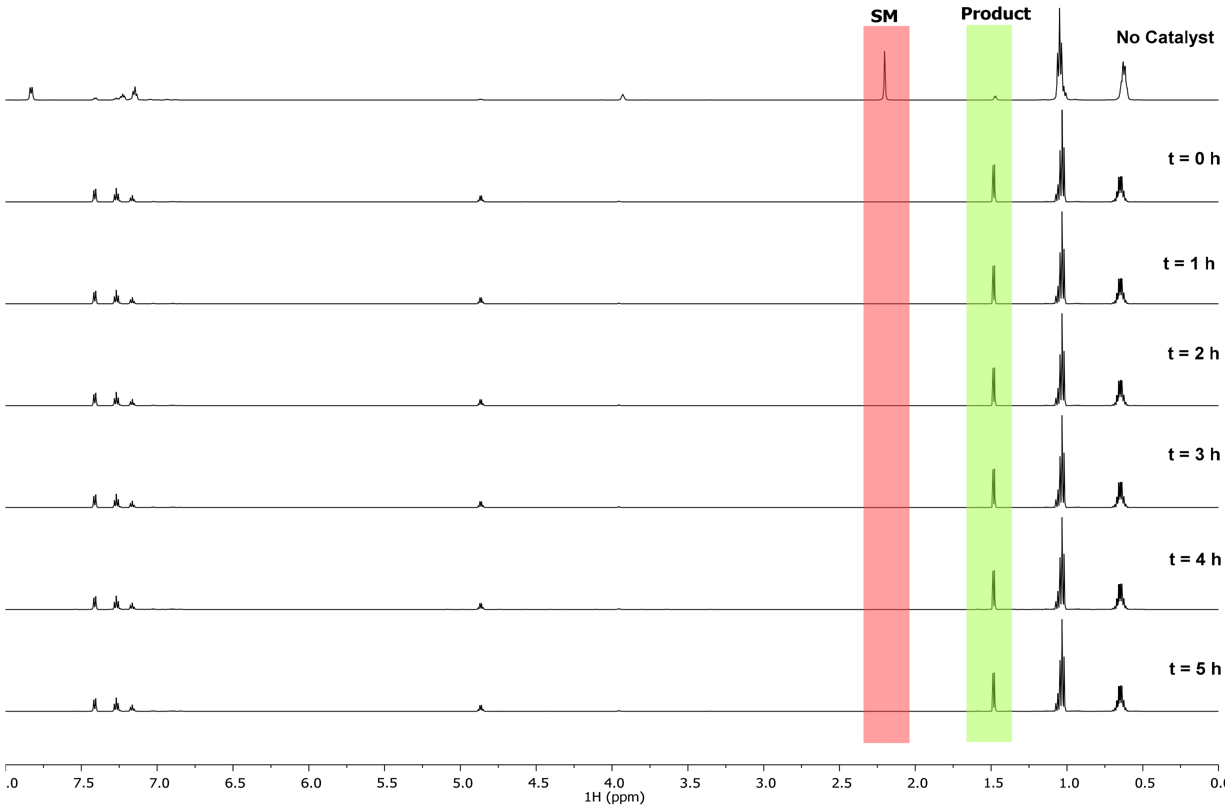


*Figure S44. Stacked [1]H NMR spectra of the hydrosilylation of acetophenone with Et_3SiH (1.1 eq.), with **4** (5 mol%) in $CDCl_3$.*

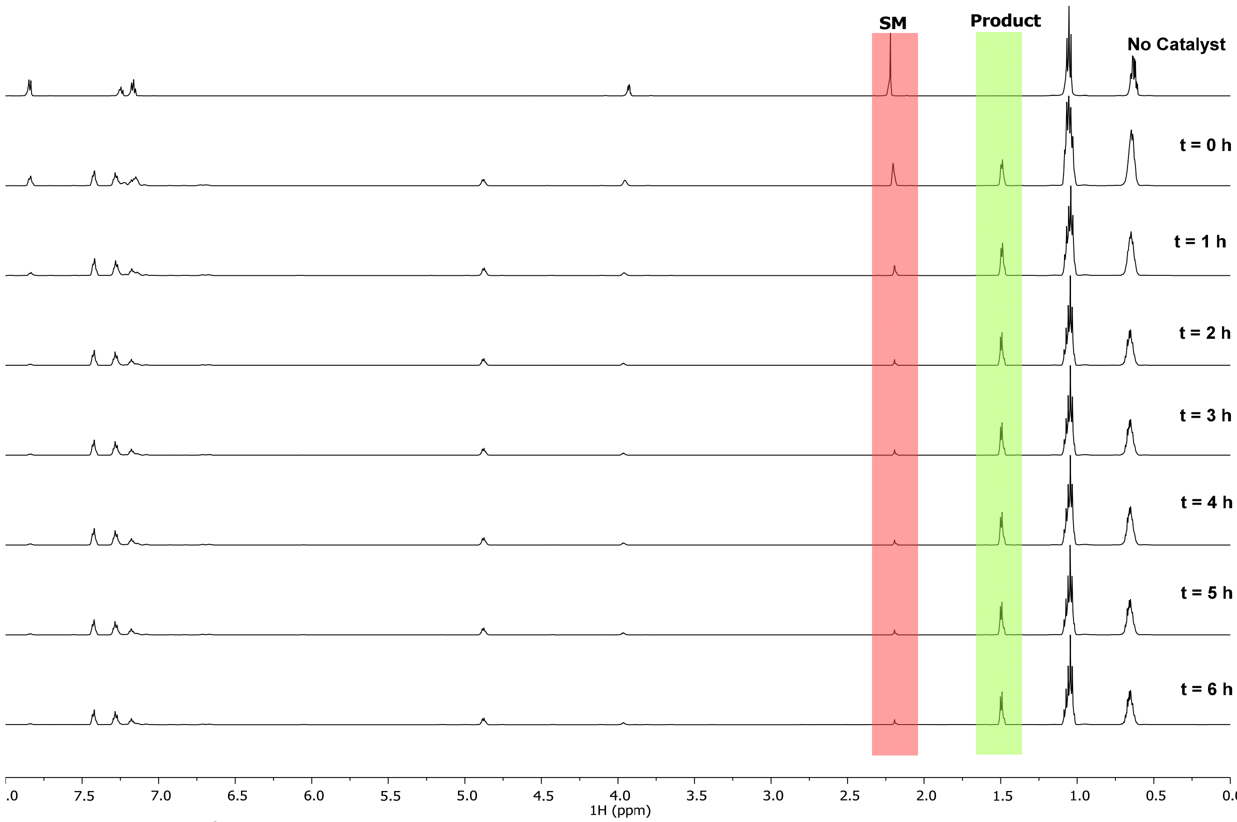


*Figure S45. Stacked [1]H NMR spectra of the hydrosilylation of acetophenone with Et_3SiH (1.1 eq.), with **5** (5 mol%) in $CDCl_3$.*

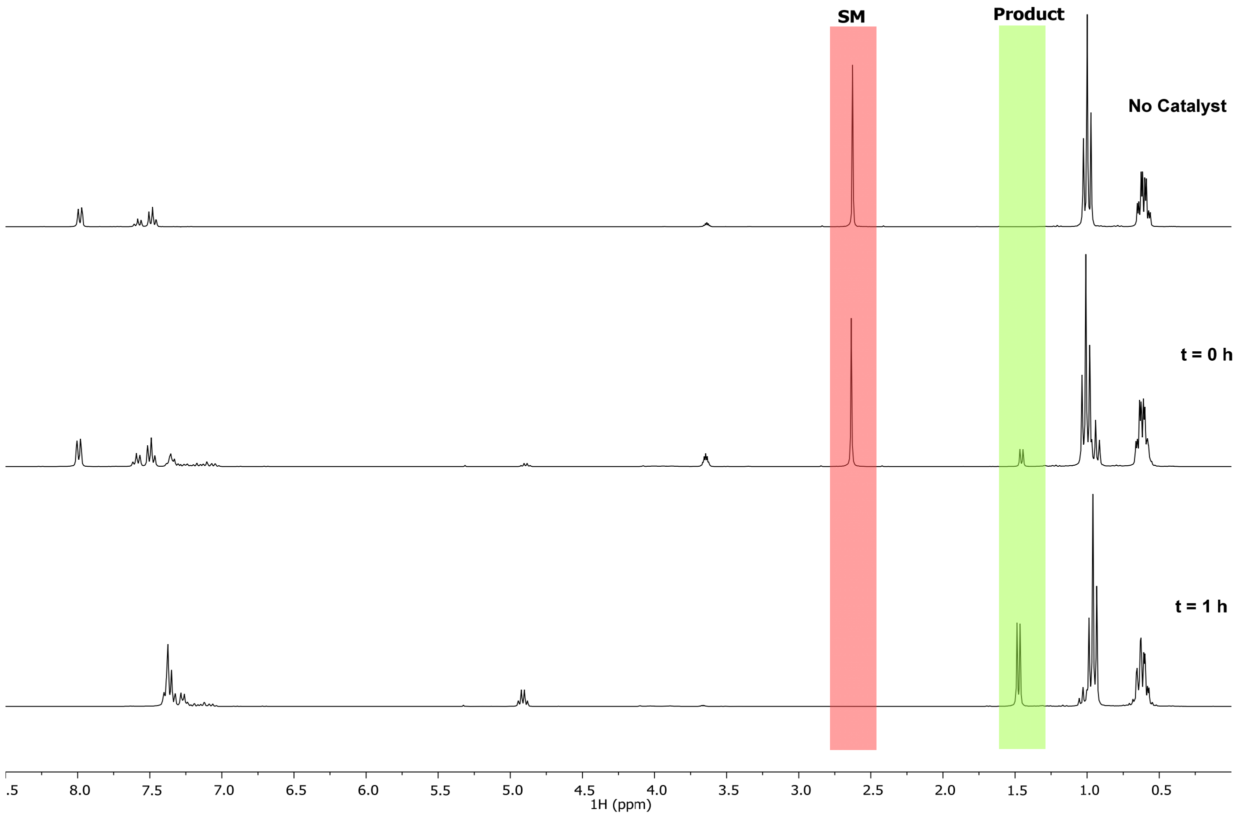


*Figure S46. Stacked [1]H NMR spectra of the hydrosilylation of acetophenone with Et_3SiH (1.1 eq.), with **6** (5 mol%) in $CDCl_3$.*

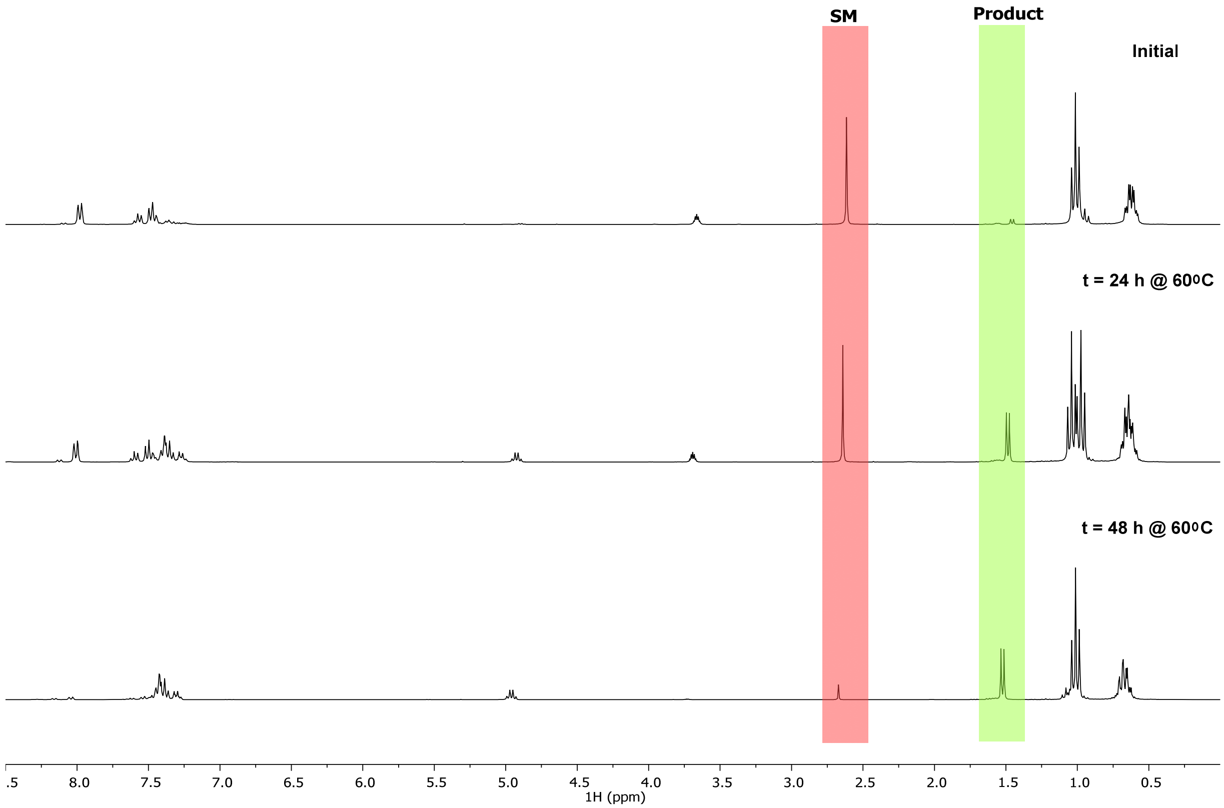


Figure S47. Stacked [1]*H NMR spectra of the hydrosilylation of acetophenone with* Et_3SiH *(1.1 eq.), with* ***5•H₂O*** *(5 mol%) in* $CDCl_3$*.*

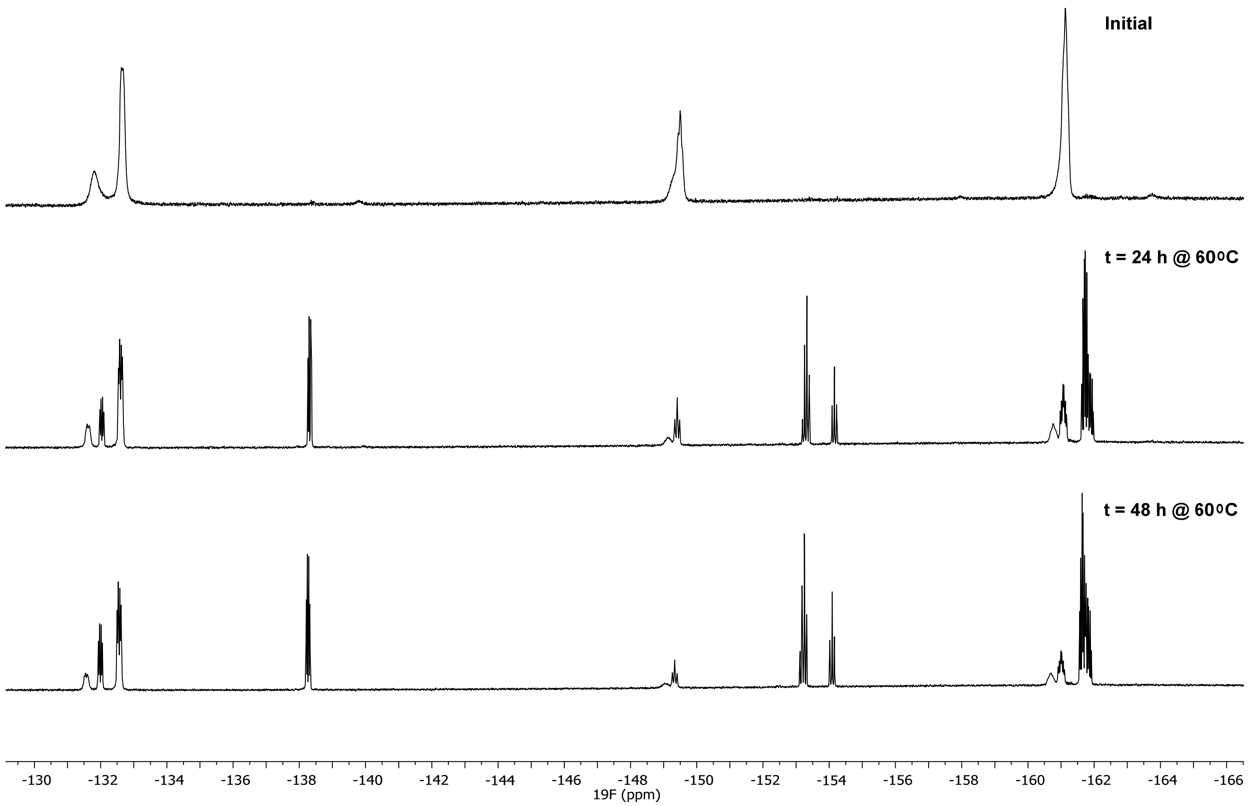


Figure S48. Stacked ^{19}F NMR spectra of the hydrosilylation of acetophenone with Et_3SiH (1.1 eq.), with ***5•H₂O*** *(5 mol%) in $CDCl_3$.*

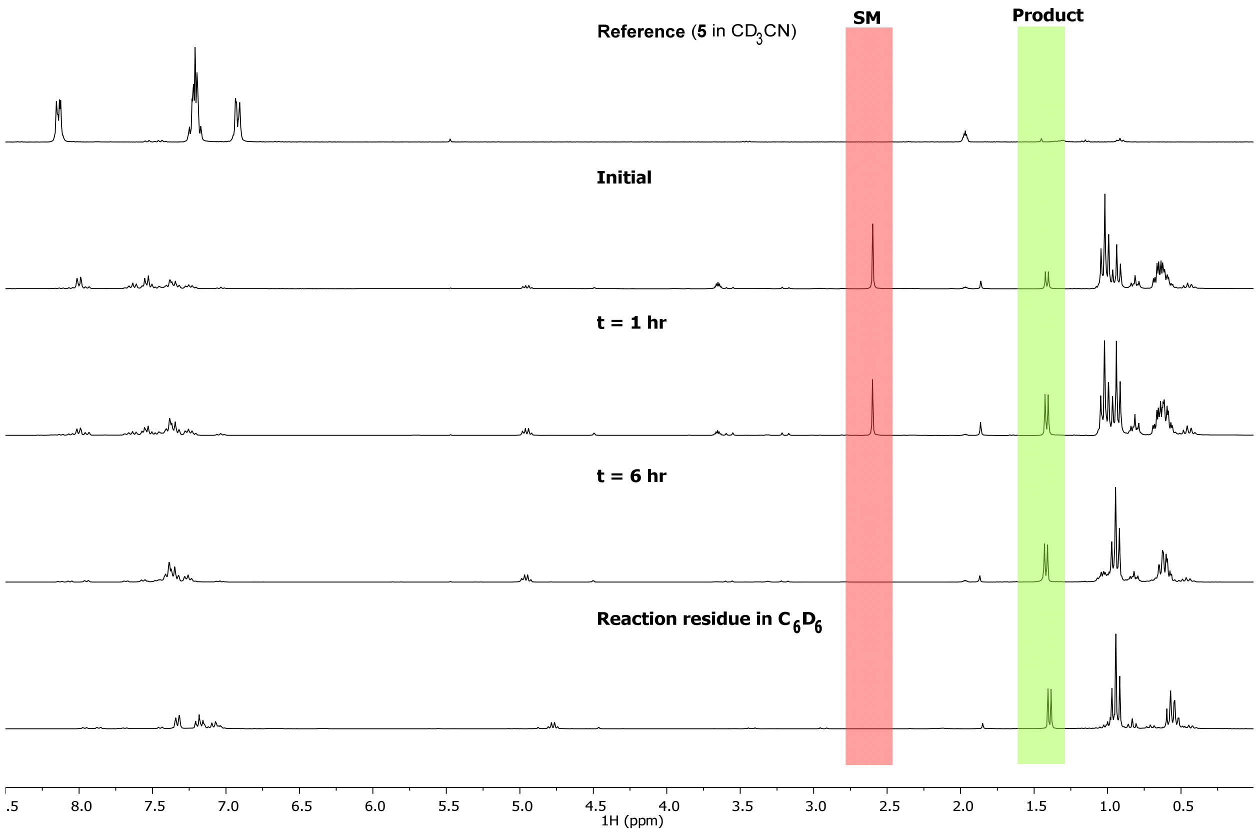


Figure S49. Stacked [1]H NMR spectra of the hydrosilylation of acetophenone with Et_3SiH (1.1 eq.), with ***5*** *(5 mol%) in CD_3CN.*

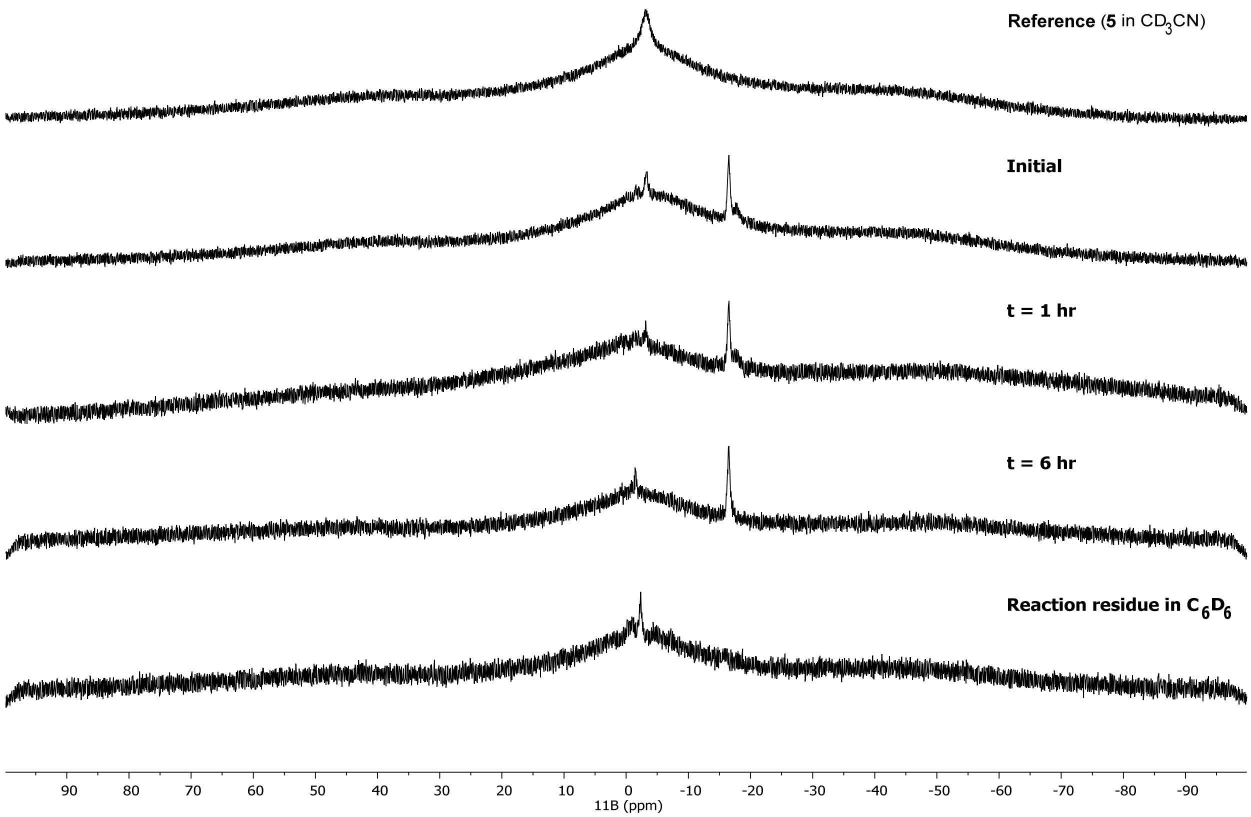


*Figure S50. Stacked ^{11}B NMR spectra of the hydrosilylation of acetophenone with Et_3SiH (1.1 eq.), with **5** (5 mol%) in CD_3CN.*

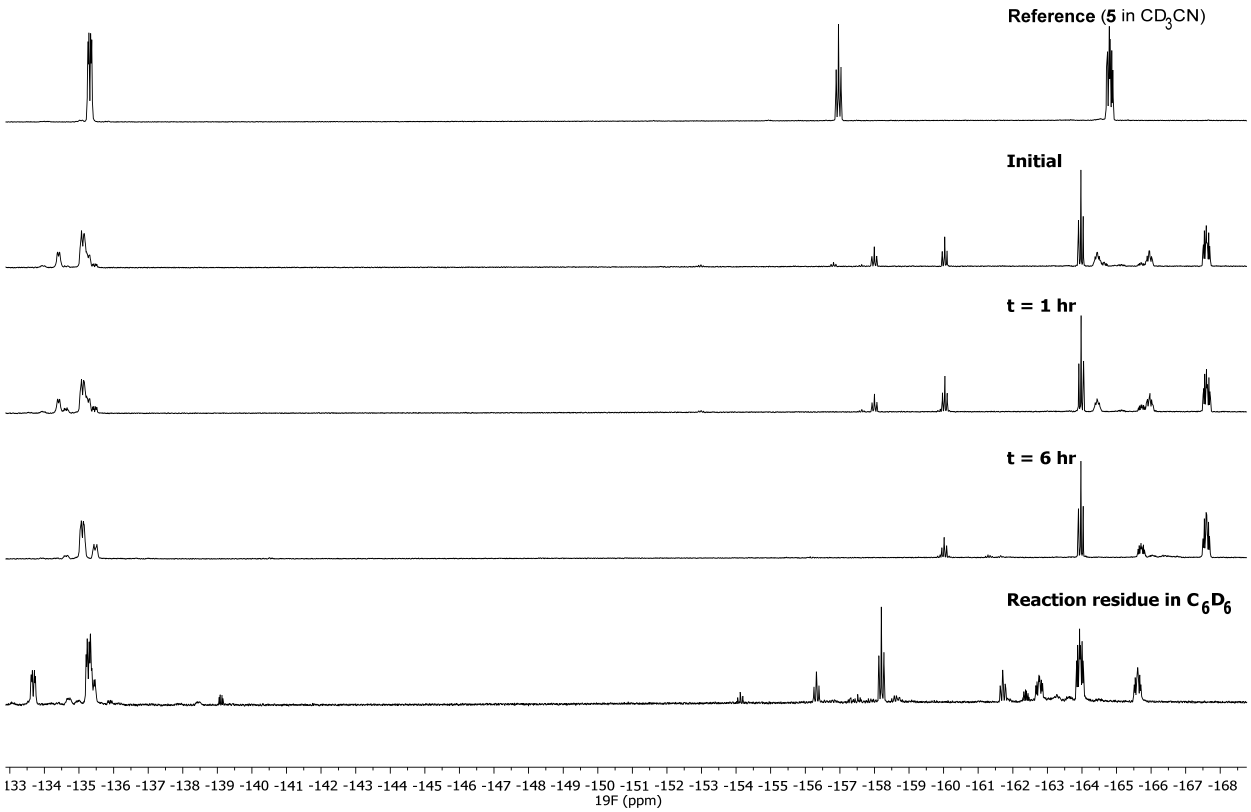
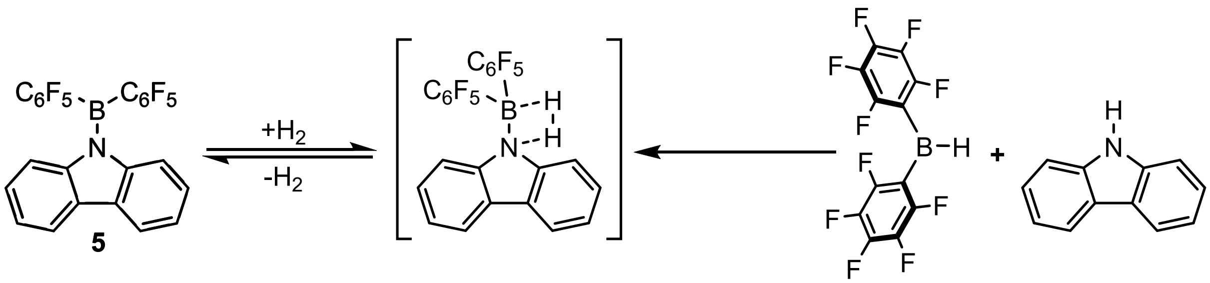


Figure S51. Stacked ^{19}F NMR spectra of the hydrosilylation of acetophenone with Et_3SiH (1.1 eq.), with ***5*** *(5 mol%) in CD_3CN.*

NMR Experiment - Reactions of aminoboranes with substrates

The following reactions were performed in a J-young tapped NMR tube with respective aminoborane (0.01 mmol) and substrate (1 eq.) in 0.5 mL of the specified solvent (see Figure captions).



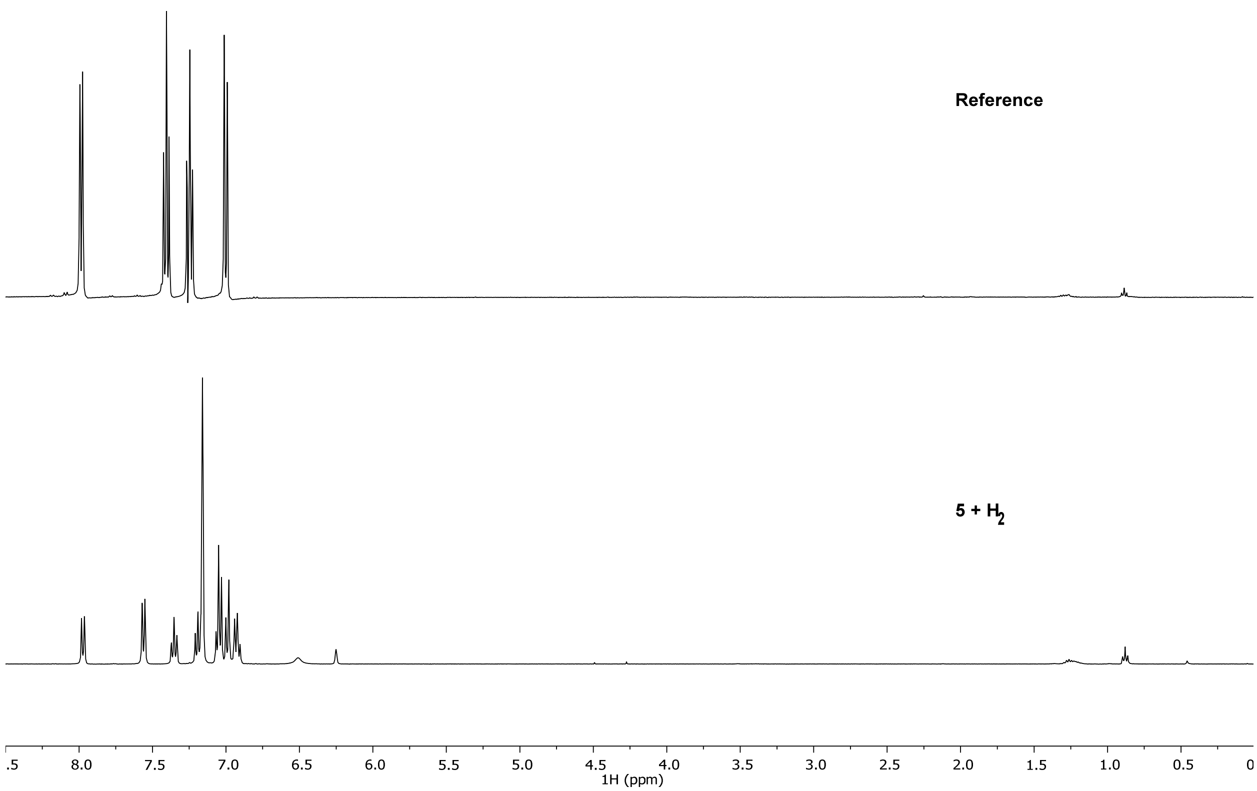


*Figure S52. Stacked ^{1}H NMR spectra of **5** referenced to the addition of H_2 sealed in a J-young tapped NMR tube in C_6D_6.*

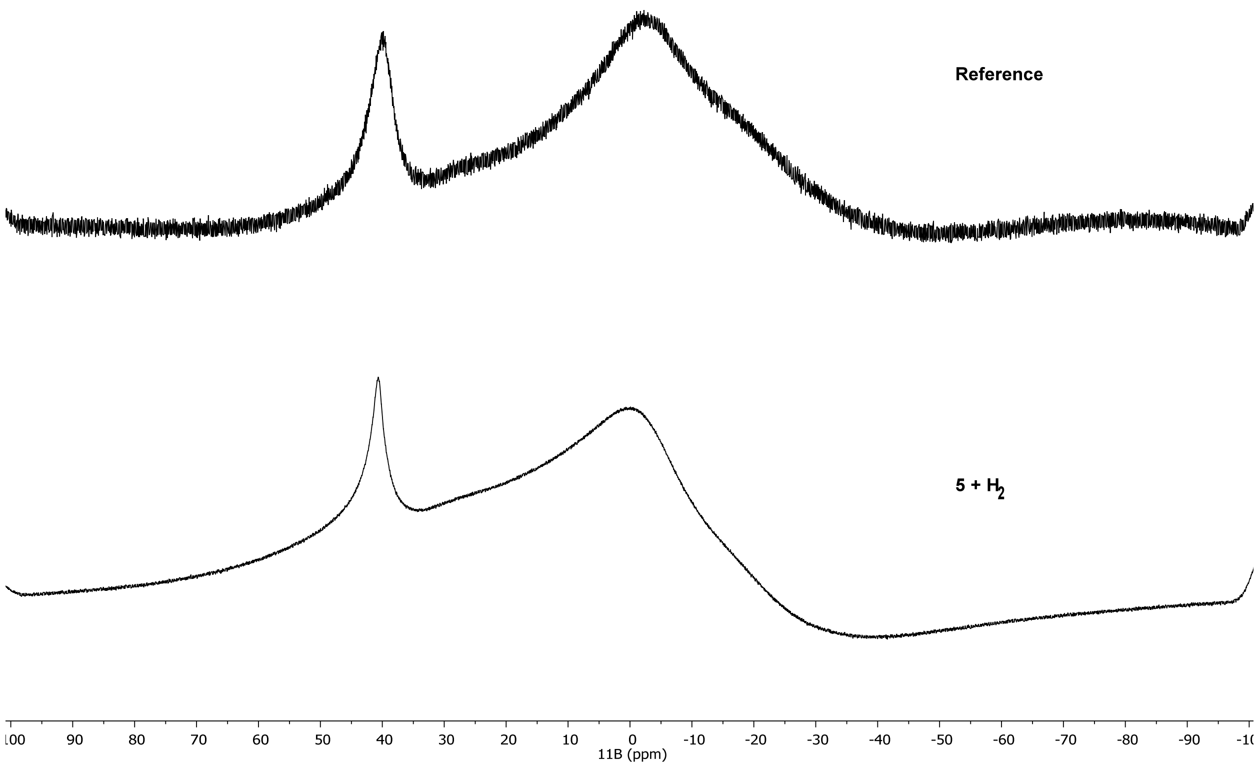


*Figure S53. Stacked ^{11}B NMR spectra of **5** referenced to the addition of H_2 sealed in a J-young tapped NMR tube in C_6D_6.*

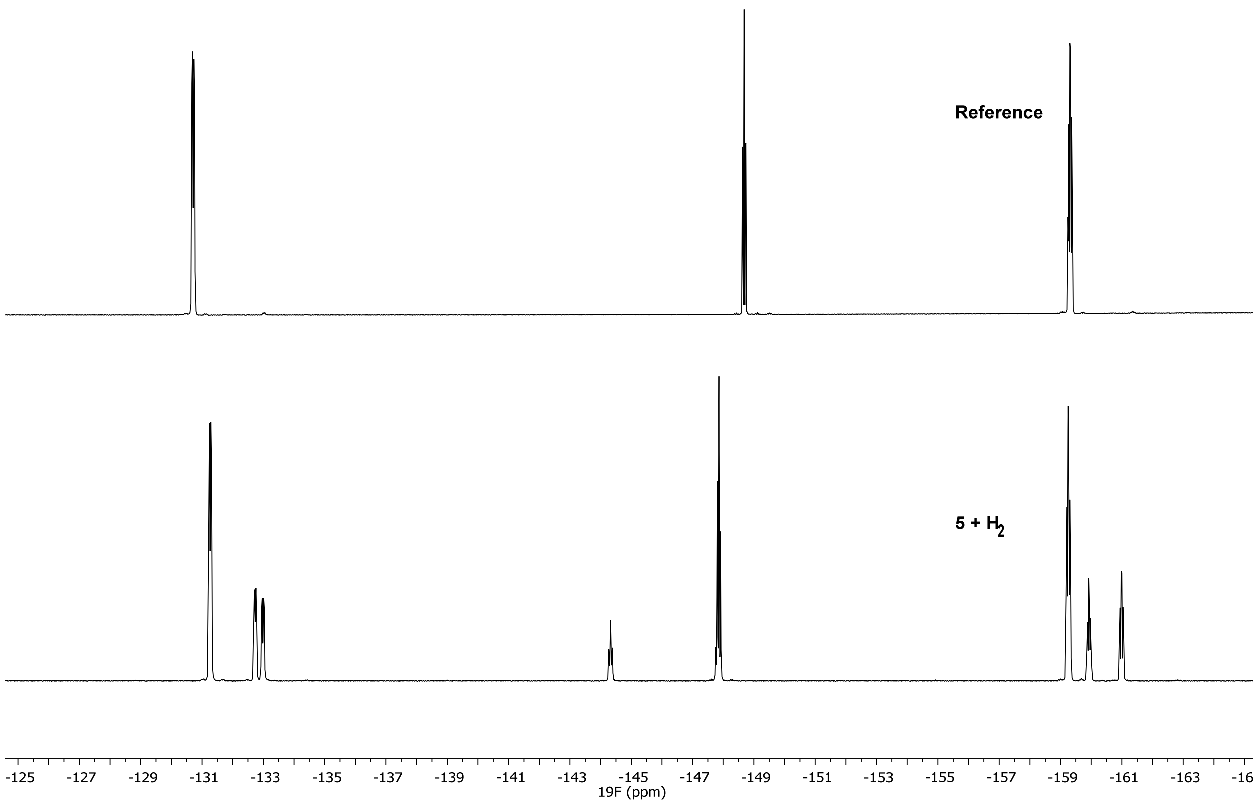
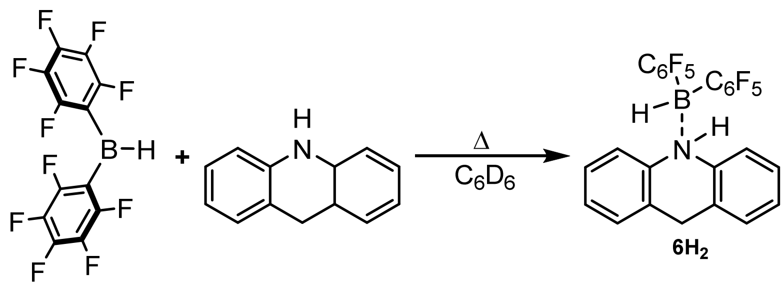


*Figure S54. Stacked ^{19}F NMR spectra of **5** referenced to the addition of H_2 sealed in a J-young tapped NMR tube in C_6D_6.*



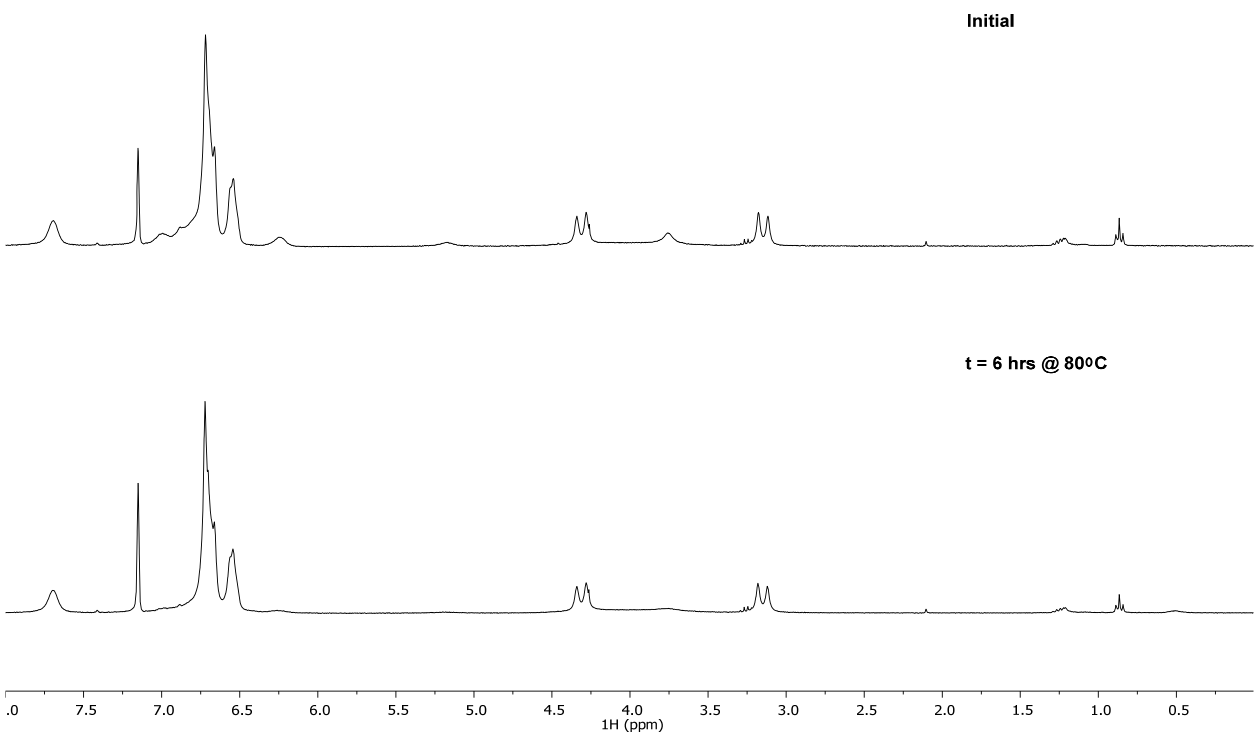


Figure S55. Stacked ^{1}H NMR spectra of $HB(C_6F_5)_2$ with acridan in C_6D_6.

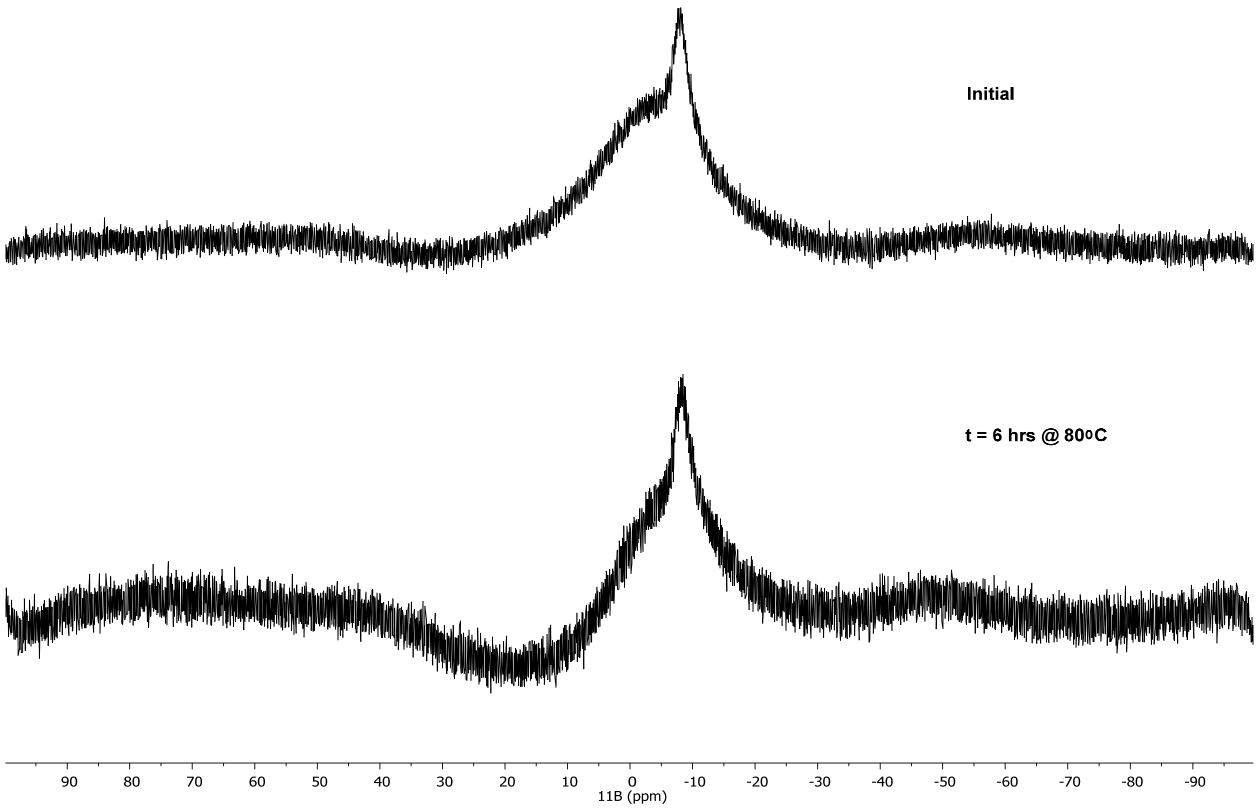


Figure S56. Stacked ^{11}B NMR spectra of $HB(C_6F_5)_2$ with acridan in C_6D_6.

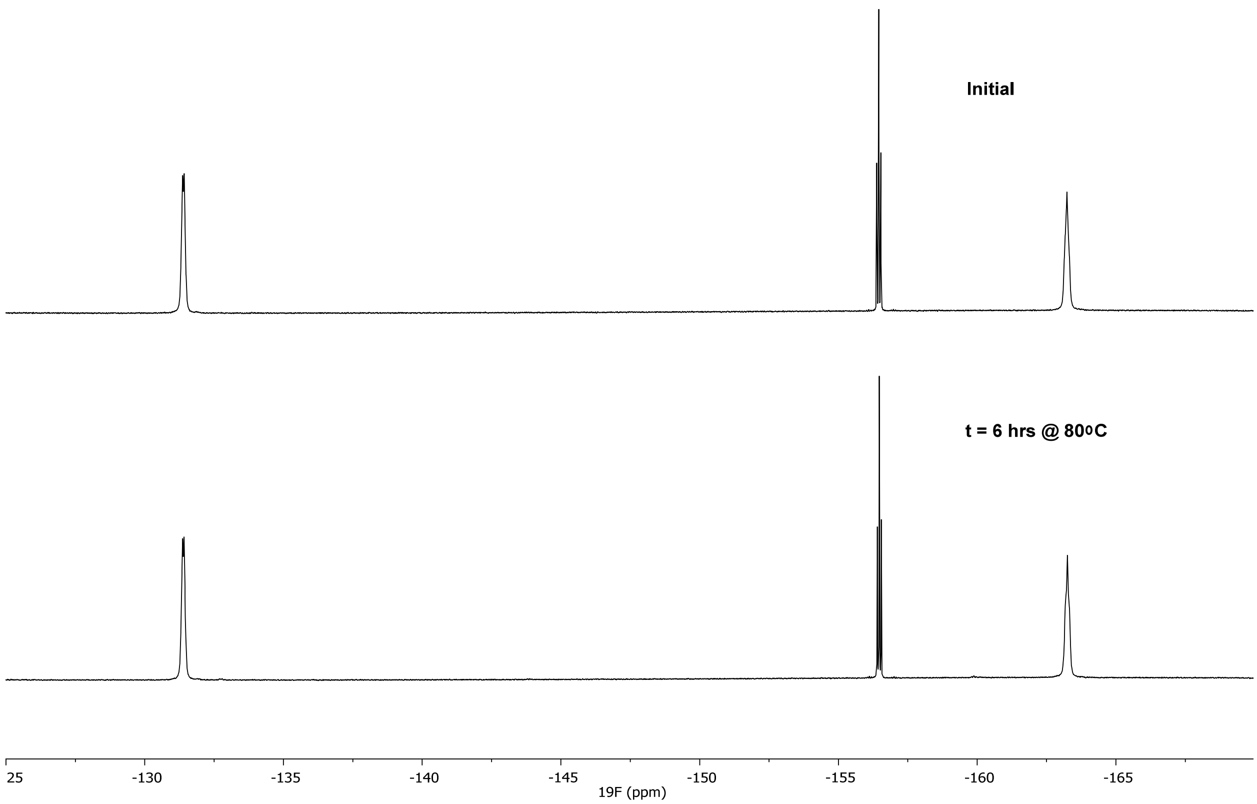
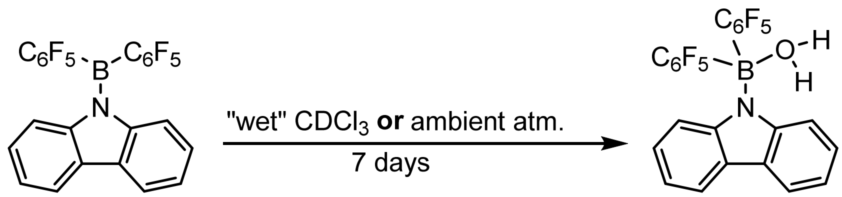


Figure S57. Stacked ^{19}F NMR spectra of $HB(C_6F_5)_2$ with acridan in C_6D_6.



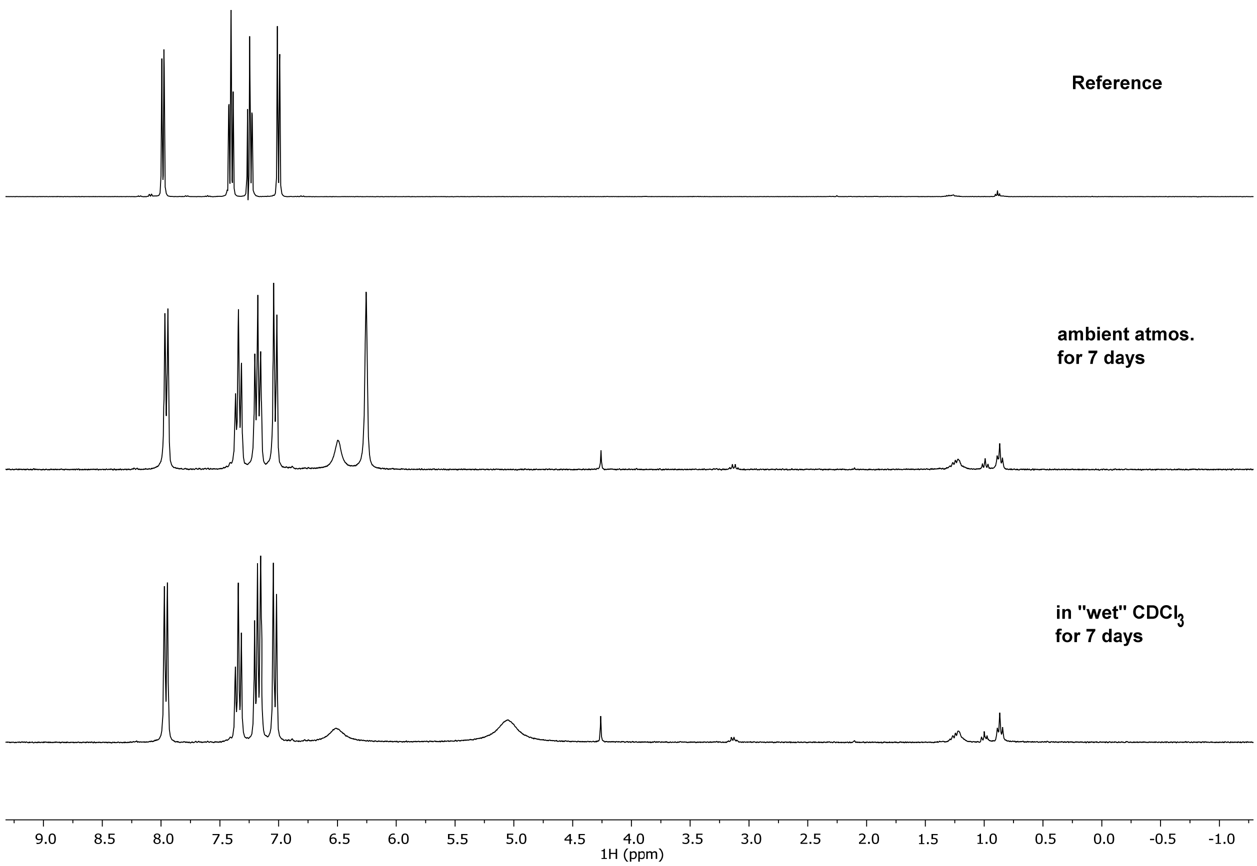


*Figure S58. Stacked ^1H NMR spectra of **5** exposed to moisture in $CDCl_3$.*

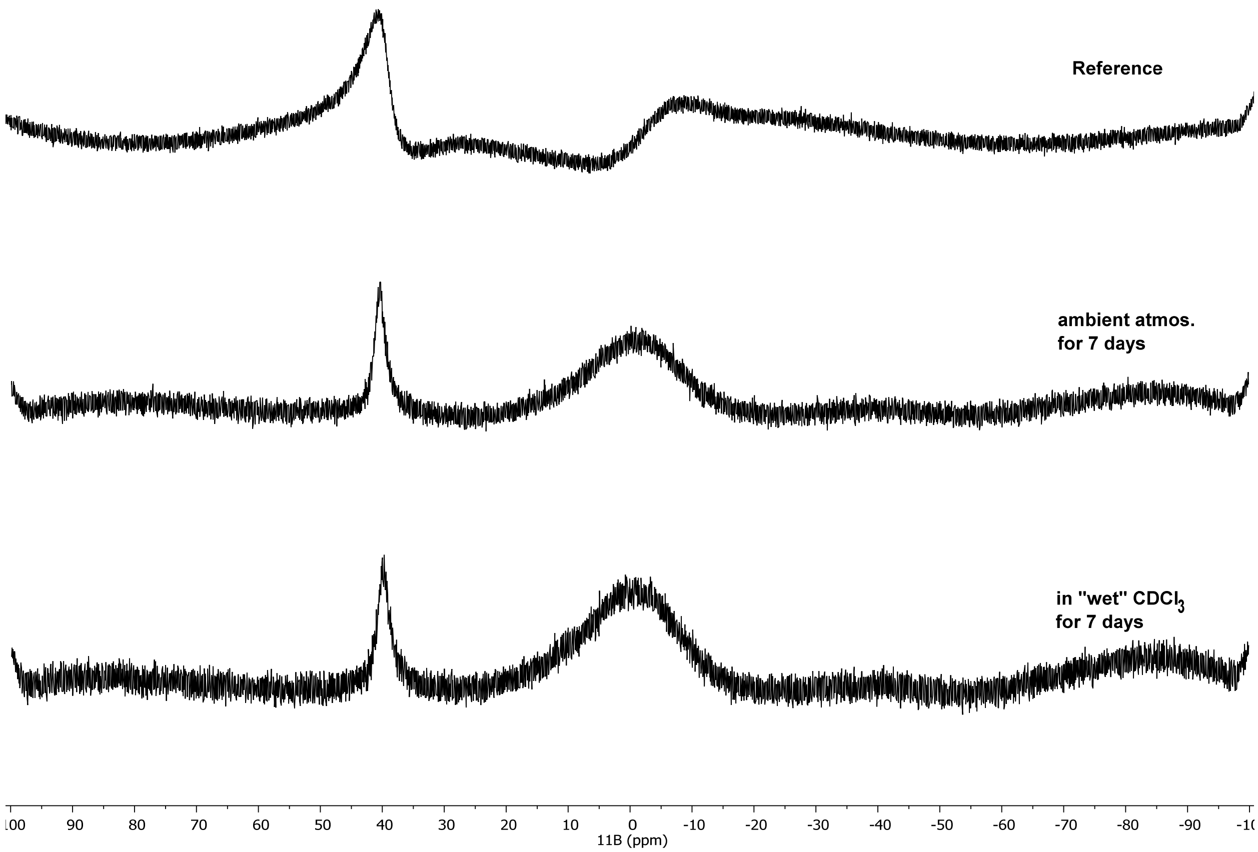


*Figure S59. Stacked ^{11}B NMR spectra of **5** exposed to moisture in $CDCl_3$.*

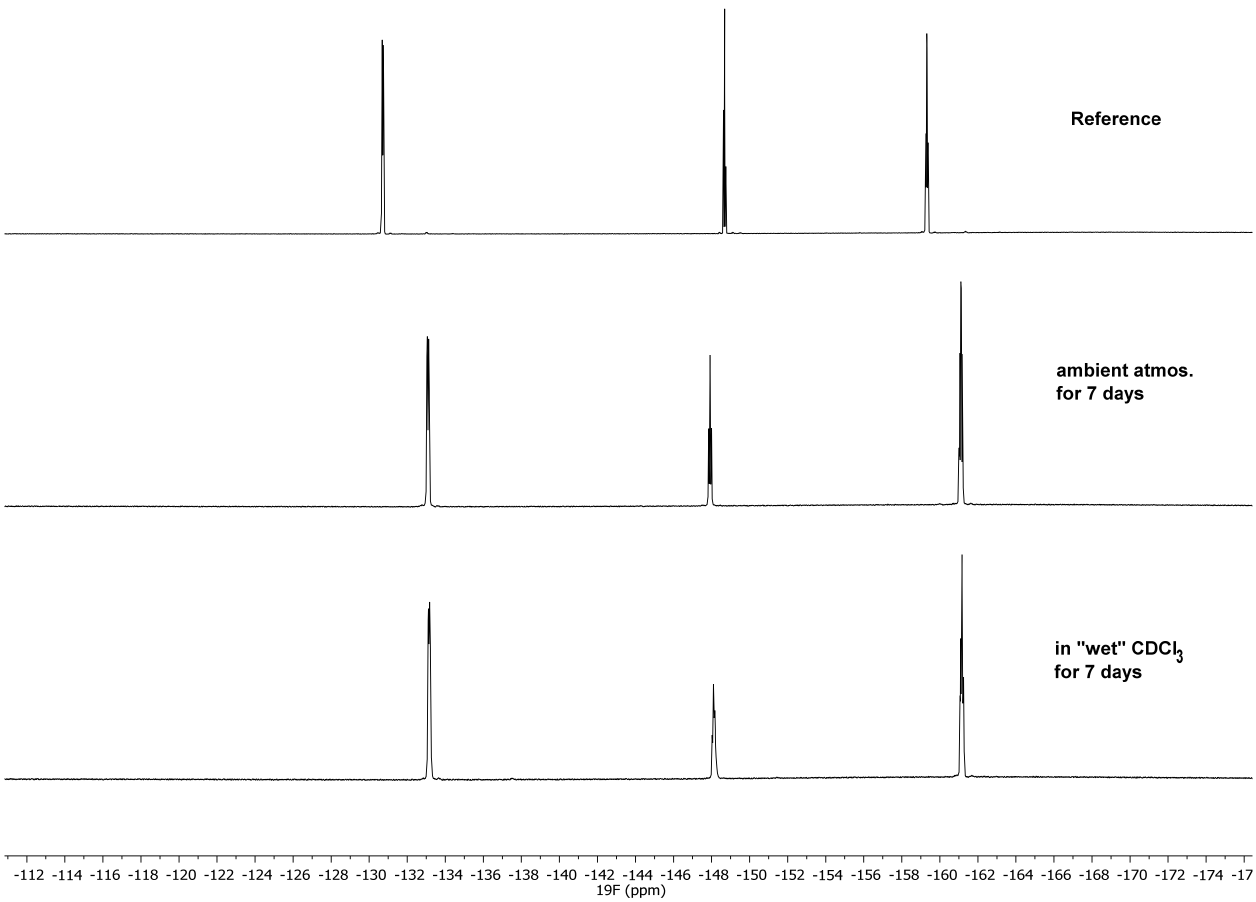


*Figure S60. Stacked ^{19}F NMR spectra of **5** exposed to moisture in $CDCl_3$.*

Structures of Aminoborane Derivatives Determined by X-ray Diffraction

*Table S4. Crystal Data and Structure Refinement of **2**, **4**, **5**, **6H2** , and **7***

	2	**4**	**5**	**6•H2**	**7**
Identification Code	JNB018_0m_a	JNB035_0m_a	JNB036_0m_a	JNB064_0m_a	JNB056_0m_a
Empirical Formula	$C_{24}H_8BF_{10}NO$	$C_{18}H_{18}BF_{10}NSi_2$	$C_{24}H_8BF_{10}N$	$C_{25}H_{12}B_1F_{10}N_1$	$C_{62}H_{36}B_2F_{20}N_6$
Formula Weight	527.12	505.32	511.12	527.17	633.30
Temperature	173(2) K	173(2) K	173(2) K	173(2) K	173(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal System	monoclinic	monoclinic	monoclinic	triclinic	monoclinic
Space Group	$P2_1/n$	$P2_1/c$	$P2_1/n$	P-1	C2/c
Unit Cell Dimensions	a = 9.4685(5) Å; α = 90 b = 12.8091(7) Å; β = 92.621(2) c = 17.3040(10) Å; γ = 90	a = 11.0755(10) Å; α = 90 b = 11.2327(11) Å; β = 105.827(3) c = 18.6587(18) Å; γ = 90	a = 7.6108(4) Å; α = 90 b = 9.4314(7) Å; β = 94.802(2) c = 27.7355(19) Å; γ = 90	a = 11.1178(6) Å; α = 83.703(2) b = 12.3316(6) Å; β = 89.331(2) c = 15.8444(8) Å; γ = 89.752(2)	a = 30.583(10) Å; α = 90 b = 14.745(5) Å; β = 122.794(12) c = 17.429(6) Å; γ = 90
Volume	2096.5(2)	2233.3(4)	1983.9(2)	2159.01(19)	6607(4)
Z	4	4	4	2	4
Density (calculated)	1.670	1.503	1.711	1.622	1.273
Absorption Coefficient	0.163	0.247	0.166	0.155	0.115
F(000)	1048	1024	1016	1056.0	2560.0
Crystal Size	0.2 x 0.15 x 0.1 mm3	0.2 x 0.2 x 0.15 mm^3	0.2 x 0.1 x 0.1 mm^3	0.2 x 0.2 x 0.1 mm^3	0.24 × 0.2 × 0.2 mm^3
Theta range for data collection	4.814 – 55.122	4.278 – 55.256	5.23 – 55.016	4.43 to 55.066	3.618 – 55.05
Index Ranges	-12 ≤ h ≤ 12, -16 ≤ k ≤ 16, -22 ≤ l ≤ 22	-14 ≤ h ≤ 14, -14 ≤ k ≤ 14, -24 ≤ l ≤ 24	-9 ≤ h ≤ 9, -12 ≤ k ≤ 12, -35 ≤ l ≤ 36	-14 ≤ h ≤ 14, -16 ≤ k ≤ 16, -20 ≤ l ≤ 20	-39 ≤ h ≤ 39, -19 ≤ k ≤ 19, -22 ≤ l ≤ 22
Reflections Collected	25799	76348	22903	61564	89071
Independent Reflections	4833	5127	4547	9880	7582
Completeness to theta = 25.242 °	0.998	0.980	0.998	0.992	0.998
Absorption Correction	N/A	N/A	N/A	N/A	N/A
Max. and min. Transmission	0.7456 / 0.6270	0.7456 / 0.6247	0.7456 / 0.6420	0.7456 / 0.5593	0.6925 / 0.5962
Refinement Method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / Restraints / Parameters	4833 / 0 / 334	5127 / 0 / 295	4547 / 0 / 325	9880 / 0 / 675	7582 / 0 / 408

Goodness-of-fit on F^2	1.041	1.060	1.065	1.051	1.012
Final R Indices [I>2sigma(I)]	R_1 = 0.0392, wR_2 = 0.1006	R_1 = 0.0466, wR_2 = 0.1050	R_1 = 0.0455, wR_2 = 0.1029	R_1 = 0.0470, wR_2 = 0.1075	R_1 = 0.0613, wR_2 = 0.1460
R Indices (all data)	R_1 = 0.0497, wR_2 = 0.1080	R_1 = 0.0525, wR_2 = 0.1108	R_1 = 0.0578, wR_2 = 0.1087	R_1 = 0.0603, wR_2 = 0.1199	R_1 = 0.0931, wR_2 = 0.1670
Extinction coefficient	N/A	N/A	N/A	N/A	N/A
Largest diff. peak and hole (e.Å^{-3})	0.31 / -0.20	0.48 / -0.59	0.29 / -0.26	0.33 / -0.26	0.35 / -0.27

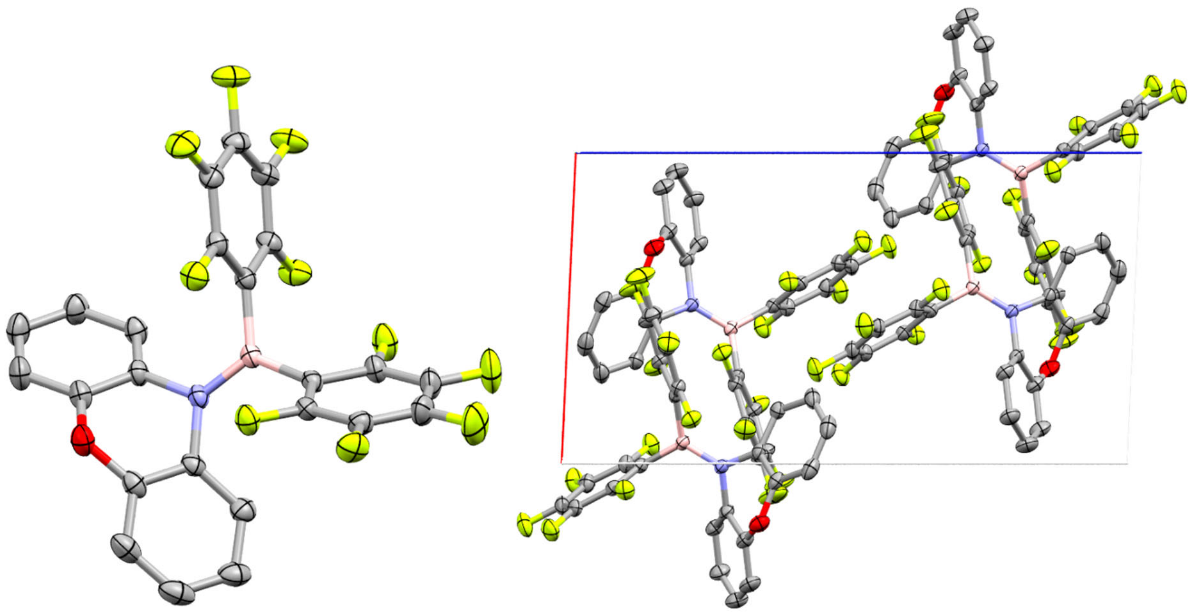


*Figure S61. Packed unit cell of **2** with significant contacts highlighted. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity. B: pink, C: grey, N: blue, F: yellow-green, O: red.*

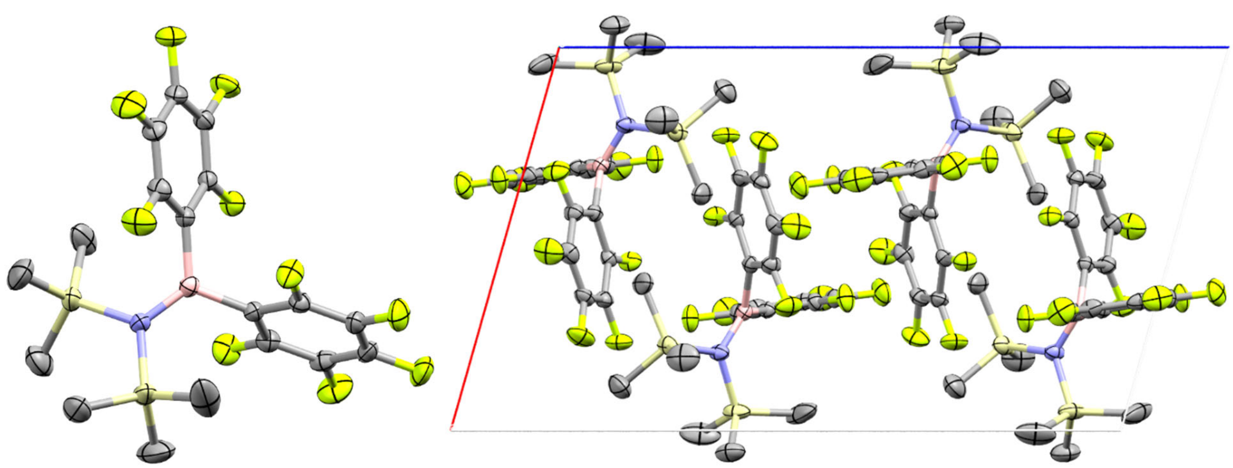


*Figure S62. Packed unit cell of **4** with significant contacts highlighted. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity. B: pink, C: grey, N: blue, F: yellow-green, Si: beige.*

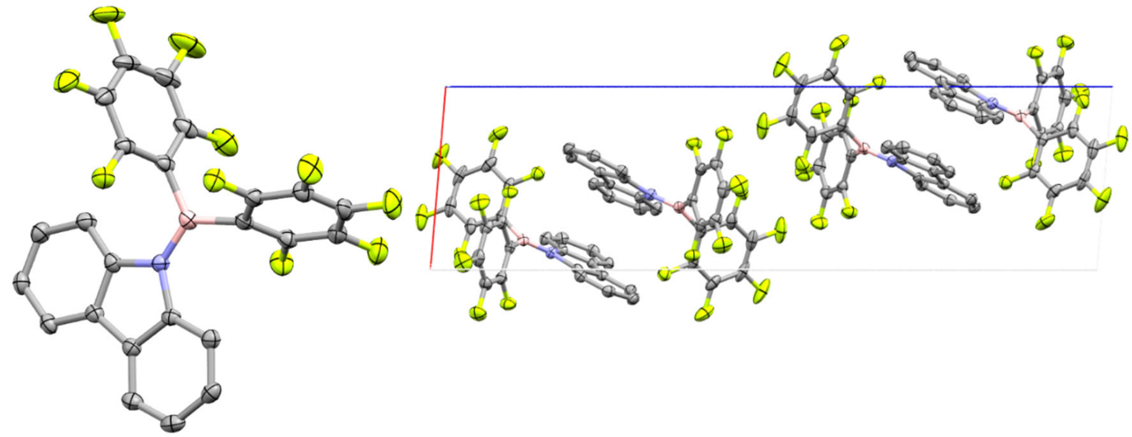


Figure S63. Packed unit cell of ***5*** *with significant contacts highlighted. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity. B: pink, C: grey, N: blue, F: yellow-green, S: yellow.*

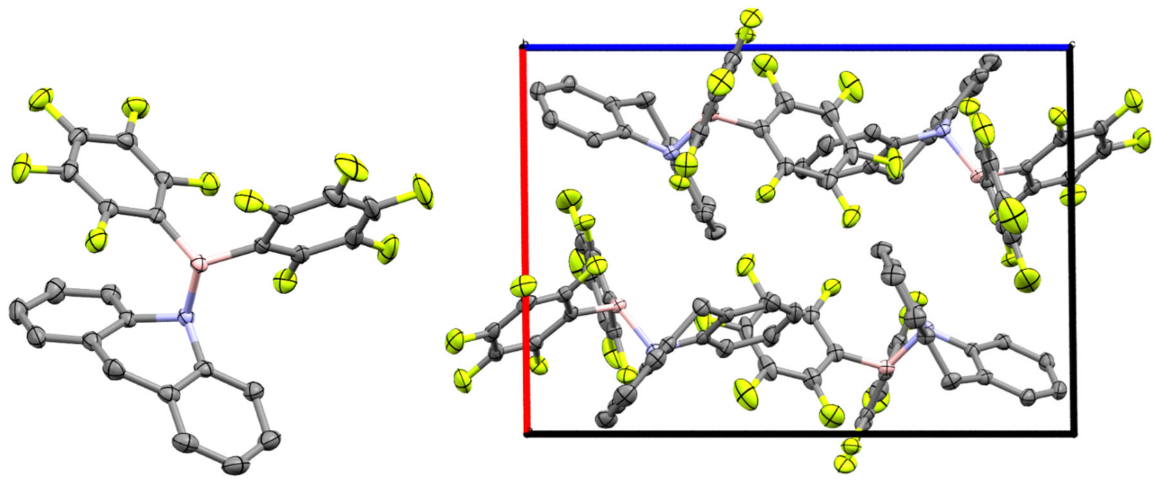


Figure 64. Packed unit cell of $\boldsymbol{6\bullet H_2}$ *with significant contacts highlighted. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity. B: pink, C: grey, N: blue, F: yellow-green, S: yellow.*

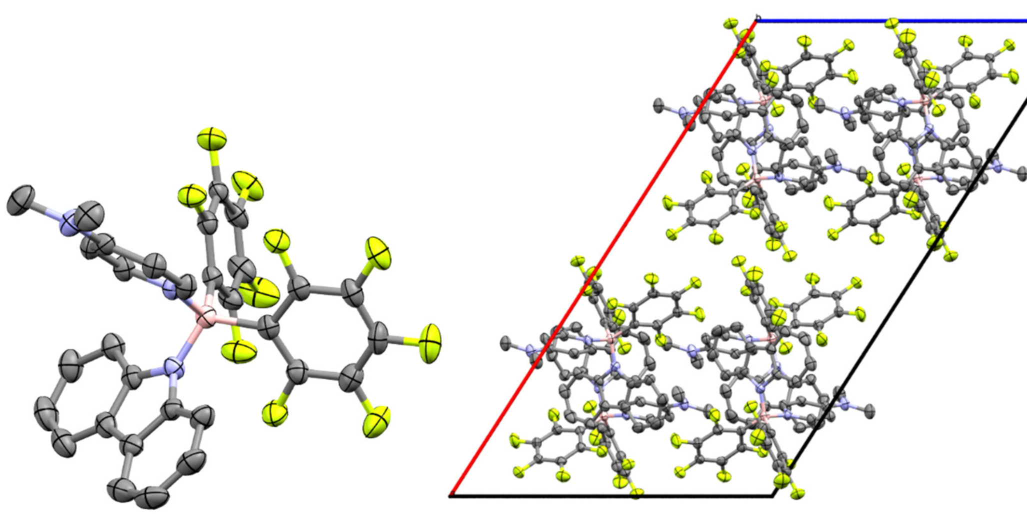


Figure S65. Packed unit cell of ***7*** *with significant contacts highlighted. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity. B: pink, C: grey, N: blue, F: yellow-green.*

Computations

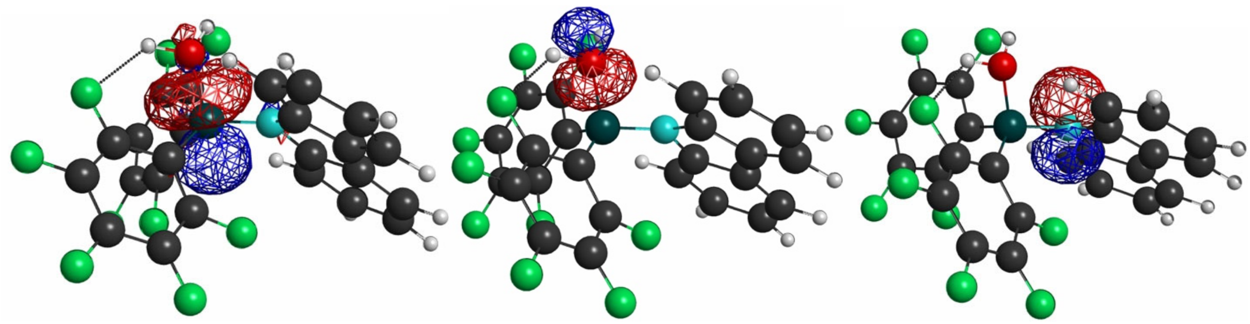


*Figure S66. From left to right, the B vacant orbital, the O lone pair orbital, and the N lone pair orbital obtained from NBO analysis of the **5•H₂O** adduct.*

Coordinates (Å) of DFT-optimized structures discussed in the main text.

1:

F	0.134913	2.740724	1.596526
F	1.553621	4.990395	1.173015
F	2.827682	5.357836	-1.185706
F	2.674682	3.477073	-3.126333
F	1.224326	1.230049	-2.697619
F	-1.033552	-1.154466	-2.521292
F	-4.832698	2.285548	-0.795679
F	-2.396094	2.289772	0.350425
N	0.323075	-0.521994	0.244085
C	1.688208	-0.630272	0.637529
C	2.248259	0.193066	1.600924
H	1.629184	0.908621	2.121004
C	3.597453	0.084921	1.900729
C	4.378662	-0.869795	1.266826
C	3.806985	-1.740457	0.353311
H	4.399964	-2.518953	-0.108246
C	2.460550	-1.621776	0.038709
C	-1.609072	-1.831869	0.988791
H	-2.005227	-0.959555	1.492053
C	-0.394937	-1.746761	0.327063
C	0.642686	1.926039	-0.545381
C	0.742494	2.908558	0.420520
C	1.472032	4.066509	0.224532
C	2.124254	4.255263	-0.981815
C	2.044193	3.293801	-1.974604
C	1.301697	2.151764	-1.739380
C	-1.643422	0.559955	-1.038226
C	-1.953529	-0.308980	-2.072448
C	-3.198590	-0.326994	-2.674339
C	-3.897571	1.442962	-1.214147
C	-2.640154	1.433603	-0.641027
B	-0.207652	0.605916	-0.386825
H	4.034796	0.740540	2.641419
H	5.429654	-0.958878	1.505931
S	1.698854	-2.723025	-1.105550

C	-2.309355	-3.027939	0.989615
C	0.147952	-2.872058	-0.284655
F	-3.465996	-1.171318	-3.661332
C	-4.173540	0.553192	-2.237745
H	-3.263232	-3.090189	1.495271
C	-1.781342	-4.143683	0.356222
C	-0.544906	-4.073708	-0.266564
F	-5.371767	0.545140	-2.799236
H	-2.323570	-5.079506	0.365641
H	-0.115641	-4.949885	-0.734175

2:

F	-0.016497	2.815296	1.593813
F	1.320217	5.120068	1.164810
F	2.656961	5.486429	-1.159533
F	2.644228	3.560475	-3.059684
F	1.272561	1.264392	-2.626811
F	-0.848467	-1.235784	-2.422780
F	-4.829299	2.225028	-1.226378
F	-2.497963	2.336762	0.122873
N	0.281820	-0.449004	0.356809
C	1.642220	-0.593608	0.749598
C	2.340469	0.324522	1.515217
H	1.832187	1.182540	1.927138
C	3.689563	0.125552	1.769451
C	4.333189	-1.001281	1.281215
C	3.625783	-1.957702	0.569152
H	4.102550	-2.860715	0.212104
C	2.282252	-1.751471	0.317016
C	-1.718503	-1.790008	0.906710
H	-2.229340	-0.911879	1.278576
C	-0.416332	-1.682655	0.449947
C	0.593545	1.983576	-0.510776
C	0.618281	2.991046	0.433817
C	1.305364	4.174113	0.235346
C	1.989890	4.362018	-0.953494
C	1.983380	3.376044	-1.925480
C	1.280850	2.209367	-1.688307
C	-1.609846	0.544660	-1.095788
C	-1.816968	-0.384100	-2.103624
C	-3.003703	-0.456842	-2.808801
C	-3.849304	1.378979	-1.515008
C	-2.645954	1.423994	-0.836263
B	-0.227451	0.647513	-0.345204
H	4.233511	0.851824	2.357102
H	5.385379	-1.154023	1.478584
O	1.572088	-2.711540	-0.341397
C	-2.354733	-3.021837	0.879842
C	0.266900	-2.818384	0.034712
F	-3.172903	-1.356413	-3.768147
C	-4.023477	0.429458	-2.507023

H	-3.376233	-3.106099	1.223833
C	-1.679435	-4.143000	0.419208
C	-0.357194	-4.051410	0.010963
F	-5.167050	0.369569	-3.170265
H	-2.176725	-5.103205	0.398832
H	0.188538	-4.923068	-0.324127

3:

F	0.720895	2.096666	1.632732
F	2.111360	4.401584	1.462533
F	2.794559	5.382381	-0.964501
F	2.087851	4.064048	-3.219998
F	0.699537	1.750518	-3.036785
F	-0.972923	-1.312003	-2.670336
F	-4.752701	2.232736	-1.110369
F	-2.312409	2.259642	0.047809
N	0.370087	-0.584714	0.047594
C	1.730997	-0.641981	0.466315
C	2.039164	-0.855399	1.804184
H	1.242633	-0.979189	2.526302
C	3.362991	-0.897637	2.207715
C	4.383931	-0.725240	1.282936
C	4.073936	-0.521439	-0.052580
H	4.863258	-0.397888	-0.781865
C	2.749970	-0.488169	-0.464072
C	-1.591843	-1.609365	1.067298
H	-1.901321	-0.635684	1.424899
C	-0.412086	-1.736873	0.346152
C	0.677217	1.861044	-0.699383
C	1.057022	2.560899	0.432078
C	1.766483	3.745241	0.362613
C	2.111610	4.251494	-0.879085
C	1.745392	3.579701	-2.033186
C	1.029720	2.402859	-1.921232
C	-1.578878	0.472091	-1.274067
C	-1.892571	-0.440607	-2.266284
C	-3.135076	-0.472988	-2.871632
C	-3.821609	1.367660	-1.490505
C	-2.565767	1.371631	-0.914133
B	-0.154002	0.528520	-0.611116
H	3.597737	-1.057453	3.251541
H	5.417058	-0.756007	1.602177
C	-2.361347	-2.730515	1.339979
C	0.009173	-2.991441	-0.077664
F	-3.410505	-1.356016	-3.822356
C	-4.101394	0.436694	-2.476352
H	-3.280110	-2.623897	1.901206
C	-1.948097	-3.981566	0.909815
C	-0.758062	-4.108258	0.206311
F	-5.298187	0.415758	-3.041431
H	-2.546337	-4.856454	1.126166

H	-0.428070	-5.082153	-0.129498
H	2.506065	-0.353501	-1.510279
H	0.932600	-3.088554	-0.633785

4:

F	0.056090	2.060172	1.899645
F	1.066294	4.538815	2.185276
F	1.931532	5.898760	0.008559
F	1.786485	4.776889	-2.447586
F	0.788579	2.284080	-2.724649
F	-0.462251	-0.883561	-2.969227
F	-4.775872	2.174383	-1.823345
F	-2.651323	2.160145	-0.155922
N	0.296809	-0.487614	0.056404
Si	2.054026	-0.607075	0.413807
Si	-0.776372	-1.846208	0.537767
C	0.423930	2.088280	-0.418735
C	0.499878	2.701489	0.818614
C	1.004578	3.978904	0.984265
C	1.441563	4.676888	-0.127980
C	1.363735	4.102462	-1.386504
C	0.846722	2.827192	-1.508926
C	-1.508271	0.617160	-1.498117
C	-1.523272	-0.140011	-2.655404
C	-2.598387	-0.145228	-3.525860
C	-3.714907	1.426461	-2.095015
C	-2.616719	1.409210	-1.256856
B	-0.224193	0.650042	-0.570266
F	-2.582335	-0.882986	-4.628408
C	-3.699674	0.641147	-3.236406
F	-4.740034	0.646631	-4.054442
C	-2.569666	-1.301720	0.708005
H	-3.075408	-2.033175	1.343380
H	-2.679523	-0.333496	1.197435
H	-3.116957	-1.271879	-0.233229
C	-0.264279	-2.397310	2.265760
H	-0.368520	-1.581294	2.982657
H	-0.934727	-3.195946	2.591220
H	0.749873	-2.785227	2.350371
C	3.079193	0.465378	-0.745209
H	2.730523	0.437395	-1.778221
H	3.142206	1.507582	-0.434919
H	4.100029	0.075267	-0.747210
C	2.609398	-2.373401	0.063679
H	2.151045	-3.143932	0.681509
H	2.442119	-2.638050	-0.981476
H	3.686321	-2.431749	0.238254
C	-0.704484	-3.302887	-0.646306
H	-1.366730	-4.093739	-0.286563
H	-1.035977	-3.038002	-1.649321
H	0.291424	-3.734437	-0.737148

C	2.487239	-0.148190	2.183570
H	2.343668	0.912756	2.384471
H	1.914607	-0.699785	2.927697
H	3.542983	-0.366866	2.358668

5:

F	0.747861	1.846566	1.890127
F	1.908671	4.272101	2.081377
F	2.304836	5.748676	-0.148946
F	1.533403	4.811369	-2.565849
F	0.360956	2.387287	-2.747428
F	-1.049996	-0.915374	-2.753401
F	-4.761448	2.599882	-0.980847
F	-2.392869	2.378955	0.294944
N	0.315313	-0.517097	-0.021294
C	1.687844	-0.791826	0.180932
C	2.803493	-0.028035	-0.133213
H	2.729938	0.945923	-0.590920
C	4.055142	-0.557585	0.137009
C	4.205450	-1.827071	0.690148
C	3.093622	-2.600223	0.968164
H	3.203792	-3.596117	1.377485
C	1.833865	-2.080238	0.704348
C	-1.760544	-1.894827	0.463461
H	-2.486711	-1.150524	0.176737
C	-0.392868	-1.670415	0.388845
C	0.530372	2.045869	-0.435327
C	0.937611	2.559460	0.785951
C	1.532254	3.801472	0.901217
C	1.731933	4.560657	-0.240521
C	1.333917	4.081712	-1.477426
C	0.731312	2.839530	-1.551517
C	-1.657915	0.723772	-1.191794
C	-1.951679	-0.050607	-2.303123
C	-3.156193	0.050960	-2.972933
C	-3.846584	1.743067	-1.411580
C	-2.625705	1.621408	-0.774396
B	-0.238433	0.679403	-0.521762
H	4.933182	0.029296	-0.096826
H	5.196275	-2.212515	0.887737
C	-2.196487	-3.117913	0.947264
C	0.510947	-2.637260	0.840261
F	-3.410675	-0.692493	-4.039869
C	-4.105277	0.952546	-2.518768
H	-3.259645	-3.308676	1.005148
C	-1.299541	-4.096998	1.368502
C	0.061244	-3.857401	1.326137
F	-5.263492	1.060127	-3.147216
H	-1.671979	-5.040524	1.743103
H	0.763695	-4.604869	1.671918

6:

F	0.067095	2.777284	1.622284
F	1.451414	5.048600	1.194973
F	2.760731	5.409889	-1.145441
F	2.674464	3.503063	-3.064920
F	1.254734	1.236945	-2.634767
F	-0.981300	-1.124019	-2.518473
F	-4.843571	2.283448	-0.868271
F	-2.442428	2.284514	0.350100
N	0.315861	-0.510806	0.267611
C	1.686165	-0.633961	0.650615
C	2.289220	0.235053	1.544577
H	1.714671	1.017398	2.016851
C	3.628808	0.066156	1.862127
C	4.349515	-0.981723	1.311776
C	3.724185	-1.874951	0.454189
H	4.278295	-2.710635	0.044258
C	2.390006	-1.710729	0.116914
C	-1.640698	-1.851689	0.900289
H	-2.106086	-0.980601	1.342231
C	-0.383777	-1.751136	0.327594
C	0.619253	1.950647	-0.502686
C	0.685589	2.945955	0.452683
C	1.399856	4.113471	0.255686
C	2.070768	4.298783	-0.940877
C	2.025465	3.323784	-1.922635
C	1.297480	2.173073	-1.686085
C	-1.641458	0.572535	-1.033073
C	-1.917995	-0.285131	-2.085674
C	-3.143520	-0.301725	-2.725505
C	-3.893068	1.448881	-1.267397
C	-2.653050	1.438294	-0.656976
B	-0.218922	0.620629	-0.349928
H	4.102715	0.746674	2.556645
H	5.392035	-1.117101	1.566183
C	1.631502	-2.658454	-0.768299
C	-2.283270	-3.080378	0.918427
C	0.258985	-2.868442	-0.195770
F	-3.376403	-1.134138	-3.731338
C	-4.134769	0.569878	-2.308630
H	-3.265644	-3.164800	1.363167
C	-1.658898	-4.199950	0.390189
C	-0.387047	-4.093368	-0.154452
F	-5.314999	0.564422	-2.907470
H	-2.156091	-5.160278	0.416009
H	0.106844	-4.970983	-0.552939
H	1.542481	-2.232813	-1.775224
H	2.162341	-3.605196	-0.874012

1•F⁻:

F	0.262872	3.249481	1.787379

F	1.705460	5.236965	0.814864
F	2.822575	5.062613	-1.649269
F	2.439725	2.829742	-3.144977
F	0.965174	0.824363	-2.202433
F	-1.087526	-1.067168	-2.168161
F	-4.734730	2.773507	-1.106545
F	-2.598851	2.575659	0.441222
N	0.332834	-0.649001	0.291950
C	1.697933	-0.687127	0.576992
C	2.290755	0.190607	1.488953
H	1.669867	0.882762	2.037902
C	3.657318	0.167600	1.715910
C	4.463659	-0.770088	1.087776
C	3.882257	-1.696933	0.236733
H	4.484229	-2.461518	-0.238517
C	2.521621	-1.644130	-0.025645
C	-1.579326	-2.046014	0.892202
H	-2.044901	-1.212717	1.397534
C	-0.326223	-1.876891	0.299255
C	0.519097	1.926502	-0.168765
C	0.746600	3.088232	0.554376
C	1.511705	4.141136	0.075820
C	2.085749	4.056949	-1.175752
C	1.889506	2.918989	-1.932537
C	1.117760	1.891795	-1.419830
C	-1.745860	0.696247	-0.720747
C	-1.954335	-0.118523	-1.825993
C	-3.062210	-0.011116	-2.654145
C	-3.833454	1.815773	-1.341915
C	-2.716536	1.675174	-0.536442
B	-0.450990	0.676433	0.326418
H	4.089887	0.877070	2.410227
H	5.529403	-0.795757	1.274359
S	1.781886	-2.763886	-1.164759
C	-2.227385	-3.270983	0.843875
C	0.262263	-2.995623	-0.304189
F	-3.218202	-0.832433	-3.694797
C	-4.011459	0.958405	-2.408545
H	-3.206206	-3.367215	1.296894
C	-1.627155	-4.370863	0.251445
C	-0.365353	-4.230089	-0.307885
F	-5.080305	1.075717	-3.197399
H	-2.127967	-5.330056	0.230787
H	0.129391	-5.075663	-0.769656
F	-0.940844	0.900560	1.629037

2•F$^-$:

F	0.029175	3.317571	1.930645
F	1.431406	5.366401	1.028610
F	2.667842	5.246864	-1.380026
F	2.453586	3.001991	-2.893317

F	1.021052	0.933269	-2.019961
F	-0.883794	-1.065628	-2.067464
F	-4.764402	2.632762	-1.398167
F	-2.761662	2.552436	0.332780
N	0.271494	-0.580870	0.482017
C	1.653105	-0.682282	0.589350
C	2.459720	0.241676	1.249953
H	2.001080	1.066800	1.773332
C	3.842670	0.106579	1.262383
C	4.449245	-0.981671	0.660569
C	3.656775	-1.957523	0.066391
H	4.095789	-2.836102	-0.388967
C	2.286681	-1.800536	0.033618
C	-1.677789	-1.993465	0.970698
H	-2.199621	-1.162384	1.421316
C	-0.385491	-1.807864	0.487290
C	0.428826	2.014411	-0.014987
C	0.572479	3.181798	0.721098
C	1.315601	4.266722	0.279266
C	1.951178	4.210313	-0.944059
C	1.839855	3.067225	-1.710558
C	1.088165	2.008461	-1.235022
C	-1.736304	0.693426	-0.716081
C	-1.815732	-0.148301	-1.817109
C	-2.852582	-0.105480	-2.737079
C	-3.808088	1.709578	-1.533511
C	-2.758921	1.631782	-0.633400
B	-0.522989	0.735754	0.430750
H	4.440990	0.857371	1.762346
H	5.525910	-1.089881	0.667941
O	1.531581	-2.772811	-0.558101
C	-2.297329	-3.235059	0.881302
C	0.271744	-2.921374	-0.047144
F	-2.886264	-0.953189	-3.767477
C	-3.858703	0.826178	-2.592772
H	-3.310042	-3.347202	1.247124
C	-1.630105	-4.321116	0.344454
C	-0.323885	-4.162665	-0.107583
F	-4.859425	0.882699	-3.472450
H	-2.110199	-5.288842	0.279444
H	0.225062	-4.991473	-0.536510
F	-1.117942	0.962997	1.684208

3•F$^-$:

F	0.891901	2.192521	2.190262
F	2.651043	4.139815	1.813216
F	3.317412	4.925535	-0.694534
F	2.176748	3.704923	-2.834443
F	0.417539	1.752996	-2.488221
F	-0.920771	-1.331454	-2.118013
F	-4.454363	2.755459	-2.310748

F	-2.595654	2.743741	-0.411548
N	0.110577	-0.617766	0.387840
C	1.520590	-0.646234	0.371225
C	2.236873	-0.643672	1.566588
H	1.687725	-0.647578	2.499129
C	3.622405	-0.623939	1.560005
C	4.316028	-0.603787	0.357507
C	3.610727	-0.618124	-0.836725
H	4.142659	-0.605033	-1.779927
C	2.223874	-0.649506	-0.830625
C	-1.920723	-1.824792	0.975398
H	-2.490689	-0.909795	1.003991
C	-0.540114	-1.792636	0.700590
C	0.512621	1.901704	-0.127554
C	1.140130	2.545727	0.929991
C	2.074579	3.553562	0.761193
C	2.419680	3.955781	-0.513423
C	1.834142	3.335520	-1.597449
C	0.904746	2.331884	-1.383719
C	-1.700902	0.669945	-1.110868
C	-1.786729	-0.315967	-2.080483
C	-2.741493	-0.315355	-3.084605
C	-3.588776	1.740548	-2.233405
C	-2.622181	1.698518	-1.242810
B	-0.616772	0.720411	0.148296
H	4.164199	-0.608071	2.497611
H	5.398259	-0.575880	0.352219
C	-2.569085	-3.016360	1.243094
C	0.136435	-3.026163	0.733033
F	-2.785484	-1.295519	-3.990645
C	-3.652867	0.718122	-3.158439
H	-3.633584	-2.990711	1.444521
C	-1.888629	-4.226089	1.271798
C	-0.526484	-4.208134	1.015852
F	-4.577197	0.735625	-4.120316
H	-2.404591	-5.152220	1.489103
H	0.039867	-5.132328	1.023261
H	1.670217	-0.678083	-1.759460
H	1.195875	-3.066748	0.519784
F	-1.362774	1.071461	1.292098

4•F⁻:

F	0.201207	1.966533	1.889005
F	1.626650	4.201253	1.987680
F	2.241661	5.540940	-0.290206
F	1.387307	4.586668	-2.683900
F	-0.036438	2.361019	-2.816677
F	-0.852104	-1.880268	-2.158029
F	-4.254739	1.948003	-3.886271
F	-2.751813	2.430939	-1.749415
N	-0.119365	-0.490326	0.218561

Si	1.489920	-0.835118	-0.348093
Si	-0.776134	-1.478460	1.499089
C	-0.008982	2.039364	-0.467648
C	0.452798	2.574799	0.728255
C	1.204015	3.734599	0.809564
C	1.519897	4.420348	-0.347180
C	1.083722	3.930304	-1.560548
C	0.332568	2.765429	-1.595097
C	-1.712744	0.309886	-1.822729
C	-1.666828	-0.882635	-2.521479
C	-2.436022	-1.146430	-3.647693
C	-3.405711	1.016370	-3.443436
C	-2.618000	1.234986	-2.329517
B	-0.944266	0.656550	-0.377780
F	-2.336973	-2.316893	-4.285035
C	-3.314256	-0.191435	-4.109898
F	-4.062816	-0.424661	-5.189577
C	-2.111322	-0.750228	2.620679
H	-2.256975	-1.445698	3.452647
H	-1.827904	0.214459	3.038372
H	-3.068607	-0.625520	2.119285
C	0.575673	-1.948649	2.754295
H	0.954415	-1.048494	3.242832
H	0.133394	-2.574659	3.533734
H	1.433522	-2.490668	2.358088
C	1.906939	-0.142295	-2.063179
H	1.084754	-0.155503	-2.774675
H	2.284835	0.878026	-2.007112
H	2.708450	-0.754278	-2.485498
C	1.837267	-2.697877	-0.498246
H	1.640398	-3.277266	0.402614
H	1.244975	-3.138328	-1.300218
H	2.890049	-2.846101	-0.752594
C	-1.529685	-3.085508	0.827987
H	-1.924326	-3.702576	1.639010
H	-2.359284	-2.867046	0.152935
H	-0.812853	-3.686889	0.268438
C	2.842582	-0.113256	0.771093
H	2.828879	0.977234	0.736698
H	2.744082	-0.404047	1.816514
H	3.831111	-0.432445	0.430939
F	-2.024066	0.978607	0.477080

5•F$^-$:

F	-0.236682	1.660079	2.378969
F	1.104539	3.861524	3.030981
F	2.042445	5.517329	1.096971
F	1.614378	4.914015	-1.513948
F	0.291870	2.721704	-2.190309
F	-0.593119	-1.638150	-2.134320
F	-3.607933	2.413054	-4.070543

F	-2.542346	2.634626	-1.638184
N	-0.160354	-0.482166	0.320642
C	1.140114	-0.746869	-0.033227
C	1.948165	-0.122029	-0.985161
H	1.585819	0.689412	-1.596608
C	3.238895	-0.584511	-1.160225
C	3.741228	-1.661793	-0.423668
C	2.935370	-2.303776	0.497228
H	3.309179	-3.152528	1.058116
C	1.633845	-1.853099	0.689293
C	-1.750234	-1.628534	1.910245
H	-2.597271	-0.987629	1.732904
C	-0.532193	-1.428021	1.251563
C	-0.082269	2.090992	0.062644
C	0.180680	2.437601	1.381828
C	0.883484	3.572478	1.747267
C	1.364069	4.418363	0.766524
C	1.141721	4.109384	-0.559117
C	0.430337	2.964305	-0.879095
C	-1.485315	0.529752	-1.763529
C	-1.305110	-0.592733	-2.553721
C	-1.851329	-0.719969	-3.824677
C	-2.852282	1.427790	-3.579436
C	-2.289105	1.514933	-2.321416
B	-0.985942	0.722218	-0.199941
H	3.871247	-0.103021	-1.895692
H	4.757529	-1.997150	-0.586087
C	-1.850319	-2.676580	2.805734
C	0.552033	-2.296057	1.516597
F	-1.642092	-1.821179	-4.549484
C	-2.627999	0.295071	-4.339806
H	-2.792599	-2.834656	3.316507
C	-0.776827	-3.532672	3.072117
C	0.428030	-3.341789	2.425656
F	-3.160105	0.188121	-5.557663
H	-0.893328	-4.342179	3.781327
H	1.268114	-3.999023	2.620139
F	-2.161669	0.846579	0.556174

6•F$^-$:

F	0.567033	1.073370	2.450322
F	2.183338	3.066133	3.130306
F	2.873537	4.956614	1.310198
F	1.907016	4.801113	-1.222324
F	0.296859	2.820142	-1.929770
F	-0.730968	-1.272532	-2.484090
F	-4.009327	3.006926	-2.932552
F	-2.491856	2.753881	-0.755341
N	0.066387	-0.717046	0.121726
C	1.406044	-0.835367	-0.220294
C	1.952261	-0.161201	-1.317025

H	1.327734	0.464332	-1.936763
C	3.290868	-0.300613	-1.642004
C	4.114046	-1.144158	-0.911006
C	3.574454	-1.833604	0.164995
H	4.200586	-2.496449	0.752465
C	2.246342	-1.675309	0.524987
C	-1.878197	-2.160416	0.454158
H	-2.504165	-1.501635	-0.128813
C	-0.532380	-1.846994	0.671386
C	0.312592	1.856565	0.234183
C	0.846074	1.976927	1.510423
C	1.698348	2.999274	1.888349
C	2.052962	3.963774	0.965388
C	1.556298	3.882324	-0.318770
C	0.704391	2.842373	-0.653044
C	-1.534042	0.730168	-1.497454
C	-1.512783	-0.191647	-2.529924
C	-2.291588	-0.069565	-3.673482
C	-3.195319	1.956325	-2.802613
C	-2.404120	1.795892	-1.681622
B	-0.730114	0.599365	-0.051792
H	3.684584	0.239664	-2.494082
H	5.157009	-1.264162	-1.174042
C	1.649063	-2.327096	1.734319
C	-2.426626	-3.320261	0.973002
C	0.237189	-2.733212	1.438155
F	-2.236087	-0.988256	-4.640733
C	-3.138389	1.009525	-3.808768
H	-3.471549	-3.535970	0.786535
C	-1.653660	-4.209882	1.705506
C	-0.319736	-3.904322	1.926373
F	-3.892773	1.143660	-4.900303
H	-2.082309	-5.121542	2.101133
H	0.302094	-4.576573	2.507922
H	2.246937	-3.182651	2.058987
H	1.649687	-1.608986	2.564791
F	-1.725444	0.647693	0.937965

5•H_2O:

F	0.370942	2.806201	2.282217
F	1.412513	5.239684	1.859026
F	1.919017	6.097991	-0.647692
F	1.489869	4.446770	-2.747416
F	0.455066	2.031987	-2.370520
F	0.160338	-0.943896	-1.840559
F	-4.744335	1.160923	-2.596243
F	-3.241233	2.077547	-0.593523
N	0.185720	-0.228731	0.775769
C	1.543184	-0.556953	0.613389
C	2.650729	0.259373	0.424044
H	2.571620	1.332041	0.392780

C	3.891572	-0.334977	0.270957
C	4.049203	-1.719839	0.294129
C	2.954484	-2.533727	0.491644
H	3.062699	-3.609110	0.514718
C	1.707013	-1.953209	0.660788
C	-1.845153	-1.675545	1.167521
H	-2.547015	-0.866111	1.266365
C	-0.491572	-1.446237	0.957430
C	0.302620	2.324709	-0.034301
C	0.617531	3.184498	1.005804
C	1.161612	4.439872	0.829597
C	1.436615	4.879214	-0.450070
C	1.199276	4.040605	-1.515594
C	0.647789	2.792265	-1.291706
C	-1.486715	0.555547	-1.073206
C	-1.058617	-0.418674	-1.957953
C	-1.820562	-0.888890	-3.002681
C	-3.532364	0.646268	-2.398566
C	-2.732708	1.077381	-1.357762
B	-0.539515	0.955361	0.195971
H	4.757621	0.294529	0.125399
H	5.027264	-2.156285	0.153473
C	-2.282473	-2.982723	1.265670
C	0.401279	-2.521556	0.878849
F	-1.365310	-1.863472	-3.781357
C	-3.068461	-0.348933	-3.231530
H	-3.332447	-3.171207	1.435830
C	-1.400082	-4.056009	1.169309
C	-0.051280	-3.829460	0.984177
F	-3.798094	-0.771082	-4.254512
H	-1.776447	-5.065149	1.248930
H	0.641763	-4.655394	0.908920
O	-1.632957	1.323968	1.358212
H	-2.317839	1.950572	1.078411
H	-1.212949	1.634904	2.173380

H_2O:

O	-3.014751	1.293785	0.885635
H	-3.049302	2.224381	0.652060
H	-2.885765	1.277873	1.837734

$SiMe_3^+$:

Si	-0.039939	0.782441	-0.085534
C	0.428163	-0.394928	-1.410125
H	0.088384	-1.408500	-1.184716
H	0.055426	-0.102831	-2.390554
H	1.520677	-0.459139	-1.477507
C	0.234373	0.301862	1.662659
H	-0.142523	1.036807	2.372187
H	-0.226717	-0.665819	1.879891
H	1.304135	0.164310	1.853974

C	-0.761892	2.420333	-0.475181
H	-0.759995	2.652150	-1.538665
H	-1.798258	2.461916	-0.119969
H	-0.241204	3.216728	0.064108

SiMe3F:

Si	-0.590797	0.526806	-0.082305
F	-2.100692	-0.083192	-0.143251
C	0.428571	-0.371236	-1.370181
H	0.454349	-1.446273	-1.187192
H	0.034617	-0.219873	-2.376084
H	1.461547	-0.018201	-1.371484
C	0.078500	0.227536	1.640070
H	-0.520779	0.726123	2.402846
H	0.103678	-0.835256	1.884256
H	1.099170	0.603522	1.735236
C	-0.701244	2.356864	-0.458574
H	-1.114413	2.543523	-1.450644
H	-1.329503	2.881447	0.262261
H	0.285258	2.823229	-0.427491