Supporting Information for:

Air-Stable, Zn^{+2} - Based Catalyst for Hydrosilylation of Alkenes and Alkynes

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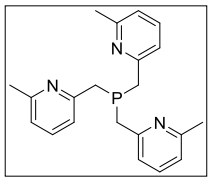
General Considerations

All experiments were carried out under an anhydrous N_2 atmosphere using standard Schlenk and glovebox techniques. All glassware was oven dried and cooled under vacuum before use. Commercial reagents were purchased from Sigma Aldrich, Strem or Apollo Scientific and used without further purification unless indicated otherwise. Dichloromethane (DCM), toluene and hexane were dried using Vacuum Atmospheres solvent purification system. 1,2-Dichlorobenzene (DCB), 1,2-difluorobenzene (DFB) and acetonitrile, were dried over CaH_2 and distilled from it. Potassium tetrakis(pentafluorophenyl)borate was prepared according to previously reported procedure.[1, 2] NMR spectra were recorded at room temperature in $CDCl_3$ solution or non-deuterated solvent, using DMSO capillary in J. Young NMR tubes, using a Bruker AvanceIII - 400 MHz spectrometer. Data for ^1H NMR are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, m = multiplet, b = broad), coupling constant (Hz), integration.

Preparation of TmPPh



An n-BuLi solution (20 mL, 31.9 mmol, 1.6 M in hexane) was added dropwise to a degassed solution of lutidine (2.8 mL, 24.4 mmol) in 100 mL of THF at −78 °C under N_2 and magnetic stirring. After one hour stirring at −78 °C, degassed chlorotrimethylsilane (3.1 mL, 24.4 mmol) was added dropwise to the solution and the system was allowed to reach room temperature overnight. The precipitated LiCl was removed by filtration and to the remained solution of lutidinetrimethylsilane in tetrahydrofuran (50 mL) at −78 °C, phosphorus trichloride (0.69 mL, 8.1 mmol) was slowly added and the system was allowed to warm to room temperature and stirred overnight. The solvent was then removed and orange residue was obtained. This residue was tritulated with boiling hexane and after cooling, **TmPPh** precipitated as white powder (1.2 g, 3.4 mmol, 42%). **TmPPh** was crystallized from hexane and its molecular structure was determined by X-ray crystallography.

^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 7.41 (t, J = 7.7 Hz, 1H), δ 7.06 (d, J = 7.6 Hz, 1H), δ 6.90 (d, J = 7.6 Hz, 1H), δ 3.04 (s, 2H) , δ 2.49 (s, 3H); **^{31}P NMR** ($CDCl_3$, 161.99 MHz): δ -13.8; **^{13}C NMR** ($CDCl_3$, 100.61 MHz): δ= 159.3 (d, J=4.5 Hz), 159.1, 137.7, 122.2 (d, J=4.2), 121.6, 37.3 (d, J=21.3), 26.0; HRMS (EI): m/z cacld. for [$C_{21}H_{25}N_3P$]: 350.1786 ($M+H^+$); found: 350.1791

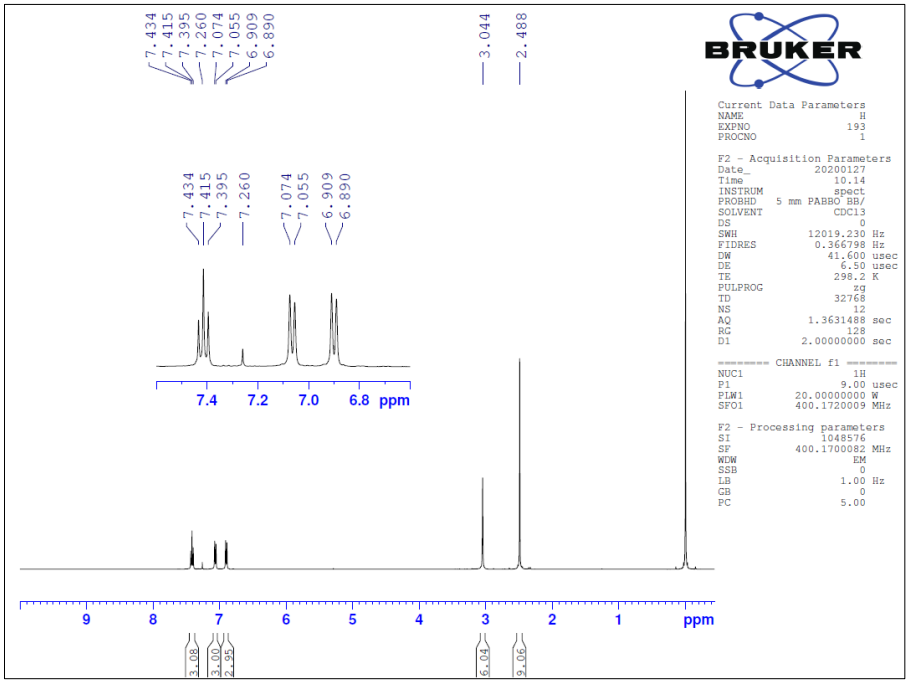


Figure S1. ^{1}H NMR spectrum of **TmPPh** ($CDCl_3$, 400.13 MHz).

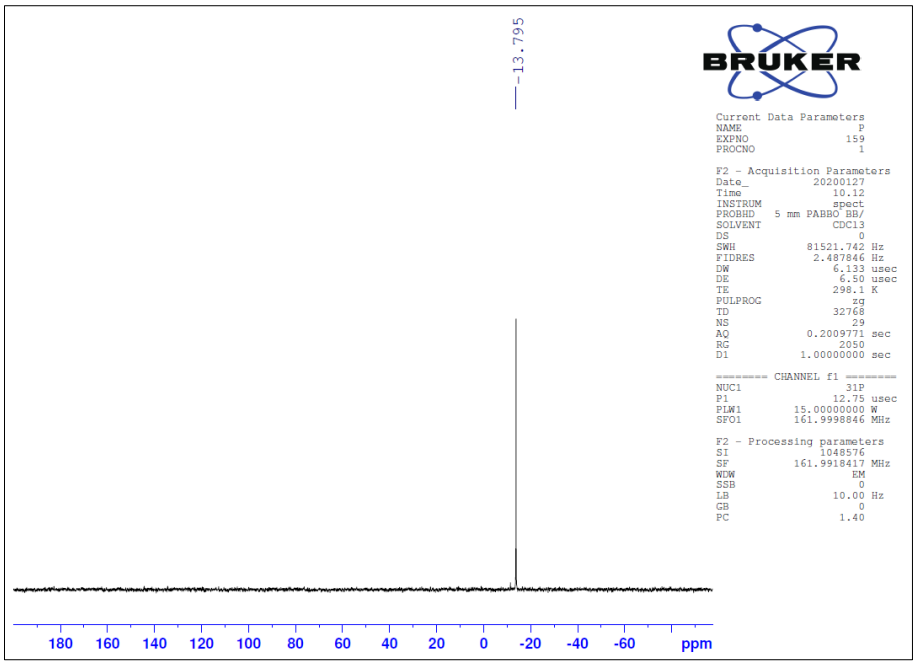


Figure S2. ^{31}P NMR spectrum of **TmPPh** ($CDCl_3$, 161.99 MHz).

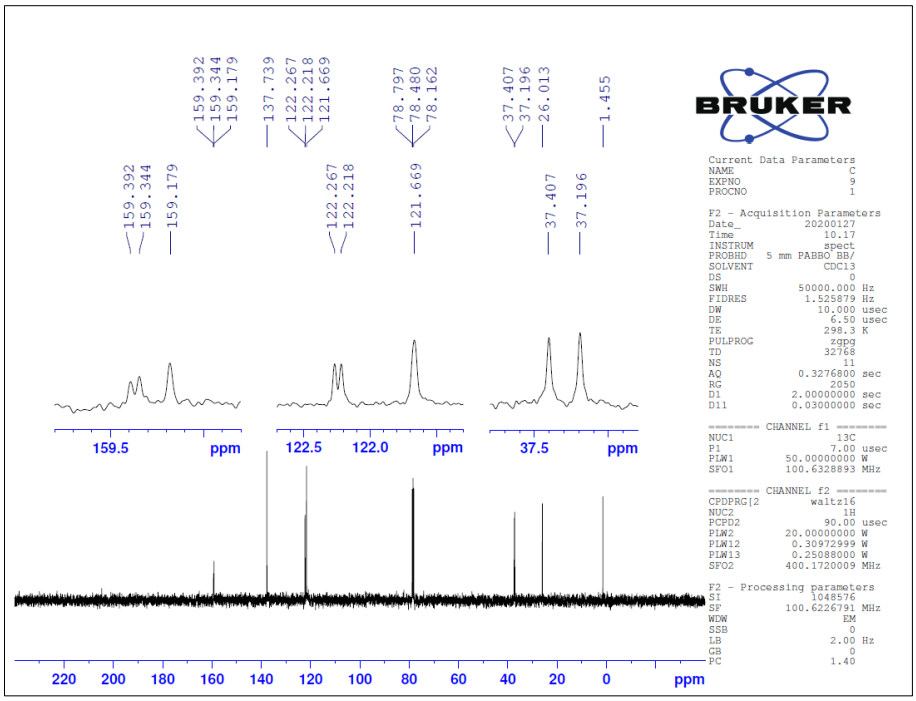
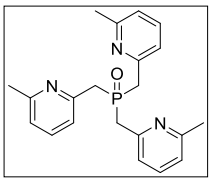


Figure S3. ^{13}C NMR spectrum of **TmPPh** ($CDCl_3$, 100.61 MHz).

Preparation of TmPPh-oxide



NMR tube containing the $CDCl_3$ solution of **TmPPh** was kept open to air overnight, resulting in a quantitative transformation to **TmPPh-oxide**.

^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 7.50 (t, J = 7.4 Hz, 1H), δ 7.26 (d, 1H), δ 7.00 (d, J = 7.6 Hz, 1H), δ 3.44 (d,J = 14.8 Hz, 2H) , δ 2.52 (s, 3H); **^{31}P NMR** ($CDCl_3$, 161.99 MHz): δ -13.8; **^{13}C NMR** ($CDCl_3$, 100.61 MHz): δ= 158.0, 152.4, 136.8, 122.03 (d, J=4.2), 121.2, 38.3 (d, J=60.1), 24.3; HRMS (EI): m/z cacld. for [$C_{21}H_{25}N_3PO$]: 366.1735 ($M+H^+$); found: 366.1736

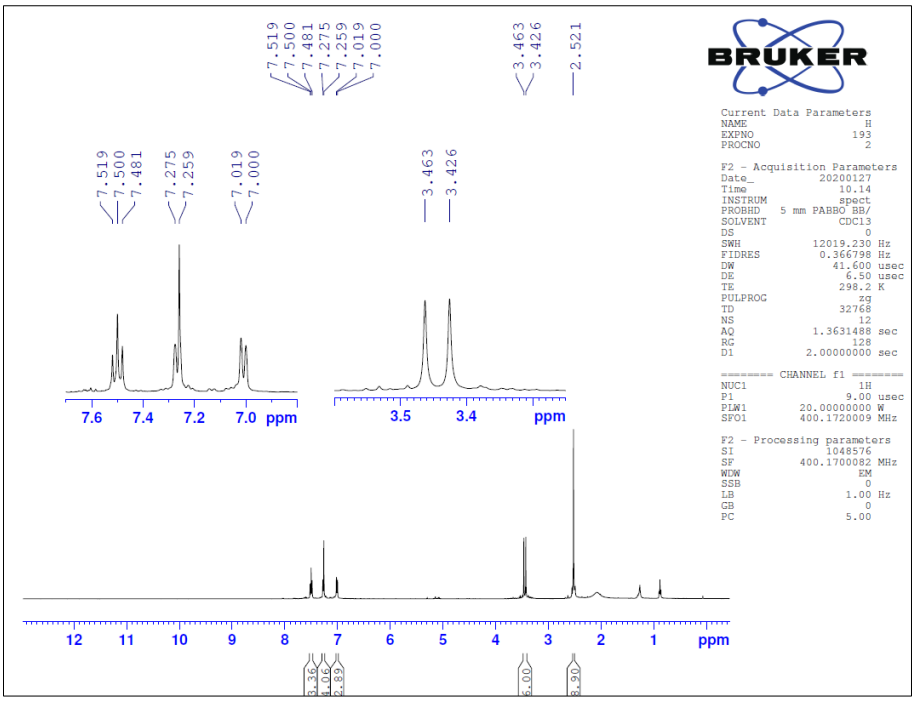


Figure S4. ^{1}H NMR spectrum of **TmPPh-oxide** ($CDCl_3$, 400.13 MHz).

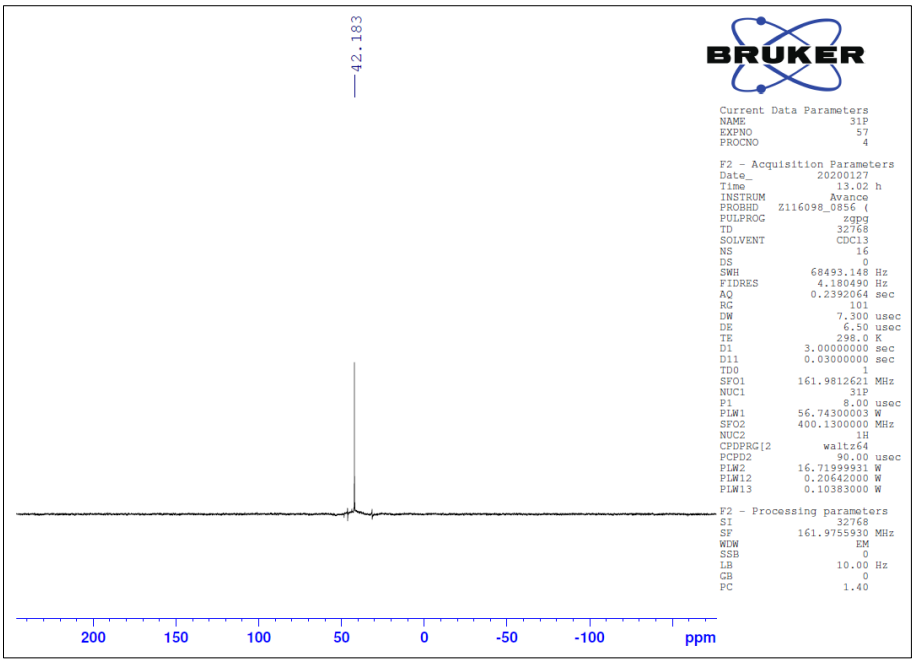


Figure S5. ^{31}P NMR spectrum of **TmPPh-oxide** ($CDCl_3$, 161.99 MHz).

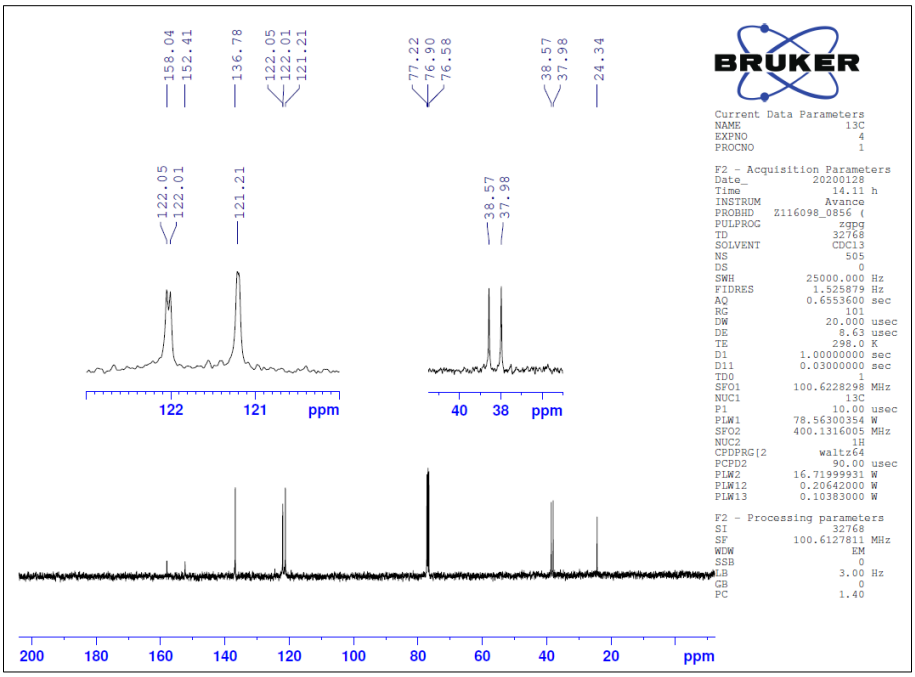
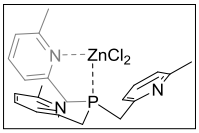


Figure S6. ^{13}C NMR spectrum of **TmPPh-oxide** ($CDCl_3$, 100.61 MHz).

Preparation of TmPPh·$ZnCl_2$ (2)



Zinc chloride (0.36 g, 1.2 mmol) was added to solution of **TmPPh** (0.43 g, 1.2 mmol) in dry tetrahydrofuran (15 mL) under N_2 and magnetic stirring. After 2 h of stirring, tetrahydrofuran was removed under reduced pressure, and 15 mL of dichloromethane were added. **2** was crystallized from a concentrated tetrahydrofuran in 95 % yield, and its molecular structure was determined by X-ray crystallography.

^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 7.57 (t, J = 7.64 Hz, 1H), δ 7.16 (d, J = 7.70 Hz, 1H), δ 7.06 (d, J = 7.58 Hz, 1H), δ 3.50 (d, J = 7.47 Hz, 2H), δ 2.65 (s, 3H); **^{31}P NMR** ($CDCl_3$, 161.99 MHz): δ -23.8; **^{13}C NMR** ($CDCl_3$, 100.61 MHz): δ= 158.9, 153.4, 138.2, 122.7, 122.1, 30.4 (d, J=13.7), 24.5;

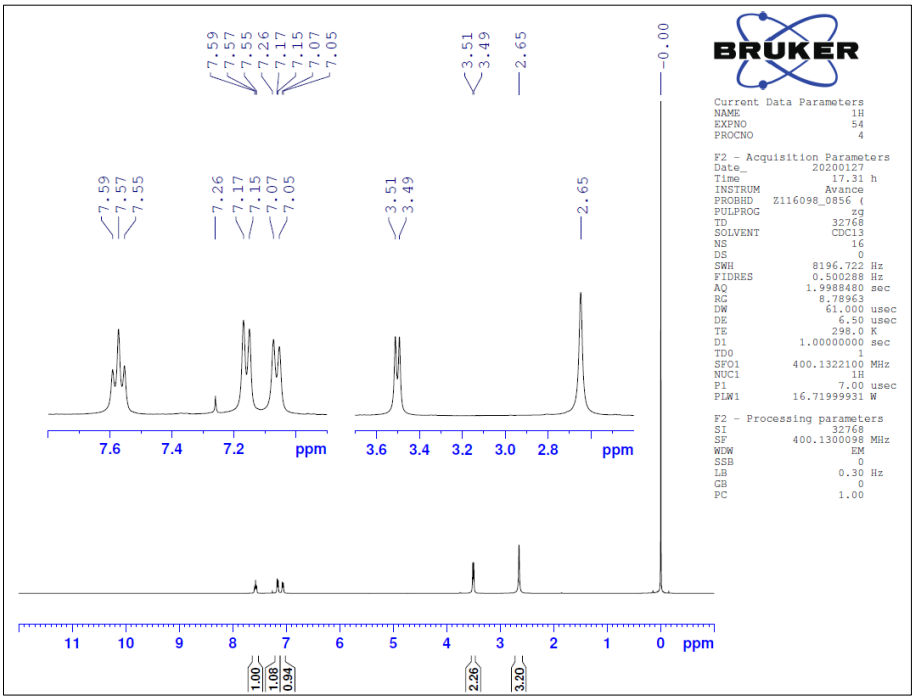


Figure S7. ^{1}H NMR spectrum of TmPPh·$ZnCl_2$ (**2**) ($CDCl_3$, 400.13 MHz).

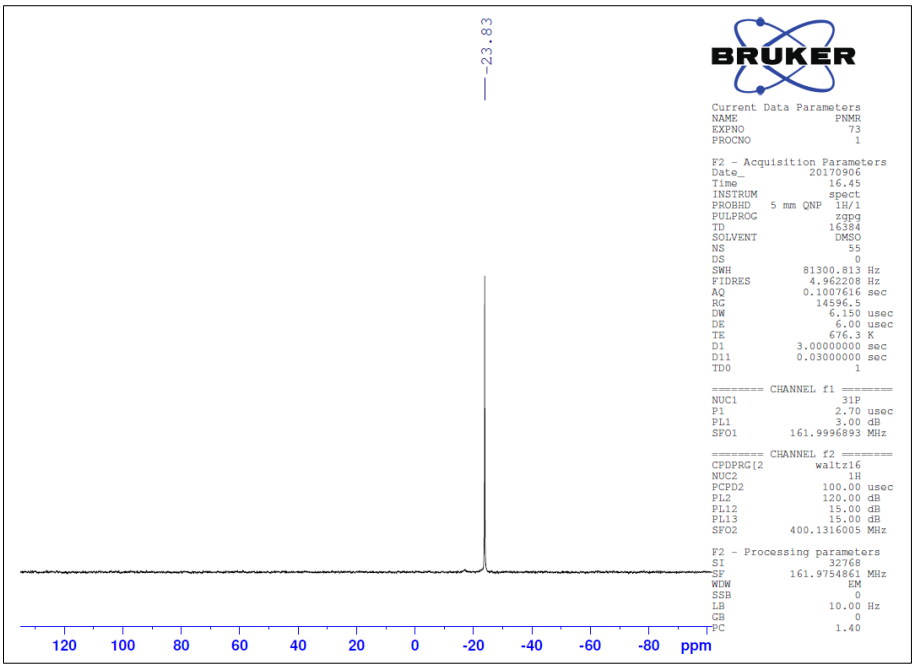


Figure S8. ^{31}P NMR spectrum of TmPPh·$ZnCl_2$ (**2**) ($CDCl_3$, 161.99 MHz).

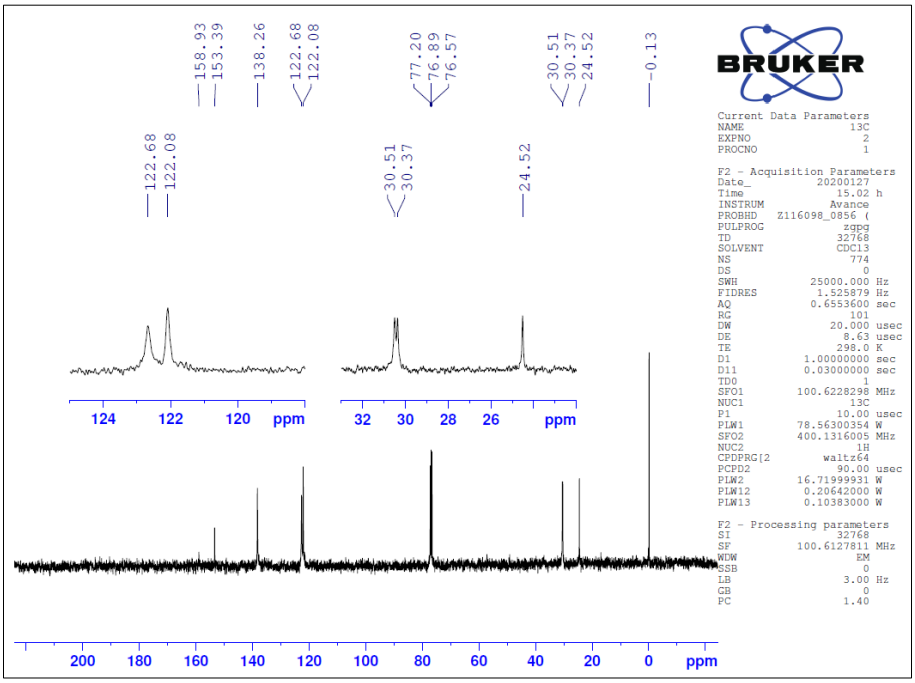
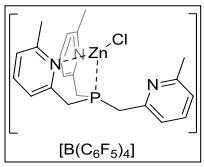


Figure S9. ^{13}C NMR spectrum of TmPPh·$ZnCl_2$ (**2**) ($CDCl_3$, 100.61 MHz).

Preparation of [TmPPh·ZnCl][B(C_6F_5)$_4$] (3)



Potassium tetrakis(pentafluorophenyl)borate (0.86 g, 1.2 mmol) was added to solution of **2** (0.79 g, 1.2 mmol) in dry dichloromethane under N_2 and magnetic stirring. The solution was left to stir overnight. The precipitated KCl was removed by filtration and the solvent was evaporated yielding **3** in 96% yields.

^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 8.00 (t, J = 7.6 Hz, 1H), δ 7.49 (d, J = 7.9 Hz, 1H), δ 7.46 (d, J = 7.9 Hz, 1H), δ 3.89 (d, J = 9.2 Hz, 2H), δ 2.93 (s, 3H); **^{31}P NMR** ($CDCl_3$, 161.99 MHz): δ -42.6; **^{13}C NMR** ($CDCl_3$, 100.61 MHz): δ= 158.8, 153.7, 149.2, 146.7, 140.1, 137.2, 134.8, 124.2, 123.1 (d, J=6.4 Hz), 30.7 (d, J=24.6 Hz), 25.5; **^{19}F NMR** ($CDCl_3$, 376.53 MHz): δ 133.6, 164.1 (t, J=15.1 Hz), 168.0; **^{11}B NMR** ($CDCl_3$, 128.37 MHz): δ -16.7; HRMS (EI): m/z cacld. for [$C_{21}H_{24}N_3PZnCl$]: 448.0688 (M); found: 448.0683

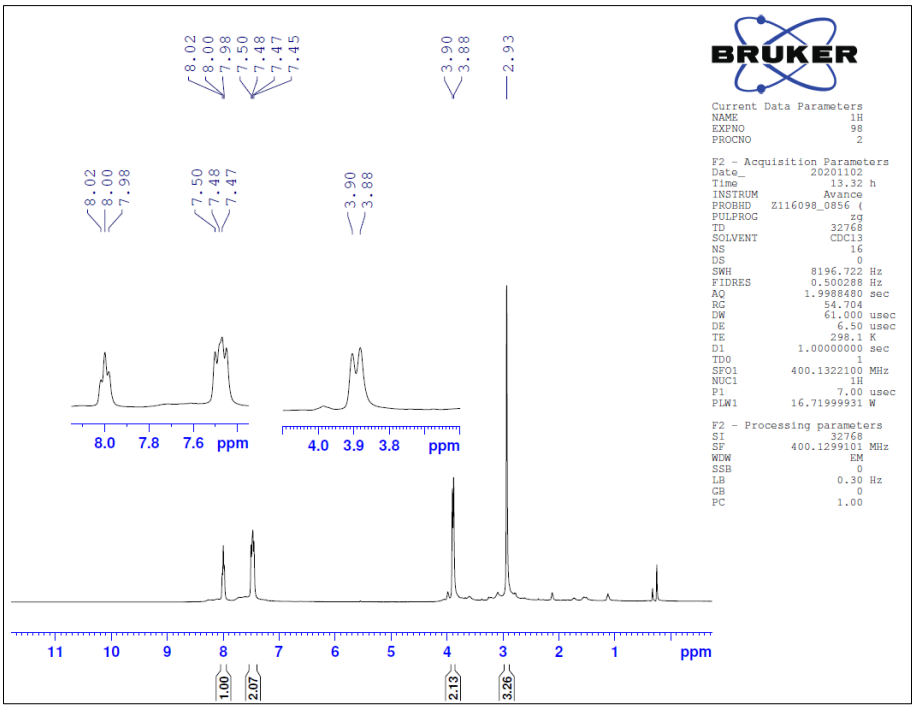


Figure S10. ^{1}H NMR spectrum of [TmPPh·ZnCl][B(C_6F_5)$_4$] (**3**) ($CDCl_3$, 400.13 MHz).

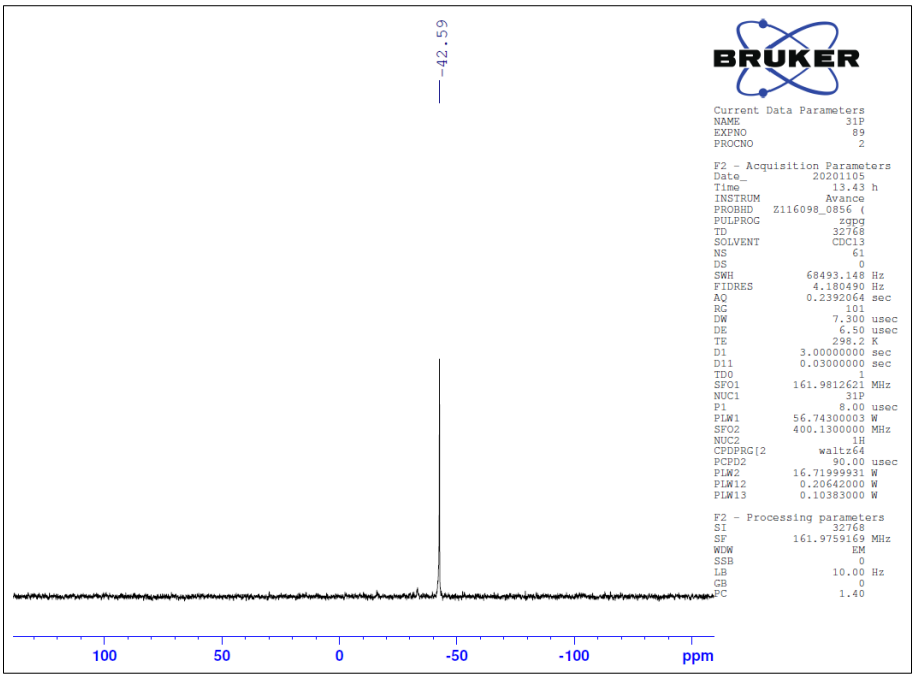


Figure S11. ^{31}P NMR spectrum of [TmPPh·ZnCl][B(C_6F_5)$_4$] (**3**) ($CDCl_3$, 161.99 MHz).

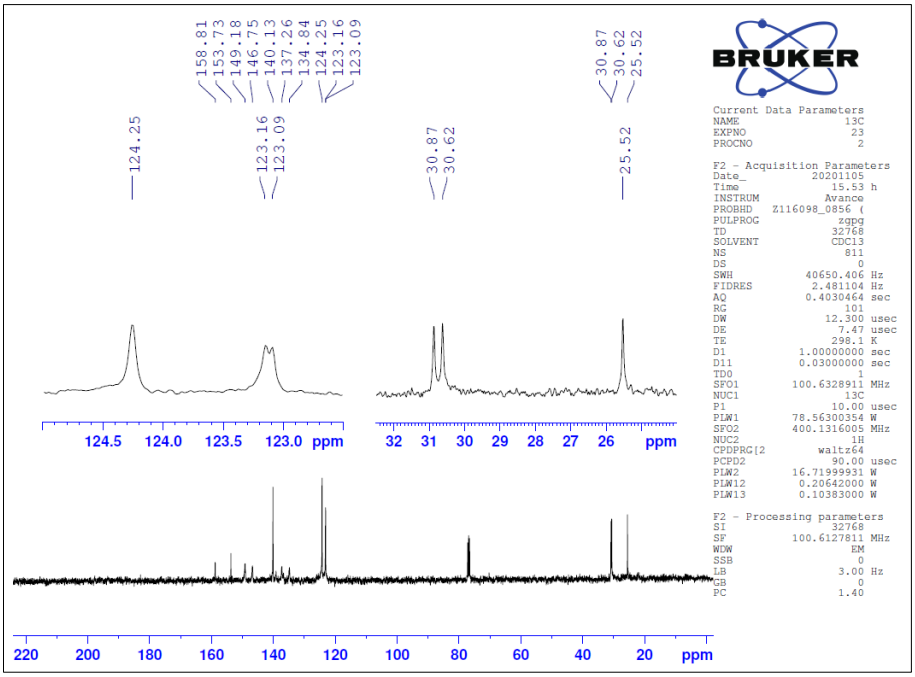


Figure S12. ^{13}C NMR spectrum of [TmPPh·ZnCl][B(C_6F_5)$_4$] (**3**) ($CDCl_3$, 100.61 MHz).

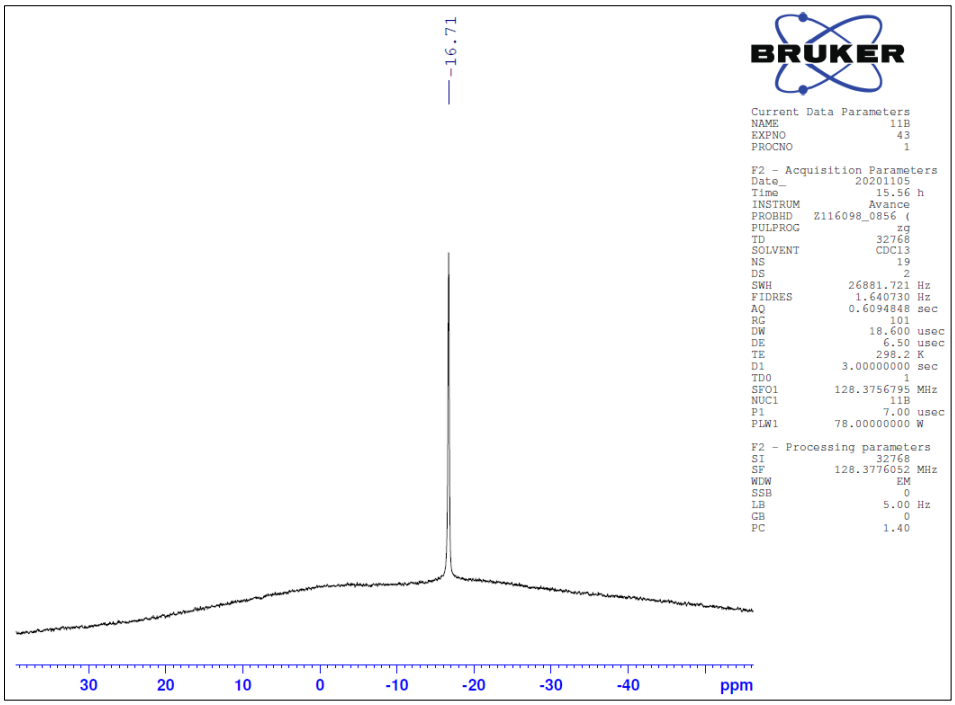


Figure S13. ^{11}B NMR spectrum of [TmPPh·ZnCl][$B(C_6F_5)_4$] (**3**) ($CDCl_3$, 128.37 MHz).

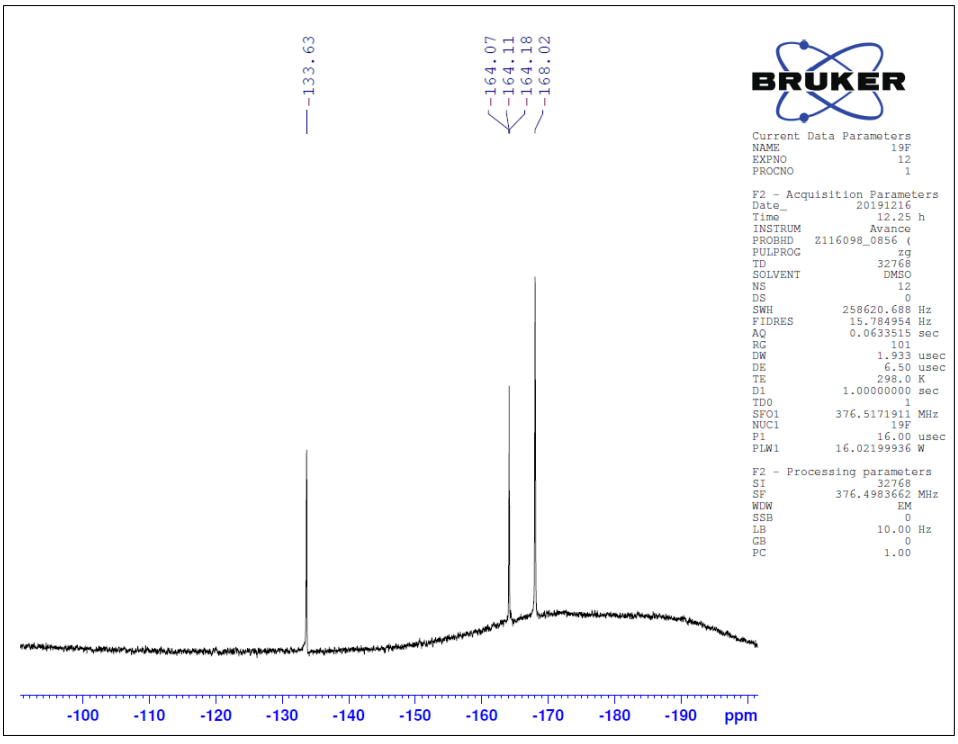
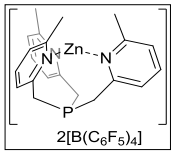


Figure S14. ^{19}F NMR spectrum of [TmPPh·ZnCl][$B(C_6F_5)_4$] (**3**) ($CDCl_3$, 376.53 MHz).

Preparation of [TmPPh·Zn][B(C_6F_5)$_4$]$_2$ (1)



Potassium tetrakis(pentafluorophenyl)borate (0.86 g, 1.2 mmol) was added to solution of **3** (0.79 g, 1.2 mmol) in dry 1,2-dichlorobenzene. The reaction mixture was left to stir overnight at 120 °C. The precipitated KCl was removed by filtration and the solvent was evaporated to obtain **1** in 95% yield.

^{1}H NMR (DMSO-d_6 capillary in dichloromethane, 400.13 MHz): δ 8.56 (t, J = 8.0 Hz, 1H), δ 7.99 (d, J = 7.8 Hz, 1H), δ 7.75 (d, J = 7.8 Hz, 1H), δ 3.44 (d, J = 5.1 Hz, 2H), δ 3.20 (s, 3H); **^{31}P NMR** (DMSO-d_6 capillary in DCM, 161.99 MHz): δ -12.6; **^{13}C NMR** (DMSO-d_6 capillary in DCM, 100.61 MHz): δ= 155.2, 150.7, 148.6, 146.1, 143.9, 136.7, 134.3, 124.7, 123.5,28.8 (d, J=24.7 Hz), 20.0; **^{19}F NMR** (DMSO-d_6 capillary in DCM, 376.53 MHz): δ 134.2, 164.1 (t, J=18.5 Hz), 168.2; **^{11}B NMR** (DMSO-d_6 capillary in DCM, 128.37 MHz): δ -16.8; HRMS (EI): m/z cacld. for [$C_{21}H_{23}N_3PZn$]: 412.0921 (M-H$^+$); found: 412.0912

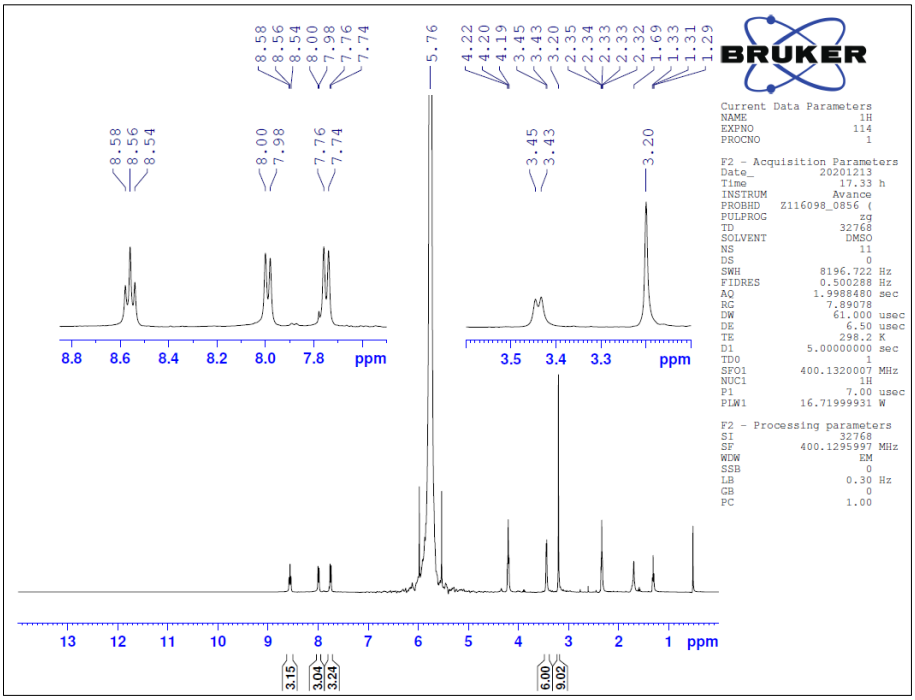


Figure S6. ^{1}H NMR spectrum of [TmPPh·Zn][B(C_6F_5)$_4$]$_2$ (**1**) ($CDCl_3$, 400.13 MHz).

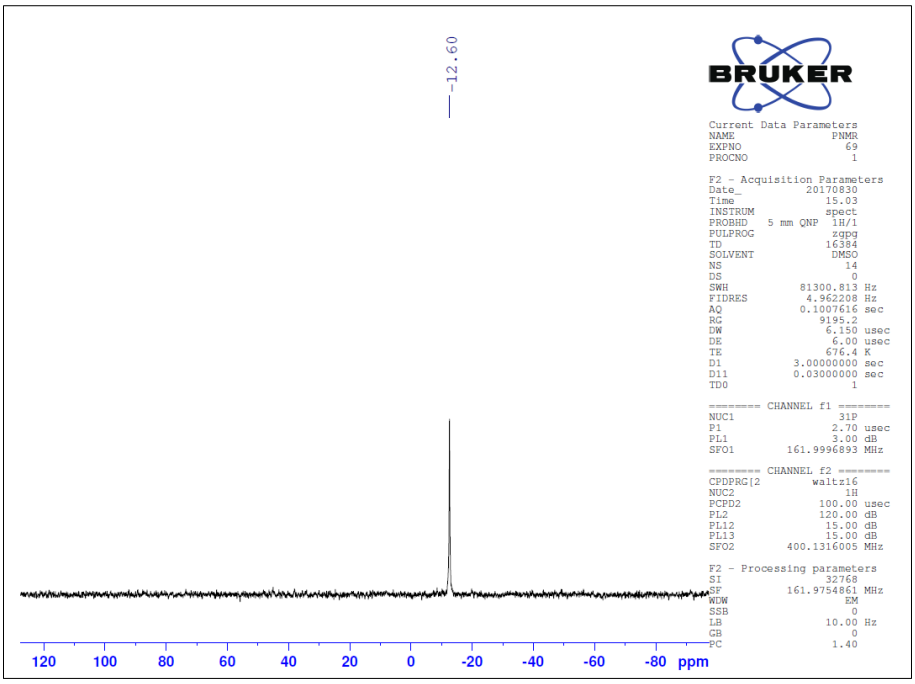


Figure S7. ^{31}P NMR spectrum of [TmPPh·Zn][B(C_6F_5)$_4$]$_2$ (**1**) ($CDCl_3$, 161.99 MHz).

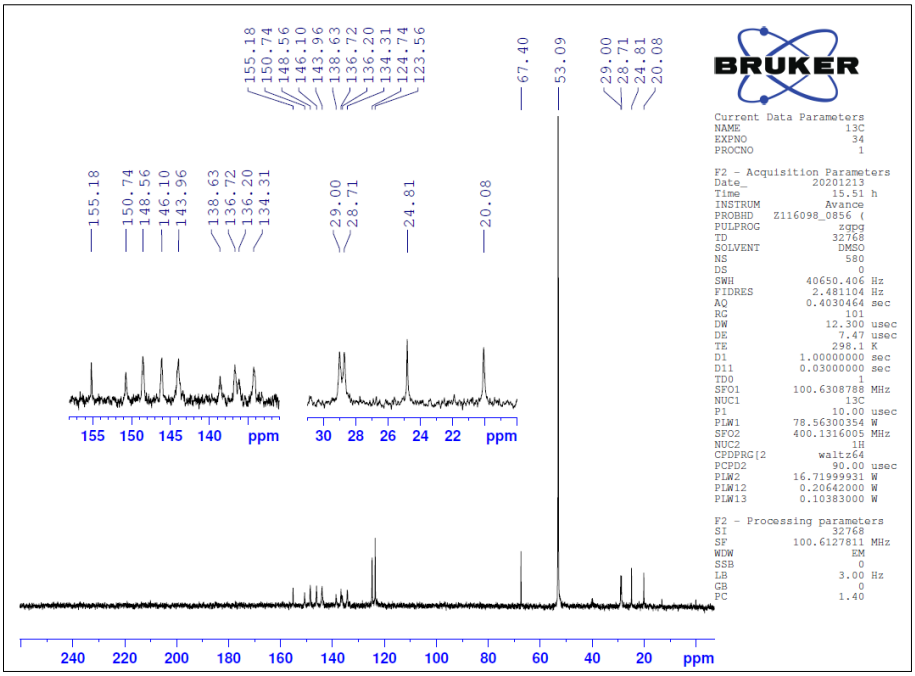


Figure S8. ^{13}C NMR spectrum of [TmPPh·Zn][B(C_6F_5)$_4$]$_2$ (**1**) ($CDCl_3$, 100.61 MHz).

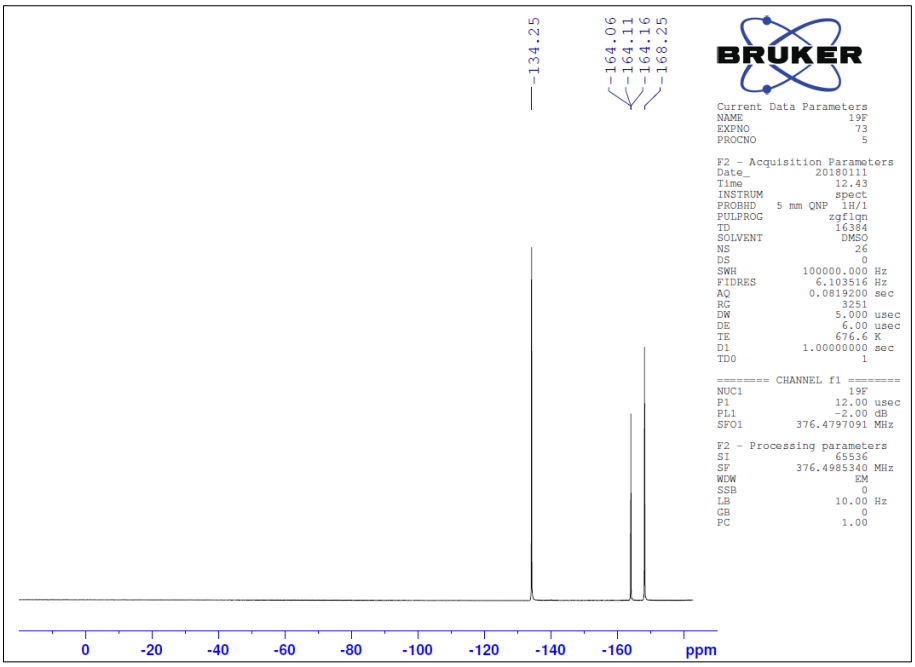


Figure S9. ^{19}F NMR spectrum of [TmPPh·Zn][B(C_6F_5)$_4$]$_2$ (**1**) ($CDCl_3$, 376.53 MHz).

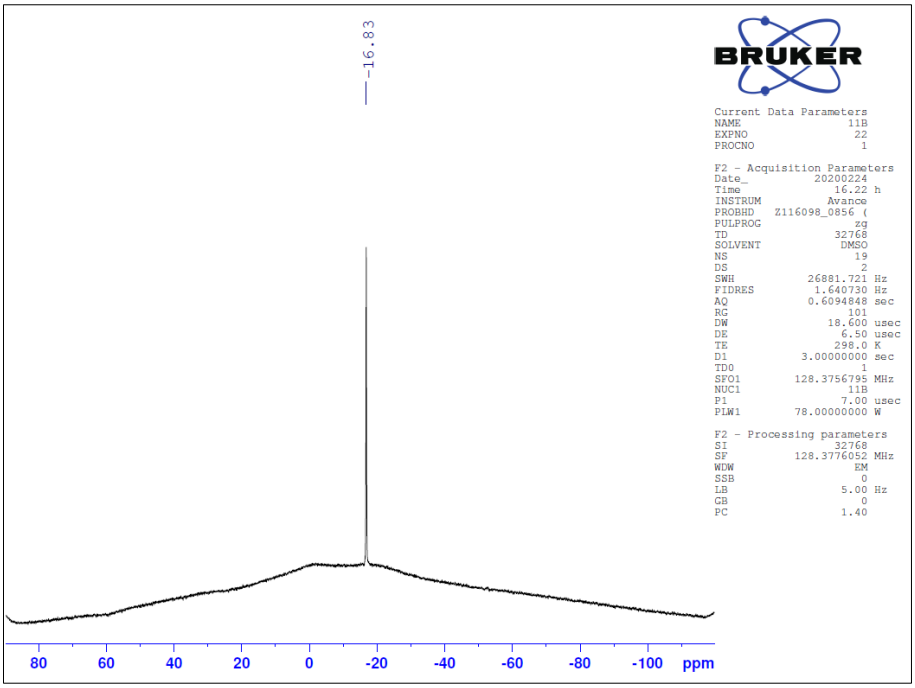


Figure S10. ^{11}B NMR spectrum of [TmPPh·Zn][B(C_6F_5)$_4$]$_2$ (**1**) ($CDCl_3$, 128.37 MHz).

Reaction of [TmPPh·Zn][B(C_6F_5)$_4$]$_2$ (1) with [N(n-Bu)$_4$]$_2$[$B_{12}I_{12}$]

1 (0.86 g, 1.2 mmol) was added to an acetonitrile solution of [N(n-Bu)$_4$]$_2$[$B_{12}I_{12}$] (1:1) under N_2. Immediately after the addition, crystalline material precipitated out of the solution and could not be redissolved in common organic solvents. A close analysis of this precipitate revealed two type of crystals. The molecular structures of both types of crystals were determined by X-ray crystallography. The first type of crystals were of [2TmPPh·Zn][$B_{12}I_{12}$] (**4**) (Figure S20, a). The second type of crystals were of [6CH_3CN·Zn][$B_{12}I_{12}$] (**5**) (Figure S20, b).

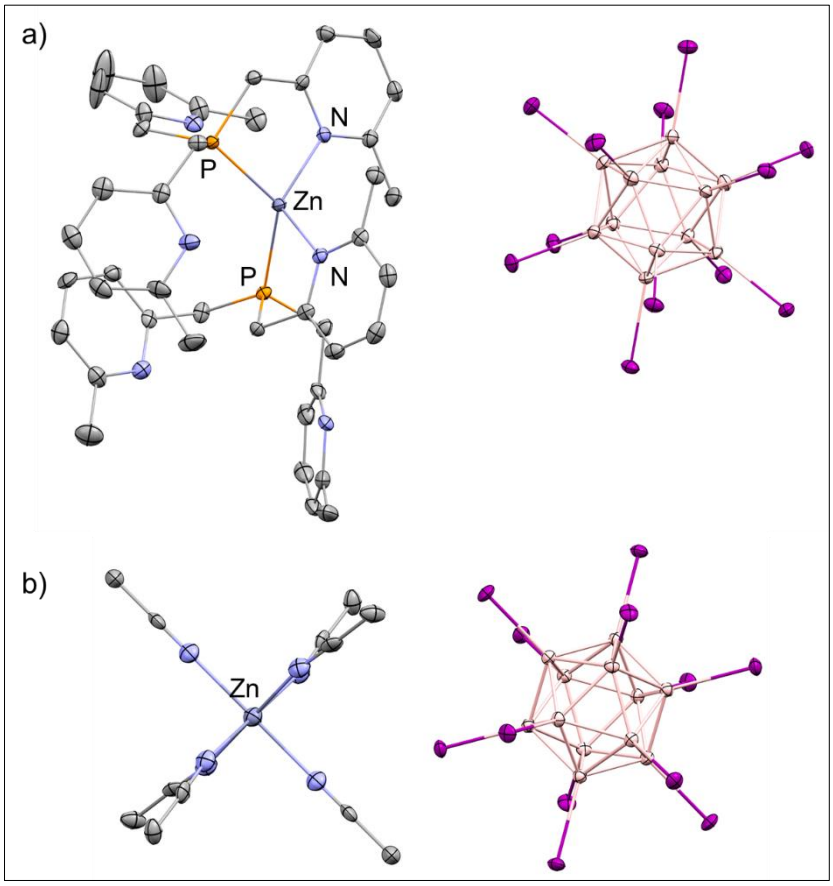
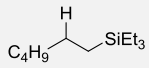
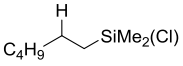
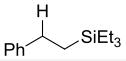
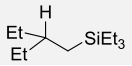
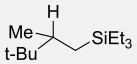
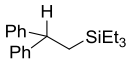
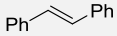
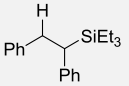
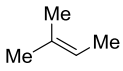
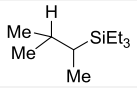
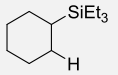
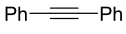
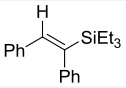
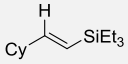


Figure S20. a) POV-ray depiction of **4** (a) and **5** (b). Thermal ellipsoids at the 50% probability level, hydrogens were omitted for clarity.

Table S1. Hydrosilylation of alkenes and alkynes catalyzed by **1**.

entry	Substrate	Hydrosilane	Time [h] / T [°C]	Product	NMR Conversion [%]	Isolated Yield [%]
1		Et_3SiH	3 / 120		99%	90%
2		$PhSiH_3$	3 / 100	Mixture of a single hydrosilylation products due to isomerization	99%	-
3		Ph_2SiH_2	3 / 100	Mixture of a single hydrosilylation products due to isomerization	99%	-
4		Me_2ClSiH	3 / 100		99%	-
5		Ph_2ClSiH (Neat)	3 / 100	Mixture of hydrosilylation products	99%	-
6		Et_3SiH	3 / 120		99%	95%
7		Et_3SiH	3 / 120		99%	93%
8		Ph_2ClSiH (Neat)	3 / 100	Mixture of hydrosilylation products	99%	-
9		Et_3SiH	3 / 120		99%	89%
10		Et_3SiH	3 / 120		99%	91%
11		Et_3SiH	3 / 120		99%	83%
12		Et_3SiH	3 / 120		99%	-
13		Et_3SiH	3 / 120		99%	90%
14		Et_3SiH	3 / 80		99%	95%
15		Et_3SiH	3 / 80		99%	93%

Hydrosilylation of alkenes and alkynes:

To a 1:1 solution of alkene/alkyne and Et_3SiH in 1,2-difluorobenzene in J-Young tube, **1** (0.5 mol%) was added and the reaction mixture was stirred for the indicated period of time at the required temperature (see Table S1). The conversion was determined by ^1H NMR spectroscopy. The products of hydrosilylation were purified by filtration of the reaction mixture through celite column, followed by evaporation of all the volatiles.

Hydrosilylation of 1-hexene with Et_3SiH (Table S1, entry 1):

Reaction was performed in 1,2-difluorobenzene at 120 ºC. ^1H NMR ($CDCl_3$, 400.13 MHz): δ 1.37 (m, CH_2, 8H), 1.00 (t, J = 7.9 Hz, $SiCH_2CH_3$, 9H), 0.97 (t, J = 6.8 Hz, CH_3, 3H), 0.58 (q, J = 7.9 Hz, $SiCH_2CH_3$, 6H), 0.58 (obscured, $SiCH_2$, 2H). ^{13}C NMR ($CDCl_3$, 100.61 MHz): 33.51 (CH_2), 31.48 (CH_2), 23.69 (CH_2), 22.53 (CH_2), 14.03 (CH_3), 11.19 ($SiCH_2$), 7.35 ($SiCH_2\mathit{C}H_3$), 3.20 ($Si\mathit{C}H_2CH_3$). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ 6.0 (Et_3SiR).

Hydrosilylation of 1-hexene with Et_3SiH under aerobic conditions:

Et_3SiH and 1-hexene (1:1) and **1** (0.5 mol%) were dissolved in 1,2-difluorobenzene under aerobic conditions and placed in a J-Young NMR tube. Afterwards, the J-Young NMR tube solution was degassed and left for heating at 120 ºC for 3 h. The results were similar in both aerobic and anaerobic conditions.

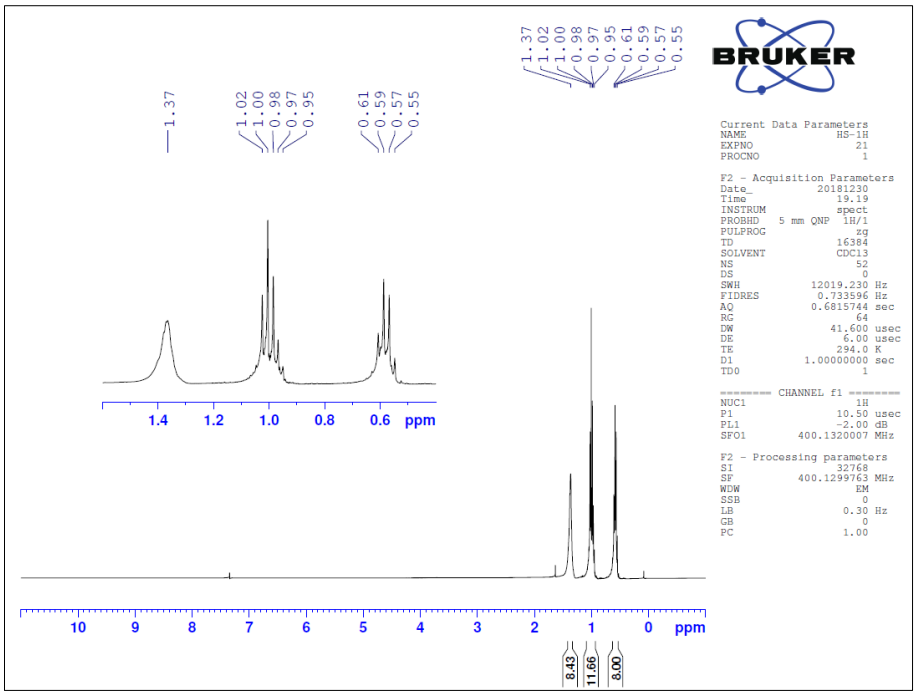


Figure S21. ^1H NMR spectrum of 1-hexene hydrosilylation product (Table S1, entry 1) ($CDCl_3$, 400.13 MHz).

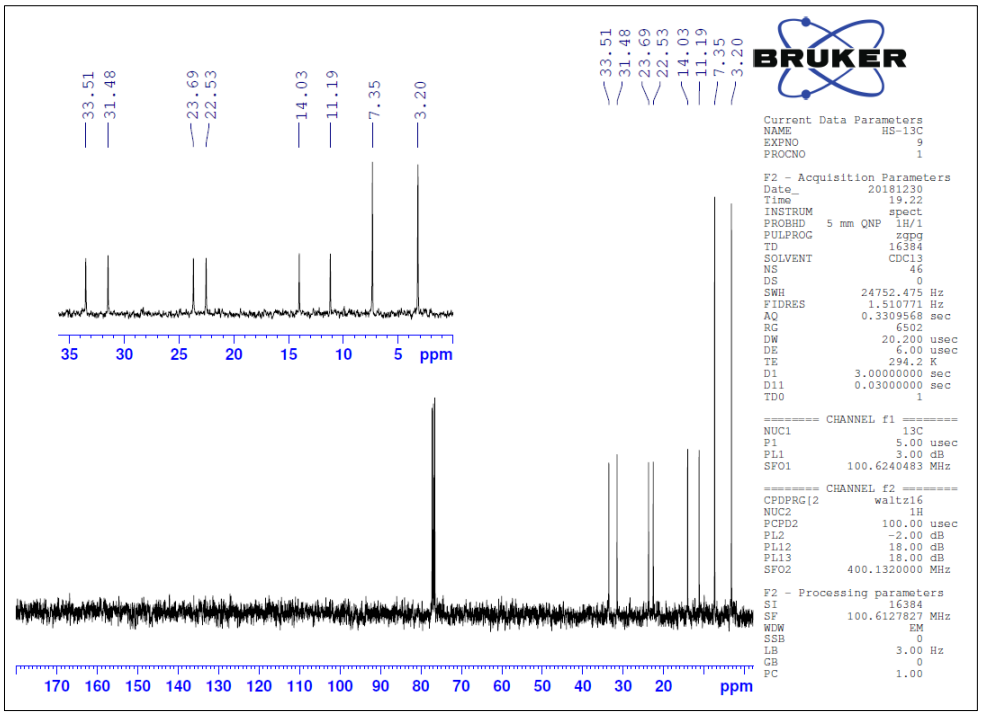


Figure S22. ^{13}C NMR spectrum of 1-hexene hydrosilylation product (Table S1, entry 1) ($CDCl_3$, 100.61 MHz).

Hydrosilylation of 1-hexene with $PhSiH_3$ (Table S1, entry 2):

Reaction was performed in 1,2-difluorobenzene at 100 ºC. According to ^{13}C NMR a mixture of hydrosilylation products was obtained. ^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 0.56-1.34 (m, $CH_3(CH_2)_4CH2Si$, 13H), 3.50 (s, SiH_2, 2H), 3.72 (s, SiH_2, 2H), 3.80 (s, SiH_2, 2H), 4.32 (s, SiH_2, 2H), 7.28-7.57 (m, Ar-H, 10H), 6.88-7.05 (m, DFB solvent). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ -32.0 (PhH_2SiR).

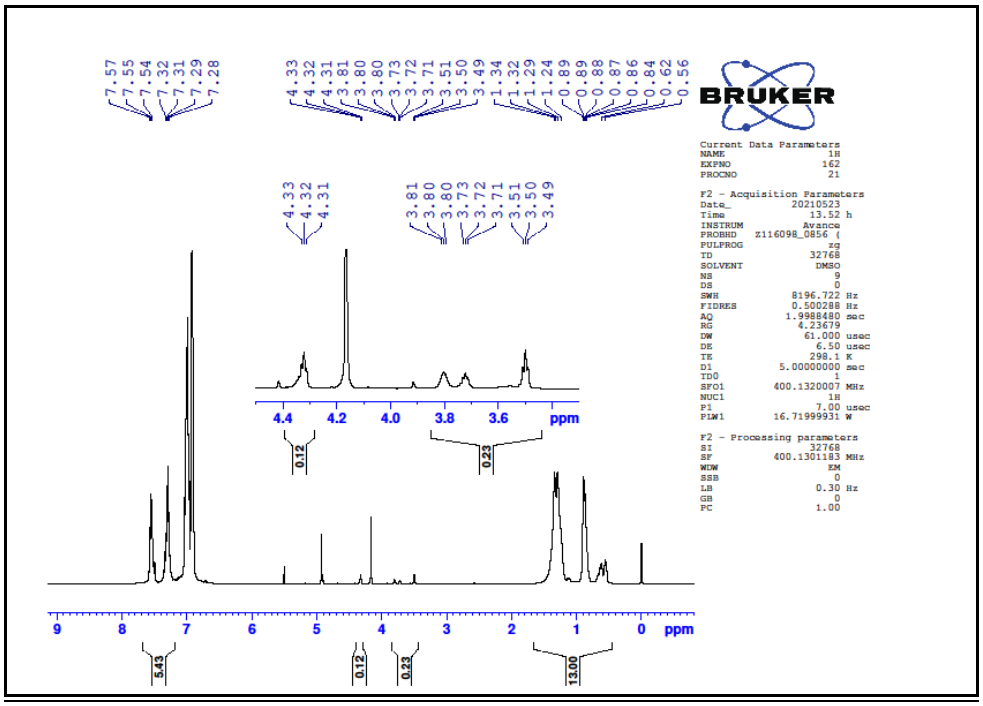


Figure S23. ^{1}H NMR spectrum of 1-hexene hydrosilylation product (Table S1, entry 2) ($CDCl_3$, 400.13 MHz).

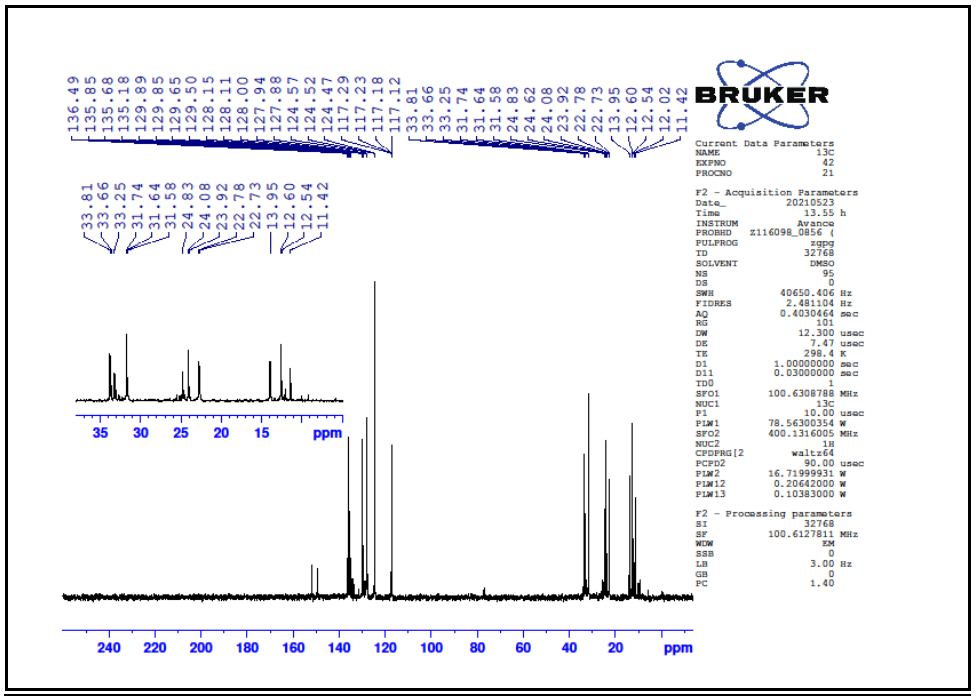


Figure S24. ^{13}C NMR spectrum of 1-hexene hydrosilylation product (Table S1, entry 2) ($CDCl_3$, 100.61 MHz).

Hydrosilylation of 1-hexene with Ph_2SiH_2 (Table S1, entry 3):

Reaction was performed in 1,2-difluorobenzene at 100 ºC. According to ^{13}C NMR a mixture of hydrosilylation products was obtained. ^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 0.50-1.48 (m, $CH_3(CH_2)_4CH2Si$, 13H), 3.48 (t, SiH, 1H), 3.66 (t, SiH, 1H), 3.71 (t, SiH, 1H), 4.29 (t, SiH, 1H), 4.87 (t, SiH, 1H), 7.33-7.58 (m, Ar-H, 10H), 6.98-7.15 (m, DFB solvent). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ -17.3 (Ph_2HSiR).

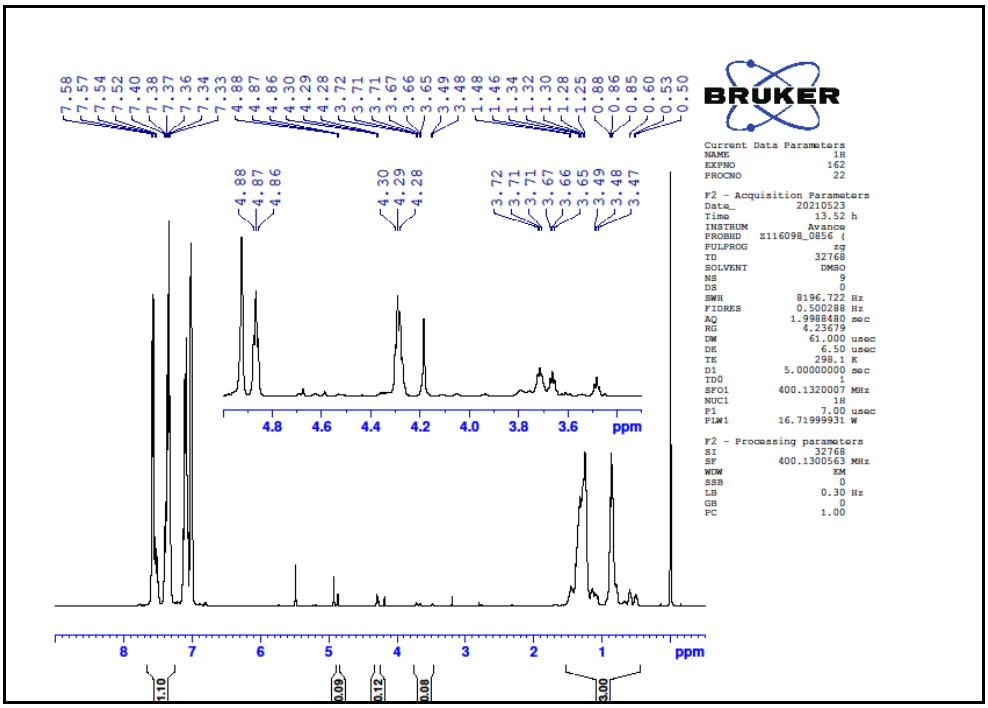


Figure S25. ^{1}H NMR spectrum of 1-hexene hydrosilylation product (Table S1, entry 3) ($CDCl_3$, 400.13 MHz).

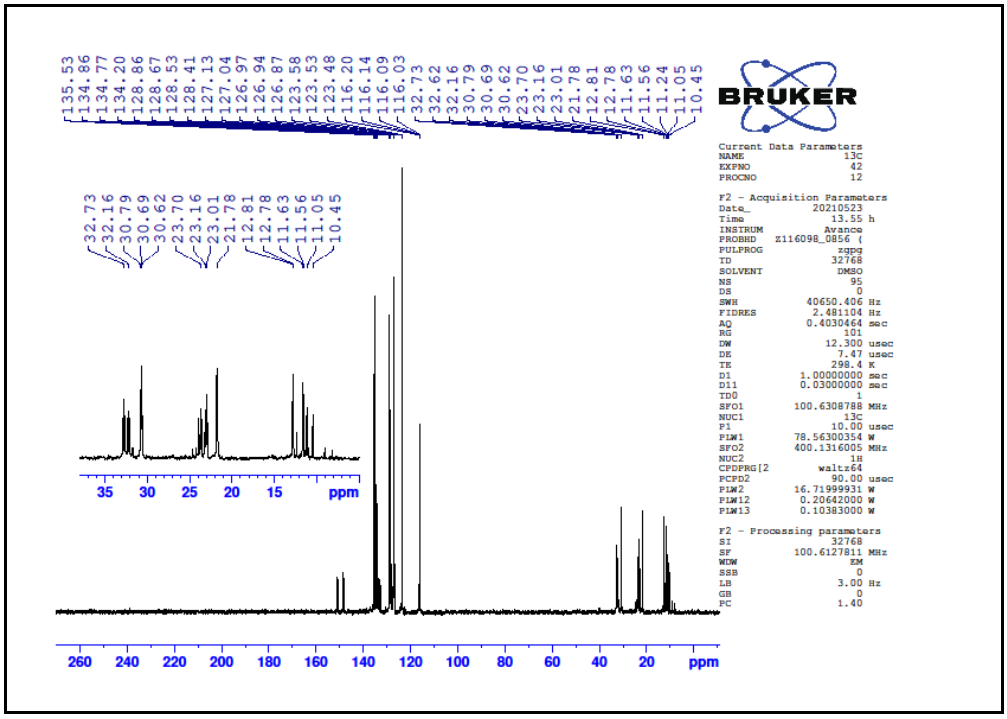


Figure S26. ^{13}C NMR spectrum of 1-hexene hydrosilylation product (Table S1, entry 3) ($CDCl_3$, 100.61 MHz).

Hydrosilylation of 1-hexene with Me_2ClSiH (Table S1, entry 4):

Reaction was performed in 1,2-difluorobenzene at 100 ºC. ^1H NMR ($CDCl_3$, 400.13 MHz): δ 0.36 (s, $SiCH_3$, 6H), 0.75 (m, $SiCH_2$, 2H), 0.87 (t, J = 6.7 Hz, CH_3, 3H), 1.32 (m, CH_2, 8H), 6.98 (m, DFB solvent), 7.23 (m, DFB solvent). ^{13}C NMR ($CDCl_3$, 100.61 MHz): 33.16 (CH_2), 31.93 (CH_2), 23.42 (CH_2), 23.07 (CH_2), 19.31 (CH_3), 14.49 ($SiCH_2$), 1.08 ($SiCH_3$). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ 14.5 (Me_2ClSiR).

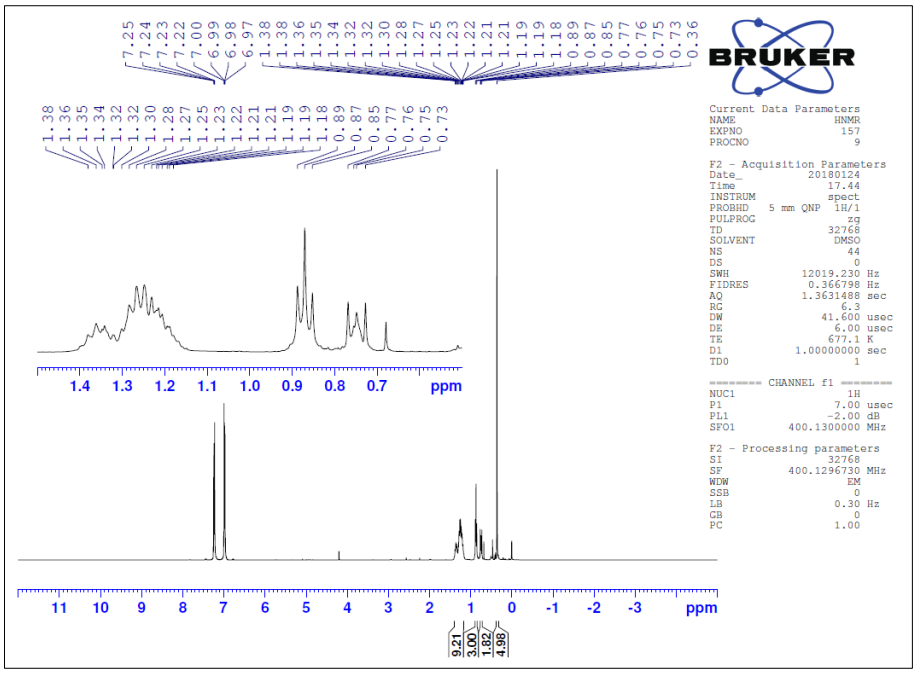


Figure S27. ^{1}H NMR spectrum of 1-hexene hydrosilylation product (Table S1, entry 4) ($CDCl_3$, 400.13 MHz).

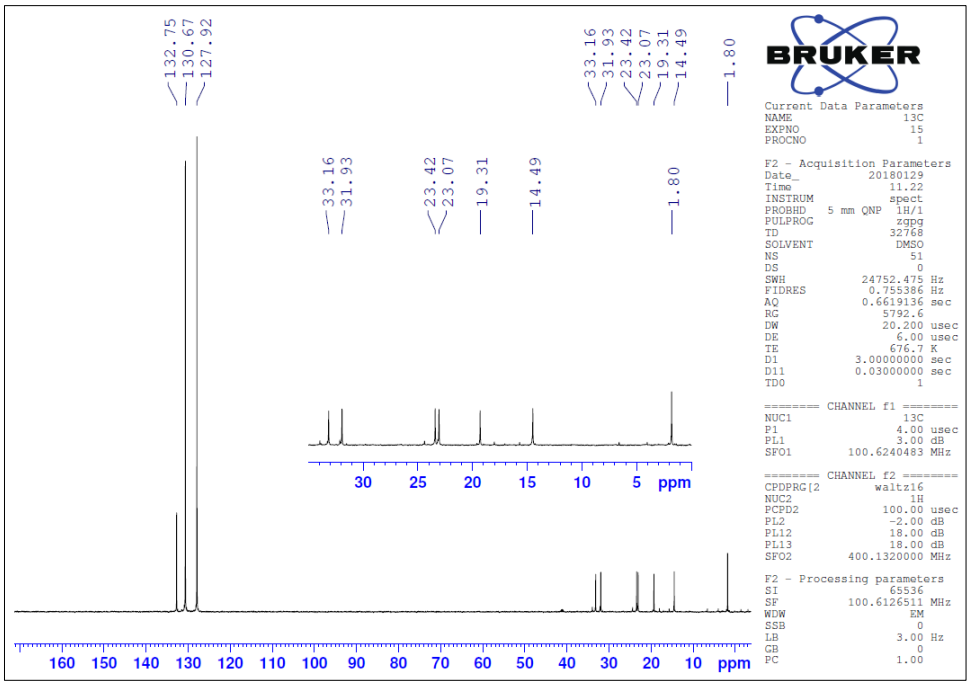


Figure S28. ^{13}C NMR spectrum of 1-hexene hydrosilylation product (Table S1, entry 4) ($CDCl_3$, 100.61 MHz).

Hydrosilylation of 1-hexene with Ph_2ClSiH (Table S1, entry 5):

Reaction was performed in neat Ph_2SiClH and 1-hexene (1:1), at 100 ºC for 3 h. According to ^{13}C NMR, there are 2 major hydrosilylation products. ^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 0.84-1.50 (m, Alk-H, 13H), 7.32-7.73 (m, Ar-H, 10H). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ 8.4 (Ph_2ClSiR).

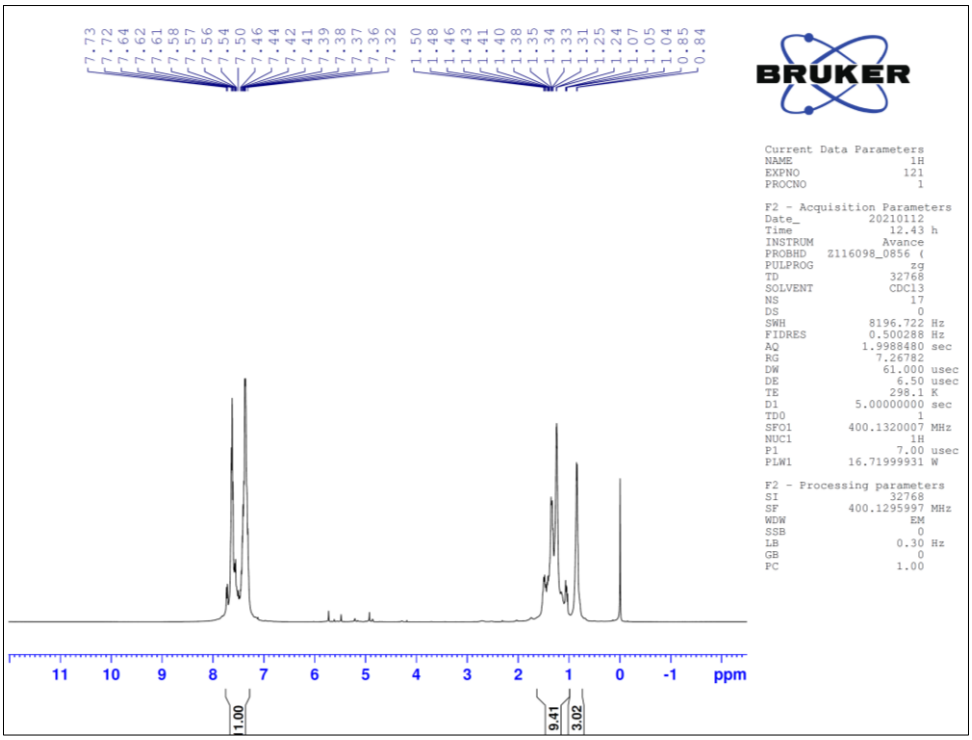


Figure S29. 1H NMR spectrum of 1-hexene hydrosilylation product (Table S1, entry 5) ($CDCl_3$, 400.13 MHz)

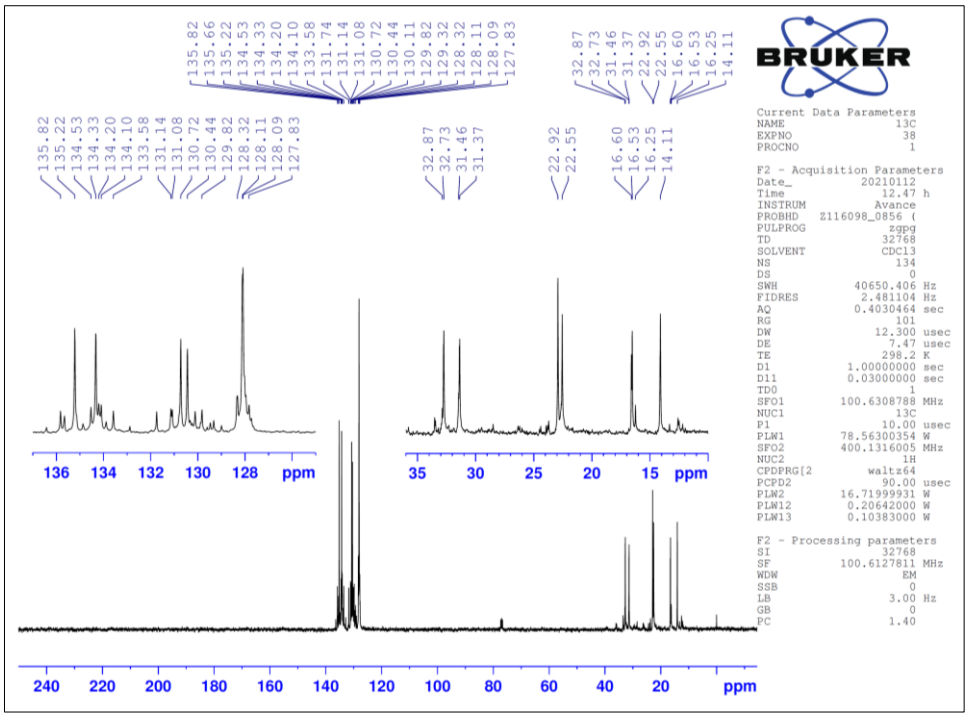


Figure S30. 13C NMR spectrum of 1-hexene hydrosilylation product (Table S1, entry 5) ($CDCl_3$, 100.61 MHz).

<u>Hydrosilylation of styrene with Et_3SiH (Table S1, entry 6):</u>

Reaction was performed in 1,2-diflourobenzene, in 120 ºC for 3 h. ^1H NMR ($CDCl_3$, 400.13 MHz): δ 7.16-7.30 (m, CH(Ph), 5H), 2.62 (m, CH_2, 2H), 0.96 (t, J = 7.8 Hz, $SiCH_2\mathit{CH_3}$, 9H), 0.89 (m, $SiCH_2$, 2H), 0.55 (q, J = 7.8 Hz, $Si\mathit{CH_2}CH_3$, 6H). ^{13}C NMR ($CDCl_3$, 100.61 MHz): 131.51 (*i*-C(Ph)), 129.76 (*m*-C(Ph)), 129.17 (*o*-C(Ph)), 126.93 (*p*-C(Ph)), 31.51 (CH_2), 15.12 ($SiCH_2$), 8.92 ($Si\mathit{CH_2}CH_3$) , 4.74 ($SiCH_2\mathit{CH_3}$). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ 6.8 (Et_3SiR).

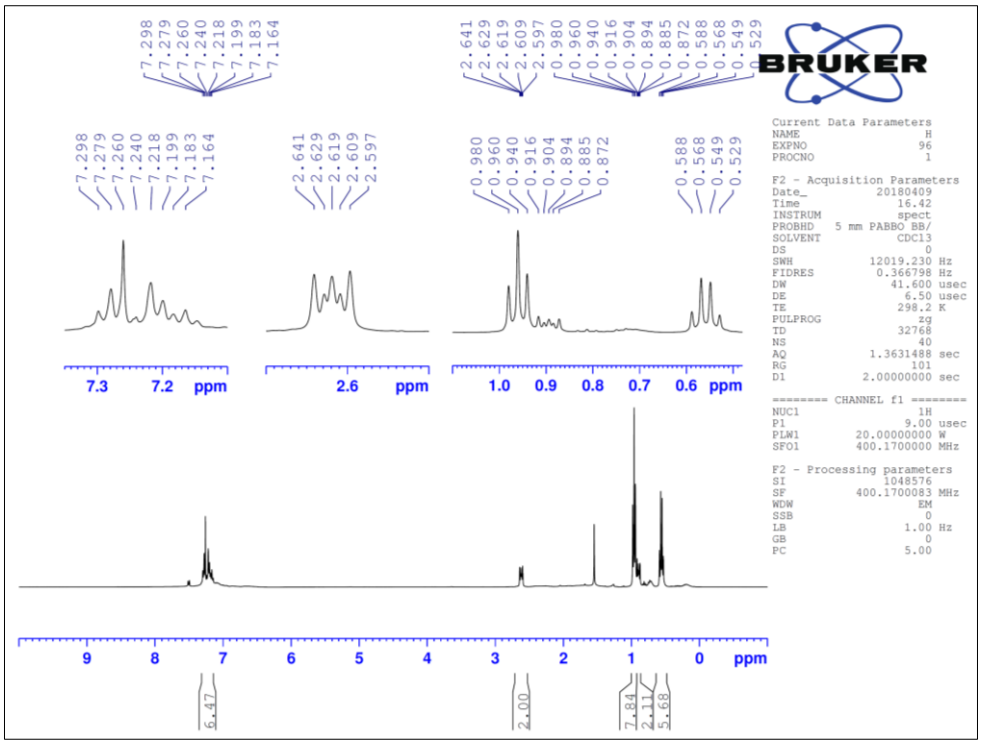


Figure S31. ^{1}H NMR spectrum of styrene hydrosilylation product (Table S1, entry 6) ($CDCl_3$, 400.13 MHz).

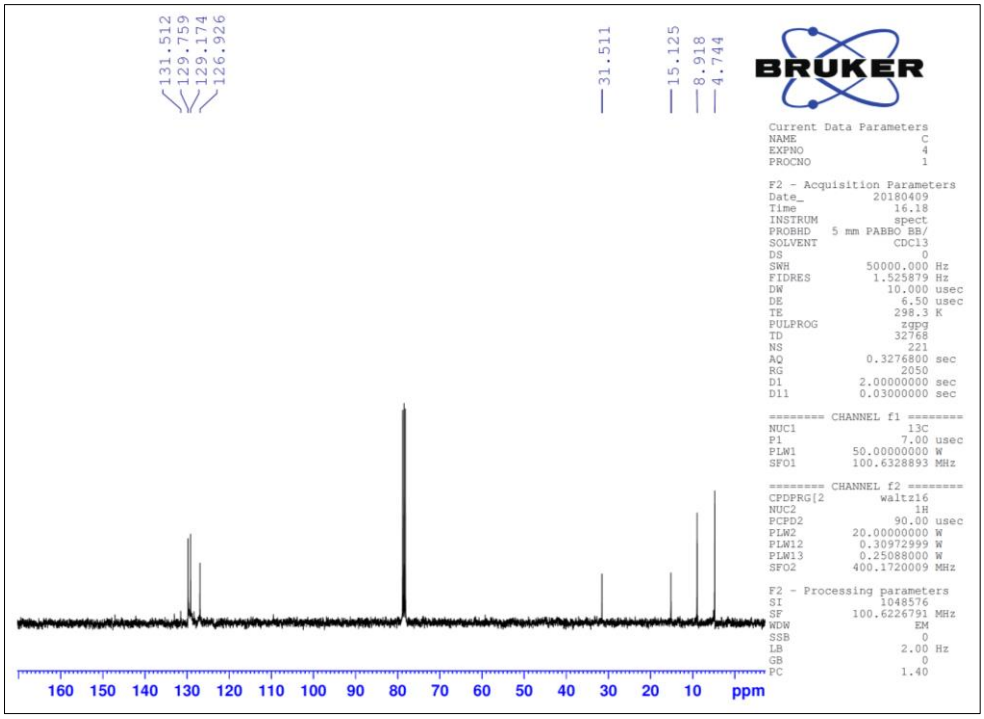


Figure S32. ^{13}C NMR spectrum of styrene hydrosilylation product (Table S1, entry 6) ($CDCl_3$, 100.61 MHz).

Hydrosilylation of 1,1-diethylethene with Et_3SiH (Table S1, entry 7):

Reaction was performed in 1,2-diflourobenzene, in 120 ºC for 3 h. ^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 1.23-1.36 (m, CH_2CH_3, 4H), 1.28 (obscured, CH, 1H), 0.93 (t, J = 7.8 Hz, $SiCH_2CH_3$, 9H), 0.83 (t, J = 7.4 Hz, CH_2CH_3, 6H), 0.51 (q, J = 7.8 Hz, $SiCH_2$, 6H), 0.49 (d, CH_2, 2H). ^{13}C NMR ($CDCl_3$, 100.61 MHz): 36.78 (CH), 28.52 (CH_2), 15.78 (CH_2), 10.96 (CH_3), 7.65 ($SiCH_2$), 4.15 ($SiCH_2CH_3$). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ 5.1 (Et_3SiR).

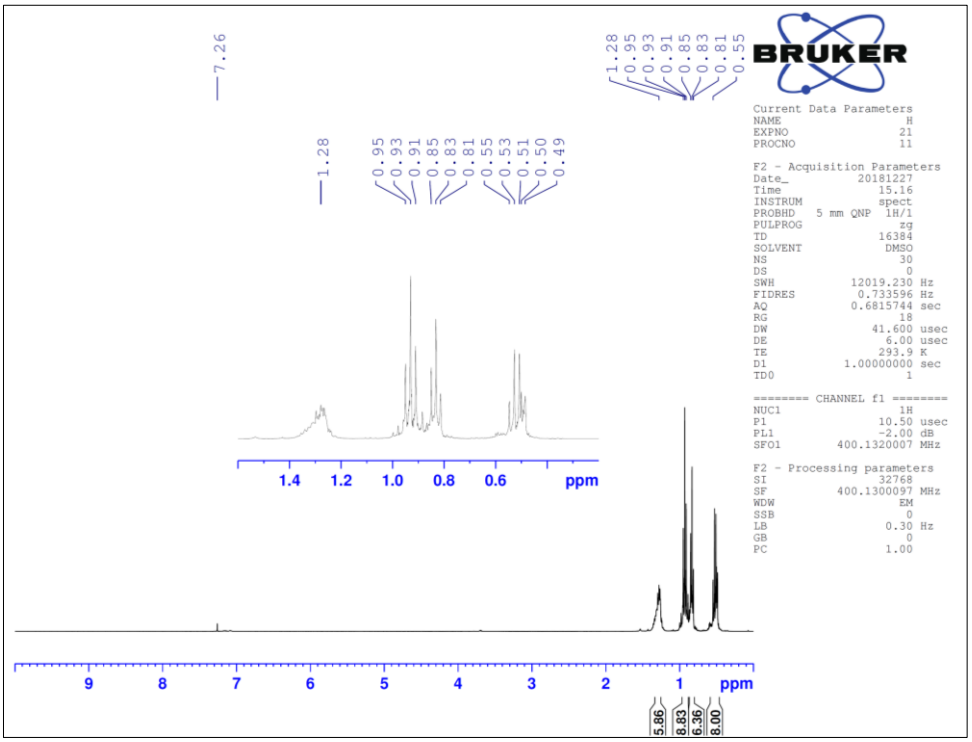


Figure S33. ^{1}H NMR spectrum of 1,1-diethylethene hydrosilylation product (Table S1, entry 7) ($CDCl_3$, 400.13 MHz).

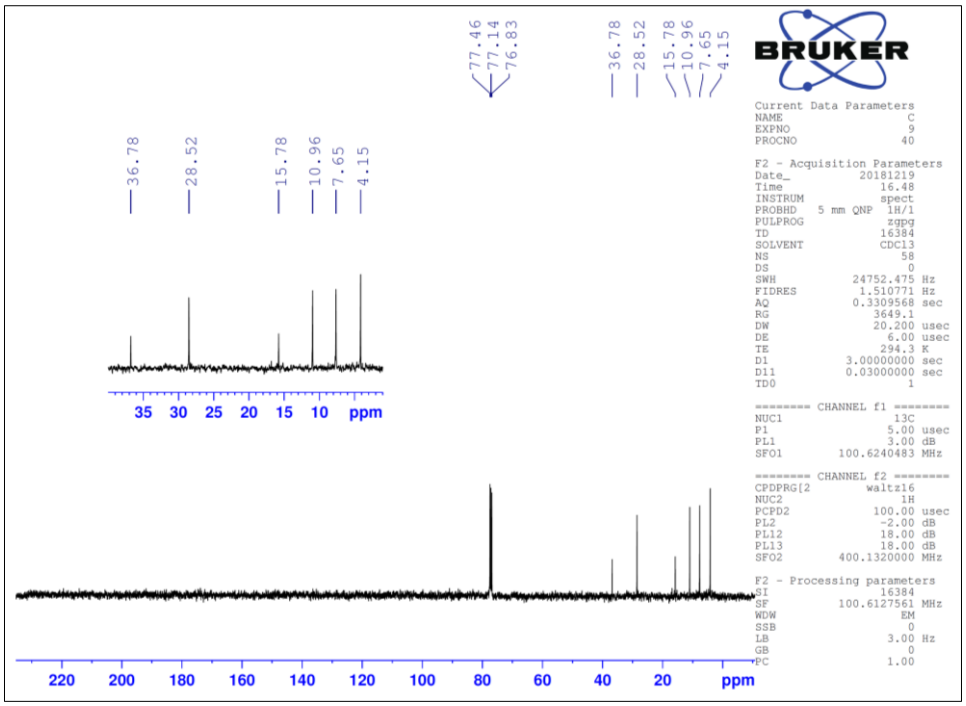


Figure S34. ^{13}C NMR spectrum of 1,1-diethylethene hydrosilylation product (Table S1, entry 7) ($CDCl_3$, 100.61 MHz).

Hydrosilylation of 1,1-diethylethene with Ph_2SiClH (Table S1, entry 8):

Reaction was performed in neat Ph_2SiClH and 1,1-diethylethene (1:1), at 100 ºC for 12 h. According to ^{13}C NMR a mixture of hydrosilylation products was obtained. ^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 0.91-1.82 (m, Alk-H, 13H), 7.44-7.82 (m, Ar-H, 10H).

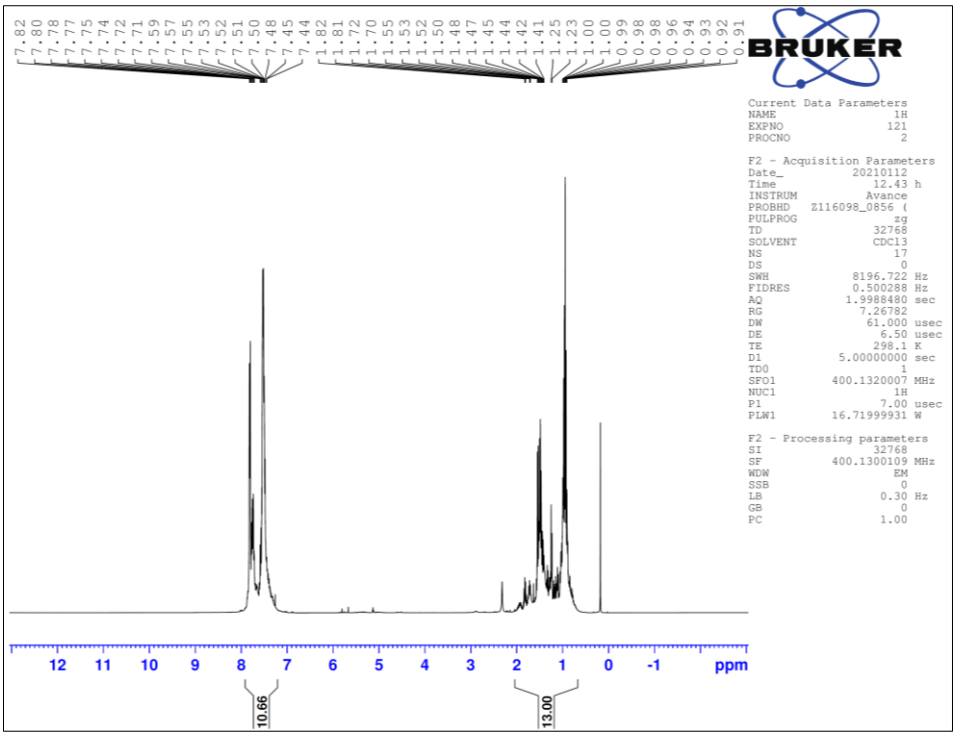


Figure S35. 1H NMR spectrum of 1,1-diethylethene hydrosilylation product (Table S1, entry 8) ($CDCl_3$, 400.13 MHz).

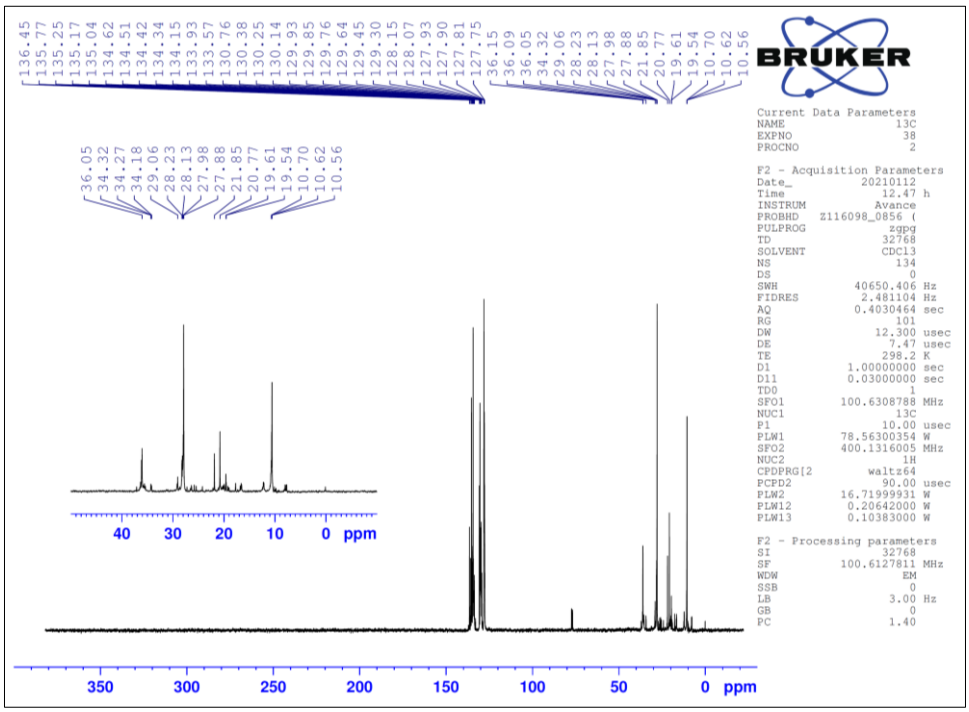


Figure S36. 13C NMR spectrum of 1,1-diethylethene hydrosilylation product (Table S1, entry 8) ($CDCl_3$, 100.61 MHz).

Hydrosilylation of 2,4,4-trimethylpent-1-ene with Et_3SiH (Table S1, entry 9):

Reaction was performed in 1,2-diflourobenzene, in 120 ºC for 3 h. ^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 1.69-1.78 (m, CH_2, 2H), 1.12-1.26 (m, CH_3, 3H), 0.94 (t, J = 7.5 Hz, $SiCH_2\mathit{CH_3}$, 9H), 0.89 (s, CH_3, 9H), 0.45-0.67 (obscured, $SiCH_2$, 2H), 0.45-0.53 (q, J = 7.5 Hz, $Si\mathit{CH_2}CH_3$, 2H). ^{13}C NMR ($CDCl_3$, 100.61 MHz): 55.39 (CH_2), 30.12 (CH_3), 25.88 (C), 25.58 ($SiCH_2$ or CH_3), 24.11 ($SiCH_2$ or CH_3), 23.00 (CH), 7.40 ($Si\mathit{C}H_2CH_3$), 4.02 ($SiCH_2\mathit{C}H_3$). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ 4.7 (Et_3SiR).

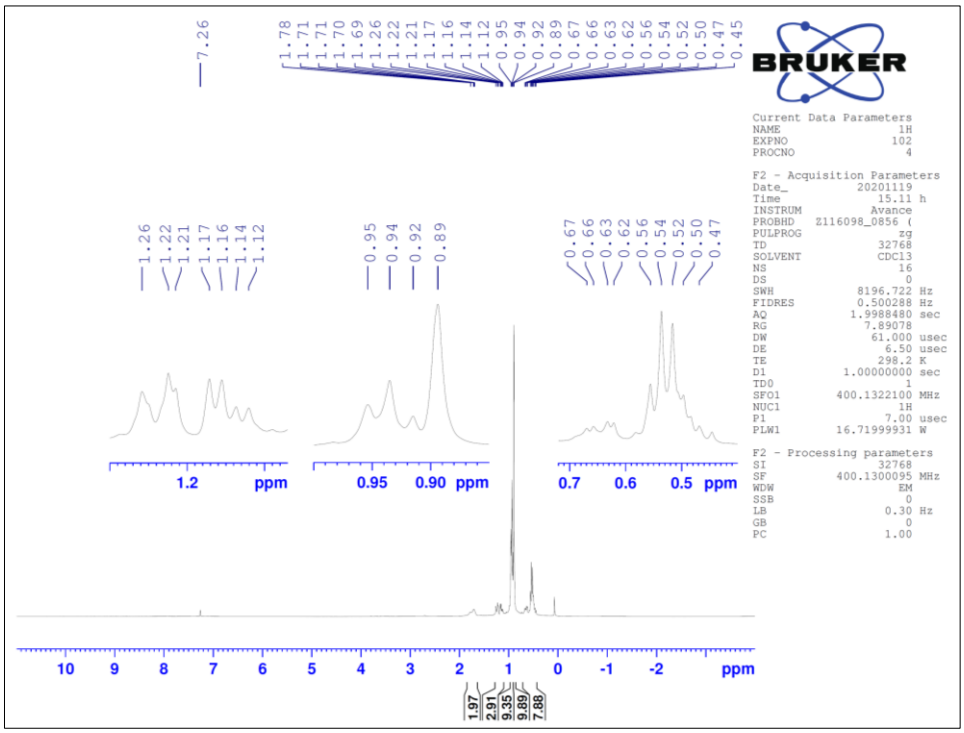


Figure S37. ^{1}H NMR spectrum of 2,4,4-trimethylpent-1-ene hydrosilylation product (Table S1, entry 9) ($CDCl_3$, 400.13 MHz).

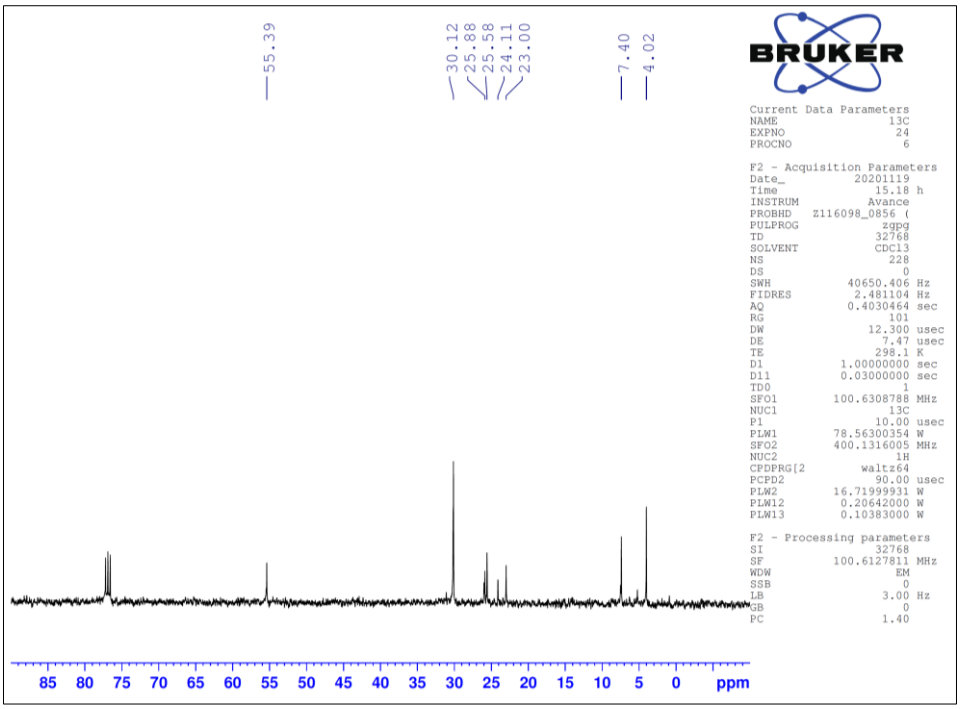


Figure S38. ^{13}C NMR spectrum of 2,4,4-trimethylpent-1-ene hydrosilylation product (Table S1, entry 9) ($CDCl_3$, 100.61 MHz).

Hydrosilylation of 1,1-Diphenylethylene with Et_3SiH (Table S1, entry 10):

Reaction was performed in 1,2-diflourobenzene, in 120 ºC for 3 h. ^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 7.13-7.35 (m, CH (Ph), 10H), 4.08 (t, J = 7.7 Hz, CH, 1H), 1.42 (d, J = 7.7 Hz, $SiCH_2$, 2H), 0.84 (t, J = 7.7 Hz, $SiCH_2\mathit{CH_3}$, 9H), 0.58 (q, J = 7.7 Hz, $Si\mathit{CH_2}CH_3$, 6H). ^{13}C NMR ($CDCl_3$, 100.61 MHz): 147.45 (*i*-C(Ph)), 128.45 (*m*-C(Ph)), 127.63 (*o*-C(Ph)), 126.11 (*p*-C(Ph)), 47.25 (CH), 19.13 ($SiCH_2$), 7.48 ($SiCH_2\mathit{C}H_3$), 3.58 ($Si\mathit{C}H_2CH_3$). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ 6.4 (Et_3SiR). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ 8.7 (Et_3SiR).

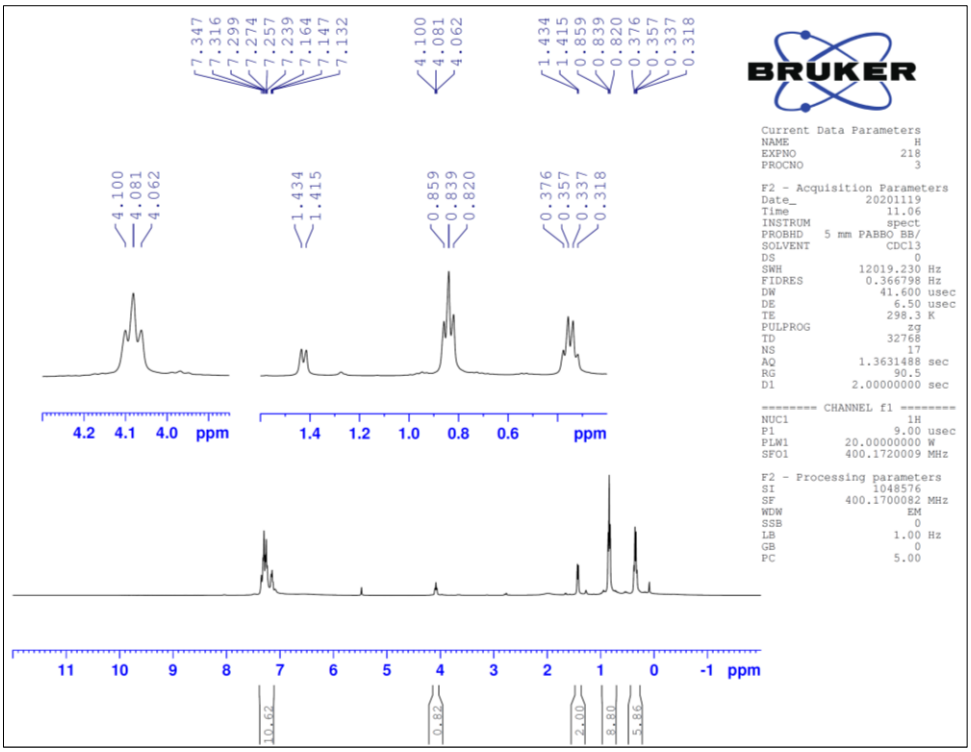


Figure S39. ^{1}H NMR spectrum of 1,1-Diphenylethylene hydrosilylation product (Table S1, entry 10) ($CDCl_3$, 400.13 MHz).

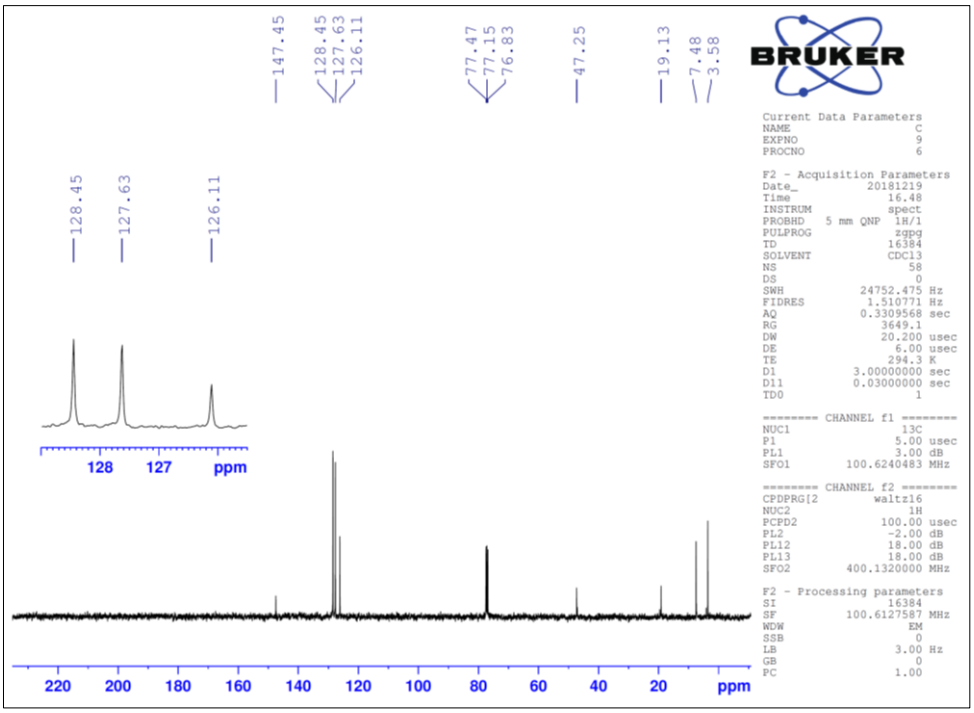


Figure S40. ^{13}C NMR spectrum of 1,1-Diphenylethylene hydrosilylation product (Table S1, entry 10) ($CDCl_3$, 100.61 MHz).

Hydrosilylation of *trans*-stilbene with Et_3SiH (Table S1, entry 11):

Reaction was performed in 1,2-diflourobenzene, in 120 ºC for 3 h. ^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 7.05-7.55 (m, CH(Ph), 10H), 3.12 (d, J = 6.2 Hz, $SiCH_2$, 2H), 2.54 (t, J = 6.2 Hz, CH, 1H), 0.95 (t, J = 7.6 Hz, $SiCH_2\mathit{CH_3}$, 9H), 0.60 (q, J = 7.6 Hz, $Si\mathit{CH_2}CH_3$, 6H). ^{13}C NMR ($CDCl_3$, 100.61 MHz): 130.18 (C(Ph)), 129.87 (C(Ph)), 129.67 (C(Ph)), 129.48 (C(Ph)), 129.12 (C(Ph)), 128.01 (C(Ph)), 127.00 (C(Ph)), 125.87 (C(Ph)), 37.73 (CH or $SiCH_2$), 37.61 (CH or $SiCH_2$), 9.03 ($SiCH_2\mathit{C}H_3$), 3.96 ($Si\mathit{C}H_2CH_3$). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ 8.6 (Et_3SiR).

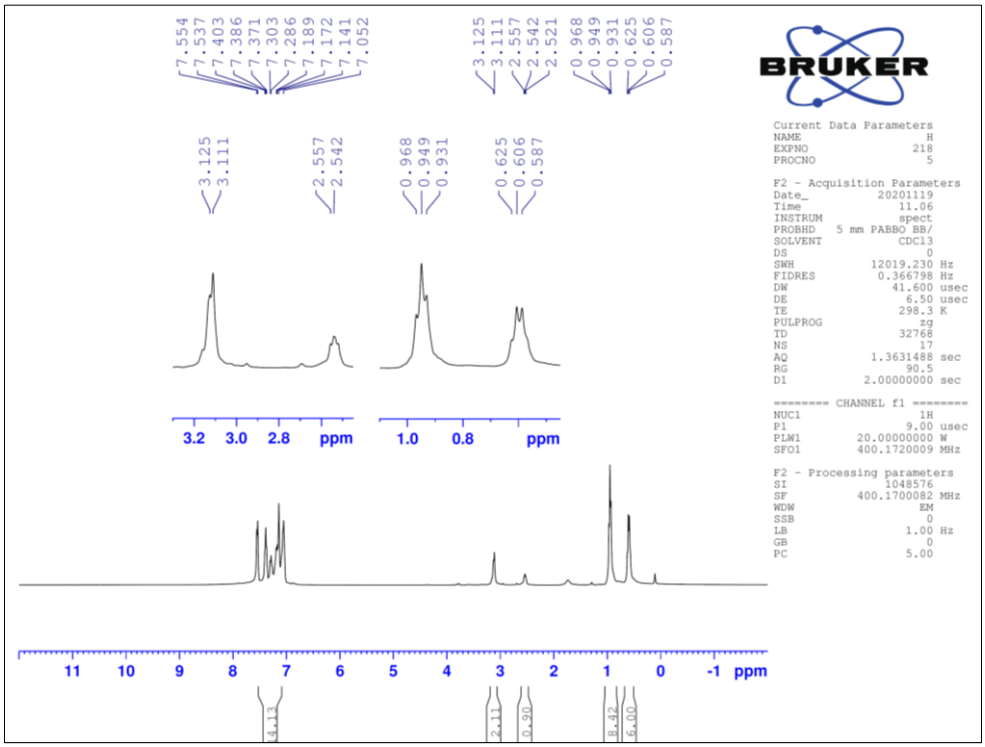


Figure S41. ^{1}H NMR spectrum of trans-stilbene hydrosilylation product (Table S1, entry 11) ($CDCl_3$, 400.13 MHz).

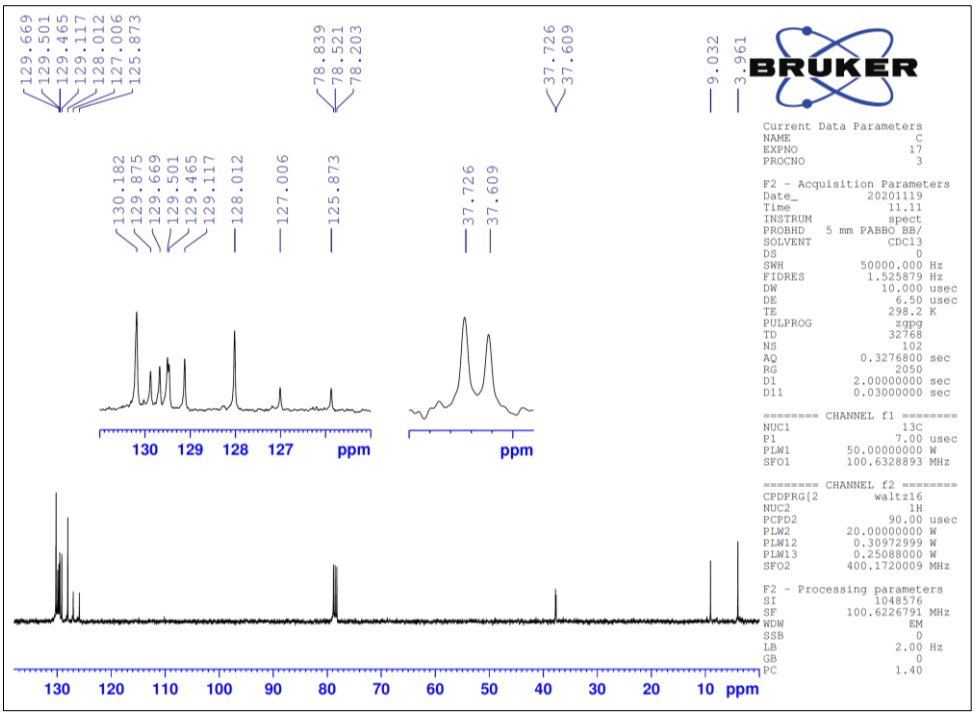


Figure S42. ^{13}C NMR spectrum of trans-stilbene hydrosilylation product (Table S1, entry 11) ($CDCl_3$, 100.61 MHz).

Hydrosilylation of 2-methyl-2-butene with Et_3SiH (Table S1, entry 12):

Reaction was performed in 1,2-diflourobenzene, in 120 ºC for 3 h. ^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 1.86-1.90 (m, CH, 1H), 0.96 (t, J = 7.8 Hz, CH, 9H), 0.96 (d, obscured, CH_3, 3H), 0.88 (m, CH_3, 6H), 0.80 (m, SiCH, 1H), 0.58 (q, J = 7.8 Hz, Si*C*$H_2$$CH_3$, 6H). ^{13}C NMR ($CDCl_3$, 100.61 MHz): 28.41 ($CH_3$), 23.88 ($CH_3$), 23.06 ($CH_3$), 19.70 (CH), 9.23 (CH), 7.63 ($SiCH_2$*C*H_3), 3.07 (Si*C*H_2CH_3). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ 5.6 (Et_3SiR).

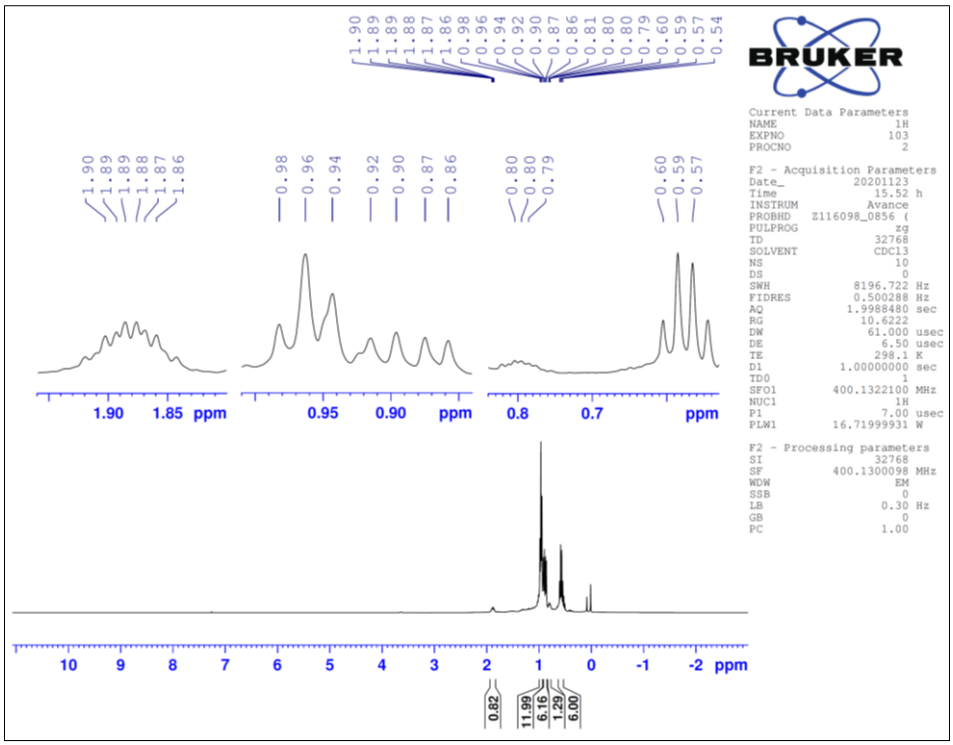


Figure S43. ^{1}H NMR spectrum of 2-methyl-2-butene hydrosilylation product (Table S1, entry 12) ($CDCl_3$, 400.13 MHz).

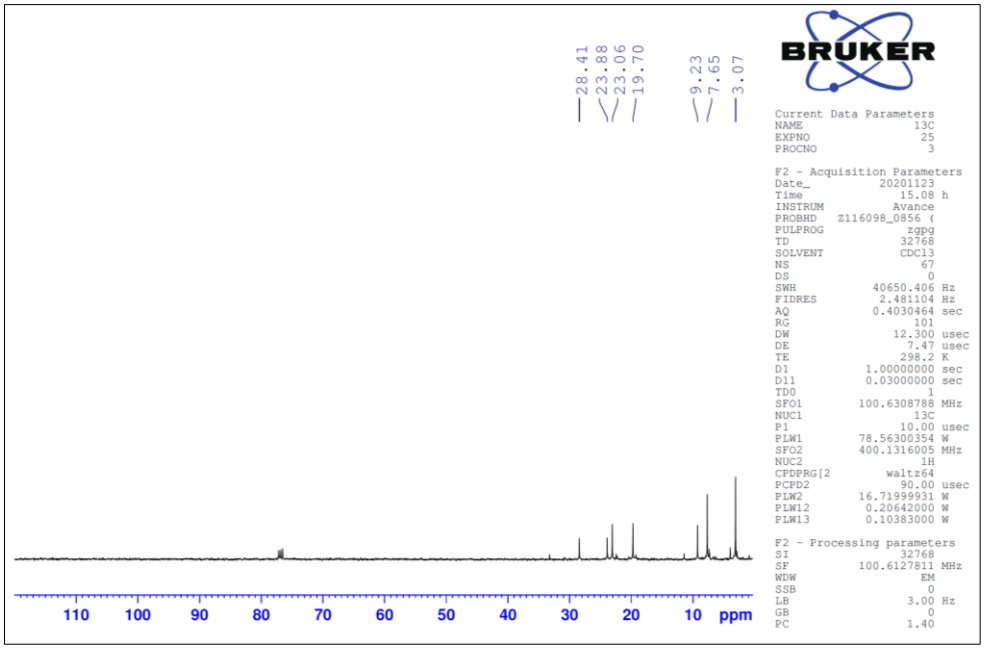


Figure S44. ^{13}C NMR spectrum of 2-methyl-2-butene hydrosilylation product (Table S1, entry 12) ($CDCl_3$, 100.61 MHz).

Hydrosilylation of cyclohexene with Et_3SiH (Table S1, entry 13):

Reaction was performed in 1,2-diflourobenzene, in 120 ºC for 3 h. ^{1}H NMR ($CDCl_3$, 400.13 MHz): δ 1.71 (m, CH_2, 5H), 1.19 (m, CH_2, 6H), 0.94 (t, J = 7.1 Hz, $SiCH_2\mathit{CH_3}$, 9H), 0.51 (q, J = 7.1 Hz, $Si\mathit{CH_2}CH_3$, 6H). ^{13}C NMR ($CDCl_3$, 100.61 MHz): 29.99 (CH_2), 29.85 (CH_2), 29.41 (CH_2), 28.62 (CH_2), 25.12 ($SiCH_2$), 9.14 ($SiCH_2\mathit{C}H_3$), 3.44 ($Si\mathit{C}H_2CH_3$). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ 5.3 (Et_3SiR).

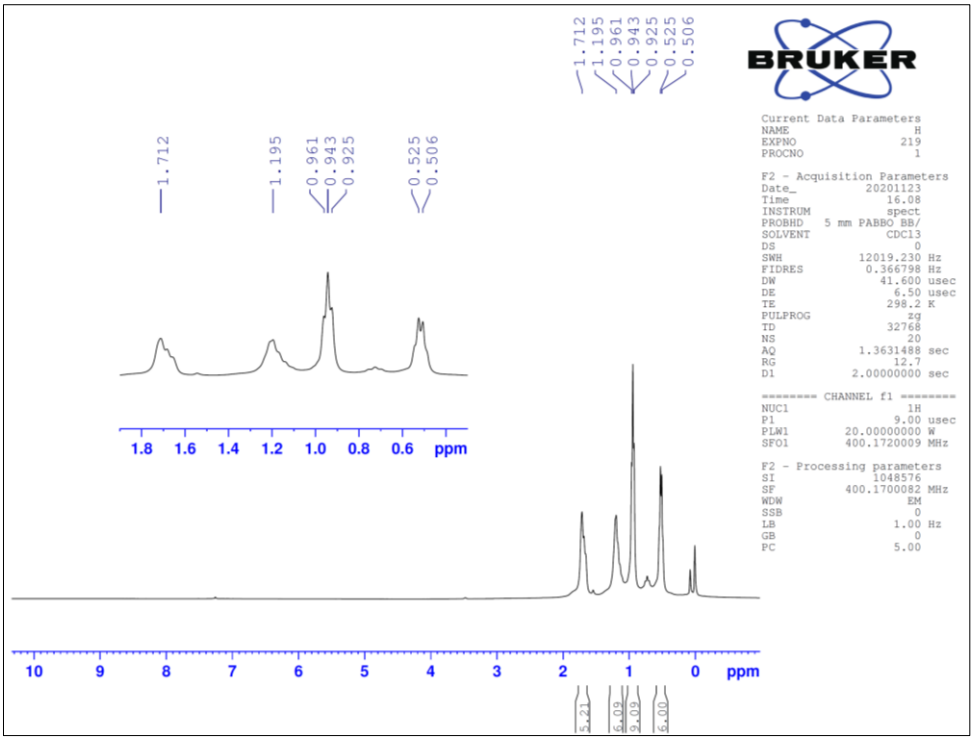


Figure S45. ^{1}H NMR spectrum of cyclohexene hydrosilylation product (Table S1, entry 13) ($CDCl_3$, 400.13 MHz).

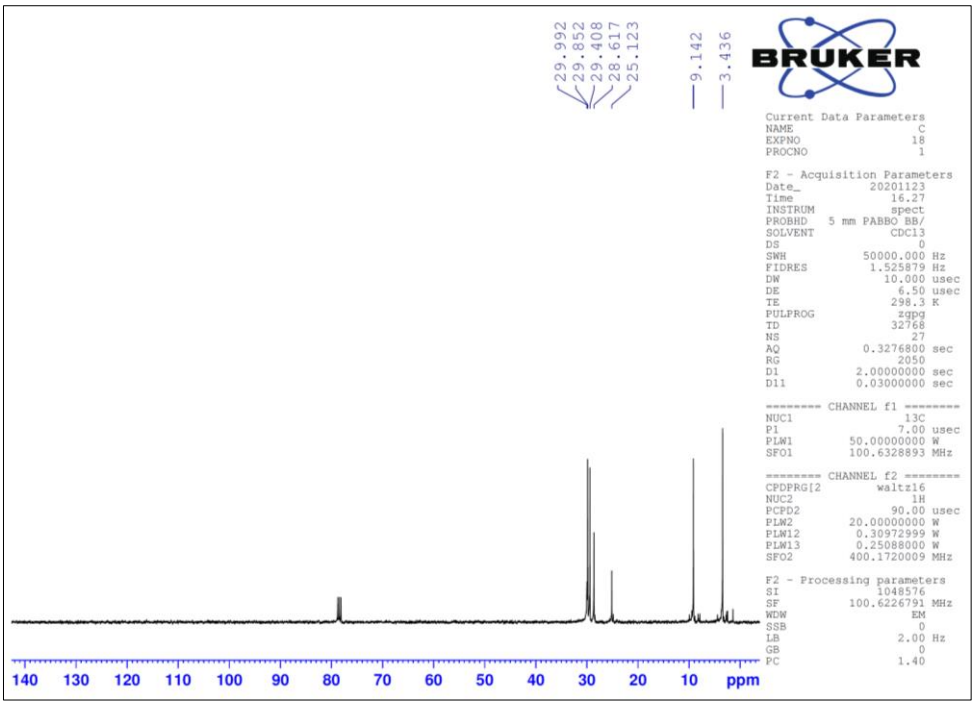


Figure S46. ^{13}C NMR spectrum of cyclohexene hydrosilylation product (Table S1, entry 13) ($CDCl_3$, 100.61 MHz).

Hydrosilylation of diphenylacetylene with Et_3SiH (Table S1, entry 14):

Reaction was performed in 1,2-diflourobenzene, in 80 ºC for 3 h. ^1H NMR ($CDCl_3$, 400.13 MHz): δ 0.49 (q, J = 7.9 Hz, Si*CH*$_2$CH$_3$, 6H), 0.89 (t, J = 7.9 Hz, SiCH$_2$*CH*$_3$, 9H), 7.27-7.64 (m, CH(Ph), 10H), 7.41 (s, CH, 1H). ^{13}C NMR ($CDCl_3$, 100.61 MHz): 147.49 (*i*-*C*(Ph)), 146.17 (C(Ph)), 145.08 (CSi(Et_3)), 139.87 (*i*-*C*(Ph)), 131.54 (CH), 128.24 (C(Ph)), 128.17 (C(Ph)), 127.79 (C(Ph)), 127.70 (C(Ph)), 127.31 (C(Ph)), 127.10 (C(Ph)), 125.51 (C(Ph)), 7.46 (SiCH$_2$), 4.60 (SiCH$_2$*C*H$_3$). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ -3.1 (Et_3SiR).

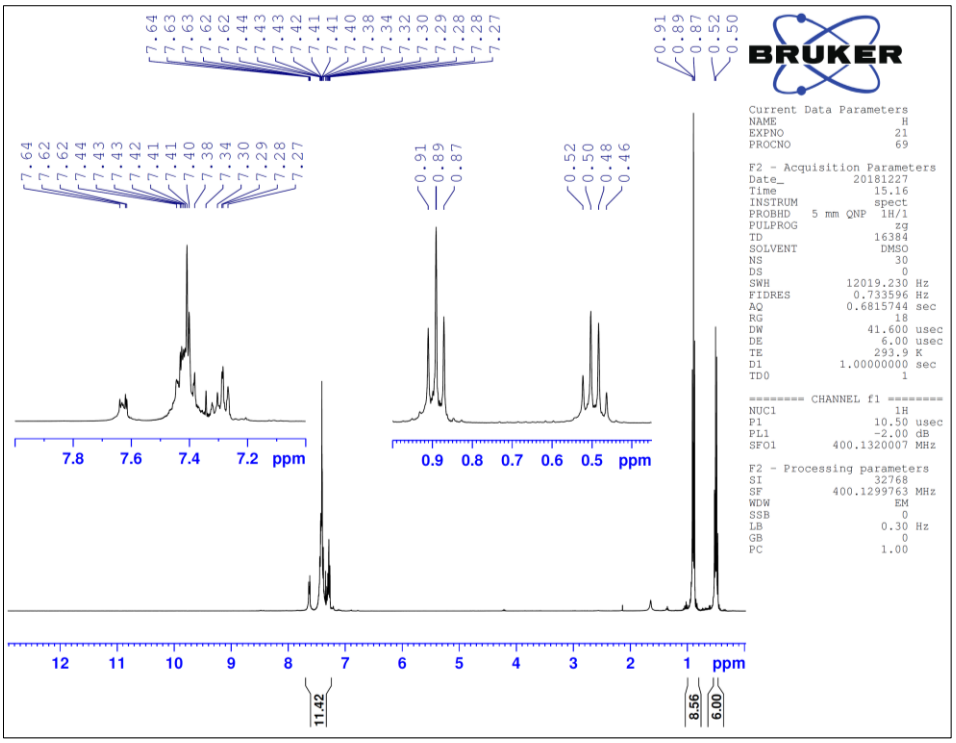


Figure S47. ^{1}H NMR spectrum of diphenylacetylene hydrosilylation product (Table S1, entry 14) ($CDCl_3$, 400.13 MHz).

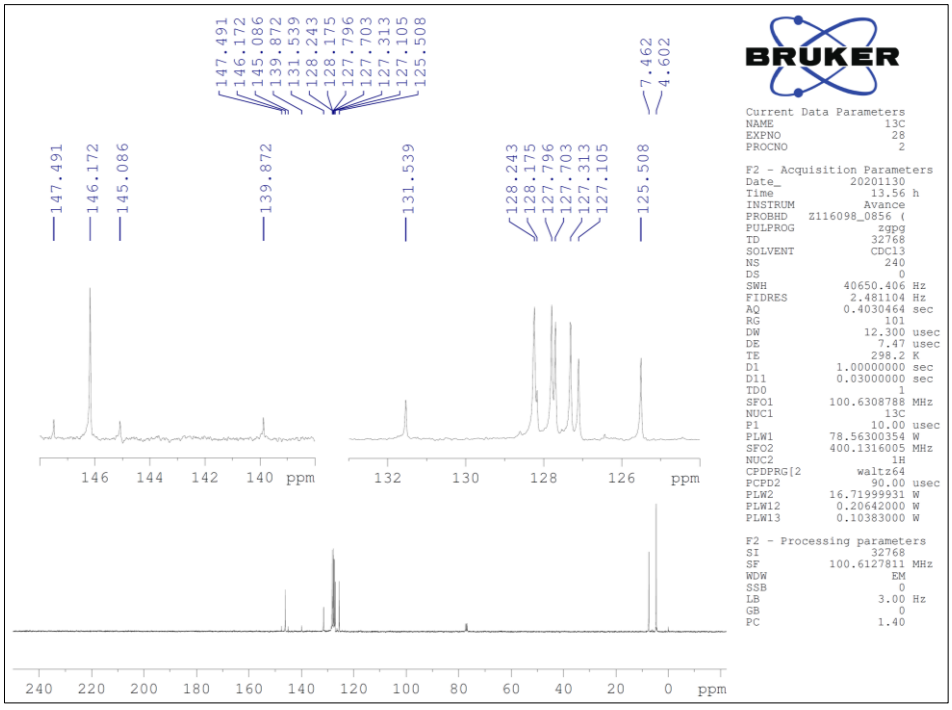


Figure S48. ^{13}C NMR spectrum of diphenylacetylene hydrosilylation product (Table S1, entry 14) ($CDCl_3$, 100.61 MHz).

Hydrosilylation of ethynylcyclohexane with Et_3SiH (Table S1, entry 15):

Reaction was performed in 1,2-diflourobenzene, in 80 ºC for 3 h. ^1H NMR ($CDCl_3$, 400.13 MHz): δ 0.60 (q, J = 7.7 Hz, Si*CH*$_2$CH$_3$, 6H), 0.95 (t, J = 7.7 Hz, SiCH$_2$*CH*$_3$, 9H), 1.07-1.31 (m, CH_2, 5H), 1.58-1.75 (m, CH_2, 5H), 2.06 (qt, J = 10.5, 3.6 Hz, CH, 1H), 5.27 (d, J = 13.9 Hz, CH=C, 1H), 6.18 (dd, J = 13.9, 10.1 Hz, CHSi, 1H). ^{13}C NMR ($CDCl_3$, 100.61 MHz): 155.76 (*C*H=C), 122.60 (Si*C*H=C), 43.28 (CH), 33.02 (CH_2), 25.85 (CH_2), 25.70 (CH_2), 7.42 (SiCH$_2$), 4.71 (SiCH$_2$*C*H$_3$). ^{29}Si NMR ($CDCl_3$, 79.5 MHz): δ -4.7 (Et_3SiR).

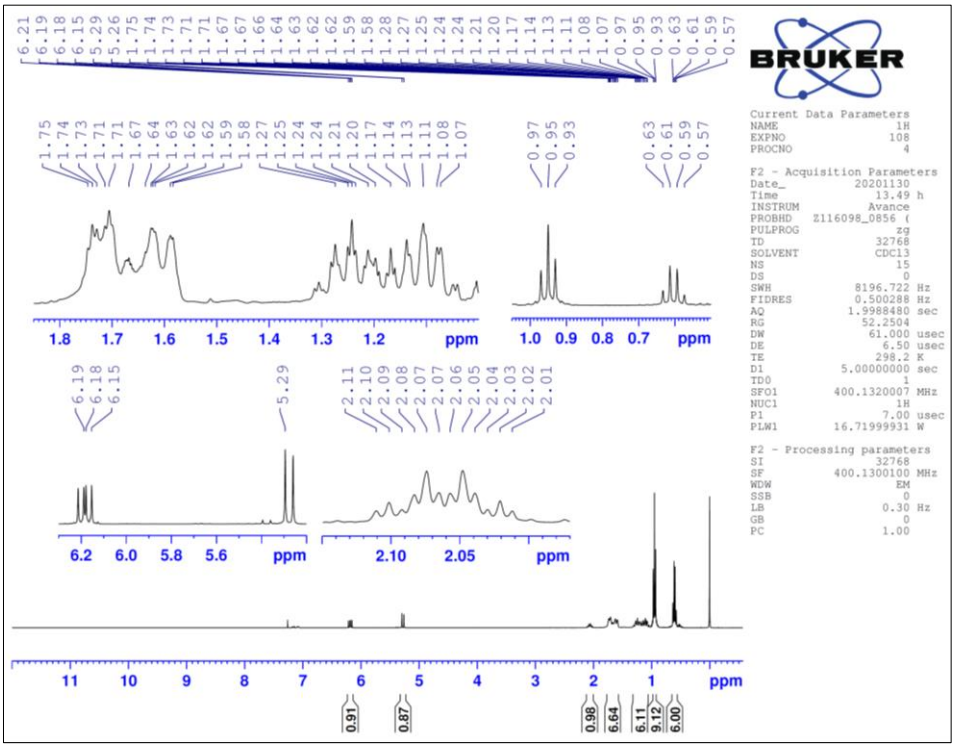


Figure S49. ^1H NMR spectrum of ethynylcyclohexane hydrosilylation product (Table S1, entry 15) ($CDCl_3$, 400.13 MHz).

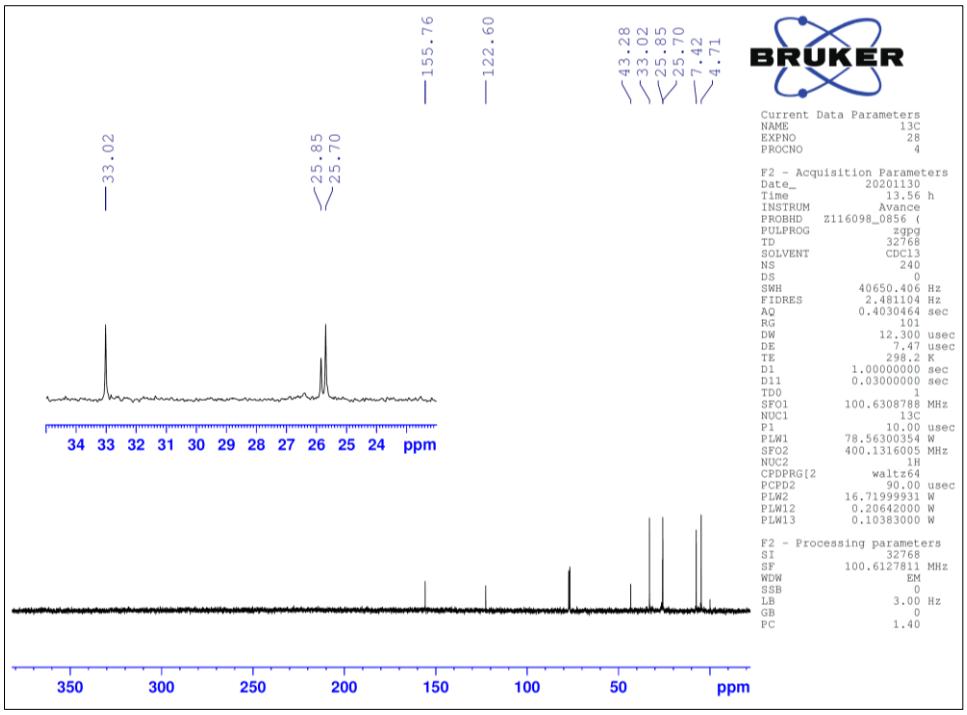
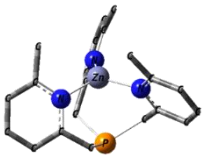


Figure S50. ^{13}C NMR spectrum of ethynylcyclohexane hydrosilylation product (Table S1, entry 15) ($CDCl_3$, 100.61 MHz).

DFT Computations

DFT calculations were performed using Gaussian 09.2.[3] Geometry optimization of all the molecules were carried out using the BP86-D3 method[4] with Ahlrichs' def2-SVP basis set,[5] and with the relativistic effect of zinc, which was accounted for by the Stuttgart-Dresden ECP,[6] implemented in the Gaussian 09 software. Thermal energy corrections were extracted from the results of frequency analysis performed at the same level of theory. Frequency analysis of all the molecules and intermediates contained no imaginary frequency showing that these are energy minima. The transition states geometries gave one imaginary frequency at expected reaction coordinates confirming that it is a first-order saddle point.

Optimized geometries



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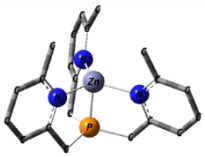

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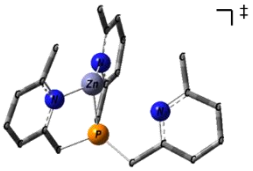

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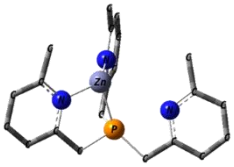

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H	4.13916	-3.03678	1.29008
C	5.14759	-0.19842	-0.35380
H	6.23674	-1.80351	0.63728
H	6.04699	0.35775	-0.65568
C	-2.61894	-2.14754	-0.19431
C	-3.83101	-2.84269	-0.33392
C	-4.95560	-2.10912	-0.74651
H	-3.89297	-3.92367	-0.13796
C	-3.57221	-0.10952	-0.83284
C	-4.82460	-0.73559	-1.00679
H	-5.92795	-2.60925	-0.87545
H	-5.68985	-0.14694	-1.34716
Zn	0.91947	0.33520	-0.66547
N	2.75684	-0.39337	-0.31848
N	-2.49754	-0.82222	-0.41829
N	-0.16315	1.63274	0.38681
P	-0.04572	-1.49698	0.31397
C	1.56082	-2.36026	0.71846
H	1.56886	-3.30107	0.12317
H	1.60288	-2.67912	1.78197
C	-1.31901	-2.82421	0.19208
H	-1.37264	-3.36850	1.16107
H	-0.97948	-3.55417	-0.57603
C	-0.39516	-0.40306	1.80298
H	-1.18948	-0.86080	2.42539
H	0.53292	-0.39706	2.41828
C	3.65240	1.58393	-1.42880
H	3.04287	1.40698	-2.34365
H	3.11565	2.31178	-0.78107
H	4.59763	2.05884	-1.75085
C	0.28272	3.48984	-1.16032
H	1.24557	3.97263	-0.88570
H	0.49588	2.69729	-1.91288
H	-0.33628	4.25940	-1.66095
C	-3.36705	1.36152	-1.08697
H	-3.29691	1.91438	-0.12675
H	-2.42103	1.53186	-1.64063
H	-4.19997	1.80035	-1.66780

Sum of electronic and zero-point Energies= -1545.983943
Sum of electronic and thermal Energies= -1545.958020
Sum of electronic and thermal Enthalpies= -1545.957076
Sum of electronic and thermal Free Energies= -1546.040212

Me_3SiH

Si	0.00009	0.00007	-0.38589
H	0.00045	0.00011	-1.89615
C	-1.66526	0.66888	0.22628
H	-1.69867	0.67930	1.33688
H	-1.83798	1.70682	-0.12882

H	-2.50785	0.04128	-0.13327
C	1.41195	1.10749	0.22642
H	1.43955	1.12817	1.33700
H	2.39679	0.73966	-0.13142
H	1.28816	2.15173	-0.13043
C	0.25321	-1.77641	0.22630
H	-0.55794	-2.44503	-0.13166
H	1.21931	-2.19158	-0.13063
H	0.25752	-1.81120	1.33698

Sum of electronic and zero-point Energies= -409.591024
Sum of electronic and thermal Energies= -409.583383
Sum of electronic and thermal Enthalpies= -409.582439
Sum of electronic and thermal Free Energies= -409.621371

$H_2C=CH_2$

C	0.00000	0.67122	0.00000
H	0.93861	1.25181	0.00000
H	-0.93855	1.25188	0.00000
C	0.00000	-0.67122	0.00000
H	-0.93861	-1.25181	0.00000
H	0.93855	-1.25188	0.00000

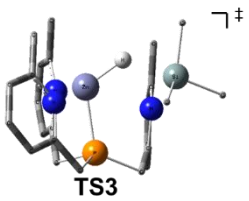
Sum of electronic and zero-point Energies= -78.476182
Sum of electronic and thermal Energies= -78.473102
Sum of electronic and thermal Enthalpies= -78.472158
Sum of electronic and thermal Free Energies= -78.497755

INT2−H−$SiMe_3$

C	-0.82262	2.21106	0.79915
C	-1.66033	3.32928	0.91474
C	-0.45377	2.66539	-1.50240
C	-1.88083	4.14374	-0.20693
H	-2.12700	3.56376	1.88265
C	-1.26937	3.81016	-1.42132
H	-2.53086	5.02932	-0.13294
H	-1.42726	4.42401	-2.32026
C	2.64398	-0.27672	1.87548
C	3.86884	-0.21897	2.56223
C	3.68215	0.50657	-0.11222
C	5.02265	0.19721	1.88324
H	3.91221	-0.51086	3.62225
C	4.92925	0.55919	0.53055
H	5.99068	0.24000	2.40618
H	5.81668	0.89053	-0.02819
C	-2.74156	-1.25798	1.59692
C	-3.95870	-1.90176	1.87896
C	-5.03471	-1.67103	1.00609
H	-4.06111	-2.56669	2.74978
C	-3.60436	-0.21216	-0.31120
C	-4.85620	-0.82690	-0.10270
H	-6.00767	-2.15451	1.18488
H	-5.68366	-0.64375	-0.80463
N	2.56809	0.09333	0.56273
N	-2.57830	-0.43013	0.54477
N	-0.23678	1.89473	-0.39691
P	-0.16264	-0.41855	1.66920
C	1.40273	-0.79585	2.59571
H	1.47086	-1.90511	2.66692
H	1.38405	-0.42486	3.64205
C	-1.48760	-1.45239	2.42998
H	-1.62591	-1.16154	3.49459

H	-1.14478	-2.51066	2.42766
C	-0.48342	1.38475	2.02765
H	-1.27094	1.49468	2.79909
H	0.45775	1.78387	2.46822
C	3.49272	0.90210	-1.55059
H	3.09811	0.05077	-2.14594
H	2.76018	1.73334	-1.62532
H	4.43568	1.23733	-2.01960
C	0.20198	2.28698	-2.80232
H	1.14049	2.86450	-2.94863
H	0.45280	1.20902	-2.84922
H	-0.45521	2.52315	-3.66177
C	-3.33377	0.70483	-1.47577
H	-3.24048	1.75515	-1.12814
H	-2.37289	0.43563	-1.96147
H	-4.14012	0.66661	-2.23196
Zn	0.71353	0.07468	-0.39786
Si	0.62099	-2.36000	-2.04243
C	1.36678	-2.51597	-3.75050
H	2.41866	-2.16512	-3.77742
H	1.36440	-3.58983	-4.03978
H	0.78075	-1.96131	-4.51116
C	1.68575	-3.06824	-0.66506
H	1.82376	-4.15831	-0.82725
H	2.68949	-2.59730	-0.64155
H	1.20852	-2.93165	0.32629
C	-1.20706	-2.71830	-1.88154
H	-1.59550	-2.36083	-0.90614
H	-1.78850	-2.23057	-2.69025
H	-1.38132	-3.81327	-1.95007
H	0.70175	-0.75299	-1.86006

Sum of electronic and zero-point Energies= -1955.637108
Sum of electronic and thermal Energies= -1955.602165
Sum of electronic and thermal Enthalpies= -1955.601221
Sum of electronic and thermal Free Energies= -1955.704109



TS3

C	-0.62491	-2.27069	-0.75889
C	-1.62854	-3.23450	-0.93041
C	-0.87410	-2.34931	1.59659
C	-2.27136	-3.76304	0.20085
H	-1.89619	-3.57416	-1.94174
C	-1.88588	-3.32235	1.47221
H	-3.06270	-4.52031	0.08797
H	-2.36015	-3.72876	2.37770
C	3.22720	0.06801	-1.23353
C	4.58031	-0.07455	-1.58055
C	3.72594	-0.34839	1.04875
C	5.52340	-0.34645	-0.57765
H	4.89171	0.03998	-2.62972
C	5.09334	-0.47917	0.75031
H	6.58925	-0.45305	-0.83246
H	5.80948	-0.69030	1.55778
C	-2.07703	0.69869	-1.66654
C	-3.10946	-0.02356	-2.28694
C	-4.14474	-0.55673	-1.50446
H	-3.08994	-0.17462	-3.37658
C	-3.05292	0.38667	0.45554
C	-4.09194	-0.37726	-0.11994
H	-4.96825	-1.11982	-1.96999
H	-4.86437	-0.80819	0.53377
N	2.82011	-0.08167	0.06273
N	-2.07222	0.93357	-0.31720

N	-0.27547	-1.82870	0.48748
P	0.50928	0.08083	-1.74169
C	2.21597	0.44329	-2.32599
H	2.25807	1.54269	-2.49592
H	2.48121	-0.03830	-3.28928
C	-0.85696	1.09094	-2.48048
H	-1.01015	0.89875	-3.56033
H	-0.58485	2.15756	-2.35216
C	0.13604	-1.72316	-1.96165
H	-0.39137	-1.94907	-2.90950
H	1.13059	-2.22096	-2.01484
C	3.17787	-0.50643	2.43999
H	2.57912	0.38506	2.72824
H	2.51018	-1.39326	2.48807
H	3.97623	-0.64293	3.19237
C	-0.39816	-1.89177	2.94856
H	0.47948	-2.49664	3.26498
H	-0.08645	-0.82678	2.94123
H	-1.17821	-2.02301	3.72215
C	-3.02540	0.61971	1.94032
H	-3.71460	-0.06914	2.46291
H	-2.00655	0.47978	2.34899
H	-3.35246	1.65276	2.18375
Zn	0.76327	0.01710	0.55185
Si	-0.83751	2.73322	0.71630
C	-0.73146	3.19157	2.54725
H	0.26437	2.93394	2.96023
H	-0.87305	4.29376	2.60489
H	-1.50647	2.72867	3.18661
C	0.75279	3.25103	-0.16931
H	0.86441	4.32981	0.08147
H	1.65270	2.72219	0.20344
H	0.72364	3.19608	-1.27393
C	-2.27142	3.72170	-0.01960
H	-2.37200	3.60249	-1.11691
H	-3.24774	3.47552	0.44490
H	-2.06287	4.79375	0.19309
H	-0.03265	1.11811	1.40285

Sum of electronic and zero-point Energies= -1955.601008
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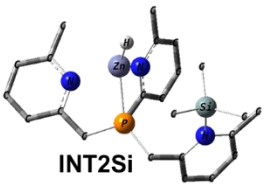
Sum of electronic and thermal Enthalpies= -1955.566687
Sum of electronic and thermal Free Energies= -1955.663587



C	-0.16251	1.20179	-1.52103
C	0.61915	1.96853	-2.39841
C	-0.32368	2.99828	0.01250
C	0.92526	3.29542	-2.05382
H	0.96245	1.53522	-3.34949
C	0.44587	3.81302	-0.84414
H	1.52609	3.92338	-2.73009
H	0.66167	4.85090	-0.55092
C	-3.22783	-1.69866	-0.40462
C	-4.42489	-2.26680	-0.86765
C	-4.35195	0.26284	0.28590
C	-5.61962	-1.54451	-0.72643
H	-4.41851	-3.26721	-1.32558
C	-5.58070	-0.26892	-0.14728
H	-6.57324	-1.97251	-1.07217
H	-6.49853	0.32607	-0.03289
C	2.24208	-1.61549	-0.99469
C	2.62123	-1.66615	-2.34619
C	3.68109	-0.88649	-2.82213
H	2.07468	-2.33686	-3.02494

C	3.95299	-0.00714	-0.56563
C	4.32610	-0.03777	-1.92246
H	3.99028	-0.93559	-3.87770
H	5.14971	0.61156	-2.25372
N	-3.19974	-0.45882	0.16070
N	-0.60690	1.70850	-0.33441
P	-0.48691	-1.30720	-0.36297
C	-1.92042	-2.46818	-0.52312
H	-1.82947	-3.20072	0.31115
H	-1.88943	-3.04971	-1.46839
C	1.02145	-2.40365	-0.59966
H	0.79202	-3.12733	-1.40634
H	1.15224	-2.98397	0.33113
C	-0.57727	-0.21451	-1.87260
H	0.00178	-0.60861	-2.73052
H	-1.64876	-0.21154	-2.17112
C	-4.24075	1.63649	0.88575
H	-3.83006	1.58101	1.91743
H	-3.54989	2.25907	0.27783
H	-5.21873	2.14960	0.92863
C	-0.83409	3.50482	1.33206
H	-1.93037	3.36340	1.41457
H	-0.38396	2.93348	2.17016
H	-0.60810	4.57757	1.47207
C	4.73009	0.90765	0.34207
H	4.15104	1.30643	1.19136
H	5.62135	0.38371	0.74649
H	5.10552	1.76943	-0.24201
Zn	-1.43102	0.36288	1.13428
H	-1.41321	0.56657	2.65674
Si	2.62226	-0.77854	1.85985
N	2.92847	-0.81442	-0.09735
C	4.29861	-1.17925	2.61277
H	4.88379	-0.28734	2.90731
H	4.11430	-1.77301	3.53288
H	4.92306	-1.80815	1.94464
C	1.90072	0.93816	2.14554
H	1.71522	1.47381	1.19295
H	0.92218	0.82654	2.65779
H	2.55483	1.56642	2.78441
C	1.42785	-2.08380	2.48797
H	0.37183	-1.94002	2.18806
H	1.75394	-3.13147	2.32938
H	1.46165	-1.91008	3.58832

Sum of electronic and zero-point Energies= -1955.626684
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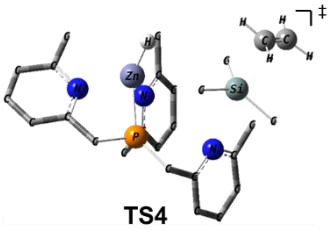
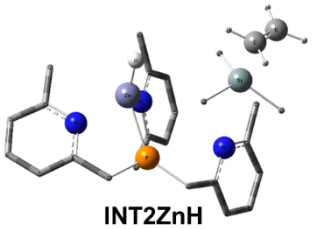
Sum of electronic and thermal Enthalpies= -1955.591623
Sum of electronic and thermal Free Energies= -1955.691228



C	0.57953	-1.99911	0.69061
C	-0.06870	-3.15659	1.14698
C	0.32332	-0.94477	2.79298
C	-0.53184	-3.19925	2.47085
H	-0.20069	-4.01339	0.47068
C	-0.32684	-2.08887	3.29990
H	-1.04328	-4.09559	2.85459
H	-0.66476	-2.09782	4.34662
C	3.49036	0.33999	-1.57978
C	4.79104	0.24423	-2.09998
C	4.32679	0.80089	0.58417

C	5.88392	0.45351	-1.24552
H	4.94109	0.01373	-3.16530
C	5.64905	0.73200	0.10809
H	6.91277	0.39229	-1.63267
H	6.48546	0.88924	0.80472
C	-1.66257	-1.39966	-1.94875
C	-1.95466	-2.67613	-2.46755
C	-2.82421	-3.51531	-1.75686
H	-1.50743	-3.00194	-3.41873
C	-3.00200	-1.77092	-0.06967
C	-3.33660	-3.06092	-0.53650
H	-3.08594	-4.51253	-2.14335
H	-4.00047	-3.69991	0.06460
N	3.27274	0.61453	-0.26225
N	0.74757	-0.90935	1.49544
P	0.78989	-0.25788	-1.47044
C	2.28531	0.13372	-2.48743
H	2.05710	1.07330	-3.03985
H	2.49758	-0.64415	-3.25053
C	-0.63120	-0.53859	-2.64485
H	-0.25989	-1.03094	-3.56566
H	-1.03574	0.45235	-2.93505
C	1.15091	-1.92188	-0.71008
H	0.79952	-2.76101	-1.34146
H	2.25922	-1.98587	-0.64740
C	4.00404	1.05677	2.02986
H	3.36406	1.95932	2.13560
H	3.43881	0.19559	2.44591
H	4.91491	1.19982	2.63944
C	0.58778	0.25310	3.66325
H	1.66547	0.30180	3.92826
H	0.34861	1.19945	3.13764
H	0.01470	0.20448	4.60756
C	-3.51537	-1.31435	1.27140
H	-4.14429	-2.09138	1.74395
H	-2.67003	-1.09797	1.95527
H	-4.12918	-0.39610	1.18797
N	-2.19415	-0.93978	-0.78451
Zn	1.28202	0.96328	0.54292
H	0.89440	2.35111	1.09092
C	-3.52786	4.51800	-0.09679
H	-2.59542	5.01698	0.21721
H	-3.82906	4.64680	-1.15119
C	-4.32671	3.89283	0.80623
H	-4.06051	3.85338	1.87570
H	-5.30727	3.47442	0.52314
Si	-2.74792	1.96281	-0.31155
C	-1.42003	2.67984	-1.41648
H	-0.56155	1.97596	-1.39251
H	-1.76178	2.84093	-2.45763
H	-1.02615	3.63010	-1.00582
C	-2.17597	1.67010	1.43900
H	-1.60077	2.55814	1.77043
H	-2.99286	1.45897	2.15340
H	-1.47642	0.81080	1.41662
C	-4.32231	1.36611	-1.12595
H	-4.76656	2.18928	-1.72302
H	-4.08944	0.53186	-1.81720
H	-5.07650	1.01252	-0.39560

Sum of electronic and zero-point Energies=	-2034.092220
Sum of electronic and thermal Energies=	-2034.054400
Sum of electronic and thermal Enthalpies=	-2034.053456
Sum of electronic and thermal Free Energies=	-2034.161966



INT2ZnH

C	1.01104	-2.08545	0.59820
C	0.82377	-3.36417	1.14583
C	0.86914	-1.08727	2.73664
C	0.66423	-3.50093	2.53255
H	0.81142	-4.24421	0.48617
C	0.68433	-2.35251	3.33135
H	0.52153	-4.49515	2.98364
H	0.55910	-2.42101	4.42228
C	3.29635	0.53811	-1.79445
C	4.57784	0.51496	-2.36928
C	4.19515	1.06907	0.32756
C	5.69160	0.79598	-1.56417
H	4.69559	0.28457	-3.43863
C	5.49795	1.07441	-0.20395
H	6.70508	0.79120	-1.99428
H	6.35201	1.28880	0.45501
C	-1.89010	-1.28809	-2.08840
C	-3.01101	-1.73138	-2.81508
C	-4.05118	-2.36209	-2.11087
H	-3.06059	-1.60212	-3.90706
C	-2.77696	-2.05443	-0.06344
C	-3.93086	-2.53271	-0.72405
H	-4.94189	-2.72933	-2.64410
H	-4.71884	-3.04499	-0.15070
N	3.12025	0.81010	-0.47102
N	1.03252	-0.96963	1.38634
P	0.65619	-0.30641	-1.56357
C	2.06508	0.25691	-2.63895
H	1.73042	1.19091	-3.14465
H	2.30153	-0.47289	-3.44130
C	-0.69317	-0.66650	-2.78231
H	-0.30095	-1.34200	-3.57464
H	-0.95576	0.28621	-3.29380
C	1.26141	-1.93492	-0.88914
H	0.82306	-2.78465	-1.44810
H	2.35951	-1.96083	-1.06816
C	3.92047	1.31794	1.78444
H	3.19677	2.15137	1.90985
H	3.46599	0.41323	2.24033
H	4.84180	1.56304	2.34376
C	0.91204	0.14676	3.59967
H	1.87384	0.19513	4.15411
H	0.81448	1.07628	3.00763
H	0.10873	0.11952	4.36283
C	-2.59780	-2.25271	1.42101
H	-2.55823	-3.33491	1.66540
H	-1.65771	-1.79187	1.77333
H	-3.44951	-1.83024	1.99377
N	-1.78843	-1.42873	-0.74651
Zn	1.13805	0.95248	0.40546
H	0.66808	2.29176	1.01694
C	-3.84377	4.26194	0.51776
H	-2.97421	4.93957	0.46771
H	-4.52686	4.26181	-0.35041
C	-4.12874	3.55408	1.65097
H	-3.50151	3.64359	2.55429
H	-5.05584	2.96028	1.74245
Si	-2.95983	2.02680	0.19954
C	-1.74116	2.75932	-1.01198
H	-1.14587	1.88751	-1.36522
H	-2.22795	3.24737	-1.87870
H	-1.02055	3.44523	-0.52598

C	-2.17707	1.23129	1.69205
H	-1.46162	1.91172	2.19180
H	-2.91700	0.83408	2.41314
H	-1.58808	0.38328	1.27620
C	-4.41927	1.15809	-0.56405
H	-4.98789	1.81206	-1.25563
H	-4.02088	0.31076	-1.16406
H	-5.11008	0.73519	0.19203

Sum of electronic and zero-point Energies= -2034.097457
Sum of electronic and thermal Energies= -2034.058517
Sum of electronic and thermal Enthalpies= -2034.057573
Sum of electronic and thermal Free Energies= -2034.169592

$Me_3Si(H)_2C\text{-}CH_3$

Si	-0.42426	-0.00125	0.00000
C	-0.53004	1.09099	1.54861
H	-1.49391	1.64198	1.58343
H	-0.45394	0.48091	2.47386
H	0.28790	1.84204	1.56853
C	-1.85572	-1.24661	-0.00009
H	-2.83792	-0.72770	0.00010
H	-1.81781	-1.89989	-0.89775
H	-1.81763	-1.90021	0.89733
C	-0.53071	1.09199	-1.54786
H	0.28721	1.84309	-1.56766
H	-0.45494	0.48251	-2.47353
H	-1.49462	1.64296	-1.58197
C	1.22522	-0.95643	-0.00068
H	1.22353	-1.63219	0.88534
H	1.22353	-1.63084	-0.88772
C	2.49126	-0.07973	-0.00005
H	2.53315	0.57935	0.89355
H	3.42211	-0.68690	-0.00074
H	2.53289	0.58102	-0.89242

Sum of electronic and zero-point Energies= -488.116803
Sum of electronic and thermal Energies= -488.105907
Sum of electronic and thermal Enthalpies= -488.104963
Sum of electronic and thermal Free Energies= -488.151774

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