Efficient and Selective Alkene Hydrosilation Promoted by Weak, Double Si–H Activation at an Iron Center

Supporting Information

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Contents:

Comparison to previously reported iron hydrosilation catalysts for primary silanes.

Table S1: Comparison of reported iron catalysts for hydrosilation of 1-octene by $PhSiH_3$ to produce the anti-Markovnikov product. [a] No 1-octene data presented; substrate was 1-hexene [b] No 1-octene data presented; substrate was 5-mesyl-1-pentene; the study was attempting to optimize for the Markovnikov product.

Catalyst	Loading	Time	Yield
1 + $Ph_3CBAr^F_4$	0 .1 %	6 h	> 99 %
(pyridyldiimine)Fe$(N_2)_2$[1]	0.3 %	1 h	98 % [a]
($R_2P(CH_2)$-pyridylimine)$FeCl_2$ $NaBHEt_3$[2]	1 % 2 %	3 h	50–98 %
(oxazolinepyridylimine)$FeCl_2$ NaO^tBu[3]	5 % 15 %	2 h	2–77 % [b]
(pyridyldiimine)Fe$(OTf)_2$ $^iPr_2EtN$[4]	2 % 25 %	1 h	95 %
(R_2P-O-pyridylimine)$FeCl_2$ $NaBHEt_3$[5]	1 % 2 %	3 h	0–99 %

General Considerations. All manipulations were carried out using standard Schlenk or inert atmosphere glovebox techniques with an atmosphere of dry dinitrogen. Pentane was dried over activated alumina and stored over molecular sieves (4 Å) prior to use. Benzene-d_6 was degassed with 3 freeze-pump-thaw cycles and stored over activated molecular sieves (4 Å) for 24 h prior to use. Fluorobenzene was purchased from Sigma Aldrich, dried by distillation from calcium hydride, and stored over molecular sieves. 3-Hexyne, 4-methyl-1-pentene, R-(+)-limonene, styrene, methylenecyclopentane, 3, 3-dimethyl-1-butene and 1-octene were purchased from Sigma-Aldrich. Phenylsilane was purchased from Oakwood Chemicals. *p*-Tolylsilane was purchased from Gelest. All liquid reagents were subjected to three freeze-pump-thaw cycles and stored over activated molecular sieves overnight. The preparations and characterization of Cp*(^{i}Pr$_2$MeP)FeH(N_2)[6] (**1**) and Cp*(^{i}Pr$_2$MeP)H_2FeSiH_2Trip[7] have been described previously.

NMR spectra were recorded using Bruker AVB-400, AV-500, or AV-600 spectrometers equipped with a 5 mm broad band or TBI probe. Spectra were recorded at room temperature (ca. 22 ºC) and referenced to the residual protoisotopomer of the solvent for ^{1}H unless otherwise noted. The chemical shift of the most intense resonance of neat fluorobenzene was determined to be 6.90 ppm vs. $SiMe_4$, against which spectra in this solvent were referenced. ^{31}P{^{1}H} NMR spectra were referenced relative to 85% H_3PO_4 external standard (δ = 0). ^{13}C{^{1}H} NMR spectra were calibrated internally with the resonance for the solvent relative to tetramethylsilane. For ^{13}C{^{1}H} NMR spectra, resonances obscured by the solvent signal were omitted. ^{29}Si NMR spectra were obtained via 2D ^{1}H ^{29}Si HMBC. Elemental analyses were performed by the College of Chemistry Microanalytical Laboratory at the University of California, Berkeley.

General synthesis of Cp*(^{i}Pr$_2$MeP)H_2FeSiH_2R (2_R). RSiH_3 (0.284 mmol) was dissolved in 2 mL of pentane and this solution was then added to Cp*(^{i}Pr$_2$MeP)FeH(N_2) (0.100 g, 0.284 mmol) in 4 mL of pentane. The resulting mixture was stirred for 18 h, over which time the color changed from orange to yellow. Volatile components were removed *in vacuo* and the resulting yellow solid was recrystallized from 2 mL 1:1 pentane/$(SiMe_3)_2O$.

Characterization data for $\mathbf{2_{Tol}}$. ^{1}H NMR (400 MHz, benzene-d_6) δ 8.14 (d, J = 7.5 Hz, 2H, p-Tol*H*), 7.23 (d, J = 7.5 Hz, 2H, p-Tol*H*), 5.23 (s, J_{SiH} = 178 Hz, 2H, Si*H*), 2.24 (s, 3H *p*-TolCH_3), 1.68 (s, 15H, Cp*), 1.51 (hept, J = 7.1 Hz, 2H, PC*H*Me_2), 1.05 – 0.93 (m, 9H, PCHCH_3 + PCH_3), 0.84 (dd, J = 13.1, 6.8 Hz, 6H, PCHCH_3), -14.18 (d, J = 54.3 Hz, 2H, Fe*H*). ^{13}C NMR (101 MHz, benzene-d_6) δ 140.68, 137.05, 136.32, 128.51, 87.36, 29.12 (d, J = 26.0 Hz), 21.51, 17.99 (d, J = 2.4 Hz), 17.10, 11.16, 7.13 (d, J = 12.0 Hz). ^{31}P NMR (162 MHz, benzene-d_6) δ 76.67. ^{29}Si NMR (79 MHz, HMBC, benzene-d_6) δ -6.7 (J_{SiH} = 12 [8.14 ppm], 179 [5.23 ppm], 16 [-14.18 ppm] Hz). Anal Calcd. for $C_{24}H_{43}FePSi$: C, 64.56; H, 9.71. Found: C, 64.39; H, 9.53.

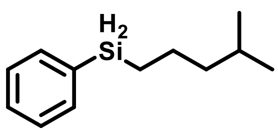
Characterization data for $\mathbf{2_{Mes}}$. ^{1}H NMR (400 MHz, benzene-d_6) δ 6.79 (s, 2H, Mes*H*), 5.20 (d, J = 5.9 Hz, 2H, Si*H*), 2.78 (s, 6H, *o*-MesCH_3), 2.17 (s, 3H, *p*-MesCH_3), 1.75 (s, 15H, Cp*), 1.28 (d, J = 6.9 Hz, 2H, PC*H*Me_2), 0.90 (dd, J = 14.6, 7.0 Hz, 6H, PCHCH_3), 0.74 (dd, J = 12.3, 6.9 Hz, 6H, PCHCH_3), 0.39 (d, J = 7.5 Hz, 3H, PCH_3), -15.01 (dd, J = 55.9, 5.9 Hz, 2H, Fe*H*). ^{13}C NMR (101 MHz, benzene-d_6) δ 144.56, 138.40, 136.97, 128.51, 87.06, 28.28 (d, J = 21.9 Hz), 23.05, 21.30, 19.04 (d, J = 3.1 Hz), 17.65 (d, J = 2.4 Hz), 10.79, 8.78 (d, J = 20.0 Hz). ^{31}P NMR (162 MHz, benzene-d_6) δ 77.45. Anal Calcd. for $C_{24}H_{43}FePSi$: C, 65.80; H, 9.98. Found: C, 66.09; H, 9.77.

Characterization data for $\mathbf{2_{Ph}}$. ^{1}H NMR (400 MHz, benzene-d_6) δ 8.26 – 8.18 (m, 2H, Ph*H*), 7.40 (td, J = 7.1, 6.4, 1.2 Hz, 2H, Ph*H*), 7.31 – 7.26 (m, 1H, *p*-PhH), 5.22 (s, J_{SiH} = 179 Hz, 2H, Si*H*), 1.65 (s, 15H, Cp*), 1.58 – 1.41 (m, 2H, PC*H*Me_2), 1.05 – 0.91 (m, 9H, PCHCH_3 + PCH_3), 0.83 (dd, J = 13.1, 6.8 Hz, 6H, PCHCH_3), -14.20 (d, J = 54.4 Hz, 2H, Fe*H*). ^{13}C NMR (101 MHz, benzene-d_6) δ 144.50, 136.17, 127.63, 87.41, 29.11 (d, J = 26.0 Hz), 17.98 (d, J = 2.4 Hz), 17.09, 11.12, 7.11 (d, J = 12.2 Hz). ^{31}P NMR (162 MHz, benzene-d_6) δ 76.52. ^{29}Si NMR (79 MHz, HMBC, benzene-d_6) δ -7.5

(J_{SiH} = 11 [8.22 ppm], 178 [5.22 ppm], 16 [-14.20 ppm] Hz). Anal Calcd. for $C_{23}H_{41}FePSi$: C, 63.88; H, 9.56. Found: C, 63.60; H, 9.35.

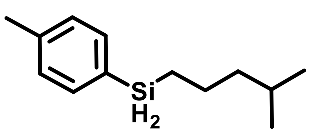
General Procedure for Hydrosilation Catalysis. Stock solution A was prepared by dissolving **1** (10 mg, 0.028 mmol) in 5.0 ml of PhF. Stock solution B was prepared by dissolving $[Ph_3C][BAr^F_4]$ (26 mg, 0.028 mmol) in 2.5 ml of PhF. Both were stored at -30 ºC, and used at that temperature. After cooling the desired silane (1.4 mmol) in a J. Young NMR tube to -30 ºC, 0.2 ml of stock solution A was added, followed by 0.1 ml of stock solution B and finally the olefin or alkyne (2.1 mmol) was added. The reaction progress was monitored by NMR spectroscopy and quenched with wet diethyl ether after completion. The product was purified by passing the reaction mixture through an alumina plug and dried under vacuum overnight.

Silane Product Characterization Data.



(4-methylpentyl)(phenyl)silane (4a) (0.27 g, > 98%).

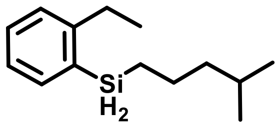
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.61 (m, 2H), 7.44 – 7.38 (m, 3H), 4.35 (t, *J* = 3.7 Hz, 2H), 1.61 – 1.58 (m, 1H), 1.53 – 1.49 (m, 2H), 1.33 – 1.27 (m, 2H), 1.00-0.93 (m, 2H), 0.91 (d, J = 6.6 Hz, 6H).; ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.3, 132.9, 129.6, 128.1, 42.4, 27.8, 23.0, 22.7, 10.3; HRMS (EI, m/z): Calcd for $C_{12}H_{19}Si$ $[(M-H)\cdot]^+$ 191.1256, found 191.1255.



(4-methylpentyl)(p-tolyl)silane (4b) (0.29 g, > 98%).

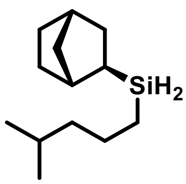
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.9 Hz, 2H), 7.24 (d, *J* = 7.5 Hz, 2H), 4.34 (t, *J* = 3.7 Hz, 2H), 2.41 (s, 3H), 1.61 (tt, *J* = 13.1, 6.5 Hz, 1H), 1.56 – 1.48 (m, 2H), 1.34 – 1.29 (m, 2H), 1.00 –

0.95 (m, 2H), 0.92 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.5, 135.4, 129.1, 128.9, 42.4, 27.8, 23.0, 22.7, 21.7, 10.5; HRMS (EI, m/z): Calcd for $C_{13}H_{22}Si$ $[M^{\cdot}]^+$ 206.1491, found 206.1487.



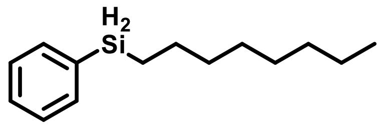
(2-ethylphenyl)(4-methylpentyl)silane (4c) (0.31 g, > 98%).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 7.3, 1.5 Hz, 1H), 7.44 (td, *J* = 7.5, 1.5 Hz, 1H), 7.32 (d, *J* = 7.6 Hz, 1H), 7.27 (td, *J* = 7.3, 1.2 Hz, 1H), 4.46 (t, *J* = 3.9 Hz, 2H), 2.86 (q, *J* = 7.6 Hz, 2H), 1.67–1.64 (m, 1H), 1.59 – 1.56 (m, 2H), 1.39 – 1.34 (m, 5H), 1.06 – 1.03 (m, 2H), 0.97 (d, *J* = 6.7 Hz, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.6, 136.6, 131.5, 130.3, 127.9, 125.3, 42.4, 29.7, 27.9, 23.3, 22.7, 16.2, 10.6; HRMS (EI, m/z): Calcd for $C_{14}H_{24}Si$ $[M^{\cdot}]^+$ 220.1647, found 220.1648.



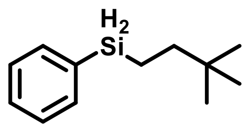
((1R,2R,4S)-bicyclo[2.2.1]heptan-2-yl)(4-methylpentyl)silane (4e) (0.29 g, > 98%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 3.59-3.48 (m, 2H), 2.26 (m, 1H), 2.16 (m, 1H), 1.56-1.51 (m, 3H), 1.46-1.44 (m, 1H), 1.42-1.35 (m, 3H), 1.33-1.31 (m, 1H), 1.25-1.19 (m, 4H), 1.16-1.14 (m, 1H), 0.87-0.85 (m, 6H), 0.77 (m, 1H), 0.67-0.62 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 42.5, 39.2, 37.5, 37.3, 34.1, 33.7, 29.3, 27.8, 23.70, 23.67, 23.4, 22.7, 9.0; HRMS (EI, m/z): Calcd for $C_{13}H_{26}Si$ $[M^{\cdot}]^+$ 210.1804, found 210.1800.



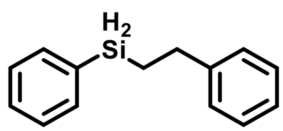
octyl(phenyl)silane (4f) (0.31 g, > 98%).

[1]H NMR (400 MHz, $CDCl_3$) 7.65 – 7.63 (m, 2H), 7.47 - 7.40 (m, 3H), 4.38 (t, *J* = 3.6 Hz, 2H), 1.57-1.50 (m, 2H), 1.45 – 1.40 (m, 2H), 1.34 (m, 8H), 1.04 – 0.95 (m, 5H); [13]C NMR (101 MHz, $CDCl_3$) δ 135.3, 133.0, 129.6, 128.1, 33.0, 32.1, 29.42, 29.40, 25.3, 22.9, 14.3, 10.2. The spectroscopic data corresponds to that previously reported.[5]



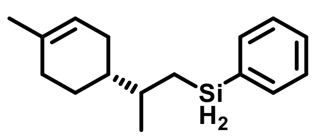
(3,3-dimethylbutyl)(phenyl)silane (4g) (0.25 g, 95%).

[1]H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.1 Hz, 2H), 7.53-7.49 (m, 3H), 4.49 (t, *J* = 3.6 Hz, 2H), 1.51 – 1.48 (m, 2H), 1.04 (s, 9H), 1.03 (m, 2H); [13]C NMR (151 MHz, $CDCl_3$) δ 135.4, 132.8, 129.6, 128.1, 39.3, 31.5, 29.0, 4.7; HRMS (EI, m/z): Calcd for $C_{12}H_{20}Si$ $[M\cdot]^+$ 192.1334, found 192.1337.



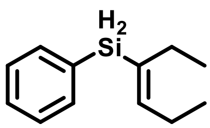
phenethyl(phenyl)silane (4h) (0.29 g, 97%).

[1]H NMR (500 MHz, $CDCl_3$) δ 7.74 (m, 2H), 7.57 – 7.50 (m, 3H), 7.45 – 7.42 (m, 2H), 7.36-7.33 (m, 3H), 4.52 (t, *J* = 3.6 Hz, 2H), 2.96 – 2.92 (m, 2H), 1.50 – 1.45 (m, 2H); [13]C NMR (151 MHz, $CDCl_3$) δ 143.9, 135.3, 132.1, 129.7, 128.4, 128.1, 127.9, 125.9, 31.2, 12.2; HRMS (EI, m/z): Calcd for $C_{14}H_{16}Si$ $[M\cdot]^+$ 212.1021, found 212.1019.



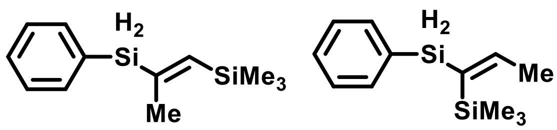
(2-(4-methylcyclohex-3-en-1-yl)propyl)(phenyl)silane (4k) (0.31 g, 92%).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.0 Hz, 2H), 7.41-7.37 (m, 3H), 5.41 (s, 1H), 4.37-4.35 (m, 2H), 2.01 – 1.96 (m, 3H), 1.76-1.73 (m, 2H), 1.67 (m, 4H), 1.45 – 1.43 (m, 1H), 1.30-1.26 (m, 1H), 1.17-1.13 (m, 1H), 1.00-0.98 (m, 3H), 0.89-0.86 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 135.3, 134.1, 133.2, 129.6, 128.1, 121.05 , 121.01 , 40.9, 40.8, 34.7, 34.6, 31.03 , 30.97, 29.2, 28.1, 26.9, 25.7, 23.6, 19.0, 18.7, 15.6, 15.2; HRMS (EI, m/z): Calcd for $C_{16}H_{24}Si$ $[M\cdot]^+$ 244.1647, found 244.1649.



(E)-hex-3-en-3-yl(phenyl)silane (4l) (0.23 g, 87%).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 – 7.69 (m, 2H), 7.49 – 7.44 (m, 3H), 6.11 (t, *J* = 6.9 Hz, 1H), 4.68 (s, 2H), 2.34 – 2.31 (m, 2H), 2.30 – 2.25 (m, 2H), 1.11 (t, *J* = 7.5 Hz, 3H), 1.07 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 147.4, 135.7, 135.1, 132.8, 129.6, 128.1, 23.4, 22.1, 14.5, 14.1; HRMS (EI, m/z): Calcd for $C_{12}H_{18}Si$ $[M\cdot]^+$ 190.1178, found 190.1178.



9 : 1

(E)-trimethyl(2-(phenylsilyl)prop-1-en-1-yl)silane (Z)-trimethyl(1-(phenylsilyl)prop-1-en-1-yl)silane (4m) (0.27 g, 89%).

(E)-trimethyl(2-(phenylsilyl)prop-1-en-1-yl)silane (E-4m)：^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 (d, *J* = 6.6 Hz, 2H), 7.51 – 7.47 (m, 3H), 6.54 (s, 1H), 4.82 (d, *J* = 4.5 Hz, 2H), 2.19 (s, 3H), 0.35 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.9, 135.4, 133.7, 132.8, 129.7, 128.2, 30.8, 0.3; HRMS (EI, m/z): Calcd for $C_{12}H_{20}Si_2$ $[M\cdot]^+$ 220.1104, found 220.1105.

(Z)-trimethyl(1-(phenylsilyl)prop-1-en-1-yl)silane (Z-4m)：^{1}H NMR (600 MHz, $CDCl_3$) δ 7.67 (d, *J* = 6.5 Hz, 2H), 7.52 – 7.48 (m, 3H), 7.17 (q, *J* = 6.6 Hz, 1H), 4.77 (s, 2H), 2.10 (d, J = 6.6 Hz, 3H), 0.28 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.4, 135.6, 134.4, 133.0, 129.5, 128.0, 22.3, 0.8; HRMS (EI, m/z): Calcd for $C_{12}H_{20}Si_2$ $[M\cdot]^+$ 220.1104, found 220.1105.

Hydrosilation of 4-methylpentene with SiH_4 to form bis(4-methylpentyl)silane. A solution of $\mathbf{2_{Mes}}$ (0.0020 g, 4.2 μmol) in 0.5 mL of PhF was cooled to -35 °C and treated with $[Ph_3C][BAr^F_4]$ (0.0039 g, 4.2 μmol) in 0.5 mL of PhF. 4-Methylpentene (0.140 g, 1.66 mmol) was added to the resulting blue-green solution, after which it became red. The solution was transferred to a PTFE-stoppered flask, the solution was frozen with liquid nitrogen, and the headspace was evacuated and backfilled with 15 % silane in nitrogen. The solution was allowed to warm to ambient temperature over 1 h after which the flask was sealed and the solution was stirred for 18 h. At this point, 4 mL of diethyl ether was added and the resulting solution was filtered through alumina and volatile components were removed *in vacuo* to give a colorless oil. While at this point the predominant component of the isolate was bis(4-methylpentyl)silane, further purification was achieved by column chromatography (silica with hexanes). Yield: 0.022 g, 2.6 %. ^{1}H NMR (500 MHz, benzene-d_6) δ 3.97 (p, *J* = 3.7 Hz, J_{SiH} = 183 Hz, 2H), 1.50 (hept, *J* = 6.7 Hz, 2H), 1.45 – 1.37 (m, 4H), 1.25 – 1.17 (m, 4H), 0.88 (d, *J* = 6.6 Hz, 12H), 0.63 (dq, *J* = 11.6, 3.6 Hz, 4H). ^{13}C NMR (126 MHz, benzene-d_6) δ 42.70, 28.07, 23.72, 22.78, 9.72. HRMS (EI, m/z): Calcd for $C_{12}H_{26}Si$: $[M\cdot]^+$ 198.1804, found 198.1802.

***In situ* yield of $\mathbf{3_{Tol}}$.** Compound $\mathbf{2_{Tol}}$ (0.0167 g, 0.0374 mmol) and C_6Me_6 (0.0052 g, 0.018 mmol) were dissolved in 0.5 mL of PhF. This solution was split into 2 equal portions (0.25 mL each); one was diluted to 0.5 mL and sealed in a J-Young tube to form the reference sample, while the other was cooled to -35 °C. $[Ph_3C][BAr^F_4]$ (0.0172 g, 0.0186 mmol) was dissolved in 0.25 mL of PhF, and this solution was cooled to -35 °C before adding it to the cooled $\mathbf{2_{Tol}}$ solution, resulting in a color change to green. The resulting solution was allowed to warm to room temperature and was transferred to a J-Young tube for spectroscopic study. The yield of $\mathbf{3_{Tol}}$, determined by relative integration of the reaction mixture vs. the reference sample, was > 99 %. ^{1}H NMR (500 MHz, fluorobenzene, 295 K) δ 5.45 (s, 1H, Ph_3CH), 2.20 (s, 3H, Tol CH_3), 2.11 (s, C_6Me_6), 1.39 (s, 15H, Cp*), 1.43-1.20 (mult, 5H, PCH_3 and $PCHMe_2$) 0.81 (dd, J = 13.9, 6.8 Hz, 6H, $PCHCH_3$), 0.67 (dd, J = 15.7, 7.0 Hz, 6H, $PCHCH_3$). ^{1}H NMR (500 MHz, fluorobenzene, 235 K) δ 5.42 (s, 1H, Ph_3CH), 2.19 (s, 3H, Tol CH_3), 2.11 (s, C_6Me_6), 1.37 – 1.16 (m, 20H, Cp* PC*H*3 $PCHMe_2$), 0.75 (dd, J = 14.1, 6.6 Hz, 6H, $PCHCH_3$), 0.62 (dd, J = 14.8, 7.6 Hz, 6H, $PCHCH_3$), -15.12 (d, J = 20.8 Hz, 2H, Fe–*H*–Si). EXSY ^{31}P NMR (202 MHz, fluorobenzene, 240 K) δ 54.04.

***In situ* characterization of $\mathbf{3_{Tol}}$ by VT NMR spectroscopy.** Compound $\mathbf{2_{Tol}}$ (0.0086 g, 0.019 mmol) was dissolved in 0.25 mL of fluorobenzene-d_5, and the resulting solution was cooled to -35 °C. A separate solution of $[Ph_3C][BAr^F_4]$ (0.0172 g, 0.019 mmol) in 0.25 mL fluorobenzene-d_5 was also cooled to -35 °C, and then added to the cooled $\mathbf{2_{Tol}}$ solution resulting in a color change to green. This solution was allowed to warm to room temperature and transferred to a J-Young tube for spectroscopic study. ^{1}H NMR (295 K, 500 MHz, fluorobenzene-d_5) δ 7.41 (d, J = 7.9 Hz, 2H, *p*-Tol*H*), 7.19 (d, J = 7.7 Hz, 2H, *p*-Tol*H*), 7.17 – 7.09 (m, 8H, $HCPh_3H$), 5.45 (s, 1H, Ph_3CH), 2.20 (s, 3H, *p*-TolCH_3), 1.38 (s, 18H, Cp* + PCH_3), 0.80 (dd, J = 14.0, 6.8 Hz, 6H, $PCHCH_3$), 0.67 (dd, J = 15.7, 7.0 Hz, 6H, $PCHCH_3$). ^{1}H NMR (235 K, 500 MHz, fluorobenzene-d_5) δ 7.44 (d, J = 7.5 Hz, 2H, *p*-Tol*H*), 7.19 (d, J

= 7.7 Hz, 2H, *p*-Tol*H*), 7.18 – 7.08 (m, 9H, $HCPh_3H$), 6.74 (s, 1H, Si*H*), 5.43 (s, 1H, Ph_3CH),), 2.19 (s, 3H, *p*-TolCH_3), 1.34 (d, *J* = 8.6 Hz, 3H, PCH_3), 1.31 (s, 15H, Cp*), 1.12 (hept, *J* = 6.0 Hz, 2H, PC*H*Me_2), 0.75 (dd, *J* = 14.0, 6.7 Hz, 6H, $PCHCH_3$), 0.62 (dd, *J* = 15.7, 6.9 Hz, 6H, $PCHCH_3$), -15.12 (d, *J* = 20.2 Hz, 2H, Fe*H*). ^{29}Si NMR (79 MHz, HMBC, fluorobenzene-d_5) δ 189 (J_{SiH} = 238 Hz [6.74 ppm], 90 Hz [-15.12 ppm]). ^{13}C NMR (126 MHz, fluorobenzene-d_5) δ 144.57 (Ph_3CH), 133.81 (p-Tol), 130.09 (Ph_3CH), 128.89 (Ph_3CH), 126.87 (Ph_3CH), 88.86 (Cp*), 57.31 (Ph_3CH), 34.73 (pentane), 29.04 (d, *J* = 25.3 Hz, $PCHMe_2$), 23.12 (pentane), 21.62, 17.49, 16.65, 14.47, 10.86 (Cp* Me), 5.56 (d, *J* = 21.4 Hz, PMe).

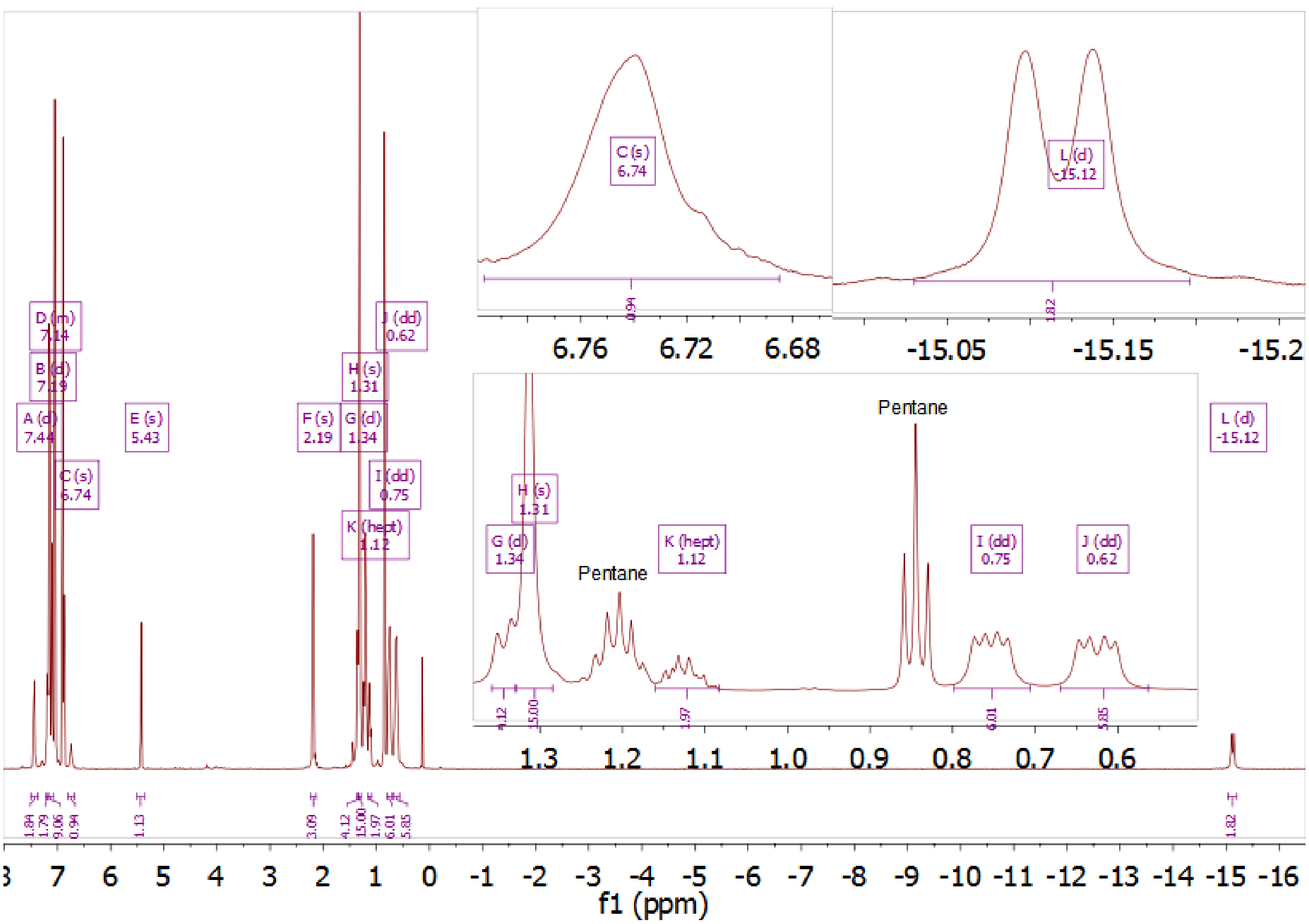


Figure S1: ^{1}H NMR spectrum of $\mathbf{3_{Tol}}$ at 235 K. The doublet emerging from the Cp* resonance has slightly higher integration than expected (4 vs. 3), likely due to residual intensity of the large Cp* resonance.

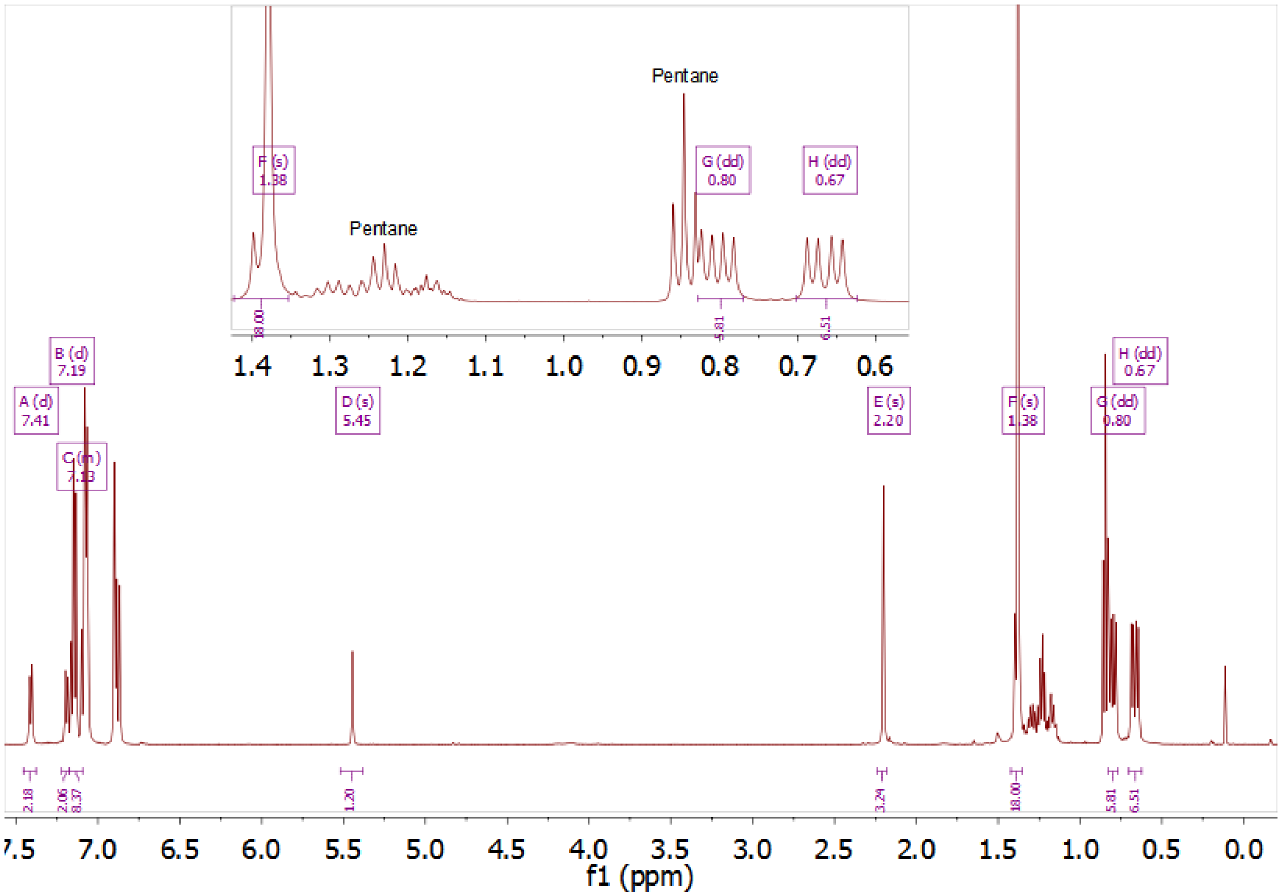


Figure S2: [1]H NMR spectrum of $\mathbf{3_{Tol}}$ at 289 K.

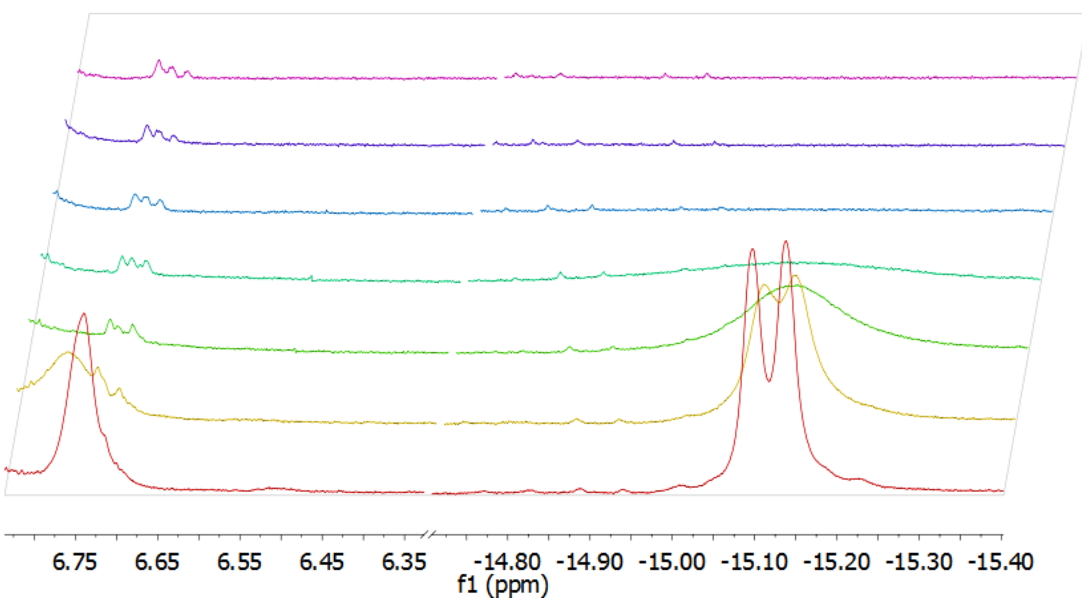


Figure S3: Coalescence behavior of the Si–H and Fe–H–Si resonances of $\mathbf{3_{Tol}}$.

Exchange kinetics of 3_{Tol} with *p*-TolSiH$_3$. Compound 2_{Tol} (0.0104 g, 23.3 µmol) and [Ph_3C][BAr^F_4] (0.0390 g, 42.3 µmol) were separately dissolved in 1.00 mL of PhF and the resulting solutions were cooled to -35 °C. 0.18 mL of the trityl solution was added to 0.33 mL of the 2_{Tol} solution at -35 °C and this mixture was allowed to warm to room temperature, forming a deep blue solution. A solution of *p*-TolSiH$_3$ (0.0106 g, 86.7 µmol) in 1 mL of PhF was prepared, 0.09 mL was added to the solution of 3_{Tol} described above, and the mixture was placed in a J-young tube for VT NMR spectroscopy. Exchange rates were determined by line-shape modeling using the text-based distribution of the MEXICO program by allowing the rate constant to freely vary. The natural linewidth was determined from line fitting of the 290 K data, then correcting it for any additional broadening by examination of the Ph_3CH resonance at each temperature. Treatment of the 321 K data was complicated by the presence of an additional, minor resonance at 1.985 ppm (visible in other spectra) that obscured the shape of the broadened line underneath. To treat this, the data were first corrected by subtraction of a Lorentzian function centered at 984 Hz and broadened by 7.34 Hz (the corrected natural linewidth at this temperature); the intensity of this function was determined empirically. The exchange constants and plots of the fits at each temperature are given in Table S2 and Figures S4-S11. Fitting of the resulting *k* values was performed using LINEST in Microsoft Excel to give the Eyring plot and activation parameters shown in Figure S5 and Table S2.

Table S2: Raw exchange data (left) and LINEST output (right) for the Eyring plot of the exchange of *p*-TolSiH3 with 3_{Tol}

T	k	1/T	ln(k/T)
300.317	3.921	0.00333	-4.33849
310.878	16.911	0.003217	-2.91144
321.439	79.686	0.003111	-1.39471
332	334.329	0.003012	0.006991
342.561	1116.682	0.002919	1.181667

	Fit	Error
slope	-13605.3	189.556
intercept	40.92684	0.591629
R2	0.999418	
ΔH‡ (kcal mol^{-1})	27.01851	0.376435
ΔS‡ (cal mol^{-1} K^{-1})	59.84474	1.1749

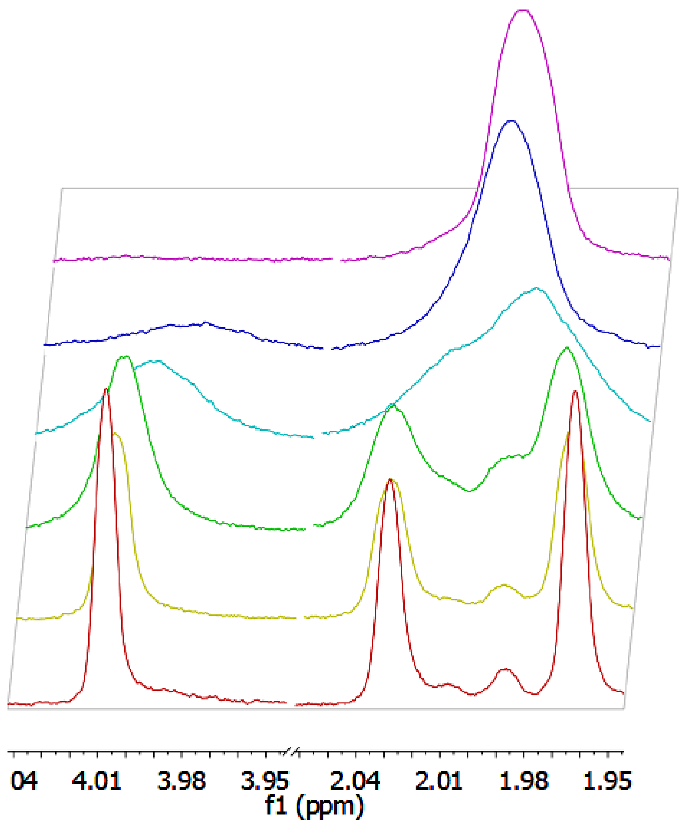


Figure S4: Broadening and coalescence behavior of the aryl methyl region and SiH_3 resonance of the exchange of *p*-TolSiH_3 with $\mathbf{3}_{\mathbf{Tol}}$.

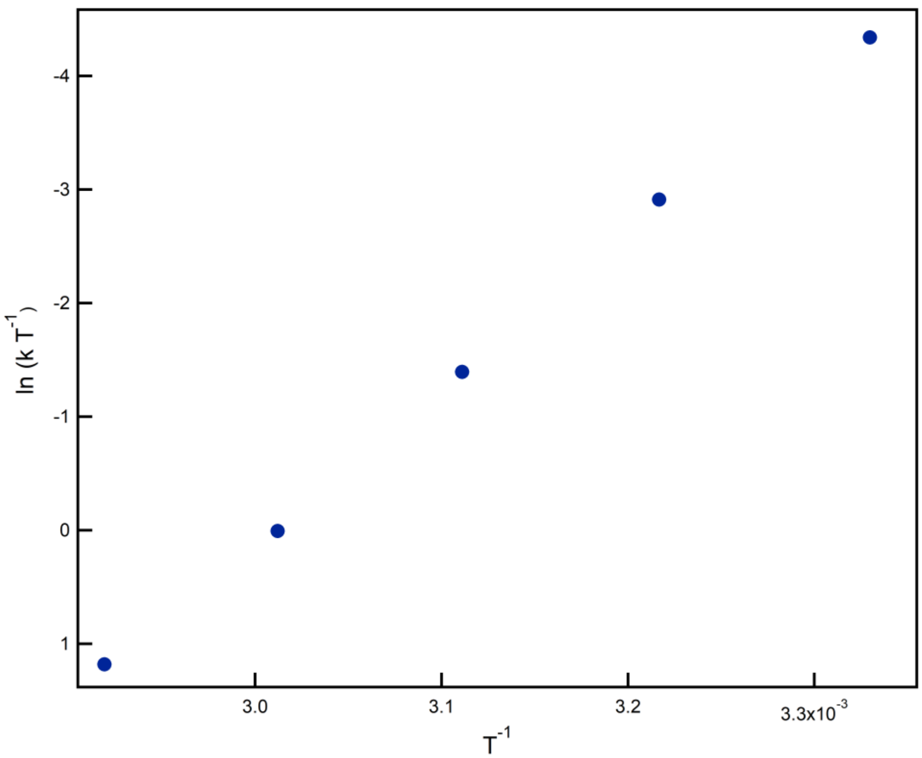


Figure S5: Eyring plot of the exchange of *p*-TolSiH$_3$ with $\mathbf{3_{Tol}}$.

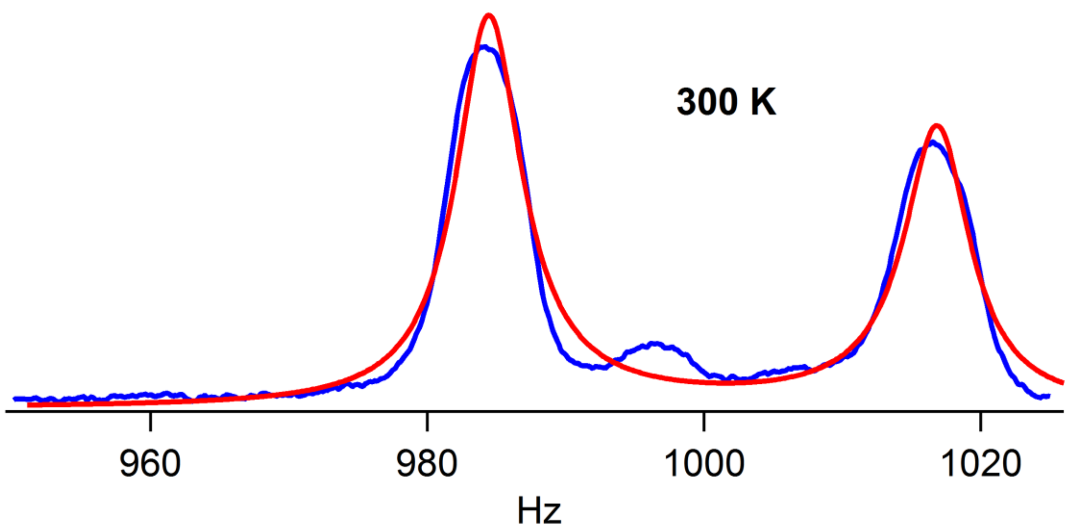


Figure S6: Experimental (blue) and MEXICO fit (red) of of the exchange of *p*-TolSiH$_3$ with $\mathbf{3_{Tol}}$ at 300 K.

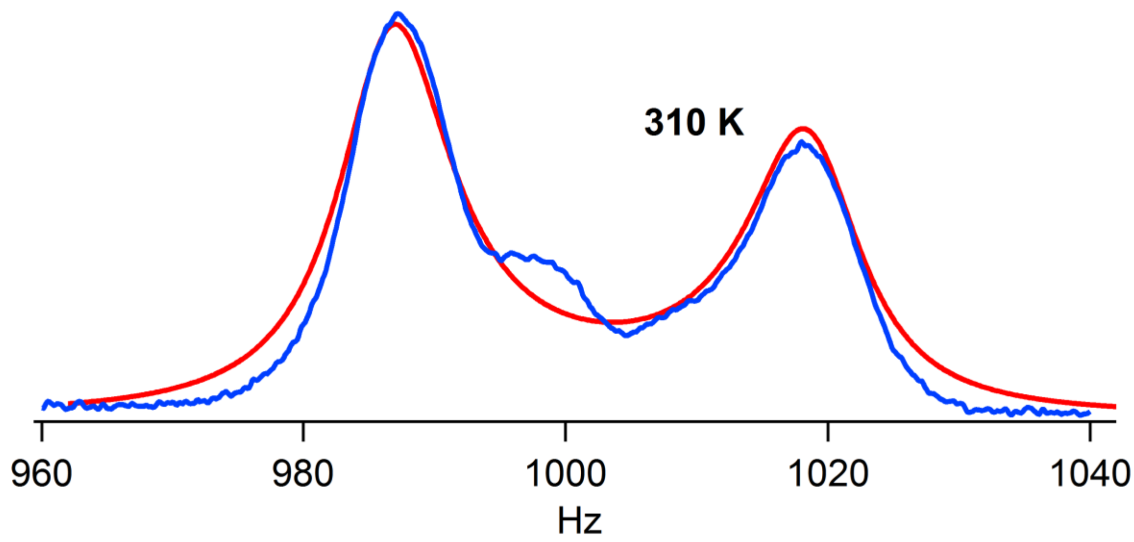


Figure S7: Experimental (blue) and MEXICO fit (red) of of the exchange of *p*-TolSiH$_3$ with **3**$_{\mathbf{Tol}}$ at 311 K.

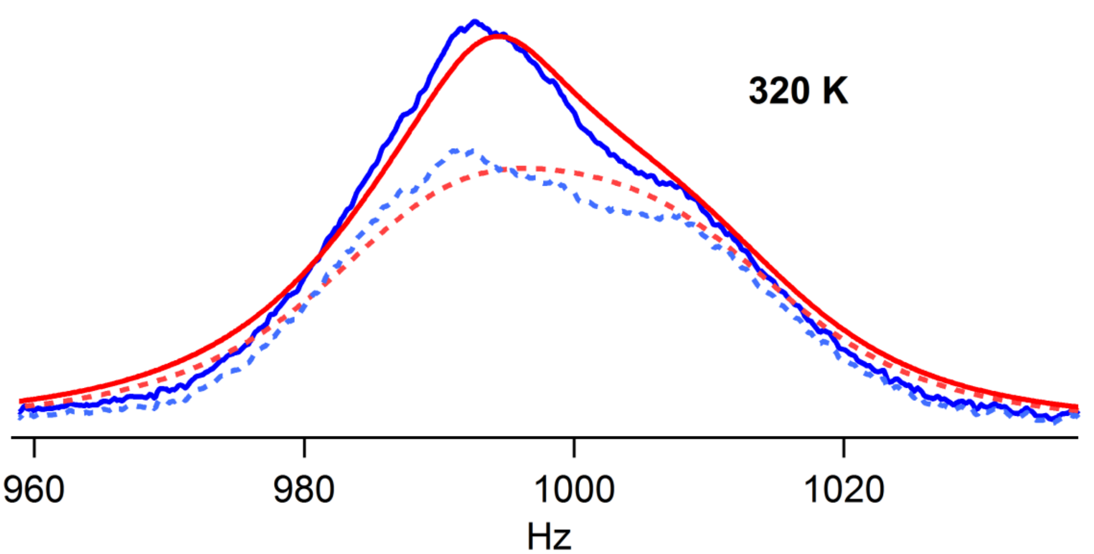


Figure S8: Solid lines are experimental (blue) and MEXICO fit plus a Lorentzian (red) of the exchange of *p*-TolSiH$_3$ with **3**$_{\mathbf{Tol}}$ at 321 K. The dashed blue line is the input used for the MEXICO program, which is the experimental data that has been modified by subtraction a 7.34 Hz wide Lorentzian at 984 Hz; the raw output from MEXICO is shown in dashed red.

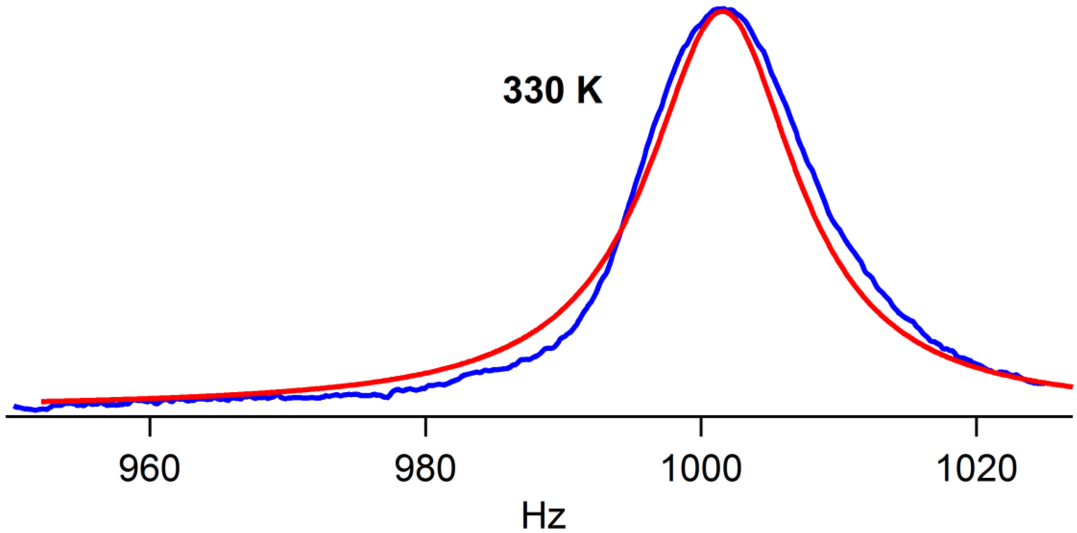


Figure S9: Experimental (blue) and MEXICO fit (red) of of the exchange of *p*-TolSiH_3 with $\mathbf{3}_{\mathbf{Tol}}$ at 332 K.

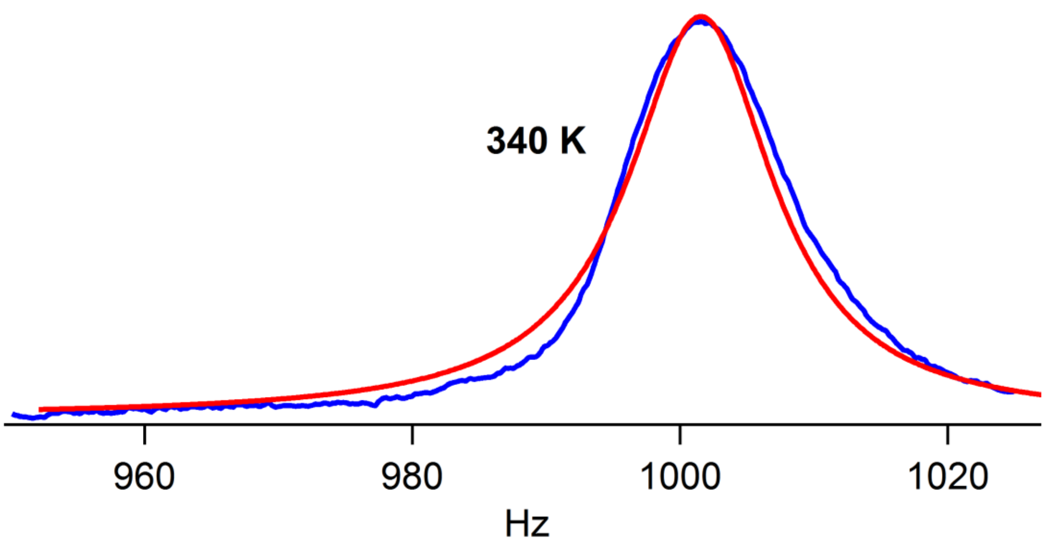


Figure S10: Experimental (blue) and MEXICO fit (red) of of the exchange of *p*-TolSiH_3 with $\mathbf{3}_{\mathbf{Tol}}$ at 343 K.

Computational details. All calculations were performed using Orca 4.2.0.[8,9] Two basis sets were utilized for different computations; for DFT optimizations and frequency calculations, the def2-TZVP basis set was used for Fe, P, and Si, as well as hydrogen atoms bound to Si and Fe. This basis set was also used for olefinic carbons and the α and β carbons of the propyl, olefinic carbons in propene, and the carbons in the 4-membered ring of **T**. For the DLPNO-CCSD(T)[10,11] single point energy calculations the def2-TZVP basis set was used for all atoms. For pure DFT functionals the RI-J approximation was used; for hybrid functionals and the Hartree-Fock SCF component of the DLPNO-CCSD(T) calculation the RIJCOSX approximation was used. Solvated free energies were corrected for standard state by subtracting 1.90214 kcal mol^{-1} from the free energy of each molecule.

Geometry optimizations. Initial geometry optimization of $\mathbf{3_{Ph}}$ was performed starting from geometries adapted from the crystal structure of $\mathbf{2_{DMP}}$[6] by replacing the Mes substituents with H, removing a single Si–bound H, and planarizing at Si. After optimizing $\mathbf{3_{Ph}}$ other geometries along the reaction coordinate were found using $\mathbf{3_{Ph}}$ as a starting point as follows: for **T**, a propylene fragment was placed in such a way to approximate a 2 + 2 cycloaddition reaction with the terminal Si–H bond; the bonds comprising the resultant 4-membered ring were fixed, and the rest of the geometry freely optimized to a minimum; this geometry was then used directly for a transition state search. The intermediate $\mathbf{3_{PhPr}}$ was found by replacing the terminal Si–H with a propyl fragment. The 14-electron intermediate following silane dissociation was optimized by simply deleting the silane residue from $\mathbf{3_{Ph}}$. For each molecule, an initial optimization was performed using the BP86 functional with the D3 dispersion correction of Grimme and coworkers, and further optimized using ωB97X-D3. Following each geometry optimization an analytic frequency calculation was performed to verify that the optimization converged to a stationary point; small imaginary frequencies (less than 25 cm^{-1}) were ignored; these likely arose from numerical noise due to the RIJCOSX approximation.

Computed Energies

Table S3: Energies computed using geometries and frequencies calculated at the ωB97X-D3-CPCM//def2-TZVP/def2-SVP with electronic energies computed at either the ωB97X-D3-CPCM//def2-TZVP/def2-SVP or DLPNO-CCSD(T)-CPCM/def2-TZVP level of theory. Energies are provided in kcal mol^{-1} except for entropy, which is cal mol^{-1} K^{-1}. All quantities were calculated at 298.15 K with a standard state of 1 M in solution.

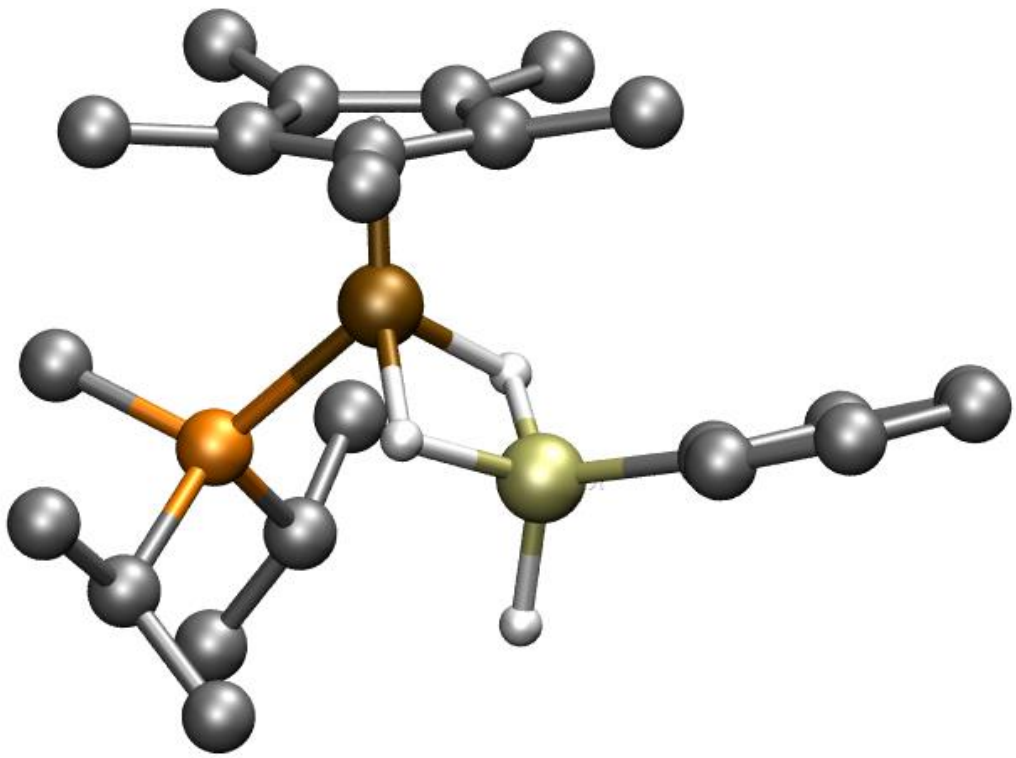
				DLPNO-CCSD(T)				
Fe	**Electronic Energy, ωB97X-D3**	**Electronic Energy, DLPNO-CCSD(T)**	**ZPE**	**H**	**S**	**G**	**ΔG_{DFT}**	**ΔG_{CC}**
3_{Ph}	-1753526.88103097	-1751688.55489955	382.31761484	-1751303.74264654	-192.07212920	-1751361.01	0.00	0.00
TS	-1827480.97343952	-1825521.34971306	435.51569753	-1825083.33937736	-201.67015931	-1825143.47	24.51	19.11
3_{PrPh}	-1827523.41790150	-1825557.13264134	439.71444851	-1825114.92355466	-208.77069331	-1825177.17	-15.85	-14.59
I_S	-1425479.62703761	-1424063.43999875	301.02681934	-1423759.91854123	-160.74657323	-1423807.85	2.68	8.87
I_T	-1425493.27602017	-1424073.75748530	301.15928042	-1423770.10356670	-168.53034912	-1423820.35	-13.16	-3.63
						ΔG_{Rxn}	-12.14	-10.66
Ru	**Electronic Energy, ωB97X-D3**	**Electronic Energy, DLPNO-CCSD(T)**	**ZPE**	**H**	**S**	**G**	**ΔG_{DFT}**	**ΔG_{CC}**
3_{RuPh}	-1020108.72419712	-1018623.23291361	380.6447296548	-1015094.66421315	188.714429791716	-1018296.35875302	0.00	0.00
TS_{Ru}	-1094071.48934616	-1092462.85393954	435.0981649248	-1088499.74423536	204.423394954553	-1092086.20997165	15.27	11.72
3_{RuPrPh}	-1094106.74754944	-1092493.36514225	437.8191361362	-1088548.81908789	207.138093926212	-1092114.80959064	-18.08	-16.88
I_{RuS}	-692056.070322383	-690995.470868244	300.6833956659	-688302.411903713	160.364889718933	-690740.105626275	8.52	11.96
I_{RuT}	-692035.286455886	-690974.291339433	300.6880078644	-688308.768329009	170.5416223297	-690721.955678093	26.27	30.11
						ΔG_{Rxn}	-12.14	-10.66
$PhSiH_3$	-328011.56672806	-327584.715609151	73.210587684	-327510.91252025	82.5789900523227	-327533.631309177		
C_3H_6	-73964.8409426762	-73838.1428816571	52.904615088	-73784.645765352	63.1374190373973	-73801.5680498815		
$PrPhSiH_2$	-402007.735084595	-401452.701861198	134.7289886163	-401317.380371365	101.900910074459	-401345.859990747		

Table S4: Results from the nudged elastic band reaction coordinate scan between the triplet state of $\mathbf{3_{Ph}}$ and $\mathbf{I_T}$.

Image	**Dist.(Ang.)**	**E(Eh)**	**dE(kcal/mol)**	**max(|Fp|)**	**RMS(Fp)**
0	0	-2793.77632	0	0.00186	0.00052
1	5.218	-2793.76944	4.32	0.00045	0.00016
2	7.771	-2793.76251	8.67	0.00138	0.00029
3	10.32	-2793.76324	8.21	0.00105	0.00023
4	12.669	-2793.76147	9.32	0.00267	0.00048
5	14.998	-2793.76241	8.73	0.00273	0.0005
6	16.781	-2793.75737	11.89	0.00051	0.00016
7	18.75	-2793.76321	8.23	0.00206	0.00047
8	21.62	-2793.76655	6.14	0.00184	0.00037
9	25.542	-2793.77018	3.86	0.00245	0.00046
10	29.897	-2793.76754	5.51	0.0009	0.00021
11	34.227	-2793.77409	1.41	0.00521	0.0013

Structures and Cartesian Coordinates Computed using the ωB97X-D3 Functional

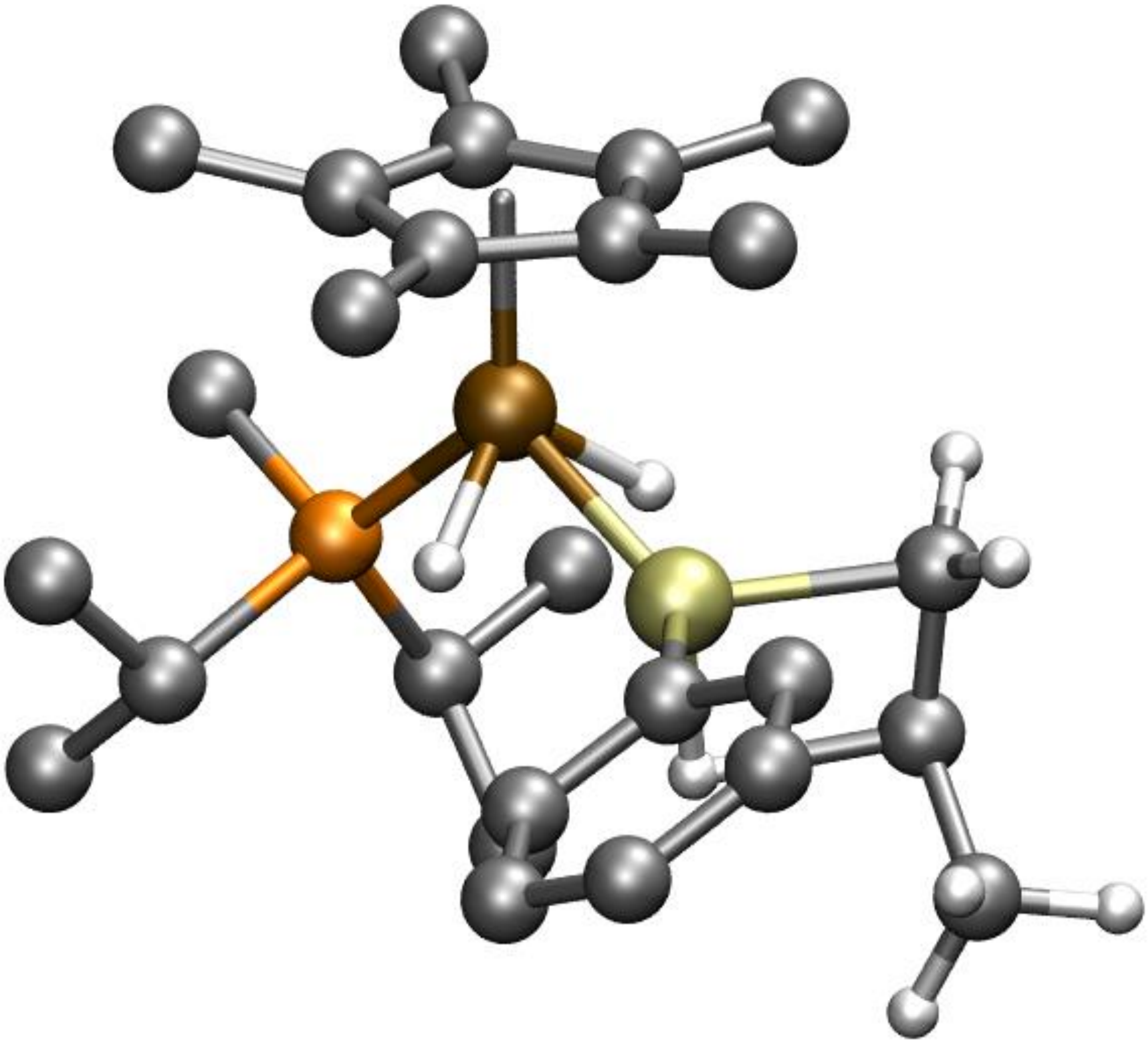
[Cp(^{i}Pr$_2$MeP)Fe(H$_3$SiPh)]$^+$ (3$_{Ph}$):



Fe	-0.20572344057939	-0.31417574569313	0.32804118565882
Si	0.81011206559548	0.89584234450181	-1.20141649085008
P	-2.13507731989916	0.93660460884013	0.34189478155358
C	0.92859373737149	-0.96122714947119	1.95399620850582
C	-3.20534082523233	0.85825745645584	-1.18189090667803
H	-4.09952960212028	1.43942042787445	-0.89603519626566
C	-2.20866645648368	-2.82372724104955	1.07845562122077
H	-3.03961768558277	-2.20570713004689	1.43762431840767
H	-2.17704563657016	-3.72107432006537	1.71580228114783
H	-2.45788485515601	-3.15674768193013	0.06230523168207
C	1.34241156847131	-1.65026259504325	0.77401434568950
C	0.21033346867061	-2.35658235463941	0.27572340508532
C	-1.07864421915679	2.85502334032459	2.05934919043951
H	-1.84098957185725	2.81587649100196	2.85334970175336
H	-0.56939875466083	3.82666793188161	2.15097908029441
H	-0.33584081466184	2.06992928876206	2.26314742507601
C	-0.42931842948800	-1.26000866636491	2.19674223847028
C	-0.89358996579808	-2.11378646598849	1.13393174715829
C	2.47749788851524	0.53294353123564	-1.88411596888518

C	2.64547513232140	-0.42668807184940	-2.89436169115444
C	0.22115697346282	-3.24722717179934	-0.92281847902597
H	-0.77714970007532	-3.36433554081904	-1.36296293337037
H	0.57975099862596	-4.24845068181774	-0.63600157909684
H	0.89259869492544	-2.86797503709130	-1.70417637945808
C	-1.72653906334389	2.71946231057441	0.67242929486456
H	-0.97028936590877	2.96952883499715	-0.08980394170452
C	3.60663064463028	1.17404628670797	-1.35233940865281
C	4.88323003641369	0.83770451657676	-1.79976808193122
H	5.75487914068304	1.33491432877753	-1.36718971114883
C	3.92101862419252	-0.75582825951453	-3.34875066518147
H	4.04702299297325	-1.50354351802077	-4.13484209115020
C	1.81302395189989	-0.12191756461044	2.82067074140748
H	2.49475608644284	0.50197582798281	2.22511303680919
H	2.43332276097982	-0.76434499455880	3.46442502993663
H	1.23207732019012	0.54085739414426	3.47496698220602
C	-3.64008326720737	-0.59181509851159	-1.44421862091850
H	-2.78746711393235	-1.21103357750846	-1.76524372620239
H	-4.38904755200052	-0.62749014985084	-2.24958680011412
H	-4.09615597458741	-1.06914373133473	-0.56580982566013
C	5.03931594070881	-0.13359111349196	-2.79217777895527
C	-3.40545180799134	0.63254210985900	1.60731096667207
H	-3.80110047763434	-0.38704208616974	1.54727450078786
H	-4.24199703901362	1.32806005002867	1.45741048898661
H	-2.98579305836496	0.78491327432037	2.60751432074255
C	-2.63914885990746	1.48195244012776	-2.45887063200648
H	-2.35368675527684	2.53777765844411	-2.33728579139712
H	-3.40427117821996	1.43759128720188	-3.24864823290506
H	-1.76547294677853	0.93267038211673	-2.84235767303837
C	-2.87134295555251	3.72170648776673	0.54673762365093
H	-3.30554589275543	3.76527548338297	-0.46250870282976
H	-2.48652549717505	4.72494099150189	0.79229162323041
H	-3.68452692736531	3.50653003923956	1.25556750257499
C	-1.14238412941941	-0.94514797088301	3.47427443477625
H	-1.06199711847486	0.11392418537723	3.75811795259582
H	-0.68780283489431	-1.52952287027551	4.28859785111146
H	-2.20512486880413	-1.21094662659145	3.43907682075777
C	2.76459332839490	-1.83081048832073	0.34658749033174
H	2.85790340404767	-2.14889343841914	-0.69877630648102
H	3.22729080072710	-2.61251664113101	0.96736438444825
H	3.36153989687923	-0.91889706637090	0.47152180476221
H	-0.25210267322027	-0.28113693231378	-1.36309692430699
H	0.68498073735454	1.09711859237957	0.37450716623970
H	1.77898504623209	-0.93598864236825	-3.32906783900605
H	3.49395673701316	1.93224015279644	-0.57018442525853
H	6.03589773653597	-0.41205189965331	-3.14598241802049
H	0.21150892089189	2.11052046838620	-1.78605755738174

[Cp(^{i}Pr$_2$MeP)Fe(H$_3$SiPh)]$^+$ + C$_3$H$_6$ Transition State (TS$_{Fe}$):

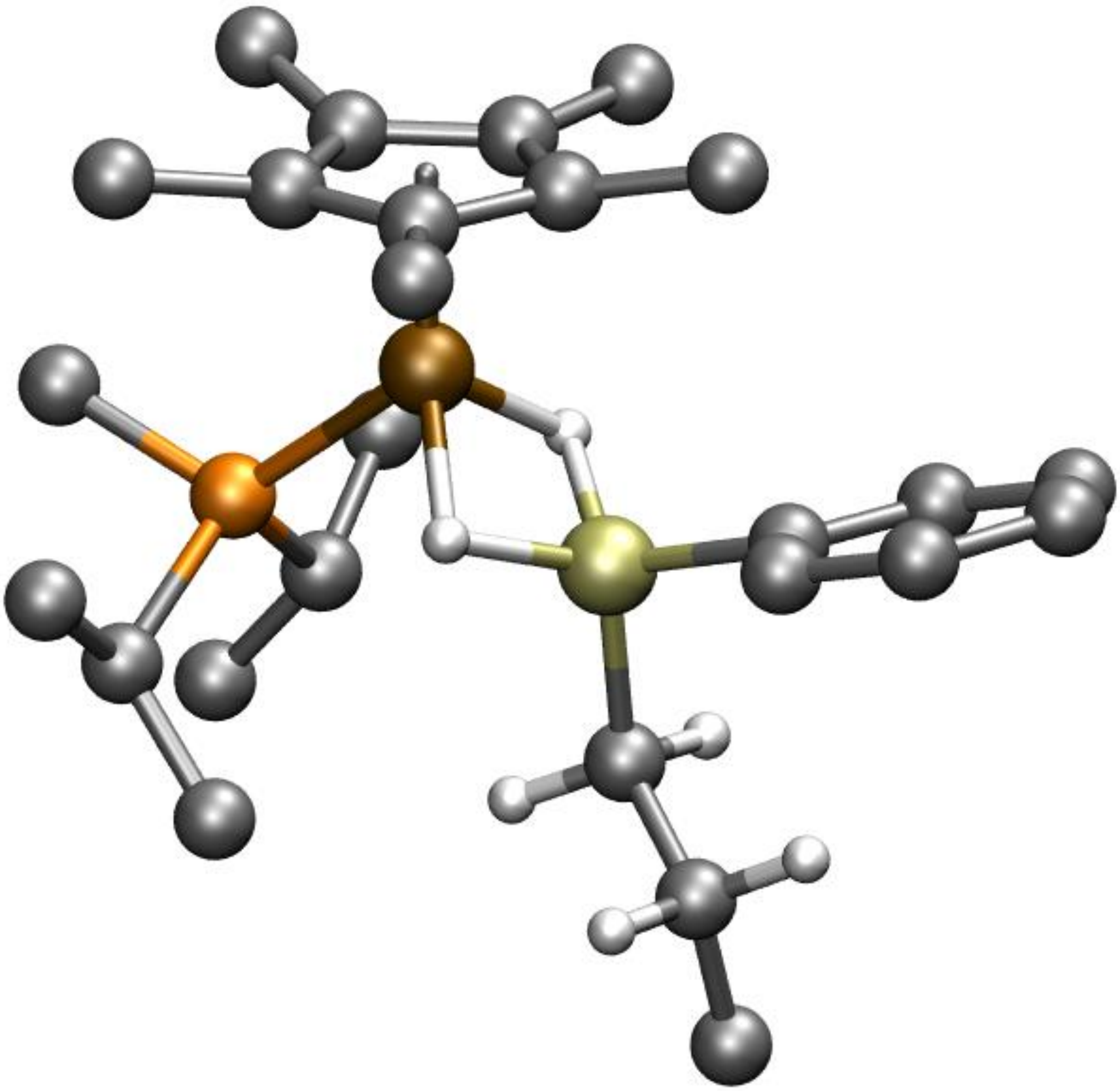


Fe	-0.00401631325520	-0.04027293984906	0.05113439421838
H	0.30096680125618	-0.01058170632868	1.53483536278206
H	1.38085050932098	0.03363367774957	-0.58333946560318
Si	1.48784677837370	1.27766834536129	0.87768184431455
H	2.82916119691009	0.63789296651954	1.26792774810703
C	3.59937650892346	1.81803524695731	0.17511248824016
H	3.97758533603241	0.95264959243291	-0.36388880715278
C	2.50122688608129	2.50040047375760	-0.38167310819882
H	2.21223531402631	2.24652032751913	-1.39432454155734

H	2.36764621152334	3.53727670445216	-0.09594321222015
C	4.49975378995210	2.42135147117013	1.19438019155609
H	5.04259443808607	1.67239916114695	1.78395429668325
H	3.96052690667040	3.10405537043772	1.86404458049867
H	5.23817196770865	3.01707226868676	0.62944678908357
C	1.31637847552118	2.33806257139111	2.42350616385398
C	1.29812968906456	3.73788318397624	2.48779582482084
H	1.34114672468742	4.33948905803066	1.57552913715510
C	1.22879340899830	4.40009361986094	3.71392368134654
H	1.21410048422748	5.49233890672197	3.74157925844705
C	1.18276877973484	3.67325584234481	4.90190301527246
H	1.13922117142474	4.19682569862868	5.85996648561036
C	1.18580804380698	2.27907711267214	4.85965828570787
H	1.14490049803520	1.69976332870799	5.78500867665850
C	1.24432221906225	1.62412745541078	3.63183624803849
H	1.23861049264365	0.52838177197091	3.61357789231635
H	-1.30295099454119	-1.52996493584246	2.58049430776702
C	-0.99916541586531	-2.58472404665147	2.63076388463898
H	-1.70793909267798	-3.17699560713073	2.03410445814905
H	-1.10527826650852	-2.92647197923154	3.67196816461998
C	0.43902731033852	-2.78274597200595	2.14681158844138
H	1.08786263739818	-2.10795453809027	2.73231926807656
C	0.88508617900810	-4.22805246913146	2.39229941471046
H	1.95257089921151	-4.39659078763721	2.18958192653409
H	0.30817163425550	-4.94173143998884	1.78689410040583
H	0.70226018426536	-4.49410117823830	3.44477269561725
P	0.62568869808243	-2.18916574828356	0.39782982209935
C	-0.26757888884004	-3.48558257128678	-0.51996138075441
H	-0.23876965215163	-3.28497429573471	-1.59554375017195
H	-1.31600519270439	-3.52698687682636	-0.20718290564930
H	0.19076252785577	-4.46614628601608	-0.33226202164545
C	2.35228082395050	-2.71788955509765	-0.03301665534642
H	2.31551226850595	-3.80642268740235	0.14101891634190
C	3.46634079912287	-2.16426064772926	0.85327693970561
H	3.66073438142971	-1.10175129296915	0.65287083039819
H	3.25252389200742	-2.26603939945655	1.92791449002094
H	4.40052933423175	-2.71046942957770	0.65166329057756
C	2.65187246826758	-2.50576729753650	-1.51607273684581
H	1.94270778196901	-3.04008810844099	-2.16180094985678
H	2.61460050180394	-1.44020876414200	-1.79359961339575
H	3.65614480992587	-2.88674938598277	-1.75963816430573
H	-2.09421582237245	-2.17999661233701	-2.28155779032023
C	-1.59773728688648	-1.25548418045311	-2.59776976220035
H	-0.63520144502745	-1.51815025024470	-3.06014154862629
H	-2.21834727837843	-0.80309558958784	-3.38720318498358
C	-1.44084937591937	-0.28477593908712	-1.47255345983788
C	-0.80123021635441	0.96168995745304	-1.60840951401997

C	-1.04399331874380	1.71805348002833	-0.41930393838513
C	-1.83505872227557	0.90780471831798	0.45742007526020
C	-2.09953620247624	-0.31622299023964	-0.19551906079644
C	-0.11940588750789	1.41268689898454	-2.86286717414926
H	0.70326061077256	0.74322681423504	-3.14905832789473
H	0.28579218751047	2.42983015451703	-2.77791931070648
H	-0.83563624915284	1.41696384614907	-3.69899230603128
C	-2.34936627017833	1.34379788996395	1.79680557853331
H	-1.57613601595227	1.87048033861179	2.37318648253160
H	-2.68301227734966	0.49002525925038	2.39995005816728
H	-3.20791127907867	2.02454642665738	1.68962919276405
C	-3.12341961531724	-1.31873070578406	0.22660775915830
H	-2.81405182400052	-2.35557209637346	0.05568232638853
H	-3.38861338017859	-1.21929171416872	1.28648123919629
H	-4.04244155963893	-1.15346067780302	-0.35700154656390
C	-0.86447692423361	3.19565775020299	-0.25562531710566
H	0.05604781696846	3.57885064243267	-0.71065916217332
H	-0.87685350078592	3.49386634790917	0.80010207904344
H	-1.70084211060010	3.71346602206638	-0.74790253736009

[Cp(^{i}Pr$_2$MeP)Fe(H$_2$Si(^{n}Pr)Ph)]$^+$ (3$_{PrPh}$):

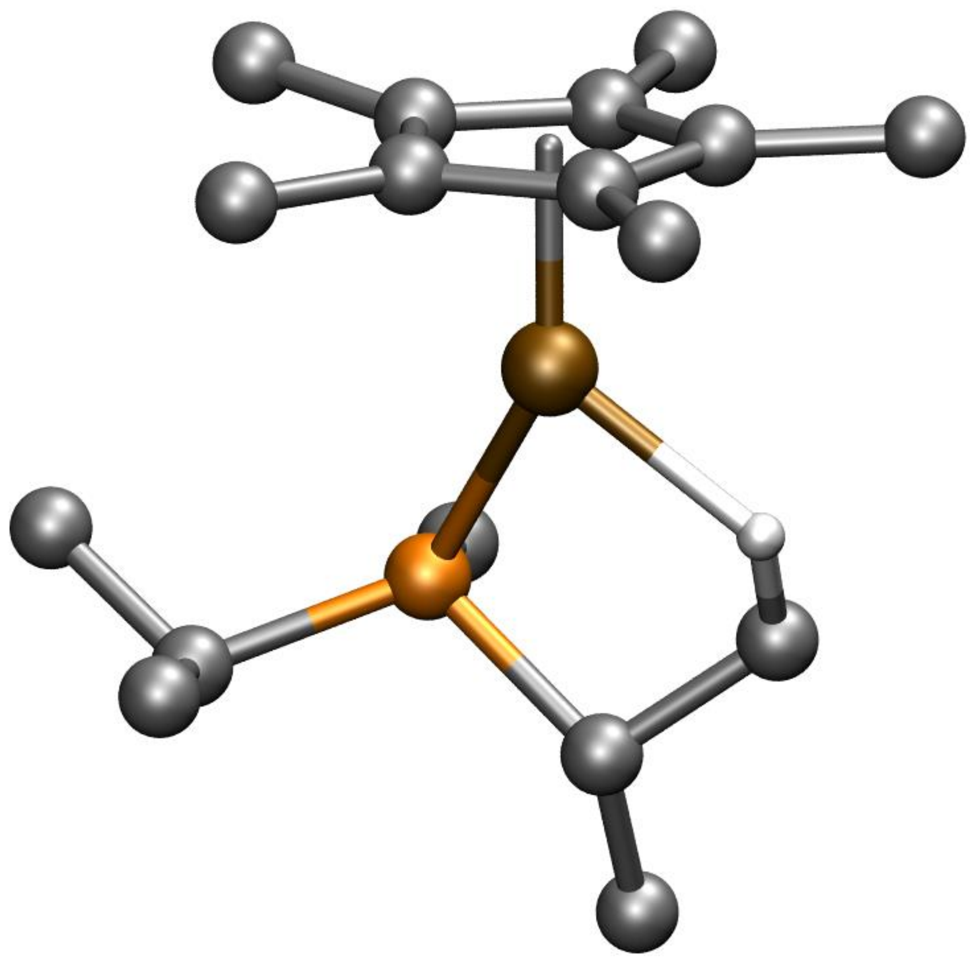


Fe	-0.19794659967891	-0.22528272287396	0.32567603164827
Si	0.89248340244577	1.05996778099938	-1.12559373150662
P	-2.17707923555154	0.93674559435663	0.38612664279671
C	0.91001547992444	-0.91708028834468	1.95841735710983
C	-3.23958454719948	0.85443397072599	-1.14510068088379
H	-4.18422368226995	1.32928702864789	-0.82879484579420
C	-2.13791981654658	-2.84881387052885	0.94823024860397
H	-3.00963106587217	-2.27073947374925	1.27546616711942
H	-2.08386646315589	-3.74159327407883	1.59094007864552

H	-2.33488668465192	-3.19869913504985	-0.07345916679074
C	1.37553075316506	-1.56122625401604	0.77350426336482
C	0.27524421952880	-2.26619036972210	0.21161819746412
C	-1.24193928611313	2.81632907230824	2.20963973084027
H	-2.00841380269242	2.70723339547455	2.99259619006727
H	-0.77666569036030	3.80451386502852	2.34679643948157
H	-0.46453490385725	2.05758838776630	2.38543709588173
C	-0.44566874509855	-1.25603877389927	2.15064778428950
C	-0.85725865841899	-2.08208190760026	1.04568520258530
C	2.54682470778875	0.53573936818890	-1.74666737822985
C	2.64875624703382	-0.40443524758906	-2.78218802669653
C	0.35014281372824	-3.11566662133396	-1.01527101679528
H	-0.63278467819727	-3.26681698512052	-1.47917445253466
H	0.75306859893676	-4.10865123006369	-0.75962020633043
H	1.01669076475887	-2.67762587874712	-1.76904035670505
C	-1.86199391471389	2.71553687543575	0.80840248652931
H	-1.09374878366084	3.02836714036199	0.08806872731720
C	3.71687755238905	1.10986959395626	-1.23045820837210
C	4.96703890339133	0.72208542438467	-1.71051179426058
H	5.86953328748257	1.17029622200686	-1.28694133402351
C	3.89701139790995	-0.78897449782662	-3.26969929700448
H	3.96806006005803	-1.52381886005822	-4.07498353694330
C	1.75465707301077	-0.08920052022938	2.87389684636528
H	2.45086144666106	0.55025599401414	2.31275433863467
H	2.35742778980868	-0.73795993260515	3.52818043186279
H	1.14615426427068	0.55783766259608	3.51927695063839
C	-3.53301040711277	-0.61584820736559	-1.47829598446910
H	-2.62432244226184	-1.13490575646889	-1.82142844717945
H	-4.27615106428441	-0.68931675350714	-2.28638526507481
H	-3.93712297212729	-1.17394619846949	-0.62316160808081
C	5.05624770172838	-0.23482897724181	-2.72500584864343
C	-3.46046878434820	0.51787545035135	1.60973759764544
H	-3.81941385157187	-0.50886757674824	1.47993080464855
H	-4.31748134292484	1.19112524867891	1.47595091295442
H	-3.07571102781959	0.62725938034902	2.62878063252403
C	-2.74629677472219	1.59393244857853	-2.38928859053210
H	-2.62329108564721	2.67470738019594	-2.22687918552257
H	-3.48347545466597	1.46967839573349	-3.19661695329135
H	-1.79540115312453	1.19042877530231	-2.77078652793476
C	-3.04403196911568	3.67247697267468	0.68747792349349
H	-3.46467625223969	3.71873357206083	-0.32770239976299
H	-2.70500351652521	4.68482179995504	0.96071144941968
H	-3.85911107789402	3.40744696282074	1.37706616638909
C	-1.19419946313332	-1.01437138117316	3.42384550314610
H	-1.16789387935592	0.03706576289699	3.74352788141764
H	-0.72627996927478	-1.60287678432725	4.22749465303110
H	-2.24196842678521	-1.32917609613554	3.36093910893487

C	2.81625146053140	-1.74775133042517	0.41931495974032
H	2.96420566752822	-2.03764975180996	-0.62723039802984
H	3.22572253890587	-2.55603176683007	1.04419358420711
H	3.42140485331995	-0.85359451384253	0.60918234772332
H	-0.21617182142217	-0.06982308530821	-1.36961938825270
H	0.64219549898755	1.19866483519710	0.45486701588101
H	1.74750418140045	-0.84902815015191	-3.21840729066351
H	3.65792574928247	1.86111358700243	-0.43491827799076
H	6.03070844022157	-0.55326748934442	-3.10569366281780
C	0.52905876509610	2.72731983949130	-1.87170090251707
C	0.97672546010023	2.89280196631551	-3.33161356059640
C	0.85177299113173	4.34293621364376	-3.77760897048241
H	1.09639411528445	3.43031228620550	-1.24290816725546
H	-0.51479906647830	3.01808563297853	-1.76908666035841
H	0.36701984100709	2.24720039196684	-3.97416836188043
H	2.00788157668342	2.55059560044562	-3.45335850340037
H	-0.18406040699703	4.70111003390529	-3.67236982821216
H	1.16145997195552	4.47536957751323	-4.82445911868835
H	1.48593119241412	4.99657017207109	-3.16140381789398

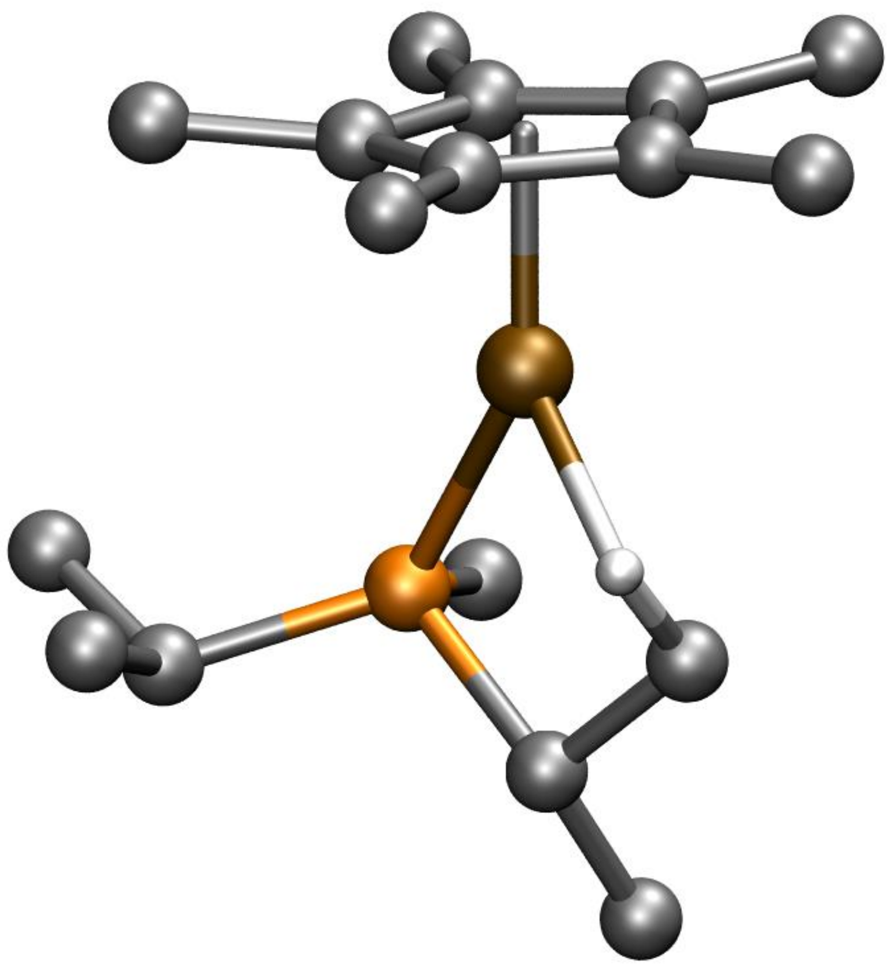
[Cp(^{i}Pr$_2$MeP)Fe]$^+$ Singlet (I$_S$):



Fe	-0.73752080213202	-0.54057499159438	0.32975796910015
C	-0.63374998169849	-1.51239109768252	2.13476863527078
C	0.00307526531975	-3.26250886873656	-1.13686292959877
H	-1.00727508901103	-3.55941275889328	-1.44658531503655
H	0.58320731752703	-4.18698140891308	-0.99184896865626
H	0.46003693750526	-2.71814113506046	-1.97463063169428
C	0.62667739132008	-0.95005283713526	1.76035097090687
C	1.02763165021833	-1.57744322042506	0.54148186270560
C	-1.04564762711533	-2.40056492323562	1.10734694068988
C	-0.00578798669704	-2.44531240281706	0.11594858535112
C	2.32964145702705	-1.33929319740210	-0.14639564942734
H	2.31898529975388	-1.68026673435808	-1.18952984078914

H	3.12435683032856	-1.89335492632688	0.37520411339110
H	2.61621095514718	-0.27764277069455	-0.12862442663005
C	-1.31143991983512	-1.28517339674207	3.44470175431419
H	-1.29440422130973	-0.23068130747783	3.75249419994675
H	-0.78235610282121	-1.85481737484123	4.22383738281264
H	-2.35343194042550	-1.62899152909757	3.44232769716601
C	-2.31746189143454	-3.18606408696365	1.09727926656538
H	-3.14399492427908	-2.63284166571327	1.56315552970269
H	-2.19194287173773	-4.12235697291113	1.66339175702278
H	-2.63060130526236	-3.46086249453155	0.08122593180561
C	1.43902814418558	0.00427813375122	2.57339407131640
H	2.05704716934439	0.65821063175941	1.94227316512768
H	2.11778304436072	-0.54367450539638	3.24569517781600
H	0.80405765192887	0.64791858298427	3.19828894026445
H	-0.05607095422892	0.37974469143477	-1.23977669894332
H	-3.47670208741588	0.07677514857218	2.72752485178570
P	-2.03716924175842	1.34461499359037	0.62870573960539
C	-3.84697061033599	1.14749074024992	0.85389884219360
H	-4.33811298423989	2.08888574340046	0.55253047622816
C	-0.21451220256615	1.49544991132011	-1.30457741175900
H	0.48708668857227	1.97032581234646	-0.60319073718674
H	0.13442440718487	1.72969076526555	-2.32239471281168
C	-1.66722023859254	1.94758198436477	-1.07511321923102
H	-2.31174252376618	1.34933612267654	-1.74107700920128
C	-4.13878622390548	0.86006232762591	2.33262903004472
H	-5.17174516880577	0.49873112757838	2.45426742433462
H	-4.01977258897989	1.75165375856956	2.96430308519790
C	-1.50022615875585	2.69194990144364	1.71654615493980
H	-1.43942859754741	2.34056461665165	2.75485808427521
H	-2.18877584018258	3.54704001012763	1.65693205364364
H	-0.49863697838842	3.02472291908451	1.41027651101909
C	-4.35100247760206	0.01452511338617	-0.04375325724558
H	-4.28650471682822	0.27027056816567	-1.11262916158462
H	-5.40732766791313	-0.20774557958888	0.17102285519022
H	-3.78401977103462	-0.91439696926516	0.13667402610742
C	-1.88472081160371	3.42760261777646	-1.37608809649379
H	-2.93694711176176	3.71958259129384	-1.23883245109308
H	-1.60578429000589	3.65578989319457	-2.41680097772209
H	-1.26987629974586	4.07181844918957	-0.73172159073699

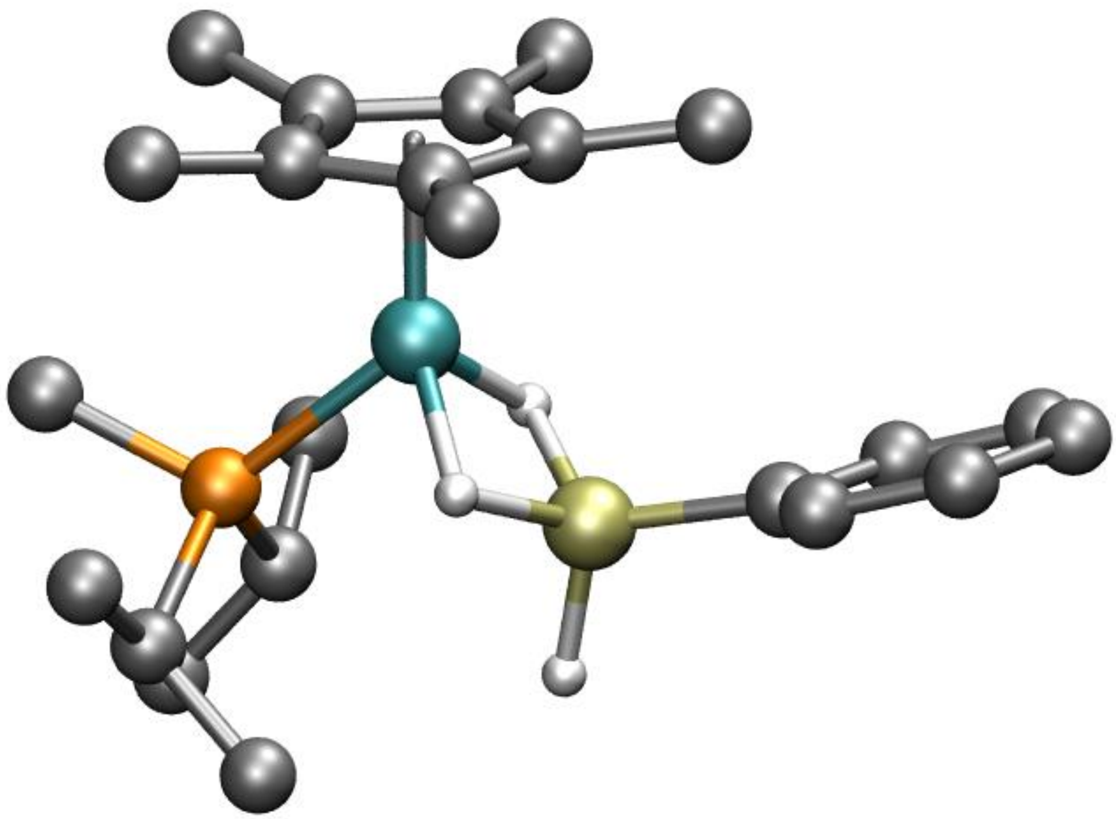
[Cp(^{i}Pr$_2$MeP)Fe]$^+$ Triplet (I$_T$):



Fe	-0.50967427358674	-0.07709961530804	0.77680658414630
C	0.49348566279334	-1.02704366893372	2.48079233047267
C	-1.62126122524031	-3.05740616318450	0.13361247911170
H	-2.65432250976540	-2.72715208010186	0.30891302837463
H	-1.52902824950883	-4.07975177454273	0.53329826957955
H	-1.46703905726959	-3.11547319900654	-0.95207093633893
C	1.31325869420220	-1.05355903487772	1.31734961415398
C	0.64596978566165	-1.80325923858143	0.28921513918894
C	-0.73151408695968	-1.64187538765666	2.14332732281086
C	-0.62428812326630	-2.15859104904375	0.78686420111210
C	1.21917549914471	-2.15797516724948	-1.05175067473244
H	0.43781310053812	-2.48800630022371	-1.74831040375382

H	1.94497893577255	-2.98130094006510	-0.96926170864101
H	1.74650038693527	-1.31232743172454	-1.51585489856558
C	0.86167043080586	-0.43761148275343	3.80701350640747
H	1.58475129509683	0.38299386083729	3.71018560914535
H	1.33090100580134	-1.20294292190948	4.44568225944598
H	-0.01185488697790	-0.04500547498019	4.34482924488358
C	-1.91240039290659	-1.84113973294397	3.03700704887645
H	-1.91959980248784	-1.12496645583186	3.86818467319874
H	-1.90723401053485	-2.85097936317440	3.47719056108706
H	-2.85506376332269	-1.73200013708911	2.48158036175520
C	2.70510461829298	-0.51635144011037	1.22538561722618
H	2.96549814719724	-0.19522447672132	0.20743119934653
H	3.42451384504423	-1.29507098382089	1.52495067670099
H	2.86379058062408	0.33867368353229	1.89423627246641
H	0.29079459846879	1.25483762895242	-0.30468145133073
H	-4.35141958435464	-1.22733758713465	0.43450326364873
P	-2.51011565525132	1.03640144709990	0.45593436570936
C	-3.77309722462463	0.50744076537865	-0.77498283224910
H	-4.27141171533636	1.42472496122346	-1.13639902962617
C	-0.12896991360154	2.21058043084001	0.13016438903112
H	0.01595114136753	2.24069941156583	1.22640419813391
H	0.57251945112642	2.94877054480179	-0.28495550741383
C	-1.58888025047777	2.47254657343476	-0.27320777398312
H	-1.67699071143065	2.33198070384990	-1.36364170557433
C	-4.82049445355871	-0.39119402565878	-0.10894144540681
H	-5.48855405988627	-0.82983428629104	-0.86574529351924
H	-5.45016781452732	0.16760016801839	0.59870452447413
C	-3.40253712024230	1.64911522846685	1.91277381827722
H	-3.88296175653890	0.80899558244362	2.43149679056846
H	-4.16920728055093	2.38971879303518	1.64393661285516
H	-2.68850044381400	2.10715624702196	2.61073608499790
C	-3.07468126072409	-0.17889890404626	-1.95345740768504
H	-2.40143760523346	0.49819226334643	-2.50108378122734
H	-3.81579745974436	-0.55131199229113	-2.67583413728365
H	-2.48099261639109	-1.03977721381452	-1.61118503320180
C	-2.03523565470669	3.88682482511175	0.08245412062739
H	-3.09021575232053	4.06444221537966	-0.17474317702237
H	-1.43754538569194	4.62209463210868	-0.47563841152093
H	-1.89260307803887	4.09974756262240	1.15344144126216

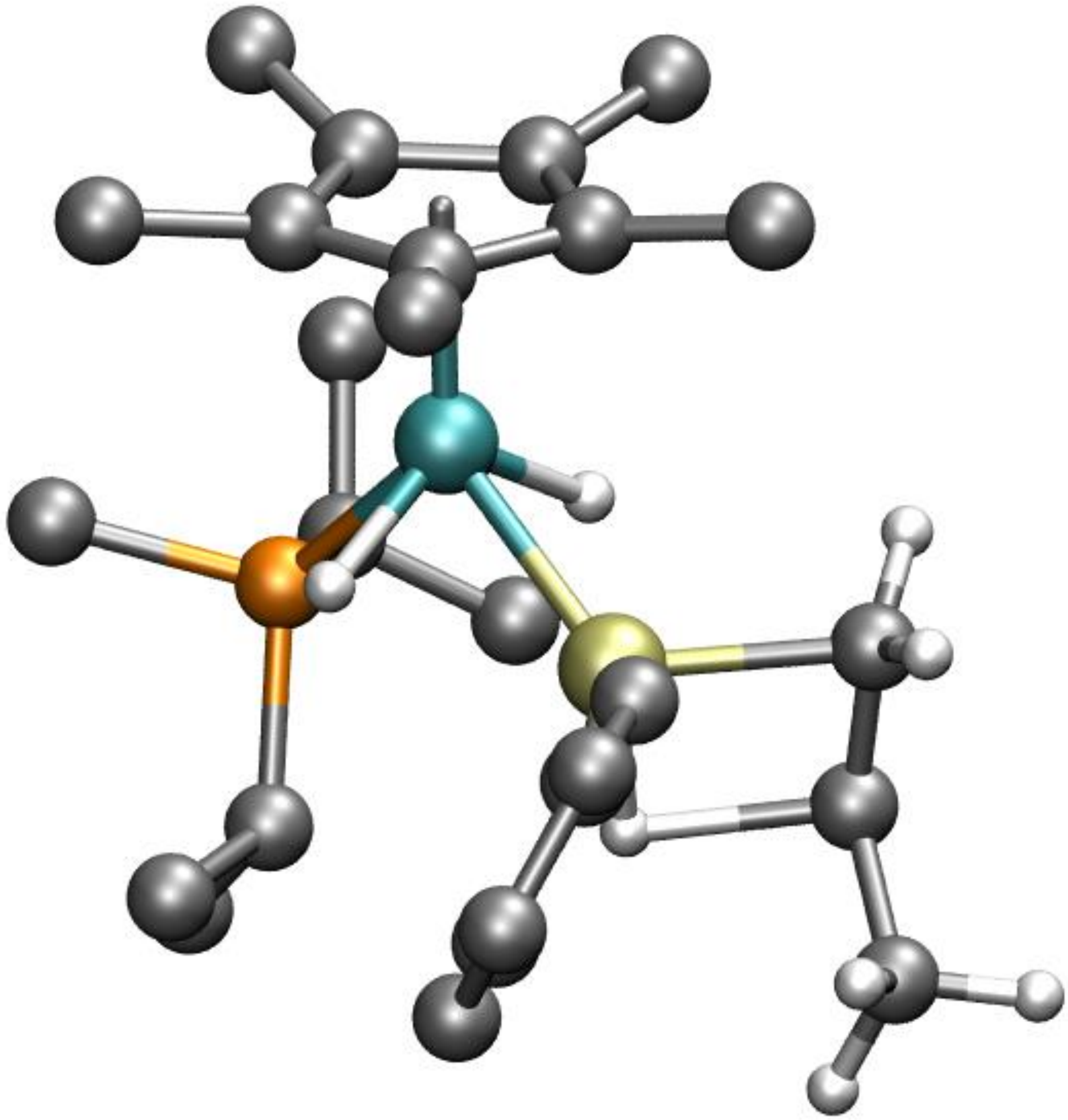
$[Cp(^{i}Pr_2MeP)Ru(H_3SiPh)]^+$ (3_{RuPh}):



Ru	-0.19281956009175	-0.27956430272914	0.28609073993877
Si	0.81568402604848	0.96656025422632	-1.29558960004933
P	-2.17166967054594	1.01332289094241	0.31402243580794
C	0.95946321395961	-1.02772557364567	2.00410915699627
C	-3.26160949477568	0.93375327763299	-1.19156664314321
H	-4.13917539891775	1.54090894775198	-0.90721183235584
C	-2.16845519706560	-2.89979983267136	1.07834438551220
H	-3.00325479340260	-2.26795681407629	1.40474772091033
H	-2.15726189194400	-3.78668600847421	1.73096559052580
H	-2.39381955953458	-3.24558534894803	0.06108914013431
C	1.40320117176930	-1.72100350743419	0.83323882165599
C	0.27810813721214	-2.42356291035029	0.30646899486984
C	-1.11527928513417	2.93957919901402	2.03573162906405
H	-1.86175243724099	2.85706647839668	2.84147004544217
H	-0.64961388005031	3.93261837326545	2.13113315037292
H	-0.33251250313376	2.18817019505041	2.21543885339876
C	-0.41189859660762	-1.33162172746109	2.22492476334377
C	-0.85661879728560	-2.18499681955625	1.14958003509051
C	2.48708959736014	0.57557764410146	-1.96613691595834

C	2.65712647959150	-0.42194287684130	-2.93931200152163
C	0.31406380076297	-3.32832273860686	-0.87992372576173
H	-0.67190017615356	-3.42917328159172	-1.35044679766558
H	0.64508632483779	-4.33118045034308	-0.56597630920948
H	1.01699201643212	-2.96705648733197	-1.64120443968445
C	-1.77846741886542	2.79731458277607	0.65634820525698
H	-1.03345791000974	3.05696045431336	-0.11514417546313
C	3.61999983372528	1.20545024812053	-1.42768582061814
C	4.89838962489976	0.82735100929281	-1.83618352174414
H	5.77136206452639	1.31661891449725	-1.39690793643838
C	3.93446475489496	-0.78918455214790	-3.35886441264958
H	4.06064384442741	-1.56311057527219	-4.11926789968764
C	1.82739655022252	-0.20302275407374	2.90033205341316
H	2.53353901716062	0.41340099771800	2.32754569633372
H	2.41727338643968	-0.85874390163213	3.55954049871540
H	1.23259799017269	0.46304114144711	3.53800730152213
C	-3.73409602323155	-0.50831007747827	-1.43615731490899
H	-2.89937828291769	-1.14953587081715	-1.76098353512987
H	-4.49265182757963	-0.52980330325974	-2.23299059193166
H	-4.19354917502020	-0.96820577224465	-0.54981008348753
C	5.05463192665491	-0.17276658018422	-2.79938949091119
C	-3.39843502496723	0.65397490338511	1.60613205739329
H	-3.76790909751884	-0.37529665477591	1.53286113733926
H	-4.25772782649684	1.33086262065483	1.50620962095645
H	-2.94430029377291	0.79075493554259	2.59414594477448
C	-2.68099767388538	1.52199765883692	-2.47782631090106
H	-2.36544906763237	2.57143335672699	-2.37435775181938
H	-3.44565344829798	1.48343487596214	-3.26822640784660
H	-1.82169186992461	0.94116455992604	-2.84701207297457
C	-2.93971211467759	3.78258542881821	0.54692172380250
H	-3.38344457962114	3.82400409357506	-0.45825305417050
H	-2.56910309148244	4.79075702769979	0.79393590354208
H	-3.74253231244460	3.55124796617937	1.26274786854477
C	-1.14516143100795	-1.03695654827617	3.49483826078093
H	-1.02853399147326	0.00744523153638	3.81666735001201
H	-0.73897580458442	-1.66905706439696	4.29933642953876
H	-2.21678368265670	-1.25480477327845	3.41946144539856
C	2.82808295337744	-1.86045456349695	0.40322523759595
H	2.92080221620068	-2.15553163825072	-0.64937926204615
H	3.31866615176524	-2.63845521893654	1.00705438011611
H	3.39666831809227	-0.93110466569434	0.53797050433301
H	-0.31035836145252	-0.25315441925999	-1.47070298867751
H	0.68086595032337	1.22362434794336	0.34968549165457
H	1.78938052231879	-0.92912730853479	-3.37449399029814
H	3.50896985672264	1.99059951661942	-0.67203805674077
H	6.05193394271031	-0.48004219910472	-3.12650188178480
H	0.24571787879594	2.18844598922389	-1.90000774850838

[Cp(^{i}Pr$_2$MeP)Ru(H$_3$SiPh)]$^+$ + C$_3$H$_6$ (TS$_{Ru}$):

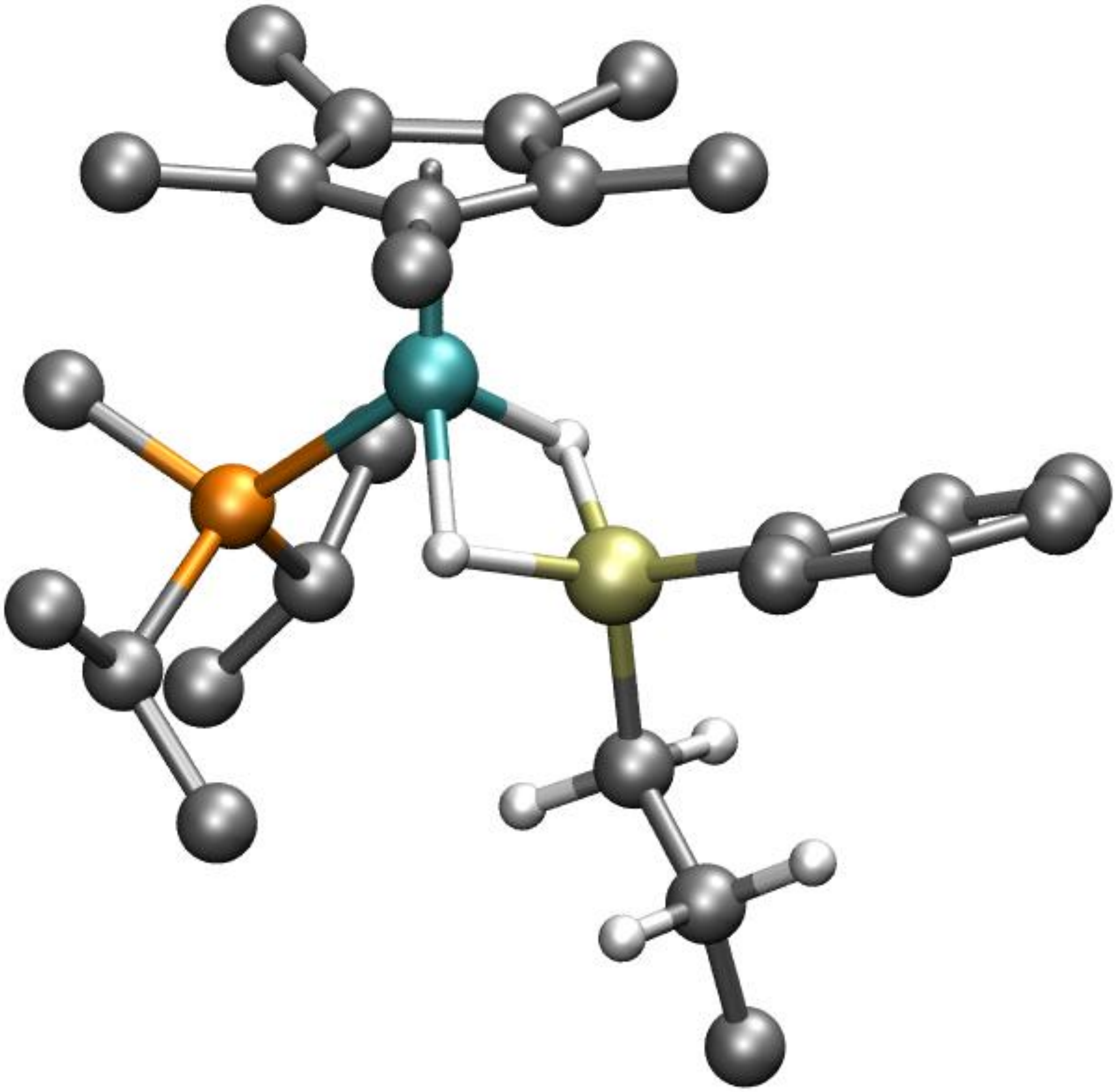


Ru	0.11107884890259	0.03534144742870	0.00594013539785
H	-0.24062175406326	-0.24940094660924	1.53596972204239
H	1.62712240215942	-0.04276856796646	-0.52256705799581
Si	1.46128152235264	1.21839579278770	1.42409057853782
H	2.69534130892664	0.45287119953036	1.96463968083572
C	3.66026264448943	1.77439090940097	1.33143076219383
H	4.18116798751851	1.00734296737142	0.76473515258553

C	2.71812290256799	2.56202293038385	0.63588653403615
H	2.70037522476511	2.47271581310278	-0.44366653670164
H	2.48472362378466	3.53831213673101	1.04926994750237
C	4.27969900331898	2.20762571340537	2.61725132039129
H	4.71203694272863	1.37565070426537	3.18592139823063
H	3.56728052463156	2.76075967034629	3.24356287114958
H	5.09371226259257	2.90245529844268	2.35213442997939
C	0.94190503171644	2.07918861677749	3.00902855928185
C	0.21614135993167	3.27830726766056	2.96320165184241
H	0.07500545204056	3.79468250948614	2.00952955448175
C	-0.34523280076193	3.83344482636858	4.11136278070357
H	-0.92975740563107	4.75405341295284	4.04325137995884
C	-0.15460510116238	3.21355184344713	5.34593293711860
H	-0.59651804735950	3.64897315010336	6.24599812502510
C	0.60635309220854	2.04670496327070	5.42344446073965
H	0.78979938252675	1.56685740532238	6.38866490173372
C	1.13427839552177	1.47960588141628	4.26408831763018
H	1.70607540178327	0.55011501578391	4.34286807247247
H	0.38310444453267	-1.26391852218454	3.32027142466390
C	0.87654527670164	-2.24628594979776	3.29716100145116
H	0.09568572480958	-3.01132379268090	3.42429659834728
H	1.53469250346161	-2.32033624364367	4.17739693904074
C	1.70377068152029	-2.49683978930674	2.03043188032010
H	2.52712650714172	-1.76187435452447	2.00220943548196
C	2.31940331493394	-3.90188455431148	2.11796954814989
H	3.04194399364856	-4.11866088445578	1.32159339185870
H	1.55118147352966	-4.69010683005614	2.10284580793170
H	2.85881323183962	-4.00877051021551	3.07205579084087
P	0.75431959921227	-2.15960691332653	0.46282962041107
C	-0.67134966319623	-3.27262942818783	0.64195400676324
H	-1.21165476690627	-3.34483718054221	-0.31016626770934
H	-1.35920819279167	-2.85935077205085	1.39091347013024
H	-0.35668697835500	-4.28053953963262	0.94958776750532
C	1.77933029418242	-3.00936543090324	-0.82273078507700
H	1.82083226612666	-4.05905862711654	-0.48663268592839
C	3.20909069444865	-2.47615964133499	-0.90668968821828
H	3.22686108195209	-1.44130347311194	-1.28509456305810
H	3.73547902213022	-2.50440662650925	0.05850530019836
H	3.79359395082672	-3.08755909112536	-1.60896643728817
C	1.11848046545135	-2.98617251746118	-2.19819237627509
H	0.12803138763322	-3.46034176723467	-2.19921302436689
H	1.01050149544062	-1.95640989245679	-2.56931045050879
H	1.73886478993229	-3.53932299635638	-2.91858758179511
H	-2.16358259225294	-2.29486872015756	-2.03211114934448
C	-1.85934250846435	-1.40169956886668	-2.59460006973871
H	-1.09992187877821	-1.69245282648477	-3.32726464427989
H	-2.74253035985506	-1.05919487702839	-3.15866866600475

C	-1.41679540333790	-0.28136782188551	-1.71269354061368
C	-0.50283915760662	0.74459772253694	-2.07137146203078
C	-0.63941194182229	1.80910720395709	-1.12574150986268
C	-1.61745816013786	1.41363361301874	-0.16154899269097
C	-2.07432393886102	0.10145784586291	-0.50561459189371
C	0.27945031038882	0.82225059052135	-3.34253831118899
H	0.64034664453706	-0.15972399663353	-3.67497553079058
H	1.15636965371794	1.47264331021240	-3.23881164913311
H	-0.35352744097346	1.23476986089605	-4.14445016557483
C	-2.27387444124057	2.30187683252426	0.84228350560564
H	-1.68117980827687	3.19724777715538	1.05123356416840
H	-2.46033351820804	1.79544796974225	1.79864423444304
H	-3.24190587026883	2.64197307953008	0.43915668578059
C	-3.26015832493490	-0.58957855703904	0.09941315979448
H	-3.23950022830504	-1.67365041062346	-0.07609823993879
H	-3.32525988371587	-0.42293168836003	1.18337970970903
H	-4.18569517659318	-0.20303073523975	-0.35773862734467
C	-0.06973397032269	3.18258545628797	-1.28074422043889
H	0.93032214485263	3.17231071239949	-1.73067159782528
H	0.00237364539755	3.71168632033097	-0.32274433432172
H	-0.71340859863451	3.78450627466010	-1.93961135852736

[Cp(^{i}Pr$_2$MeP)Ru(H$_2$Si(^{n}Pr)Ph)]$^+$ (3$_{\mathbf{RuPrPh}}$):

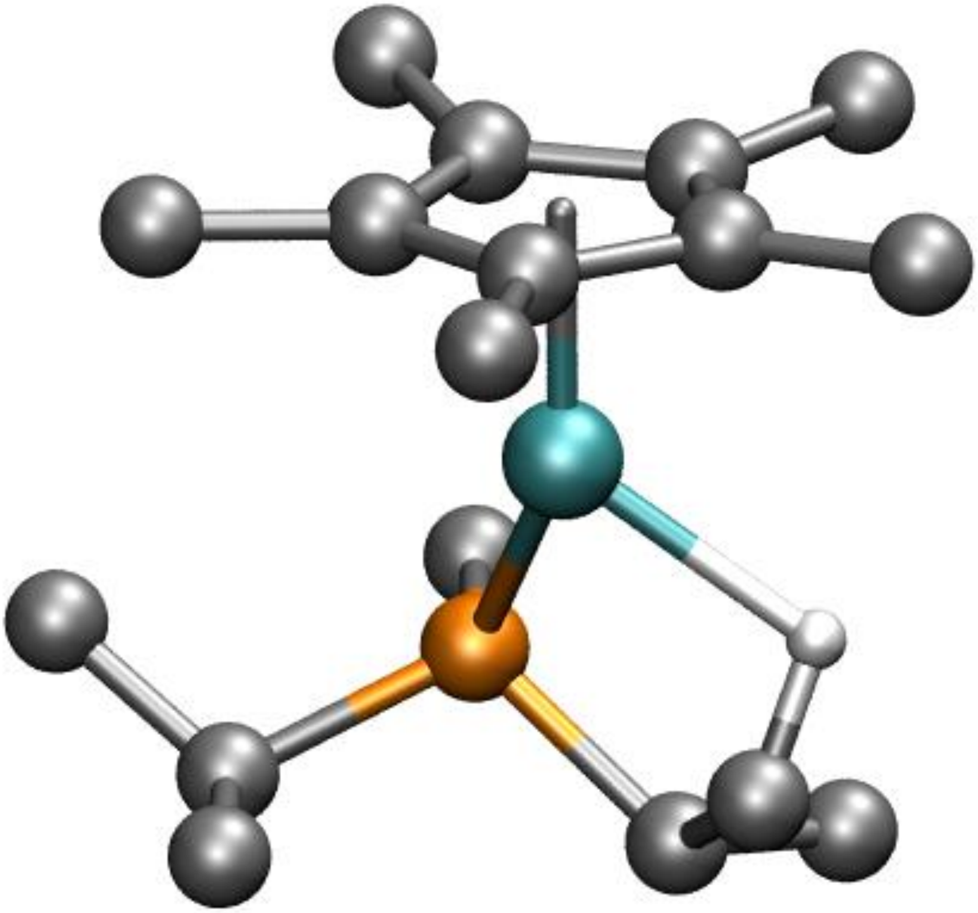


Ru	-0.19141469340716	-0.18888222414190	0.29767778804827
Si	0.92404997999096	1.13625223248696	-1.16810539819173
P	-2.23851268888928	0.98576086045570	0.35026496694547
C	0.96761751976773	-0.98419775056602	1.98725080625913
C	-3.30348755038556	0.89503777754622	-1.17195568483450
H	-4.24262028058361	1.38484427331860	-0.86076282248601
C	-2.11398107501097	-2.90868415763117	1.02722004283406
H	-2.97091604689696	-2.32763734039390	1.38724641753916
H	-2.04890643537494	-3.81165762636038	1.65475883215856
H	-2.34060197327208	-3.23740915429601	0.00459953461754

C	1.42220944051294	-1.65167742348329	0.80870309019036
C	0.30523843630382	-2.34855134936431	0.25682989193577
C	-1.34999276436463	2.89625875210173	2.17472637610912
H	-2.10085039786102	2.73742049552635	2.96425505810170
H	-0.94167650539620	3.90896261069702	2.31510039982082
H	-0.52773617959977	2.18256742872757	2.33323242262592
C	-0.40298868155093	-1.30369199704521	2.19429389177262
C	-0.82983129273769	-2.14569338431700	1.10133369666879
C	2.57408519674597	0.58283087422810	-1.78956875650801
C	2.65468858517430	-0.40968193674884	-2.77787193623909
C	0.36514637750543	-3.23931529694032	-0.94059853364941
H	-0.61927972405437	-3.37677656290565	-1.40488694355546
H	0.73758131739525	-4.23245105747330	-0.64196399145765
H	1.04762265320644	-2.84504884875828	-1.70397583995827
C	-1.97757799441567	2.77267375007460	0.77823946734586
H	-1.22627587924461	3.11084680511938	0.04849183322175
C	3.75866452248568	1.14792992710069	-1.29558169172309
C	4.99892735790714	0.70591964575348	-1.75515861797488
H	5.91231204614126	1.14653049617640	-1.34678316928139
C	3.89283578456930	-0.84162515052848	-3.25165544646575
H	3.94585422949153	-1.61224599372619	-4.02436375161705
C	1.82727920335648	-0.17318648017336	2.90401650172276
H	2.54374201941726	0.44382103916848	2.34469450994690
H	2.40482365139166	-0.83677853784971	3.56641765189900
H	1.22690166103989	0.49175331532353	3.53798456530579
C	-3.61834283316222	-0.57219188795690	-1.50210102867654
H	-2.71385366390631	-1.11094550568074	-1.82502997086384
H	-4.34985261069566	-0.63550640256721	-2.32169580049330
H	-4.05029061183809	-1.11648196849243	-0.65062117450351
C	5.06530482426460	-0.29180654012157	-2.73114627445571
C	-3.48197214362591	0.50366671616717	1.59180783692153
H	-3.82602549714585	-0.52457647795579	1.43386136710493
H	-4.35504564280410	1.16504621680017	1.51244084298724
H	-3.06534931880241	0.58244781643237	2.60185974173453
C	-2.78227339636087	1.62913756119316	-2.40799138042662
H	-2.64259194553282	2.70726506731226	-2.23775101050626
H	-3.50726103759450	1.52045932648829	-3.22836176115808
H	-1.83052255844870	1.21171581136344	-2.77250687991040
C	-3.19675978482816	3.68329018193826	0.66661419867663
H	-3.62238666285251	3.71509322813959	-0.34692997795660
H	-2.89761479347076	4.70790595999135	0.94015905215033
H	-3.99796155285005	3.38654683715817	1.35969466048756
C	-1.13600181932265	-1.05261780960546	3.47459312087466
H	-1.08371039156443	-0.00238090726772	3.79414503819090
H	-0.68174355690291	-1.65614406991670	4.27518051525739
H	-2.19228011253059	-1.33887101035664	3.41165056230816
C	2.85553067404239	-1.82135342013613	0.42115685020783

H	2.97672328798885	-2.11738600713887	-0.62739838522356
H	3.30049791379304	-2.61481915948414	1.04065916785825
H	3.44552010021912	-0.91057183734666	0.58093954692149
H	-0.25105213861401	-0.02594761930752	-1.45925194839556
H	0.59404691304063	1.32889138838245	0.48890642338142
H	1.74265061949510	-0.85714887906317	-3.18869094574861
H	3.71959124260666	1.93724093839003	-0.53653940179721
H	6.03183125428681	-0.64676766610775	-3.09959496023332
C	0.58851826482726	2.81222092997768	-1.90305149629665
C	1.05020936593452	2.98429151134563	-3.35807793399559
C	0.96402331088985	4.43964323098463	-3.79422325300833
H	1.15699313504853	3.50601426989236	-1.26466199810704
H	-0.45553550632534	3.10845211318751	-1.79946719519143
H	0.43291336367105	2.35662677617028	-4.01073277218935
H	2.07466566595136	2.61990264022399	-3.47380536889277
H	-0.06268331041643	4.82361763844284	-3.69301447879669
H	1.28447161601906	4.57027219177579	-4.83814292917177
H	1.61099051815886	5.07308280564646	-3.17020676019125

[Cp(^{i}Pr$_2$MeP)Ru]$^+$ Singlet (I$_{RuS}$):



Ru	-0.80111738550251	-0.43161144958230	0.34202366080919
C	-0.36766935341065	-1.21352485353268	2.26577616449565
C	-0.31149856251014	-3.48706155795572	-0.74427229166176
H	-1.37407505454319	-3.74049062365504	-0.85782678116788
H	0.22660733925582	-4.41889335003318	-0.51027713690891
H	0.05000656559849	-3.12436515758234	-1.71631299773556
C	0.83409737071520	-0.78329235031301	1.60146370411689
C	1.01480154364685	-1.61027684935912	0.43140925946728
C	-0.97050994210976	-2.22302304585356	1.45396738856498
C	-0.09161082958017	-2.47865582648066	0.33318077304790
C	2.18599489354710	-1.57494671392441	-0.49241654686868
H	1.95210362119504	-2.04613387815908	-1.45576134093283
H	3.03053719899184	-2.12333549133395	-0.04737090392381

H	2.52927985310421	-0.54925458412705	-0.68962633489026
C	-0.82821076480791	-0.77665142445339	3.61622900205215
H	-0.61033574654462	0.28269310143383	3.80645006130091
H	-0.30162174704816	-1.36349629298077	4.38497028690583
H	-1.90426434326643	-0.93841757459133	3.75974995247420
C	-2.21133199426373	-2.98828203353973	1.78190425335973
H	-2.90141591622502	-2.40103679899216	2.39941398797134
H	-1.95906301706424	-3.89827979464881	2.34859795301406
H	-2.75543967990633	-3.30031333389206	0.88029864995419
C	1.82209989445320	0.20342626066905	2.12377796065448
H	2.32845031398471	0.74387809499441	1.31191168206799
H	2.59645361568635	-0.32106772205759	2.70698563382455
H	1.34830717730316	0.94476121856067	2.78061530427749
H	-1.42701802512403	0.48317748014675	-1.96693148035192
H	-3.82919345254067	-0.49267850506539	2.03843424420833
P	-2.24412054972115	1.43495243509851	0.66979930531841
C	-3.99059614807658	0.93454759186773	0.39432202808370
H	-4.58195148061571	1.83988591276346	0.17268180381684
C	-0.83120619738618	1.33248817957586	-1.58100747150287
H	0.01842333213730	0.95811334190057	-0.93636072732150
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C	-1.68136045915874	2.37308813895216	-0.83156174105216
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H	-5.48746721092880	-0.23760673792459	1.46237422420534
H	-4.70687626445616	0.99413421710338	2.46988391389127
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C	-4.03590940602140	-0.00474692977467	-0.81287489335414
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H	-5.05066601425817	-0.40157781838522	-0.96715886680090
H	-3.37357883112975	-0.87857416720010	-0.65746081928309
C	-0.87935168878210	3.63550567126029	-0.51484534857262
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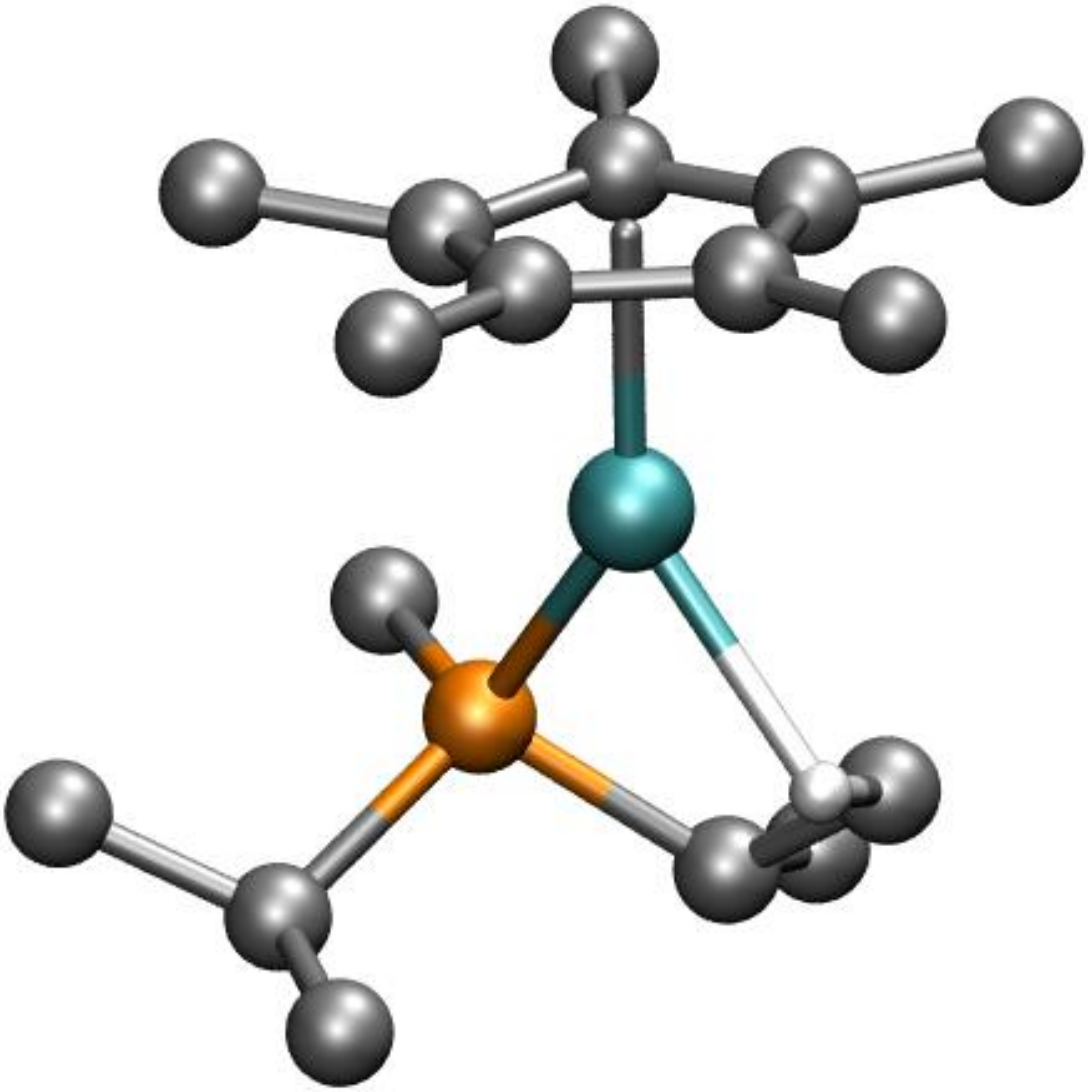
[Cp(^{i}Pr$_2$MeP)Ru]$^+$ Triplet (I$_{RuT}$):



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C	-0.84784417175750	-3.70546357107171	-0.03401525614662
H	-1.94345374411935	-3.72545197085222	0.03617939674469
H	-0.46879055993028	-4.63629653777072	0.41872262869259
H	-0.57632513685260	-3.72237711357707	-1.09825923503313
C	1.22280828159876	-0.90135463620461	1.38807136102604
C	0.96692481980303	-1.89795603987002	0.38624140924588
C	-0.83179100608029	-1.86624973004634	1.81964905329444
C	-0.26163556002545	-2.52976354168107	0.67702849970202
C	1.91672933319360	-2.28146122452025	-0.70110718317207
H	1.42562345234583	-2.86992067859310	-1.48580256637374

H	2.72835796798889	-2.89396937026894	-0.27744667010422
H	2.38304783329637	-1.40743905371645	-1.17661152072747
C	0.05022192914317	-0.16327027690560	3.59663852123182
H	0.60457429443770	0.78362390791648	3.57826986905457
H	0.47925745775523	-0.78506809147294	4.39855032476189
H	-0.98738585128459	0.06365568716858	3.87612203549319
C	-2.02810267943253	-2.32588813837299	2.58789873864502
H	-2.53042670150587	-1.49706374751915	3.10416969715196
H	-1.71320034117152	-3.05059752594273	3.35508402070199
H	-2.76511619408233	-2.82513705567663	1.94626140287568
C	2.47143110902122	-0.08579620487671	1.49064703270706
H	2.84496293363351	0.22748938449684	0.50522540418351
H	3.27117119545386	-0.66951751818849	1.97268641919384
H	2.31653108266182	0.81997948561789	2.09101763872182
H	-0.46917294979178	0.93141905249919	-1.37979714743802
H	-4.34451451993256	-1.08452645695877	0.74882362215955
P	-2.50327634023721	1.17723638956321	0.54062034426257
C	-4.05755021999743	0.77482241635469	-0.36866611778452
H	-4.60432817799026	1.72930264590233	-0.46614535265177
C	-0.35211298758378	1.94328009691743	-0.89369924528994
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H	0.14398264670971	2.53276932797182	-1.68000508783723
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H	-5.77020370989013	-0.53940880608171	-0.15871179268314
H	-5.33050340867889	0.28031522379629	1.34839156716377
C	-3.04881110399291	1.84578617089740	2.14246384533016
H	-3.44957377807246	1.02821064457550	2.75607565426584
H	-3.82979846723687	2.61245702038187	2.03416626810433
H	-2.19160023822776	2.28076558624633	2.67341806414600
C	-3.75345629862699	0.22123020665302	-1.76539419042952
H	-3.23986520256433	0.94778097921500	-2.41130742317991
H	-4.68810149508007	-0.05952591068710	-2.27468288078158
H	-3.12956719822267	-0.68735854076615	-1.71108151686656
C	-1.48192237141850	3.86658443845286	0.31621355856635
H	-2.43068857592848	4.30051539843593	0.66591507652306
H	-1.00568057282443	4.60502701343146	-0.34571805012931
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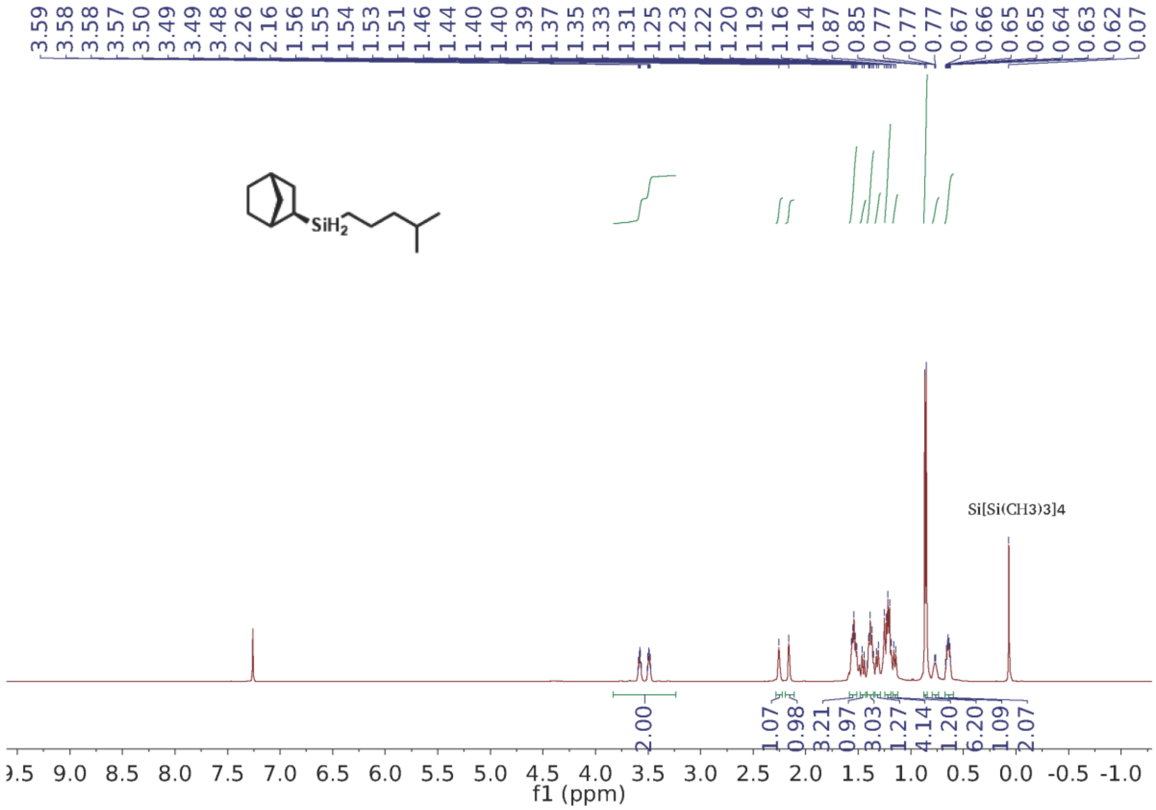
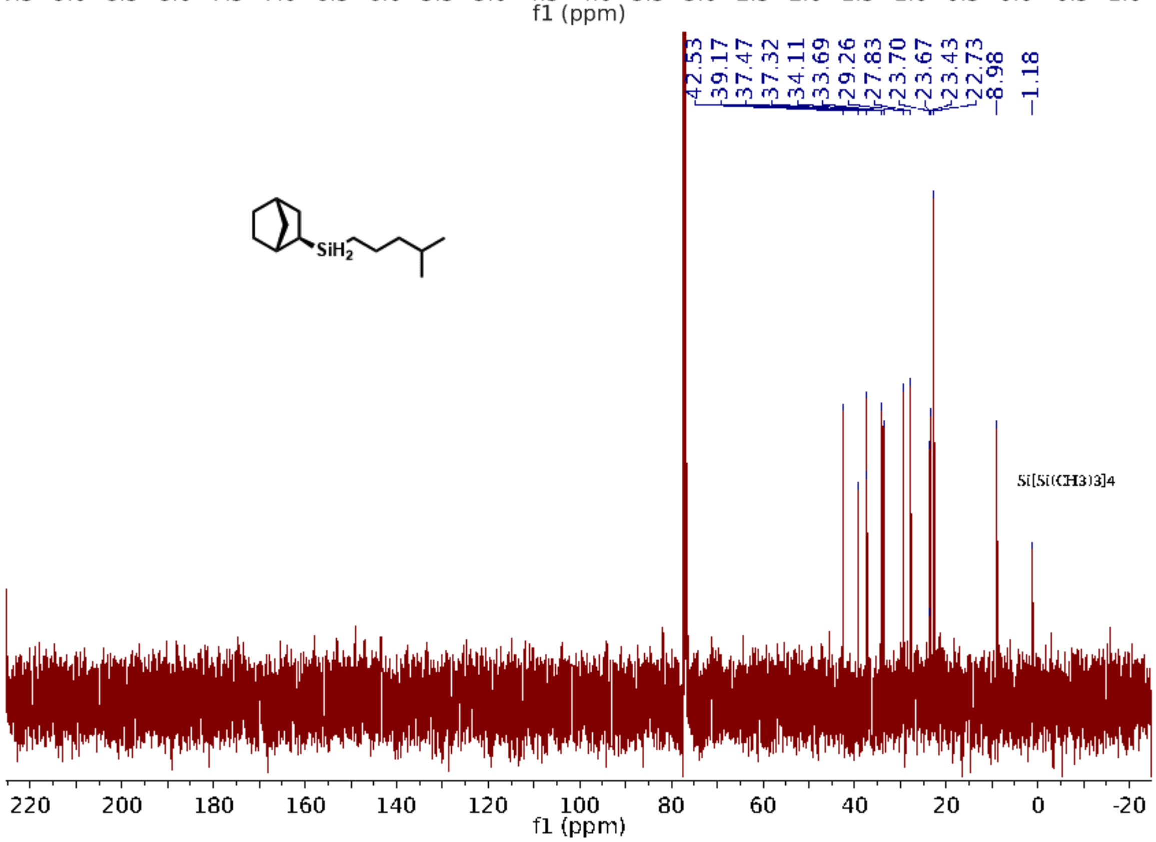
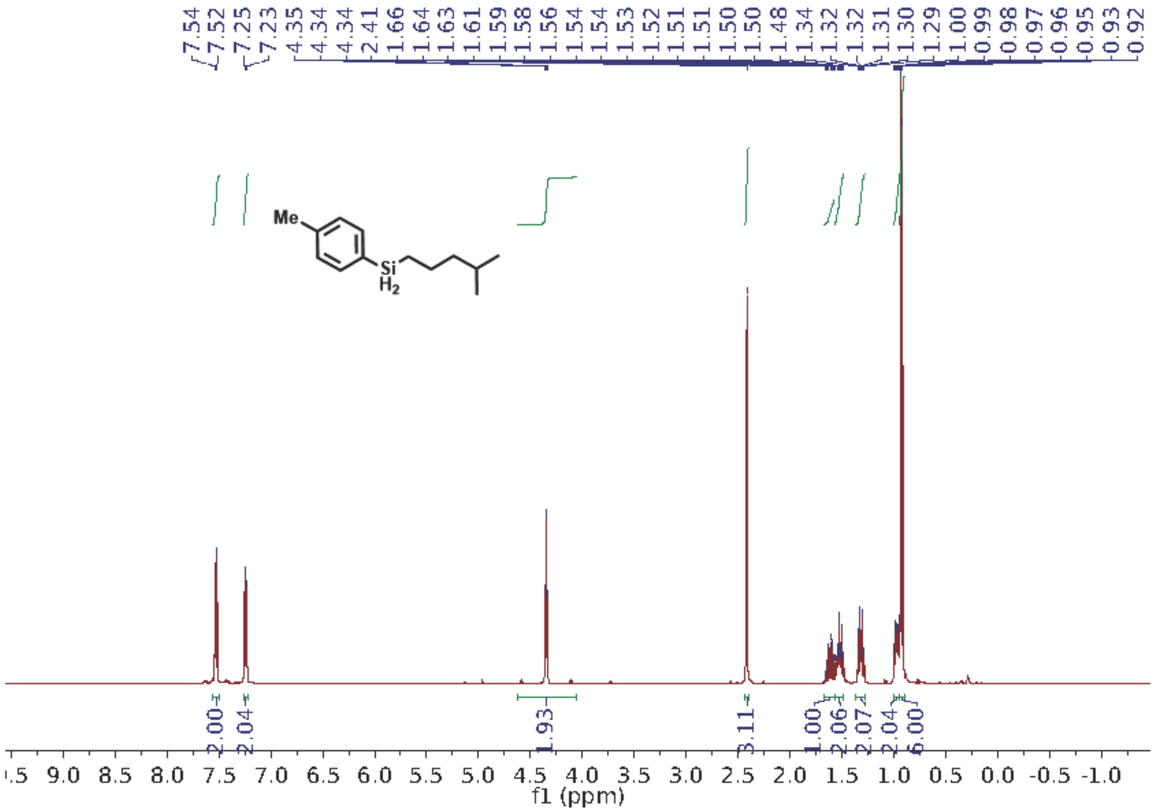
NMR spectra of silane products.



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4.34
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2.41
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1.64
1.63
1.61
1.59
1.58
1.56
1.54
1.54
1.53
1.52
1.51
1.51
1.50
1.50
1.48
1.34
1.32
1.32
1.31
1.30
1.29
1.00
0.99
0.98
0.97
0.96
0.95
0.93
0.92
Me
Si
H_2
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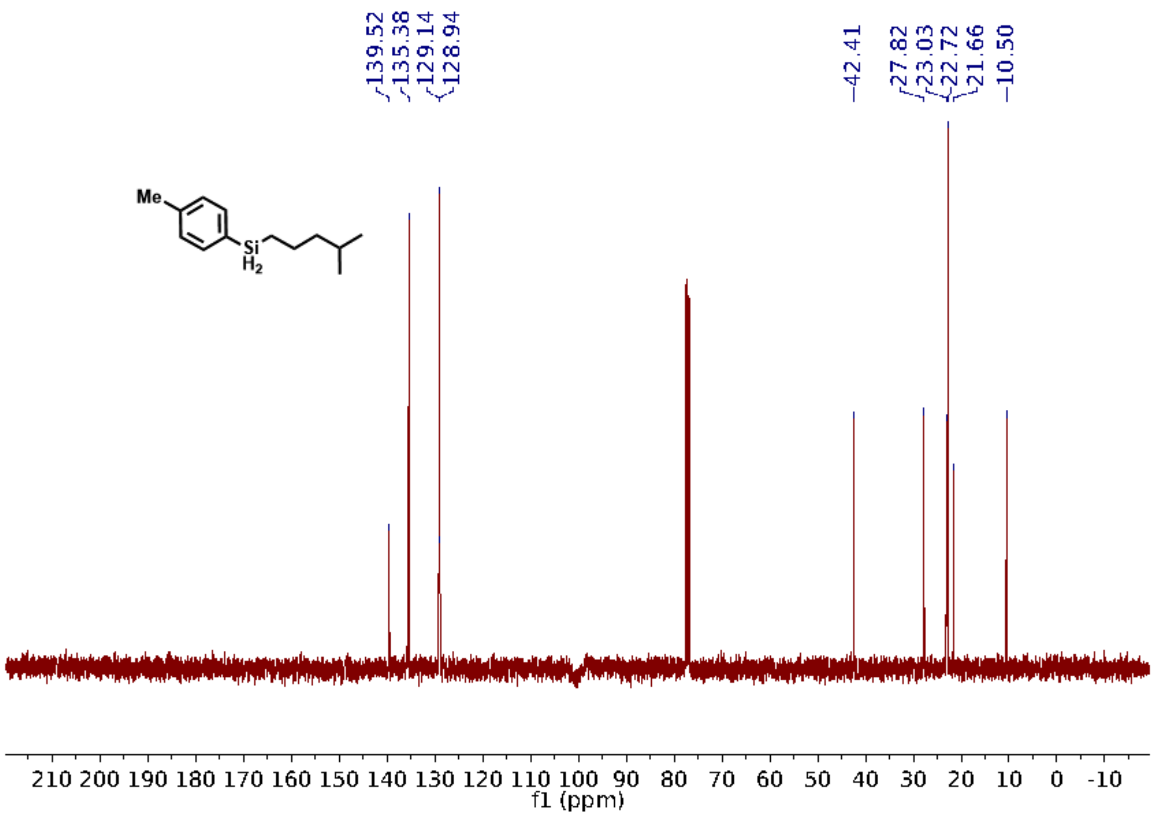
2.04
1.93
3.11
1.00
2.06
2.07
2.04
6.00
f1 (ppm)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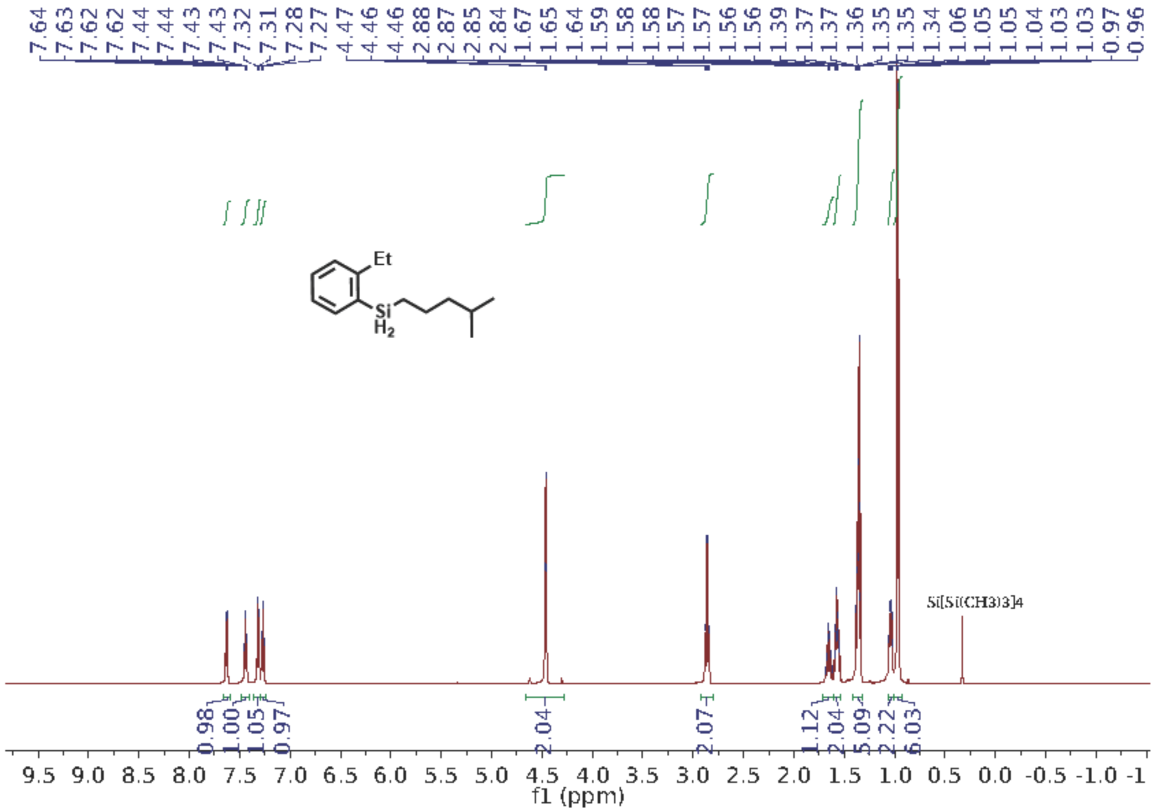
135.38
129.14
128.94
42.41
27.82
23.03
22.72
21.66
10.50
Me
Si
H_2
f1 (ppm)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7.31
7.28
7.27
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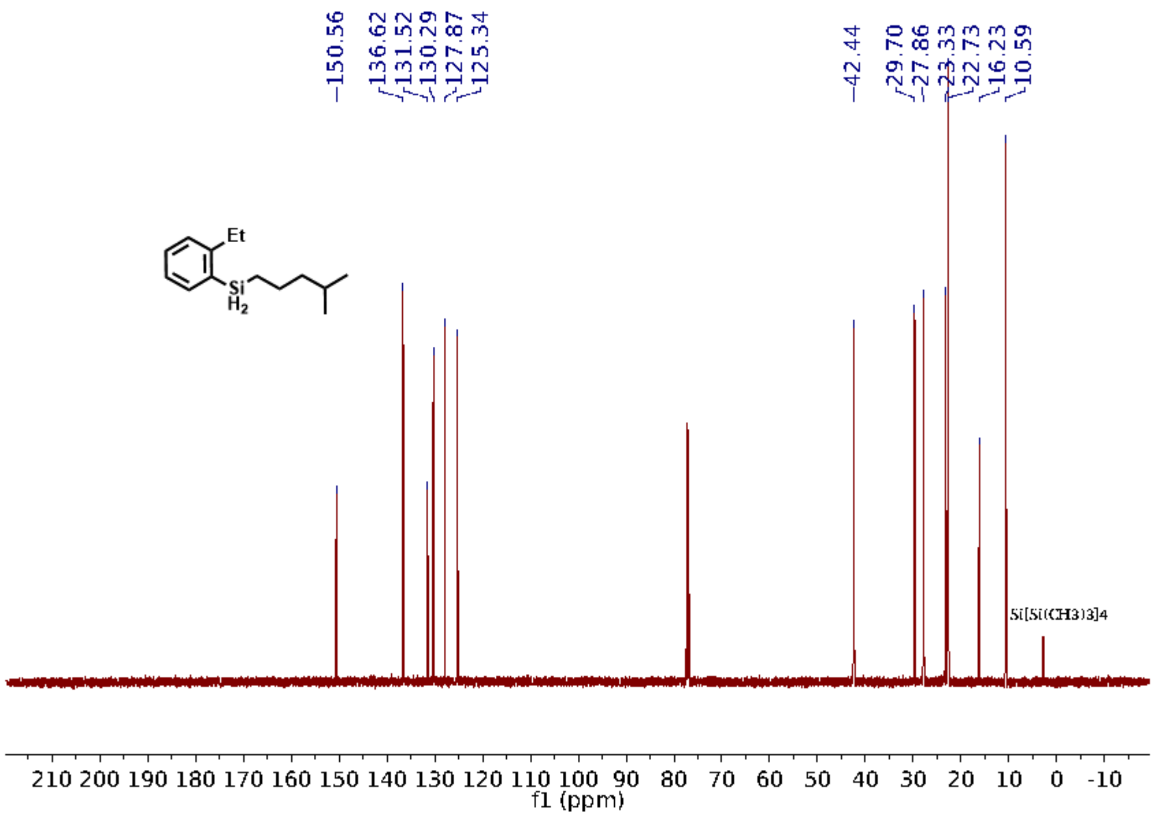
4.46
4.46
2.88
2.87
2.85
2.84
1.67
1.65
1.64
1.59
1.58
1.58
1.57
1.57
1.56
1.56
1.39
1.37
1.37
1.36
1.35
1.35
1.34
1.06
1.05
1.05
1.04
1.03
1.03
0.97
0.96
Et
Si
H2
Si[Si(CH3)3]4
0.98
1.00
1.05
0.97
2.04
2.07
1.12
2.04
5.09
2.22
6.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1
f1 (ppm)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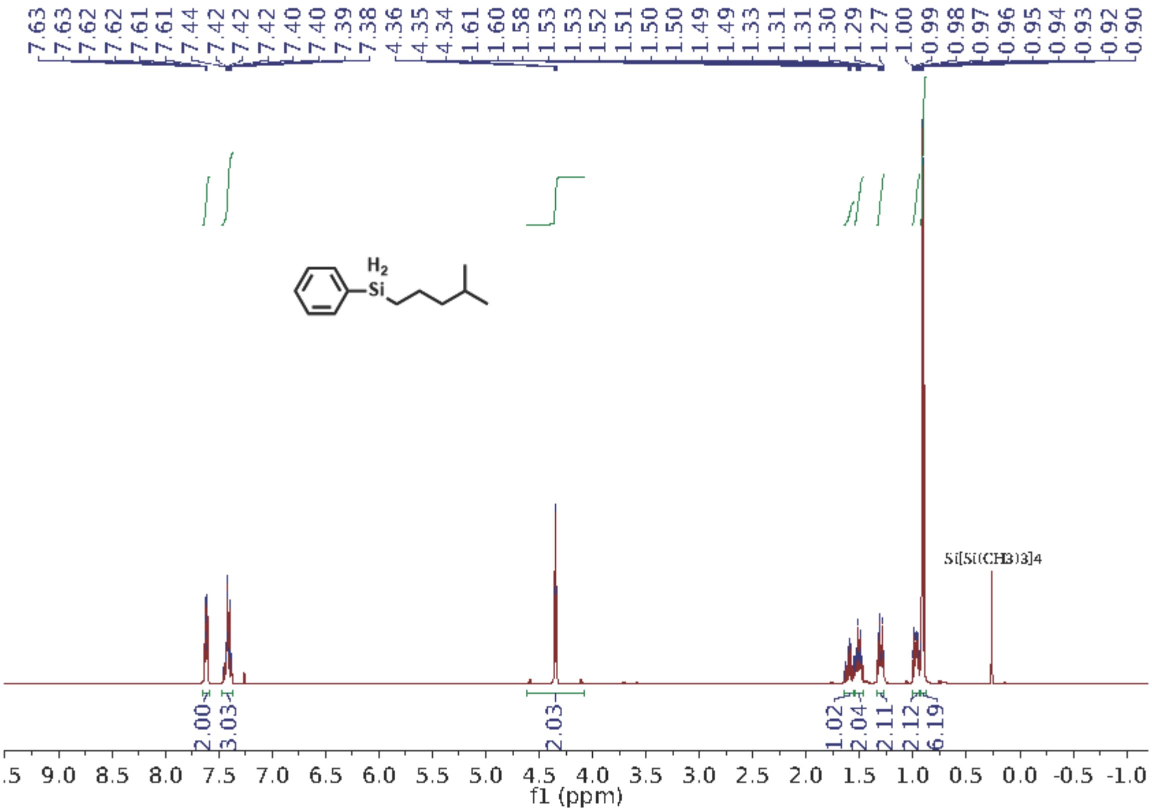
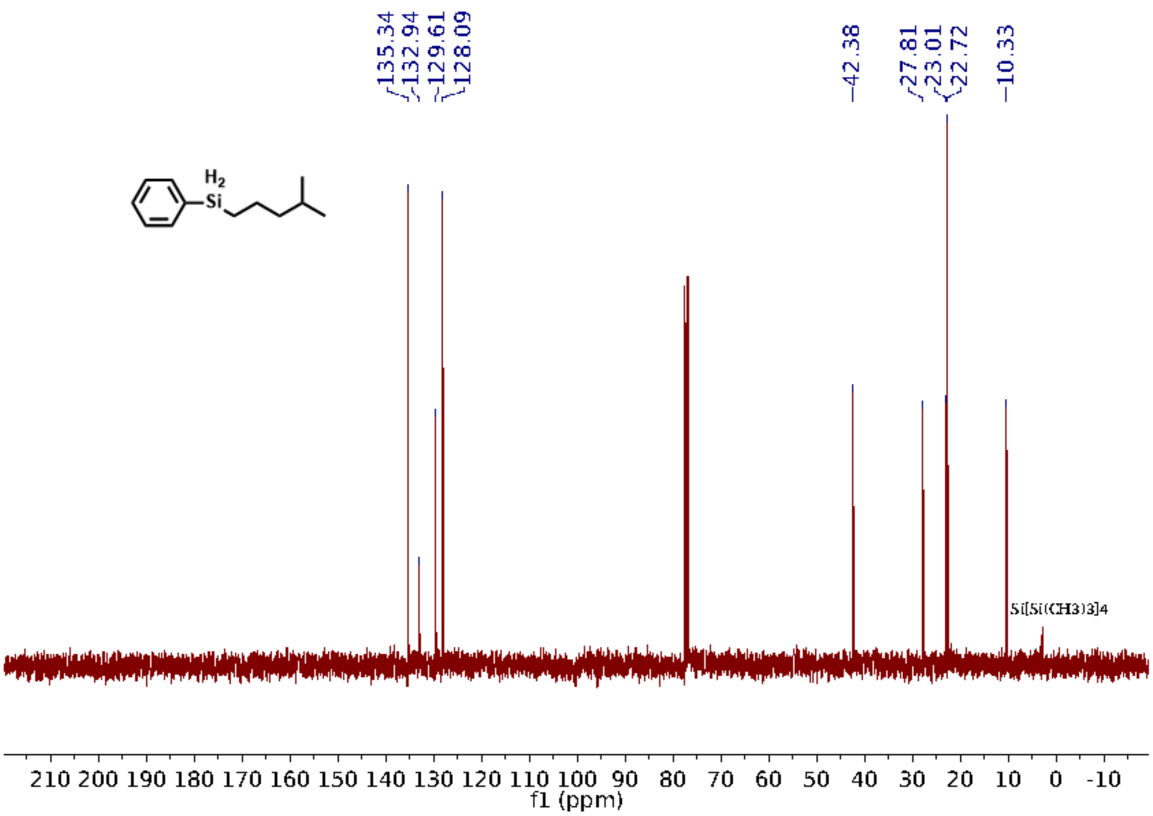
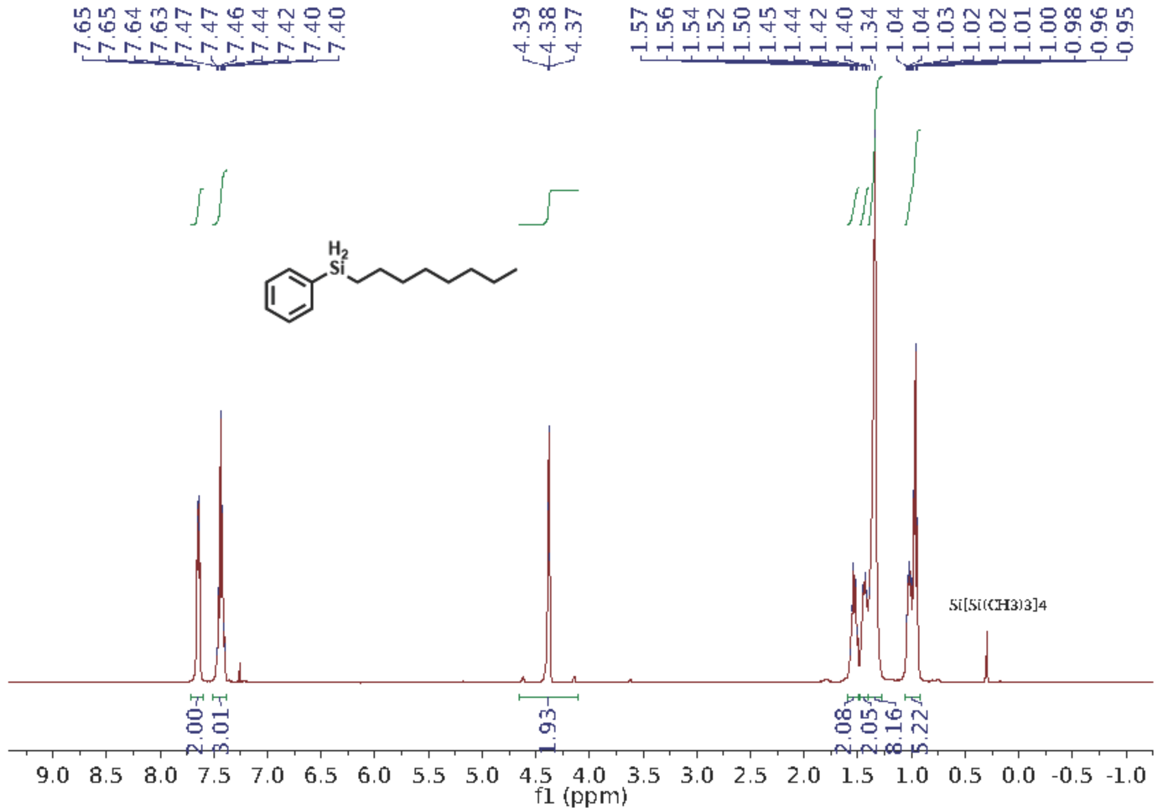
130.29
127.87
125.34
42.44
29.70
27.86
23.33
22.73
16.23
10.59
Et
Si
H2
Si[Si(CH3)3]4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



7.63 7.63 7.62 7.62 7.61 7.61 7.44 7.42 7.42 7.42 7.40 7.40 7.39 7.38 4.36 4.35 4.34 1.61 1.60 1.58 1.53 1.53 1.52 1.51 1.50 1.50 1.49 1.49 1.33 1.31 1.31 1.30 1.29 1.27 1.00 0.99 0.98 0.97 0.96 0.95 0.94 0.93 0.92 0.90
Si[Si(CH3)3]4
2.00 3.03 2.03 1.02 2.04 2.11 2.12 6.19
f1 (ppm)



135.34 132.94 129.61 128.09
42.38
27.81 23.01 22.72
10.33
Si[Si(CH3)3]4
f1 (ppm)



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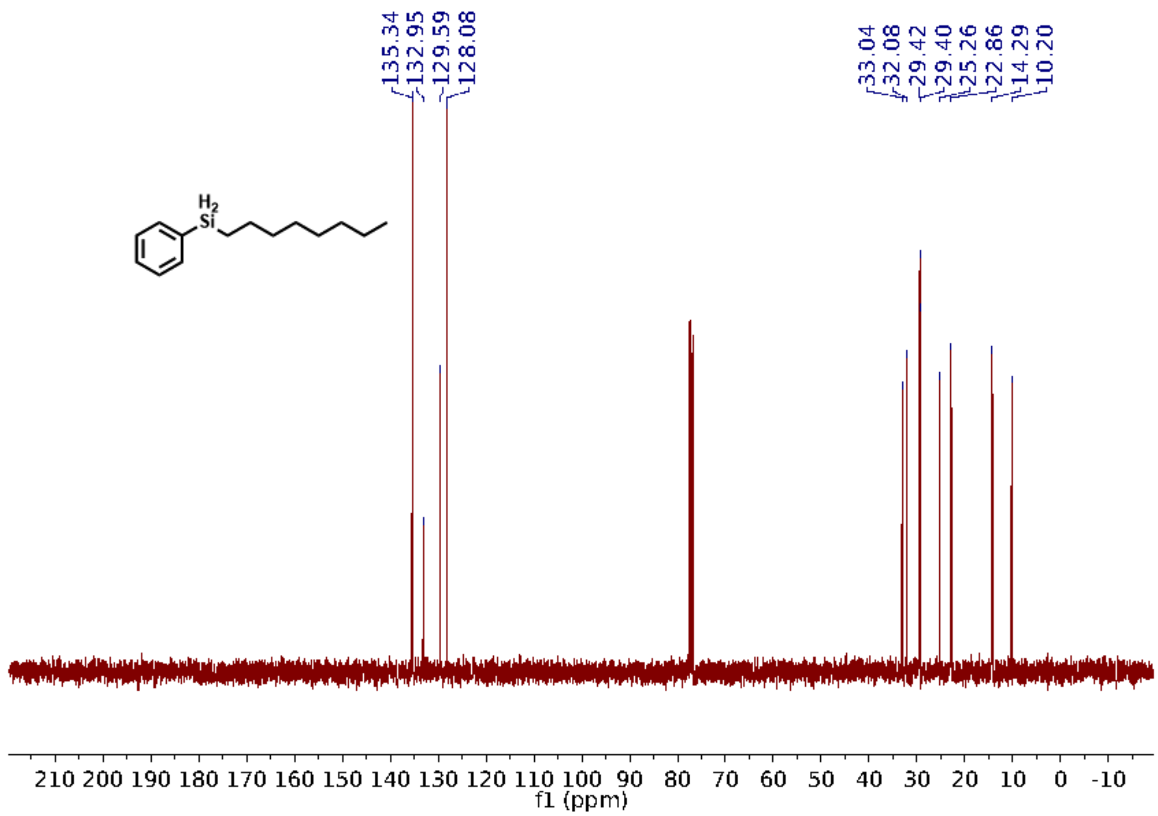
4.39 4.38 4.37
1.57 1.56 1.54 1.52 1.50 1.45 1.44 1.42 1.40 1.34 1.04 1.04 1.03 1.02 1.02 1.01 1.00 0.98 0.96 0.95
Si[Si(CH3)3]4
2.00 3.01 1.93 2.08 2.05 8.16 5.22
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)



135.34 132.95 129.59 128.08
33.04 32.08 29.42 29.40 25.26 22.86 14.29 10.20
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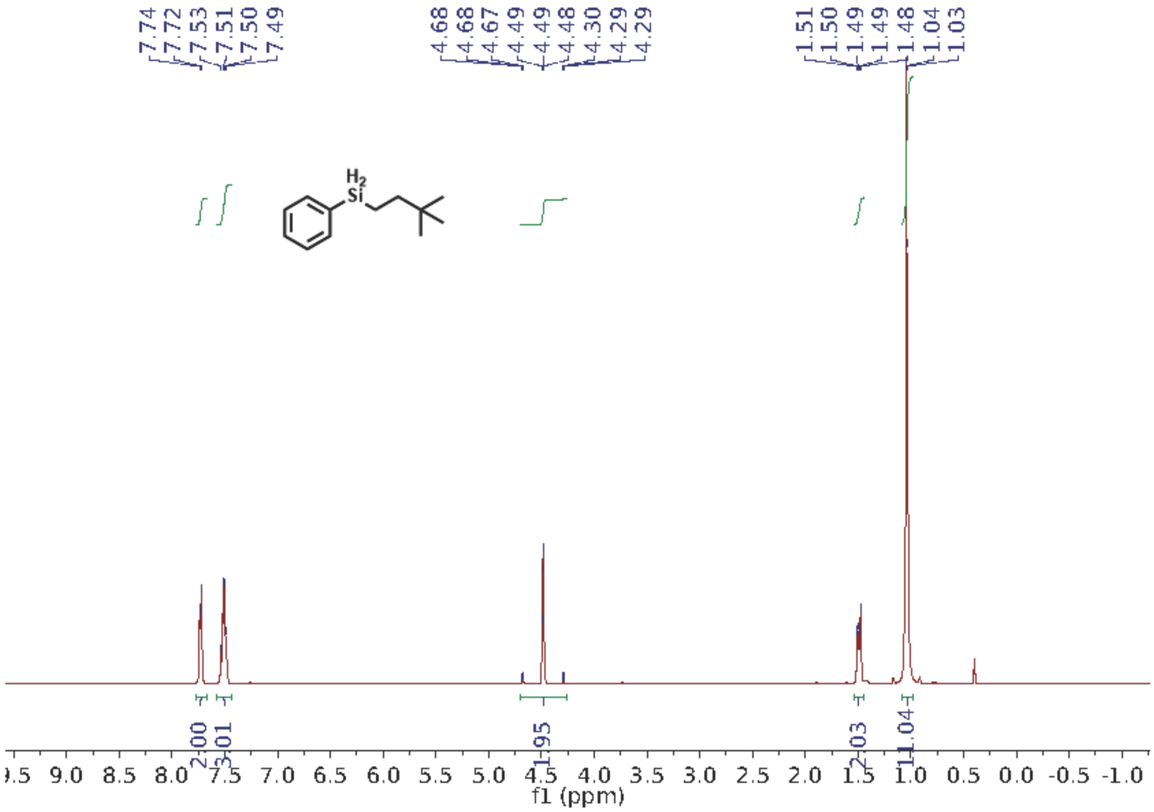
f1 (ppm)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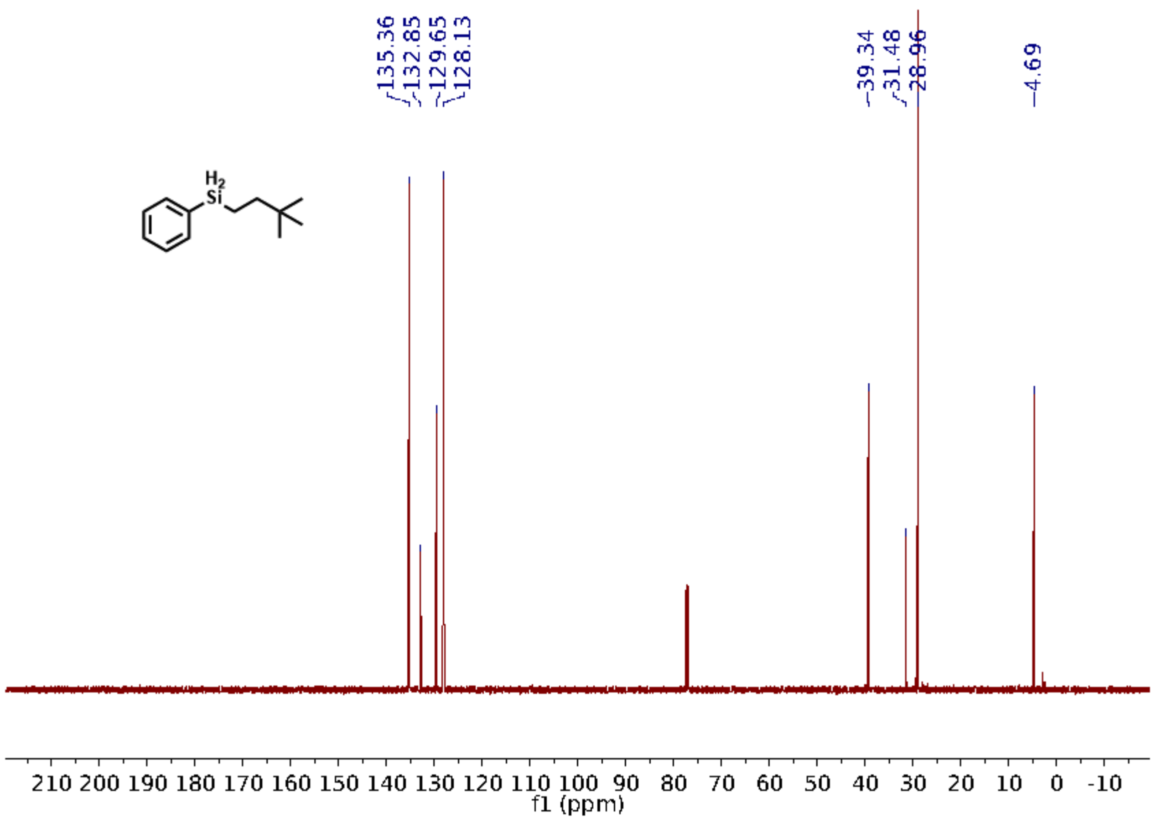
4.30
4.29
4.29
1.51
1.50
1.49
1.49
1.48
1.04
1.03
2.00
3.01
1.95
2.03
11.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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28.96
4.69
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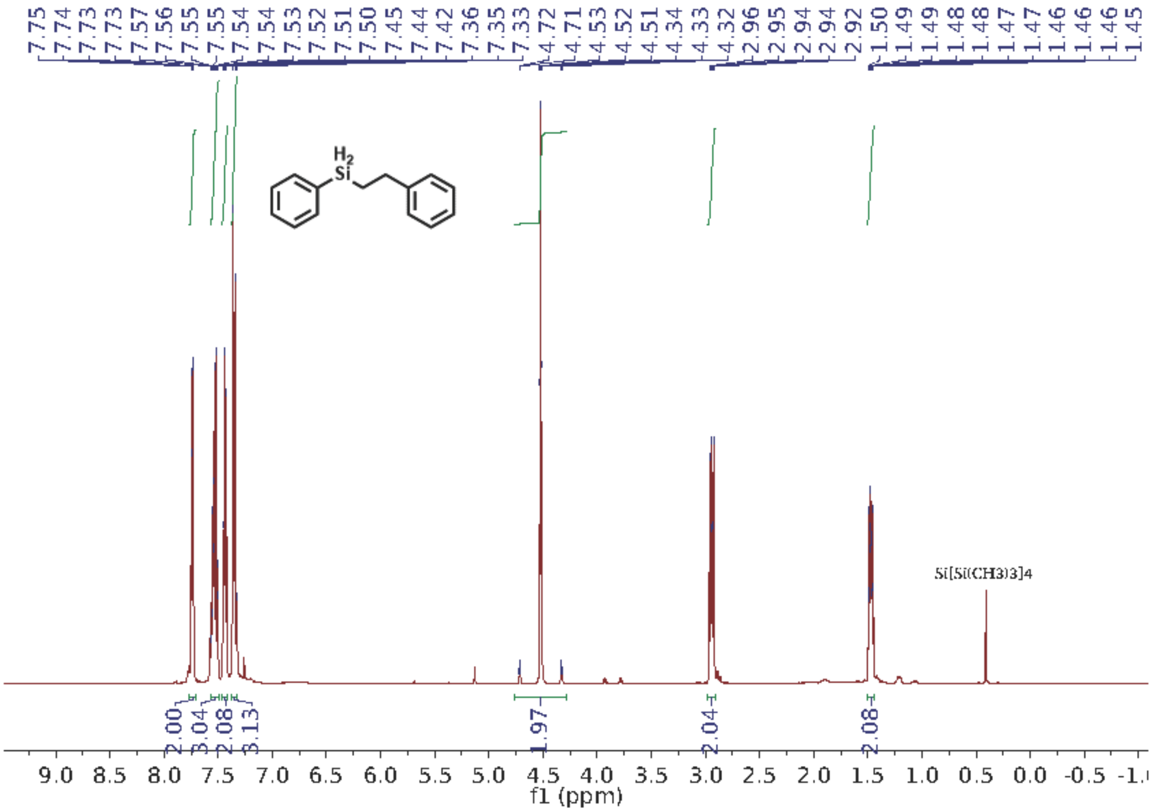
f1 (ppm)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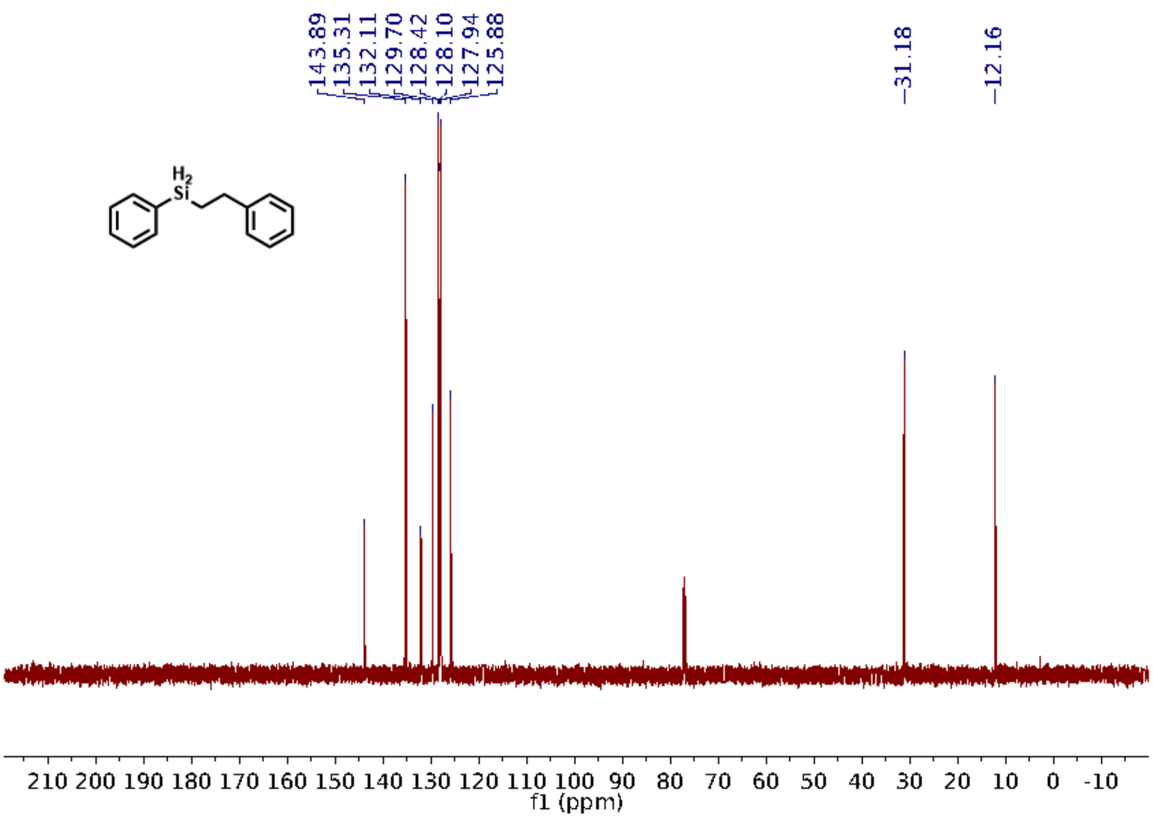
Si[Si(CH3)3]4
2.00 3.04 2.08 3.13 1.97 2.04 2.08
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


143.89 135.31 132.11 129.70 128.42 128.10 127.94 125.88
31.18
12.16
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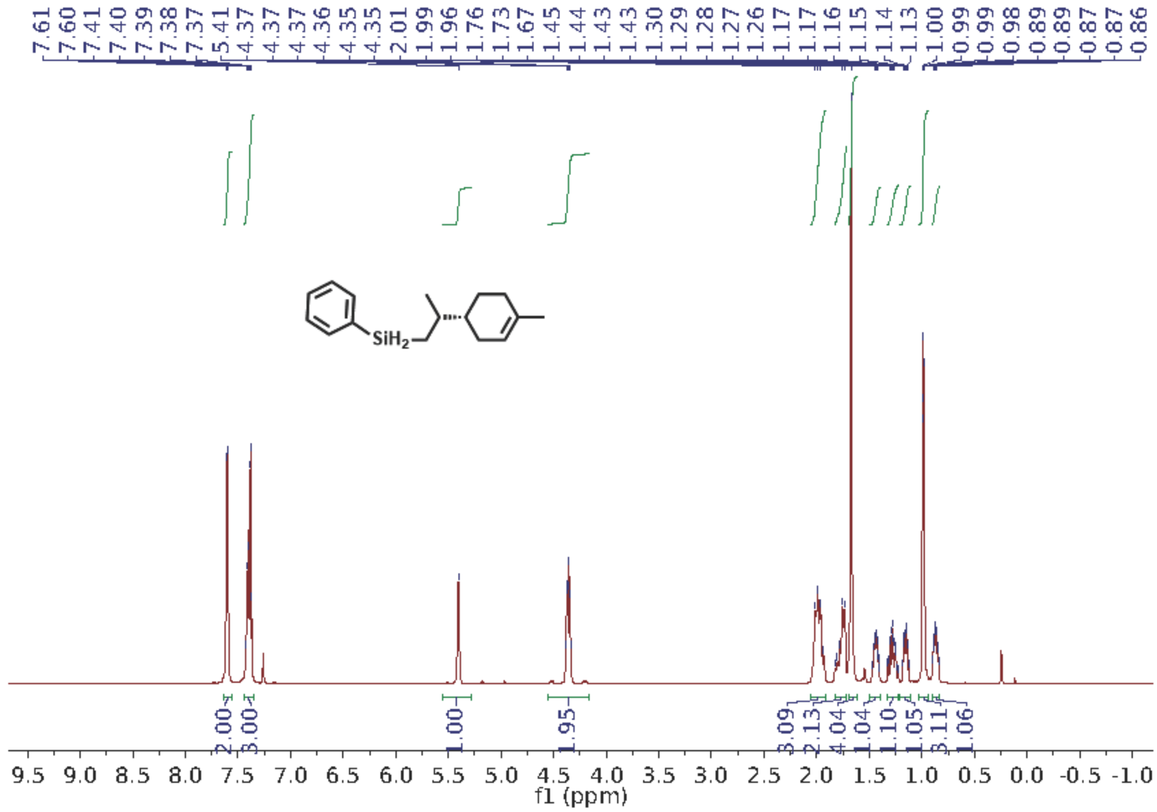
f1 (ppm)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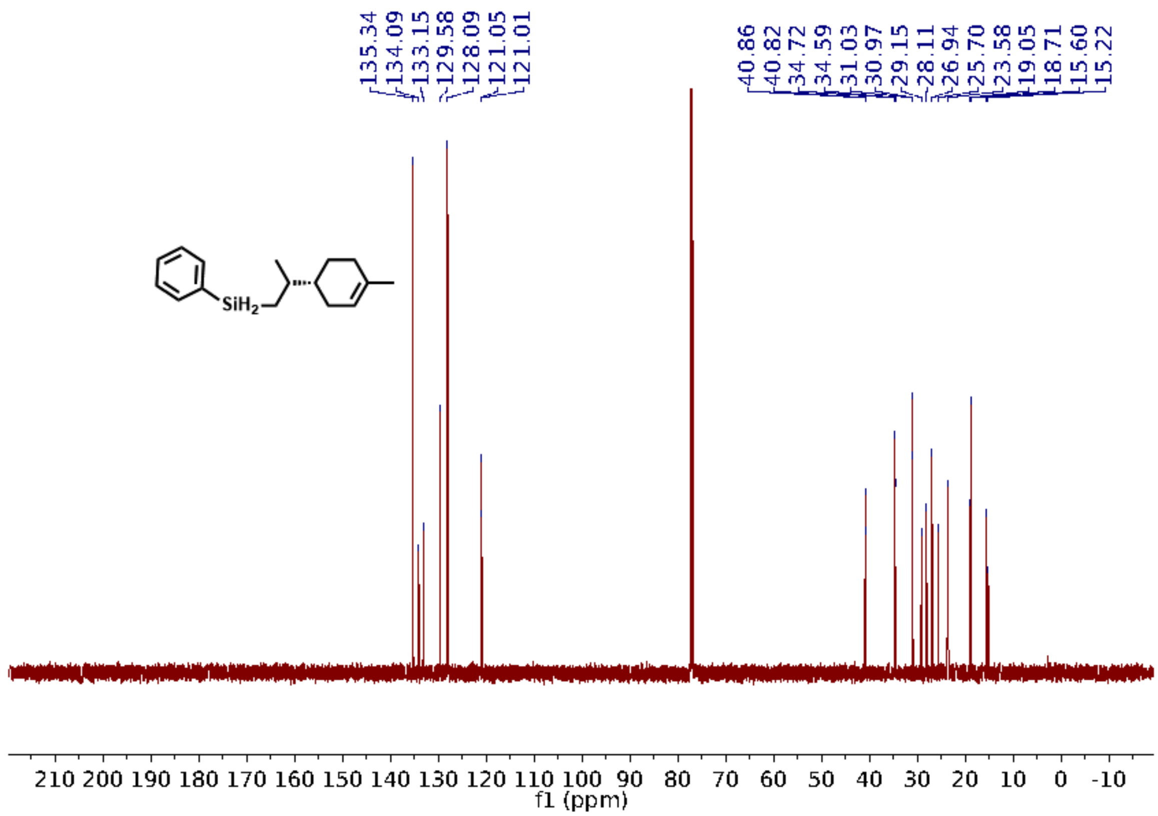
SiH2
2.00 3.00 1.00 1.95 3.09 2.13 4.04 1.04 1.10 1.05 3.11 1.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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40.86 40.82 34.72 34.59 31.03 30.97 29.15 28.11 26.94 25.70 23.58 19.05 18.71 15.60 15.22
SiH2
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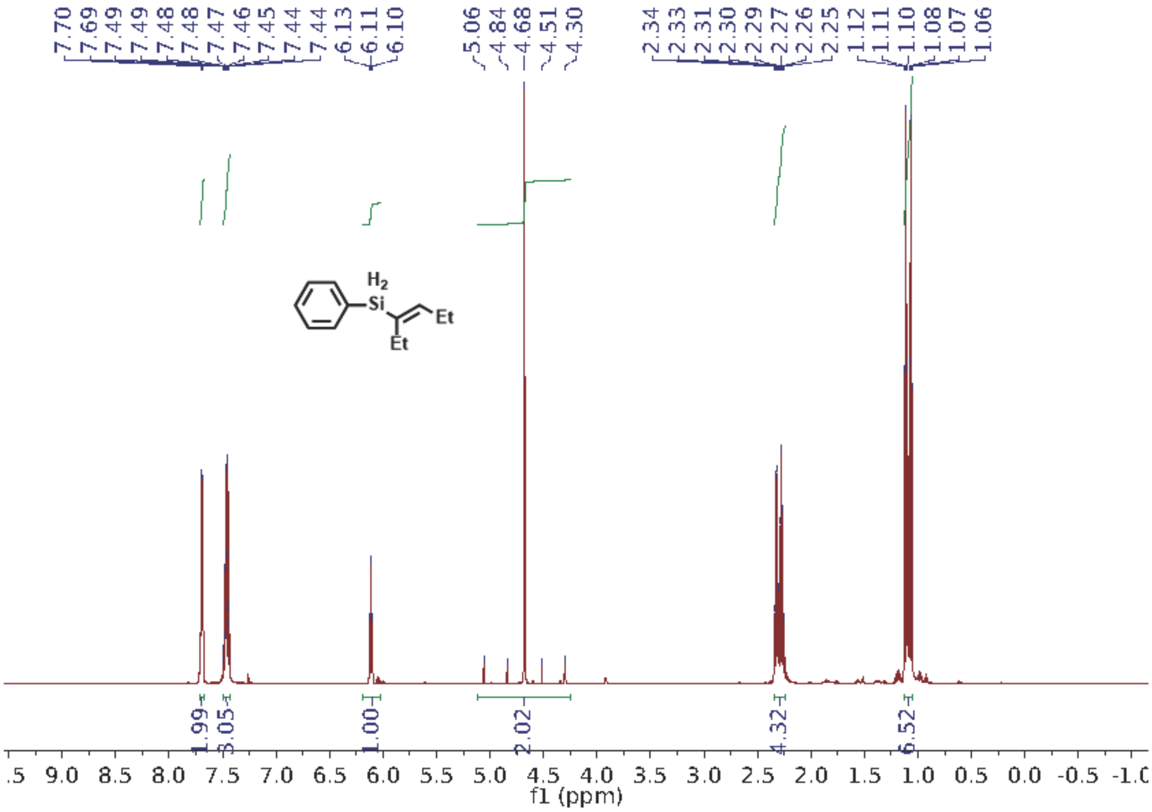
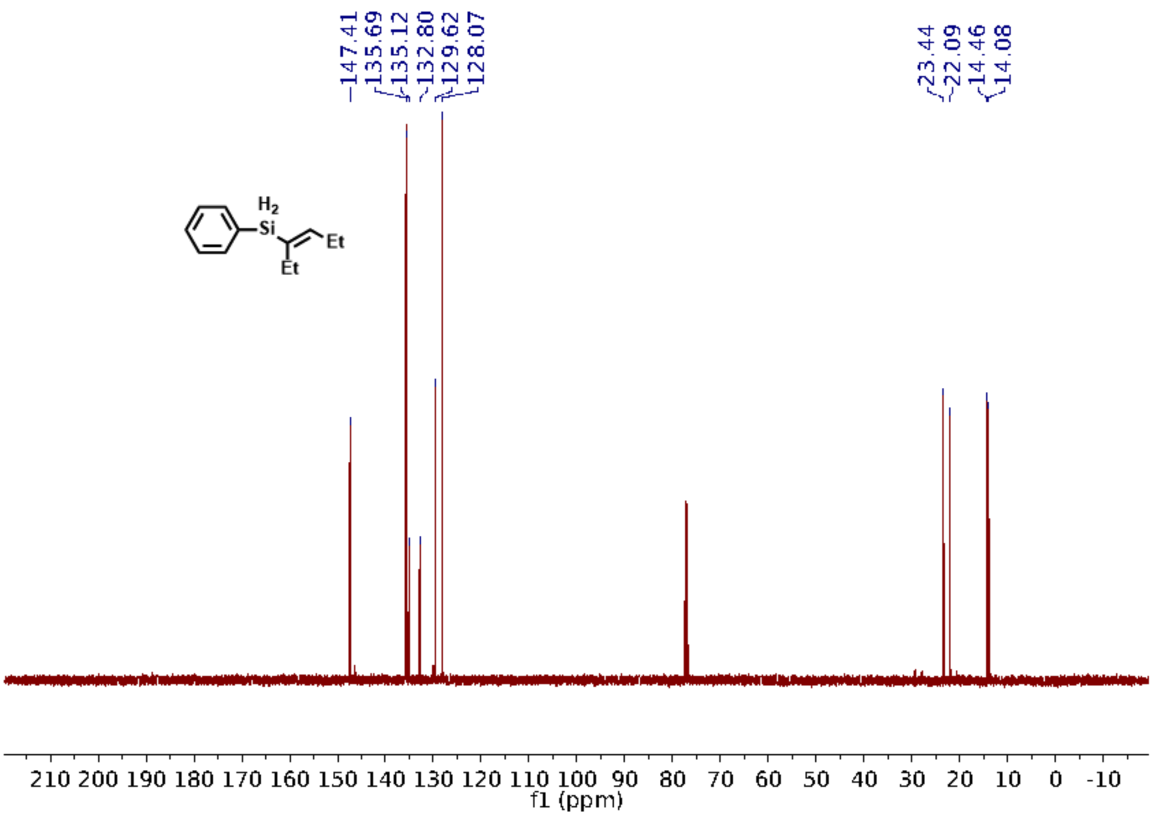
f1 (ppm)


7.70 7.69 7.49 7.49 7.48 7.48 7.47 7.46 7.45 7.44 7.44 6.13 6.11 6.10
5.06 4.84 4.68 4.51 4.30
2.34 2.33 2.31 2.30 2.29 2.27 2.26 2.25 1.12 1.11 1.10 1.08 1.07 1.06
H2
Si
Et
Et
1.99
3.05
1.00
2.02
4.32
6.52
f1 (ppm)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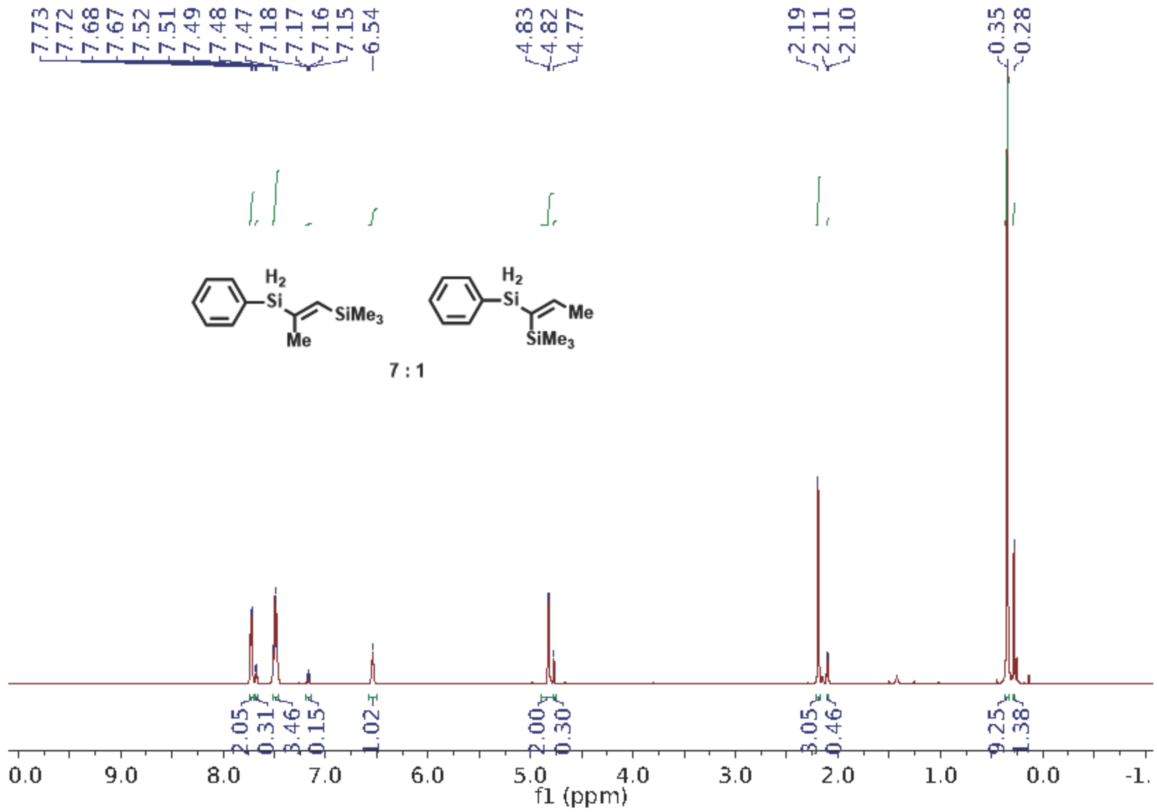
23.44 22.09 14.46 14.08
H2
Si
Et
Et
f1 (ppm)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7.51
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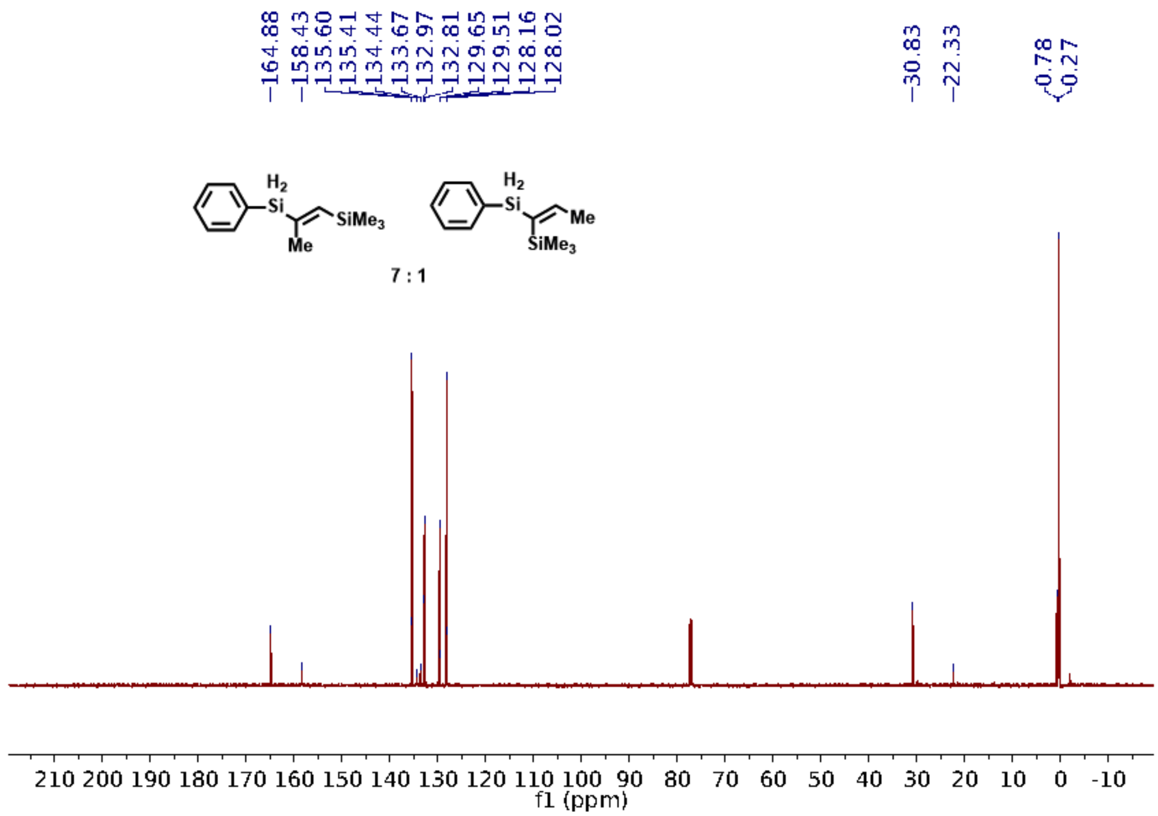
7.48
7.47
7.18
7.17
7.16
7.15
6.54
4.83
4.82
4.77
2.19
2.11
2.10
0.35
0.28
H2
Si
SiMe3
Me
7 : 1
2.05
0.31
3.46
0.15
1.02
2.00
0.30
3.05
0.46
9.25
1.38
f1 (ppm)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133.67
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132.81
129.65
129.51
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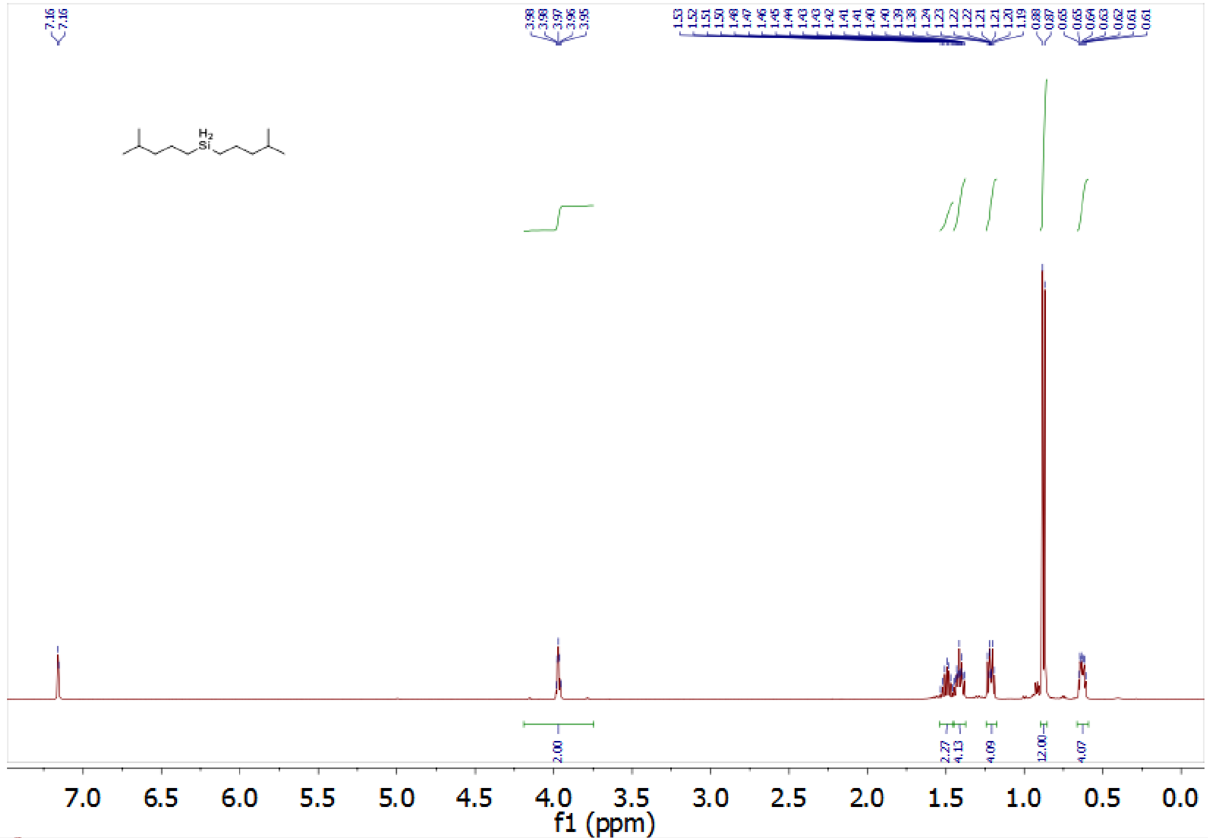
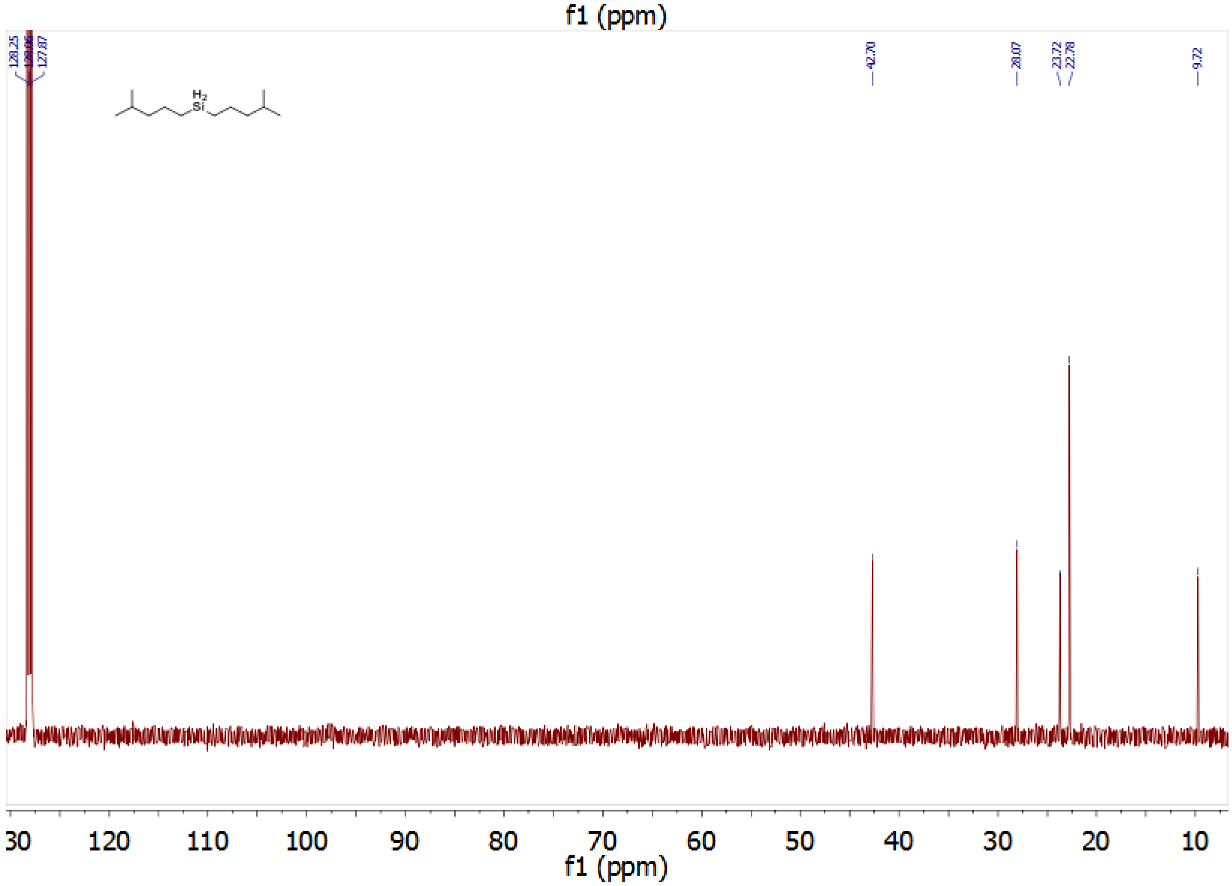
30.83
22.33
0.78
0.27
H2
Si
SiMe3
Me
7 : 1
f1 (ppm)





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