Supporting information

to the manuscript

Multiple coupling of silanes with an imido Mo complex

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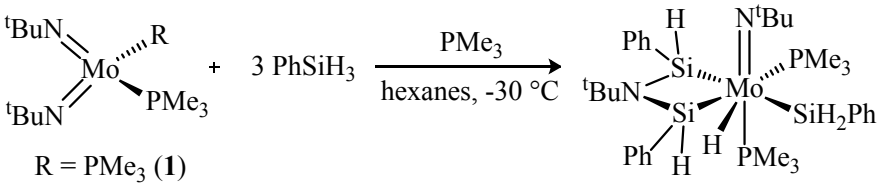
Contents

I. Experimental details

All manipulations were carried out using conventional inert atmosphere glove-box and Schlenk techniques. Dry diethyl ether, toluene, hexanes, and acetonitrile were obtained, using Grubbs-type purification columns, other solvents were dried by distillation from appropriate drying agents. NMR spectra were obtained with a Bruker DPX-300 and Bruker DPX-600 instruments (^{1}H: 300 and 600 MHz; ^{13}C: 75.5 and 151 M

Hz; ^{29}Si: 59.6 and 119.2 MHz; ^{31}P: 121.5 and 243 MHz). NMR spectra weretaken at room temperature unless specified. IR spectra were measured on a Perkin-Elmer 1600 FT-IR spectrometer. Elemental analyses were performed in "ANALEST" laboratories (University of Toronto). Preparation of (^{t}BuN=)$_2$Mo(PMe$_3$)$_2$ (**1**) and (^{t}BuN=)$_2$Mo(PMe$_3$)(η^2-C$_2$H$_4$) (**2**) was reported previously.[1] PhSiH$_3$ and PhSiD$_3$ were prepared from PhSiCl$_3$ by treatment with LiAlH$_4$ or LiAlD$_4$, respectively. Mechanistic studies were carried outunder nitrogen atmosphere, using NMR tubes equipped with Teflon valves.

Preparation of (^{t}BuN=){μ-^{t}BuN(SiHPh)$_2$}Mo(H)(SiH$_2$Ph)(PMe$_3$)$_2$ (3)



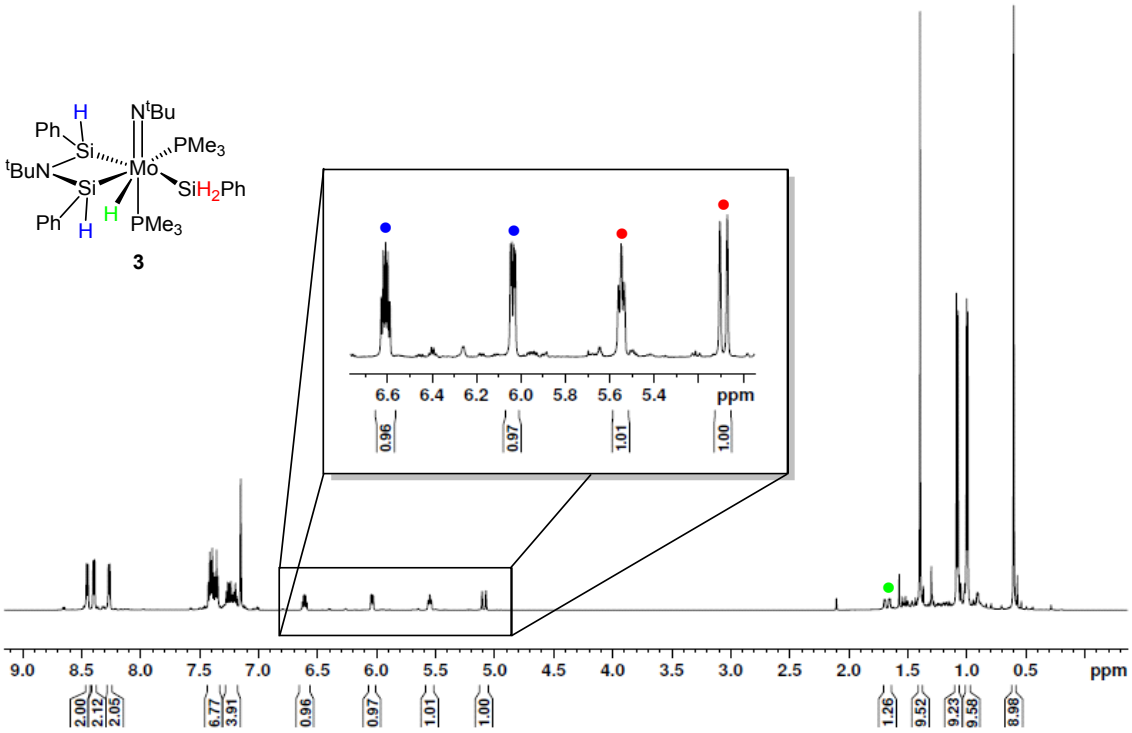
R = PMe$_3$ (**1**)
R = η^2-C$_2$H$_4$ (**2**)

3

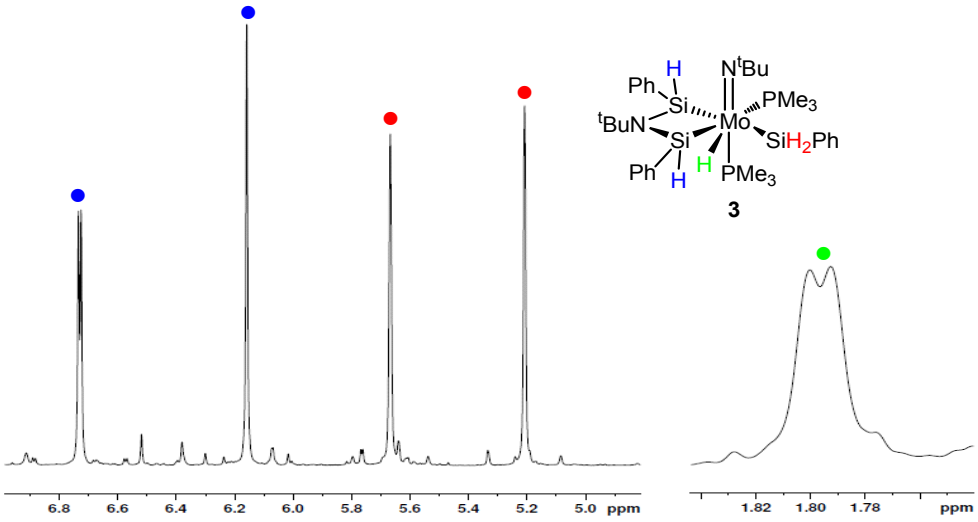
A solution of **1** (300.0 mg, 0.769 mmol) in hexanes (12 mL) was precooled to -30 °C using an acetone/CO$_2$ bath. PhSiH$_3$ (0.19 mL, 1.54) was added in one portion and the mixture stirred for 1 h 20 min at -30 °C. After this time the solution was warmed to 0/-5 °C and all volatiles removed in vacuum to give a light brown powder. Yield: 0.38 g, 82 %. Alternatively, a similar procedure using complex **2** with one equivalent of PMe$_3$ in a hexane/toluene (5:1) mixture can be employed resulting in similar yields and purity.

^{1}H-NMR (600 MHz; Toluene-d$_8$; - 28 °C; δ, ppm): 0.62 (s, 9H, ^{t}*Bu*N), 0.99 (d, $^2J_{P\text{-}H}$ = 6.0 Hz, 9H, P*Me$_3$*), 1.04 (d, $^2J_{P\text{-}H}$ = 7.5 Hz, 9H, P*Me$_3$*), 1.47 (s, 9H, ^{t}*Bu*N), 1.54 (bd, 1H, $^2J_{P\text{-}H}$ = 21.0 Hz, Mo*H*), 5.13 (bd, 1H, $^2J_{P\text{-}H}$ = 19.6 Hz, Si*H$_2$*Ph), 5.60 (dd, 1H, $^3J_{P\text{-}H}$ = 14.9 Hz, $^2J_{H\text{-}H}$ = 7.5 Hz, Si*H$_2$*Ph), 6.03 (dd, 1H, $^3J_{P\text{-}H}$ = 9.6 Hz, $^3J_{P\text{-}H}$ = 3.7 Hz, {(Si*H*Ph)$_2$(*u*-N^{t}Bu)}), 6.67 (ddd, 1H, $^2J_{H\text{-}H}$ = 5.9 Hz, $^3J_{P\text{-}H}$ = 11.6 Hz, $^3J_{P\text{-}H}$ = 17.2 Hz, {(Si*H*Ph)$_2$(*u*-N^{t}Bu)}), 7.26 (m, 2H, *p*-H, Si*Ph*), 7.32 (t, 1H, $^3J_{H\text{-}H}$ = 7.5 Hz, *p*-H, Si*Ph*), 7.40 (t, 2H, $^3J_{H\text{-}H}$ = 7.5 Hz, *m*-H, Si*Ph*), 7.46 (t, 2H, $^3J_{H\text{-}H}$ = 7.5 Hz, *m*-H, Si*Ph*), 7.49 (t, 2H, $^3J_{H\text{-}H}$ = 7.5 Hz, *m*-H, Si*Ph*), 8.32 (bs, 2H, *o*-H, Si*Ph*), 8.48 (d, 2H, $^3J_{H\text{-}H}$ = 6.6 Hz, *o*-H, Si*Ph*), 8.54 (d, 2H, $^3J_{H\text{-}H}$ = 6.7 Hz, *o*-H, Si*Ph*).**^{1}H-NMR** (600 MHz; Toluene-d$_8$; 22 °C; δ, ppm): 0.61 (s, 9H, ^{t}*Bu*N), 1.05 (d, $^2J_{P\text{-}H}$ = 6.4 Hz, P*Me$_3$*), 1.14 (d, 9H, $^2J_{P\text{-}H}$ = 7.7 Hz, P*Me$_3$*), 1.39 (s, 9H, ^{t}*Bu*N), 1.50 (bd, 1H, $^2J_{P\text{-}H}$ = 21.0 Hz, Mo*H*), 5.05 (d, 1H, $^3J_{P\text{-}H}$ = 19.4 Hz, Si*H$_2$*Ph), 5.50 (bddd, 1H, $^3J_{P\text{-}H}$ = 15.9 Hz, $^2J_{H\text{-}H}$

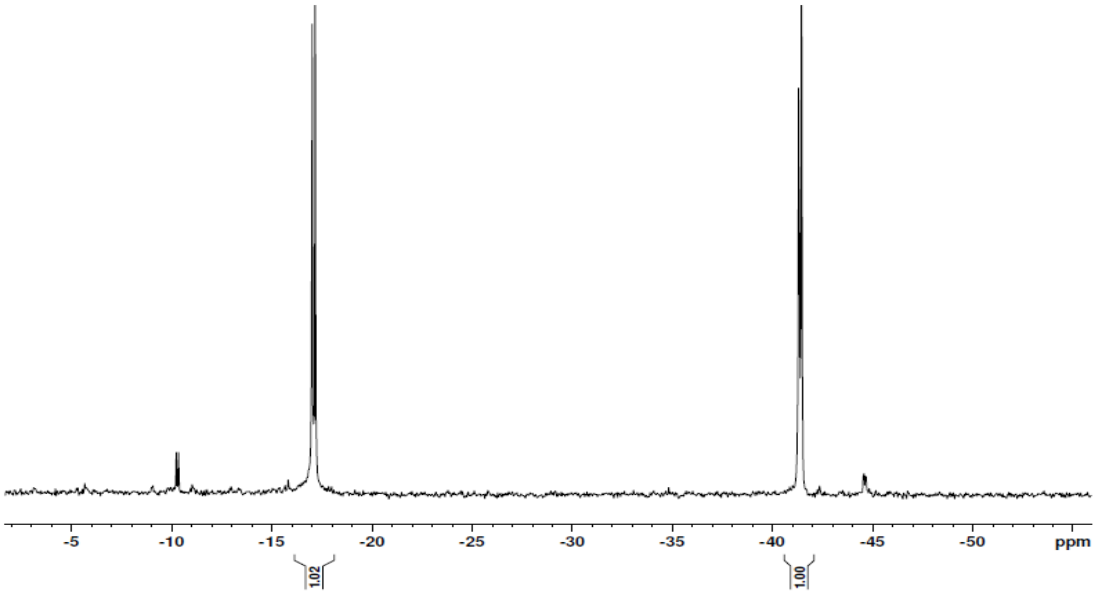
= 7.4 Hz, SiH_2Ph), 6.04 (dd, 1H, $^3J_{P\text{-}H}$ = 3.7 Hz, $^3J_{P\text{-}H}$ = 9.2 Hz, {(Si*H*Ph)$_2$(*u*-N^{t}Bu)}), 6.59 (ddd, 1H,$^2J_{H\text{-}H}$= 5.8 Hz, $^3J_{P\text{-}H}$= 11.6 Hz, $^3J_{P\text{-}H}$= 17.5 Hz, {(Si*H*Ph)$_2$(*u*-N^{t}Bu)}),7.23 (m, 3H, *p*-H, Si*Ph*),7.36 (t, 2H, $^3J_{H\text{-}H}$= 7.3 Hz, *m*-H, Si*Ph*),7.40 (t, 4H, $^3J_{H\text{-}H}$= 7.0 Hz, *m*-H, Si*Ph*),8.25 (d, 2H, $^3J_{H\text{-}H}$= 7.0 Hz, *o*-H, Si*Ph*),8.37 (d, 2H, $^3J_{H\text{-}H}$= 7.3 Hz, *o*-H, Si*Ph*),8.39 (d, 2H, $^3J_{H\text{-}H}$= 7.3 Hz, *o*-H, Si*Ph*). **^{1}H{^{31}P}-NMR** (600 MHz, Toluene-d_8, 22 °C, δ, ppm, selected signals): 6.59 (d, 1H, $^2J_{H\text{-}H}$ = 5.9 Hz, {(Si*H*Ph)$_2$(*u*-N^{t}Bu)}), 6.04 (s, 1H, {(Si*H*Ph)$_2$(*u*-N^{t}Bu)}), 5.49 (s, 1H, SiH_2Ph), 5.05 (s, 1H, SiH_2Ph), 1.55 (d, 1H, $^2J_{H\text{-}H}$= 5.9 Hz, Mo*H*). **^{31}P{^{1}H}-NMR** (243.0 MHz, Toluene-d_8, -28 °C, δ, ppm): -40.2 (d, $^2J_{P\text{-}P}$= 34.5 Hz, *P*Me$_3$), -16.3 (d, $^2J_{P\text{-}P}$= 34.5 Hz, *P*Me$_3$). **^{31}P{^{1}H}-NMR** (121.5 MHz, Toluene-d_8, 22 °C, δ, ppm): -41.5 (d, $^2J_{P\text{-}P}$= 32.0 Hz, *P*Me$_3$), -17.2 (d, $^2J_{P\text{-}P}$= 34.5 Hz, *P*Me$_3$). **^{29}Si INEPT+** (119.2 MHz, Toluene-d_8, -28 °C, *J* = 180 Hz, δ, ppm): -14.3 (tdd, $^1J_{Si\text{-}H}$ = 154.4 Hz, $^2J_{Si\text{-}P}$ = 25.0 Hz, $^2J_{Si\text{-}P}$ = 28.6 Hz, *Si*H$_2$Ph), -5.0 (d, $^1J_{Si\text{-}H}$ = 186.0 Hz,{(*Si*HPh)$_2$(*u*-N^{t}Bu)}), 1.4 (ddd, $^1J_{Si\text{-}H}$ = 166.9 Hz, $^2J_{Si\text{-}P}$ = 25.0 Hz, $^2J_{Si\text{-}P}$ = 20.3 Hz, {(*Si*HPh)$_2$(*u*-N^{t}Bu)}). **^{29}Si RF INEPT NMR** (119.2 MHz, Toluene-d_8, -18 °C, *J* = 180 Hz, δ, ppm): 1.4 (dd, $^2J_{Si\text{-}P}$ = 16.7 Hz, $^2J_{Si\text{-}P}$ = 28.6 Hz, {(*Si*HPh)$_2$(*u*-N^{t}Bu)}, "up"), -5.1 (d, $^2J_{Si\text{-}P}$ = 10.7 Hz, {(*Si*HPh)$_2$(*u*-N^{t}Bu)}, "up"), -14.7 (t, $^2J_{Si\text{-}P}$ = 23.8 Hz, *Si*H$_2$Ph, "down"). **^{1}H-^{31}P HSQC JC NMR** (243.0 Hz, Toluene-d$_8$; -20 °C; *J* = 15 Hz; ^{1}H projection; δ, ppm): 1.6 (d, $^2J_{H\text{-}P}$ = 30.0 Hz, {(Si*H*Ph)$_2$(*u*-N^{t}Bu)}). **^{13}C{^{1}H]-NMR** (151 MHz; Toluene-d$_8$; - 28 °C; δ, ppm): 14.9 (d, $^1J_{C\text{-}P}$ = 18.1 Hz, P*Me$_3$*), 19.1 (d, $^1J_{C\text{-}P}$ = 24.1 Hz, P*Me$_3$*), 30.3 (s, *C*H$_3$, ^{t}BuN), 31.7 (s, *C*H$_3$, ^{t}*Bu*N), 34.8 (s, *C*H$_3$, ^{t}BuN=Mo), 54.7 (s, *C*(CH$_3$)$_3$, N^{t}Bu), 127.3 (s, *m*-C, Si*Ph*), 127.5 (s, *m*-C, Si*Ph*), 128.1 (s, *m*-C, Si*Ph*), 128.2 (s, *p*-C, Si*Ph*), 128.4 (s, *p*-C, Si*Ph*), 133.9 (s, *o*-C, Si*Ph*), 137.1 (s, *o*-C, Si*Ph*), 137.8 (s, *o*-C, Si*Ph*), 143.2 (s, *i*-C, Si*Ph*), 147.8 (s, *i*-C, Si*Ph*), 148.8 (s, *i*-C, Si*Ph*). **IR (nujol)**: 1825 cm^{-1} (medium, Mo-H), 1890 cm^{-1} (strong, Si-H), 2037 cm^{-1} (strong, Si-H), 2142 (strong, Si-H). **Elem. Anal.** (%): calc for $C_{32}H_{56}MoN_2P_2Si_3$ (710.945) C 54.06, H 7.94, N 3.94; found C 53.99 H 7.87, N 4.22.



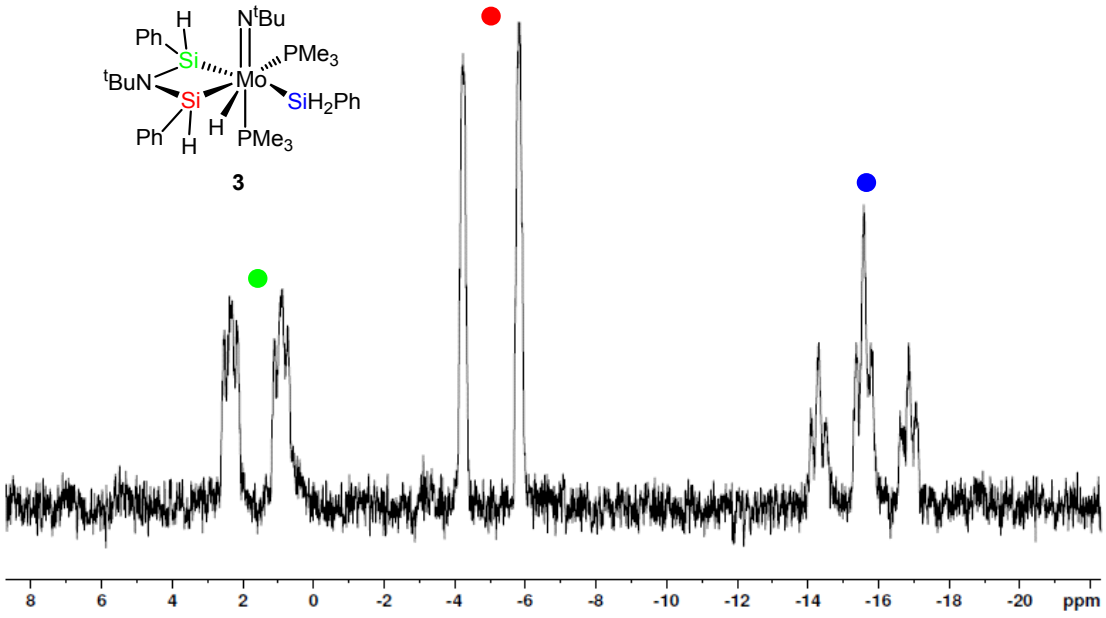
^{1}H-NMR (600 MHz, Toluene-d_8, -40°C)



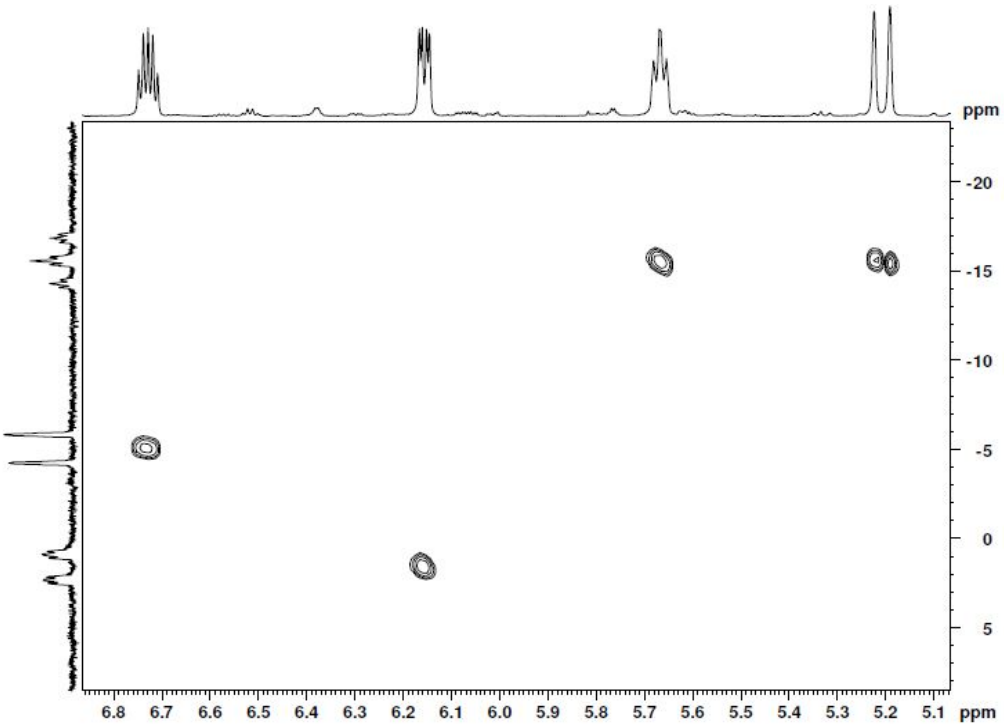
^{1}H{^{31}P}-NMR (600 MHz, Toluene-d_8, -40°C)



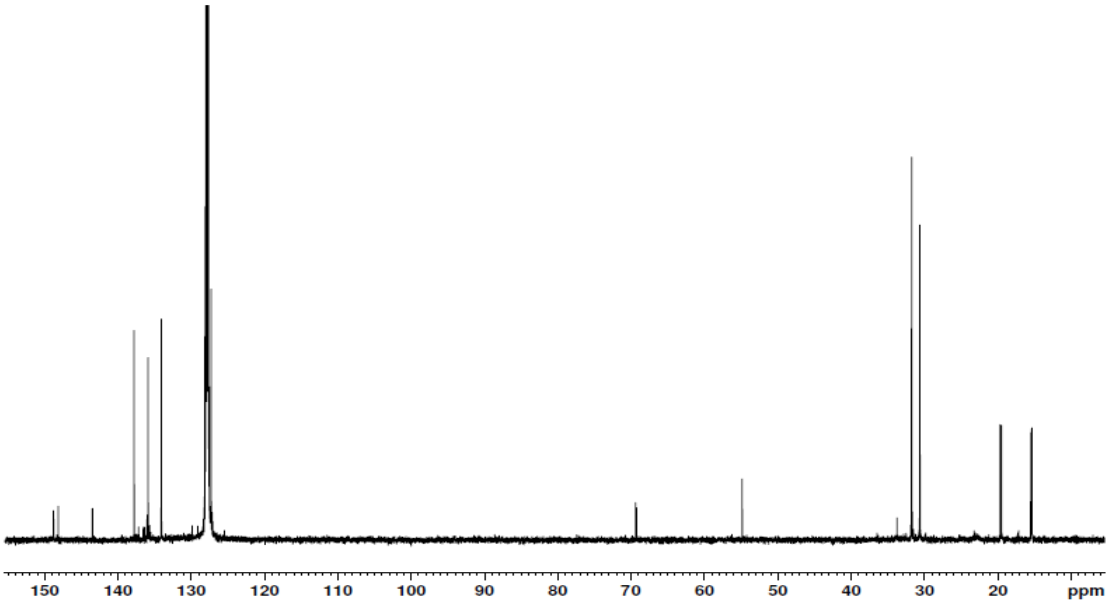
$^{31}P\{^{1}H\}$-NMR (243.0 MHz, Toluene-d_8, -40°C)



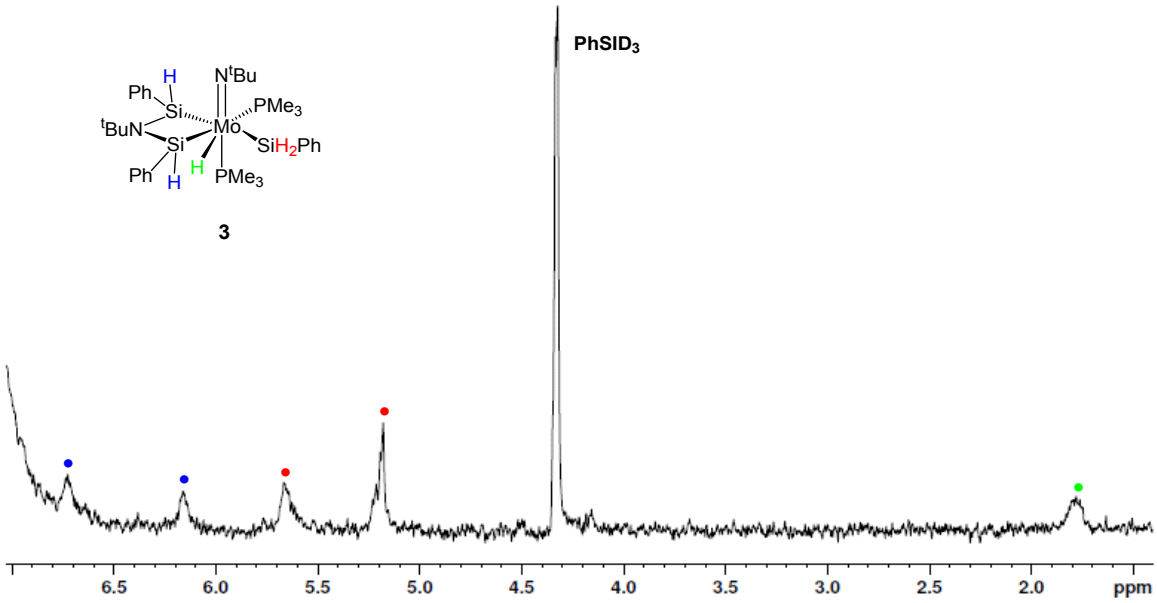
^{29}Si INEPT+ NMR (119.2 MHz, Toluene-d_8, -40 °C)



^{1}H-^{29}Si HSQC(600 MHz / 119.2 MHz, Toluene-d_8, -40 °C, J = 200 Hz**)**



^{13}C{^{1}H}-NMR(151 MHz, Toluene-d_8, -40 °C)



^{2}H-NMR (600 MHz, Toluene-d_8, RT, 30 minutes after addition of $PhSiD_3$)

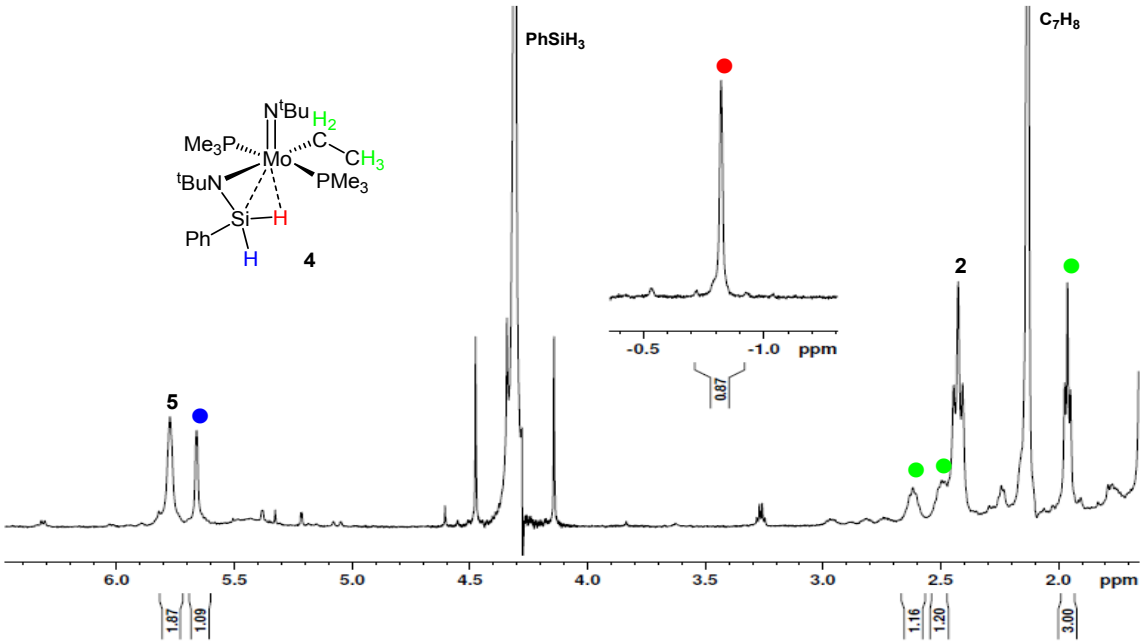
General Procedure for Addition of Silane

To a solution of (^{t}BuN=)Mo(PMe_3)(L) (L = PMe_3 (**1**), η^2-CH_2CH_2 (**2**))intoluene-d_8, $PMe_3$was added in one portion at room temperature. The sample was cooled to -196 °C using liquid nitrogen on a Schlenk line and $PhSiH_3$was directly added. The sample was quickly removed from the liquid nitrogen and inverted once, then immediately placed back. The sample was then placed into a pre-cooled NMR machine at the appropriate temperature and monitored at various temperatures. In some cases, the sample was allowed to react for 2-4 hours at -40 °C, then monitored by NMR at the appropriate temperature.

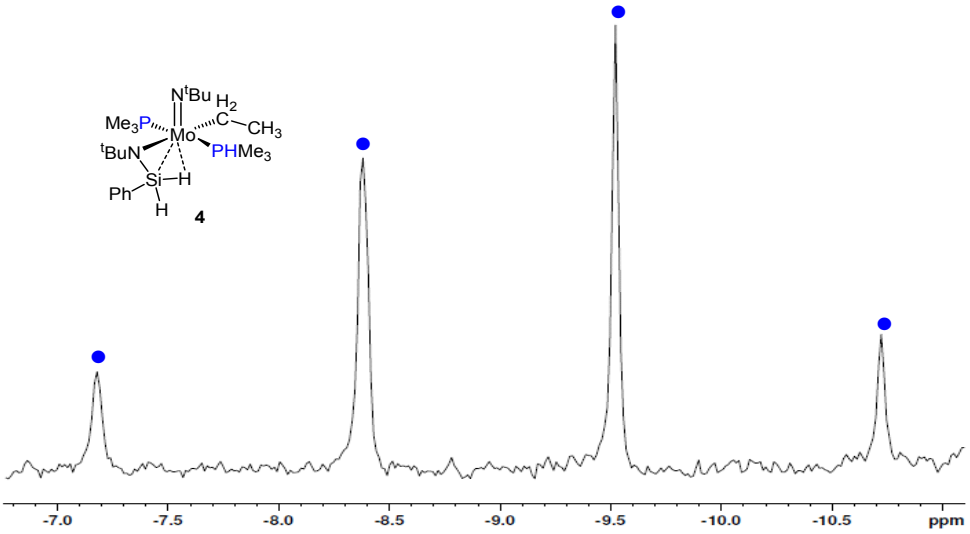
(^{t}BuN=)Mo(η^3-N^{t}Bu-SiHPh-H)(PMe_3)$_2$(Et) (4)

^{1}H-NMR (600 MHz, Toluene-d_8, -53 °C, δ, ppm): -0.82 (s, 1H, Si-H$_{agostic}$, $^{1}J_{Si\text{-}H}$ = 125.1 Hz, found by ^{1}H-^{29}Si HSQC 1D JC), 1.03 (s, 9H, 3 CH_3, ^{t}*Bu*N=Mo), 1.10 (s, 9H, 3 CH_3, Mo-N^{t}*Bu*-SiH_2Ph), 1.32 (d, 9H, PMe_3, $^{2}J_{H\text{-}P}$ = 5.22 Hz), 1.43 (d, 9H, PMe_3, $^{2}J_{H\text{-}P}$ = 5.28 Hz), 1.96 (t, 3H, CH_3, Mo-CH_2-C*H*$_3$, $^{3}J_{H\text{-}H}$ = 7.53 Hz), 2.50 (m, 1H, Mo-C*H*$_2$-CH_3), 2.61 (m, 1H, Mo-C*H*$_2$-CH_3), 5.66 (s, 1H, Si-*H*$_{class}$, $^{1}J_{Si\text{-}H}$ = 212.0 Hz, found by ^{1}H-^{29}Si HSQC 1D JC), 7.27 (m, 2H, *m*-Ph), 7.96 (d, 2H, *o*-Ph, $^{3}J_{H\text{-}H}$ = 6.9 Hz).**^{31}P{^{1}H}-NMR** (243.0 MHz, Toluene-d_8, -53 °C, δ, ppm): -7.78 (d, 1P, PMe_3, $^{2}J_{P\text{-}P}$ = 291.7 Hz), -10.12 (d, 1P, PMe_3, $^{2}J_{P\text{-}P}$ = 291.8 Hz).**^{1}H-**

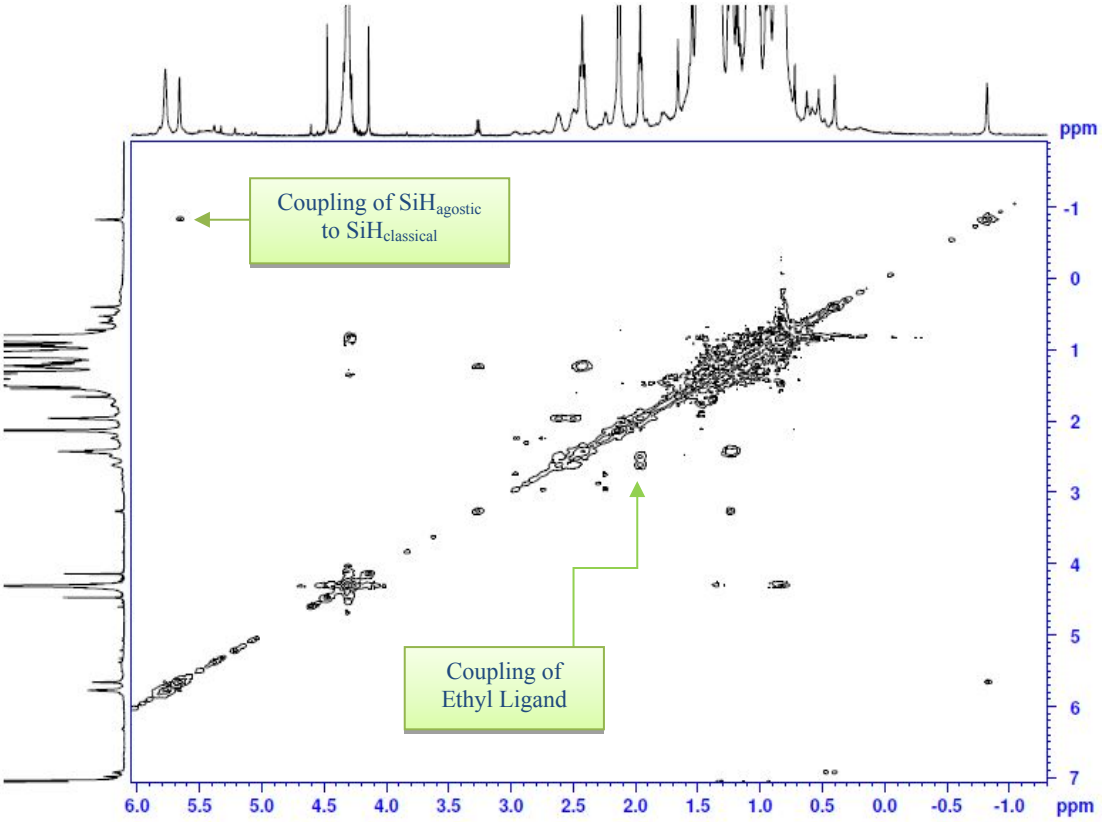
^{29}Si HSQC NMR (119.0 MHZ, Toluene-d_8; -53 °C; J = 150 Hz; ^{29}Si projection, δ, ppm): -75.4 (Mo-N^{t}Bu-*Si*H$_2$Ph).



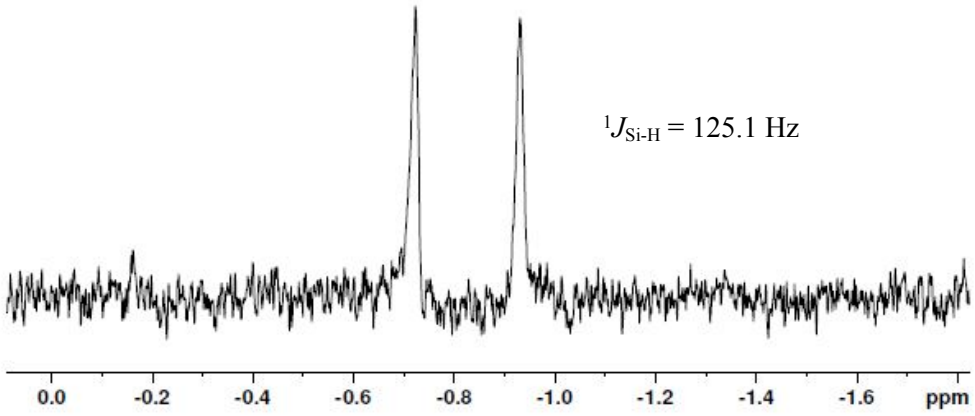
^{1}H-NMR (600 MHz, Toluene-d_8, -53 °C, after 3 hours at -40 °C; **5** – (^{t}BuN=)Mo(η^3-N^{t}Bu-SiHPh-H)(PMe$_3$)$_2$(SiH$_2$Ph))



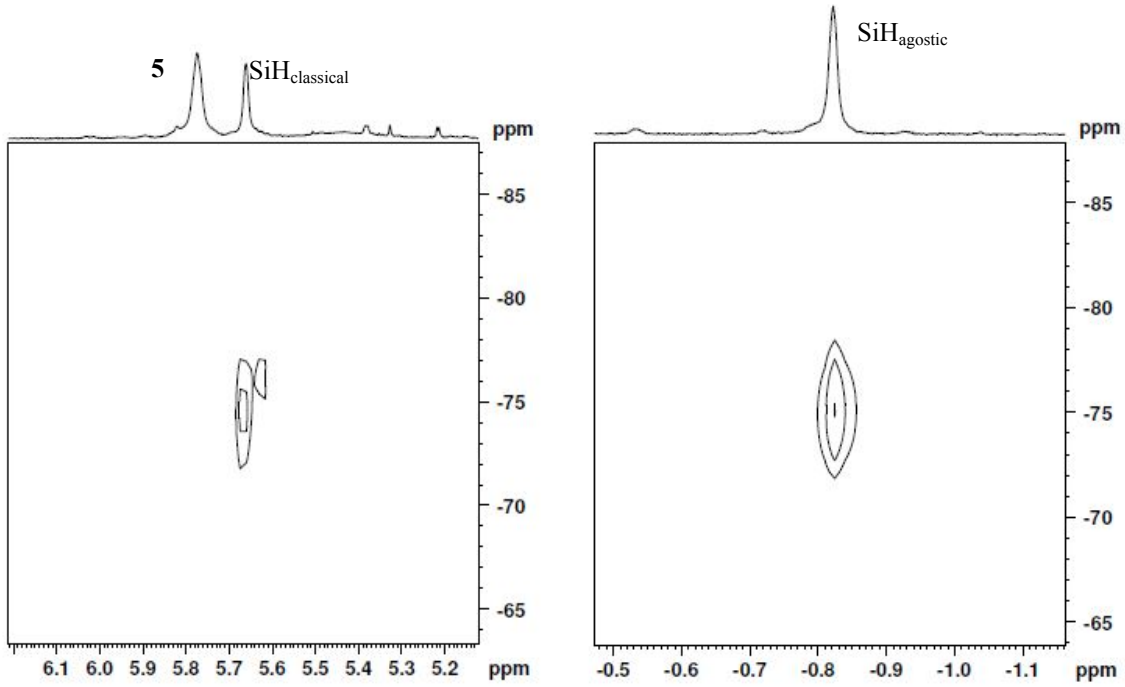
^{31}P{^{1}H}-NMR (243.0 MHz, Toluene-d_8, -53 °C, after 3 hours at -40 °C)



^{1}H-^{1}H COSY (600 MHz, Toluene-$d_{8,}$ -53 °C, after 3 hours at -40 °C)



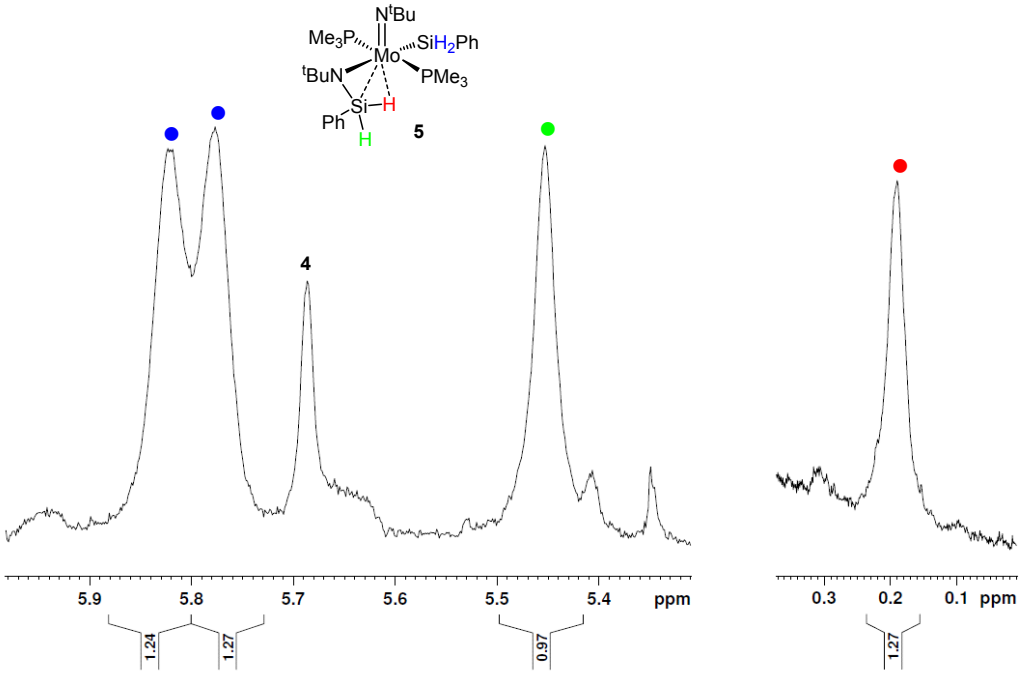
^{1}H-^{29}Si HSQC 1D JC (600 MHz / 119.2 MHz, -53 °C, after 3 hours at -40 °C)



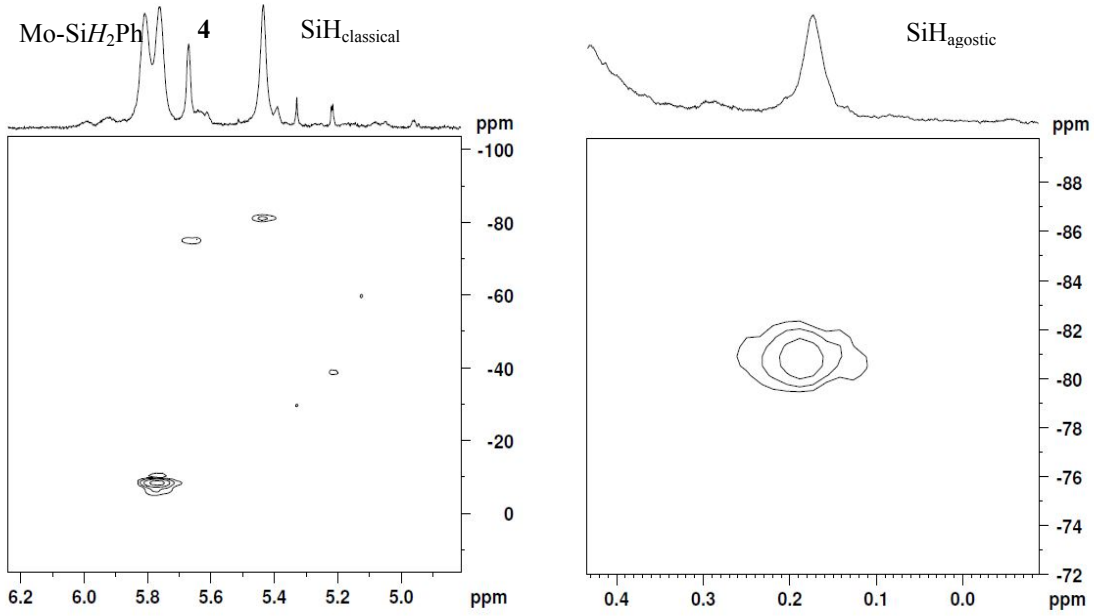
^{1}H-^{29}Si HSQC (600 MHz / 119.2 MHz, Toluene-d_8, -53 °C, after 3 hours at -40 °C; **5** – (^{t}BuN=)Mo(η^3-N^{t}Bu-SiHPh-H)(PMe$_3$)$_2$(SiH$_2$Ph))

(^{t}BuN=)Mo(η^3-N^{t}Bu-SiHPh-H)(PMe$_3$)$_2$(SiH$_2$Ph) (5)

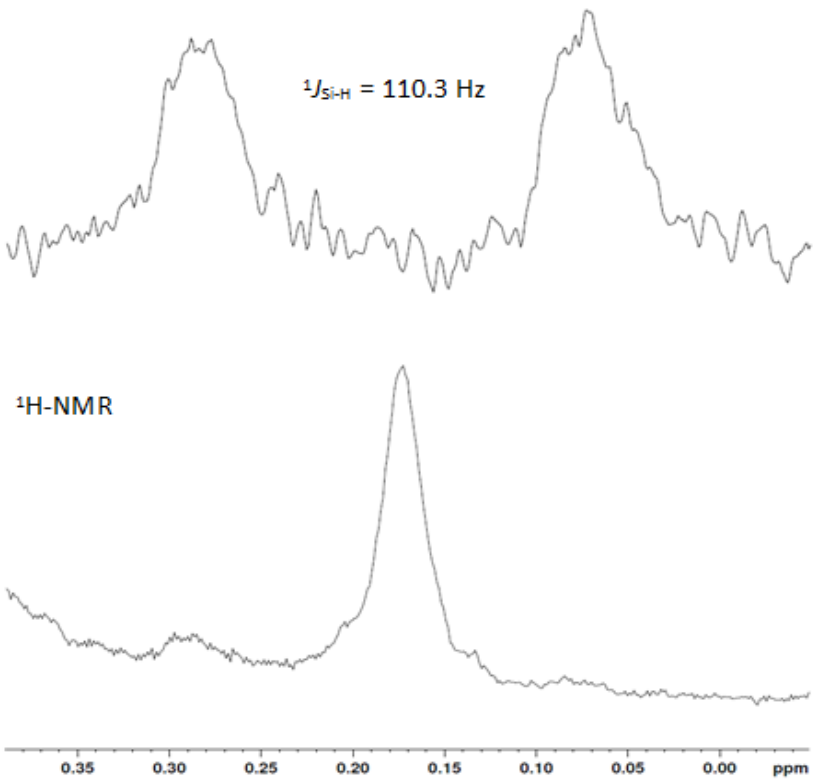
^{1}H-NMR (600 MHz, Toluene-d_8, -78 °C, δ, ppm): 0.17 (s, 1H, Si-H$_{agostic}$, $^{1}J_{Si-H}$ = 110.3 Hz, found by ^{1}H-^{29}Si HSQC 1D JC), 1.00 (s, 9H, 3 CH$_3$, ^{t}*Bu*N=Mo), 1.35 (bs, 18H, 2 P*Me$_3$*), 1.37 (s, 9H, 3 CH$_3$, Mo-N^{t}*Bu*-SiH$_2$Ph), 5.43 (s, 1H, Si-*H$_{class}$*, $^{1}J_{Si-H}$ = 226.1 Hz, found by ^{1}H-^{29}Si HSQC 1D JC), 5.76 (s, 1H, Mo-Si*H$_2$*Ph), 5.81 (s, 1H, Mo-Si*H$_2$*Ph), 7.23 (t, 2H, *m*-Ph, Mo-N^{t}BuSiH*Ph*,$^{3}J_{H-H}$ = 7.26 Hz), 7.37 (t, 2H, *m*-Ph, Mo-SiH$_2$*Ph*,$^{3}J_{H-H}$ = 7.23 Hz), 7.84 (d, 2H, *o*-Ph, Mo-N^{t}BuSiH*Ph*, $^{3}J_{H-H}$ = 6.84 Hz), 8.22 (d, 2H, *o*-Ph, Mo-SiH$_2$*Ph*, $^{3}J_{H-H}$ = 6.98 Hz).**^{31}P{^{1}H}-NMR** (243.0 MHz, Toluene-d_8, -72 °C, δ, ppm): -10.9 (d, 1P, PMe$_3$, $^{2}J_{P-P}$ = 268.2 Hz), -13.0 (d, 1P, PMe$_3$, $^{2}J_{P-P}$ = 266.8 Hz).**^{1}H-^{29}Si HSQC NMR** (119.0 MHZ, Toluene-d_8; -53 °C; J = 150 Hz; ^{29}Si projection, δ, ppm): -8.4 (Mo- *Si*H$_2$Ph), -81.1 (Mo-N^{t}Bu-*Si*H$_2$Ph).



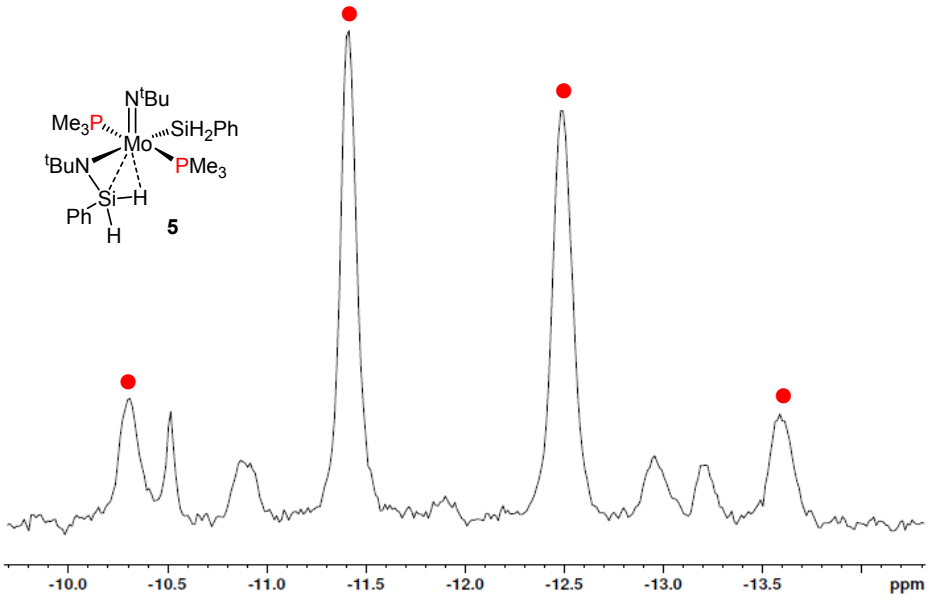
^{1}H-NMR (600 MHz, Toluene-d_8, -80 °C; **4** – (^{t}BuN=)Mo(η^3-N^{t}Bu-SiHPh-H)(PMe$_3$)$_2$(Et))



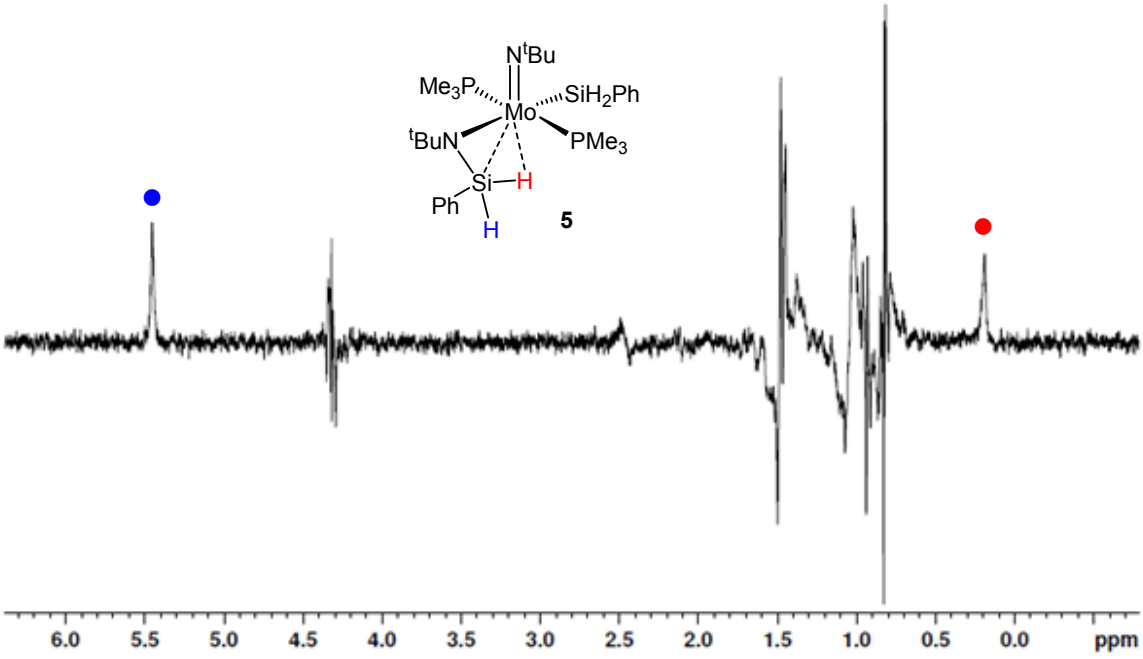
^{1}H-^{29}Si HSQC (600 MHz / 119.2 MHz, Toluene-d_8, -80 °C, **4** – (^{t}BuN=)Mo(η^3-N^{t}Bu-SiHPh-H)(PMe$_3$)$_2$(Et))



^{1}H-^{29}Si HSQC 1D JC (600 MHz / 119.2 MHz, -80 °C; *Top* - ^{1}H-^{29}Si HSQC 1D JC, *Bottom* – ^{1}H NMR)



^{31}P{^{1}H}-NMR (243.0 MHz, Toluene-d_8, -80 °C)



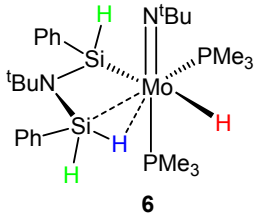
H-EXSY 1D (600 MHz, Toluene-d_8, -80 °C d8 = 100 ms, excitation of the Si-$H_{classical}$ peak @ 5.43 ppm)

**Note: Positive phase response of the Si-$H_{agostic}$signal at similar intensity indicates an exchange.*

(^{t}BuN=)Mo(H)(η^3-PhHSi-N(^{t}Bu)-SiHPh-H)(PMe_3)$_2$ (6)

^{1}H-NMR (600 MHz, Toluene-d_8, -41 °C, δ, ppm): -4.63 (dd, 1H, $^2J_{H-P}$ = 54.9 Hz,$^2J_{H-P}$ = 19.5 Hz, Mo-*H*, minor isomer), -4.43 (ddd, 1H, $^2J_{H-P}$ = 46.1 Hz,$^2J_{H-P}$ = 16.7 Hz,$^2J_{H-H}$ = 4.4 Hz, Mo-*H*, major isomer), 0.37 (dt, 1H, $^2J_{H-P}$ = 45.5 Hz,$^2J_{H-H}$ = 4.4 Hz, Si$H_{agostic}$, major isomer), 0.81(d, 9H, $^2J_{H-P}$ = 7.3 Hz, PMe_3, major isomer), 0.88 (d, 9H, $^2J_{H-P}$ = 7.3 Hz, PMe_3, major isomer), 1.36 (s, 9H, ^{t}*Bu*N=Mo, major isomer),1.44 (s, 9H, μ-N(^{t}*Bu*), major isomer), 6.84 (bd, 1H, $^2J_{H-H}$ = 5.3 Hz,Si$H_{classical}$, major isomer), 6.92 (bs, 1H, Mo-Si*H*Ph, major isomer), 7.22 (bs, 1H, Mo-Si*H*Ph, minor isomer), 7.23 (t, 1H, $^3J_{H-H}$ = 7.4 Hz, *p*-H, Mo-SiH*Ph*, major isomer), 7.27 (t, 1H, *p*-H, $^3J_{H-H}$ = 7.4 Hz, SiH_2Ph, major isomer), 7.36 (t, 1H, $^3J_{H-H}$ = 7.1 Hz, *m*-H, Mo-SiH*Ph*, major isomer),7.43 (t, 2H, *m*-H, SiH_2Ph, $^3J_{H-H}$ = 7.3 Hz, major isomer), 7.47 (t, 1H, *m*-H, Mo-SiH*Ph*, $^3J_{H-H}$ = 6.9 Hz, major isomer), 8.25 (bd, 1H, *o*-H, Mo-SiH*Ph*,

$^{3}J_{H\text{-}H}$ = 6.2 Hz, major isomer), 8.39 (bs, 2H, *o*-H, SiH$_2$*Ph*, $^{3}J_{H\text{-}H}$ = 7.3 Hz, major isomer), 8.56 (bd, 1H, *o*-H, Mo-SiH*Ph*, $^{3}J_{H\text{-}H}$ = 6.3 Hz, major isomer).**^{31}P{^{1}H}-NMR** (243.0 MHz, Toluene-d_8, -25 °C, δ, ppm): 2.4 (d, $^{2}J_{P\text{-}P}$ = 43.7 Hz, P*Me$_3$*, minor isomer), -0.8 (d, $^{2}J_{P\text{-}P}$ = 43.7 Hz, *P*Me$_3$, major isomer), -5.1 (d, $^{2}J_{P\text{-}P}$ = 43.7 Hz, *P*Me$_3$, minor isomer), -7.0 (d, $^{2}J_{P\text{-}P}$ = 43.7 Hz, *P*Me$_3$, major isomer). **^{29}Si INEPT+** (119 MHz, Toluene-d_8, -40 °C, *J* = 200 Hz, δ, ppm): -19.5 (dd, $^{1}J_{H\text{-}Si}$ = 37.3 Hz, $^{1}J_{H\text{-}Si}$ = 199.8 Hz, Si*H$_2$*Ph, minor isomer), -16.2 (dd, $^{1}J_{H\text{-}Si}$ = 34.9 Hz, $^{1}J_{H\text{-}Si}$ = 195.6 Hz, *Si*H$_2$Ph, major isomer), 5.2 (d, $^{1}J_{H\text{-}Si}$ = 172.3 Hz, *Si*HPh, major isomer), 7.5 (d, $^{1}J_{H\text{-}Si}$ = 182.7 Hz, *Si*HPh, minor isomer).**^{13}C{^{1}H}-NMR** (151 MHz; Toluene-d$_8$; - 40 °C; δ, ppm): 19.89 (d, 3C, P*Me$_3$*, $^{1}J_{C\text{-}P}$ = 23.8 Hz), 22.65 (d, 3C, P*Me$_3$*, $^{1}J_{C\text{-}P}$ = 24.8 Hz), 31.35 (s, 3C,*C*H$_3$, ^{t}BuN), 31.97 (s, 3C,*C*H$_3$, ^{t}BuN), 54.54 (s, 1C, *C*(CH$_3$)$_3$, ^{t}BuN), 65.70 (s, 1C, *C*(CH$_3$)$_3$, ^{t}BuN), 127-130 (*p*-Ph, *m*-Ph, overlapped by solvent signals, found by ^{1}H-^{13}C HSQC), 134.0 (*o*-Ph, 2C, MoSiH*Ph*), 137.1 (*o*-Ph, 2C, Si*Ph*), 149.2 (*i*-Ph, 1C, Si*Ph*), 151.0 (*i*-Ph, 1C, Si*Ph*).



6

^{1}H-NMR (600 MHz, Toluene-d_8, -40 °C)

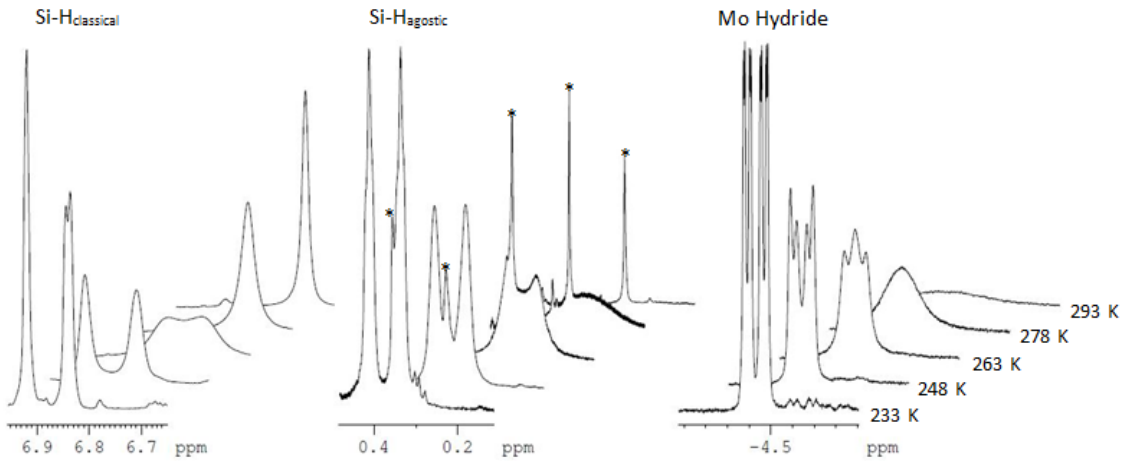
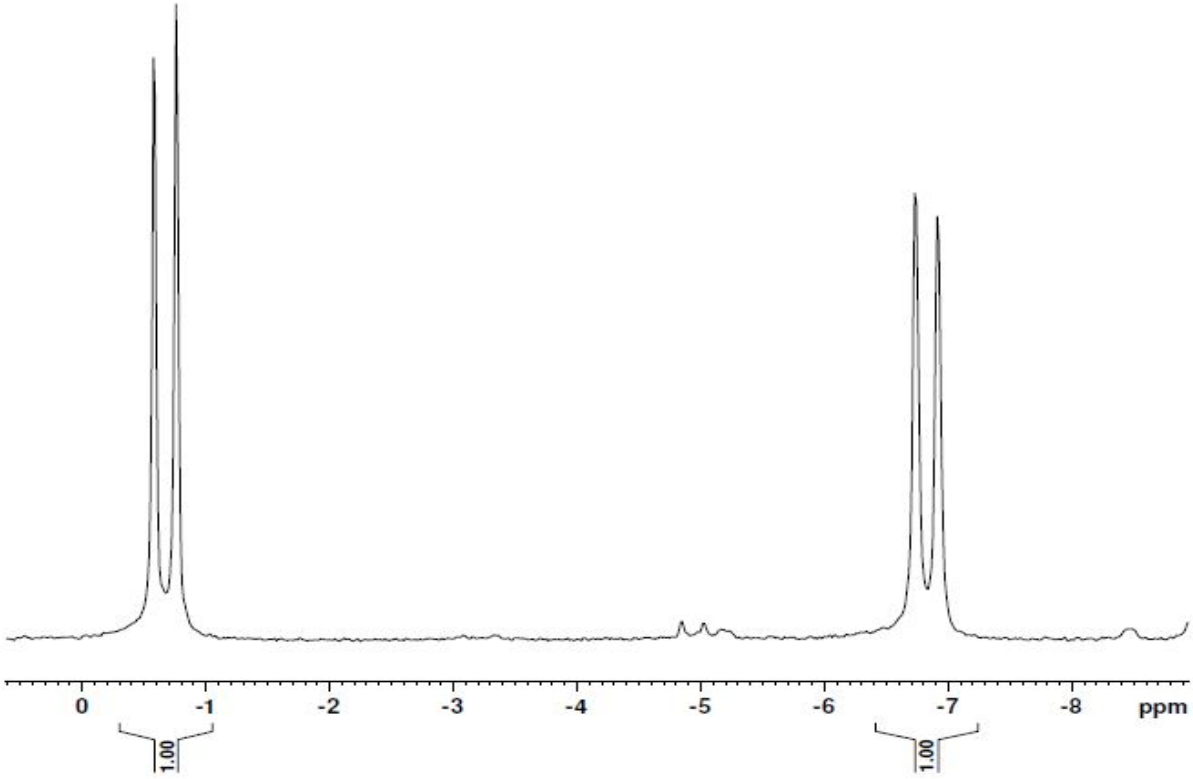


Figure S1 –Variable temperature ^{1}H-NMR for complex **6** beginning at 233 K and warming to 293 K. The respective peaks are labelled accordingly. De-coalescence is observed for Si-$H_{agostic}$ and Mo-H at approximately 278 K. Coalescence of all Si-$H_{classical}$ signals are observed upon warming to room temperature (* - residual silicon grease peak).



^{31}P{^{1}H}-NMR(243.0 MHz, Toluene-$d_{8,}$ -40 °C)

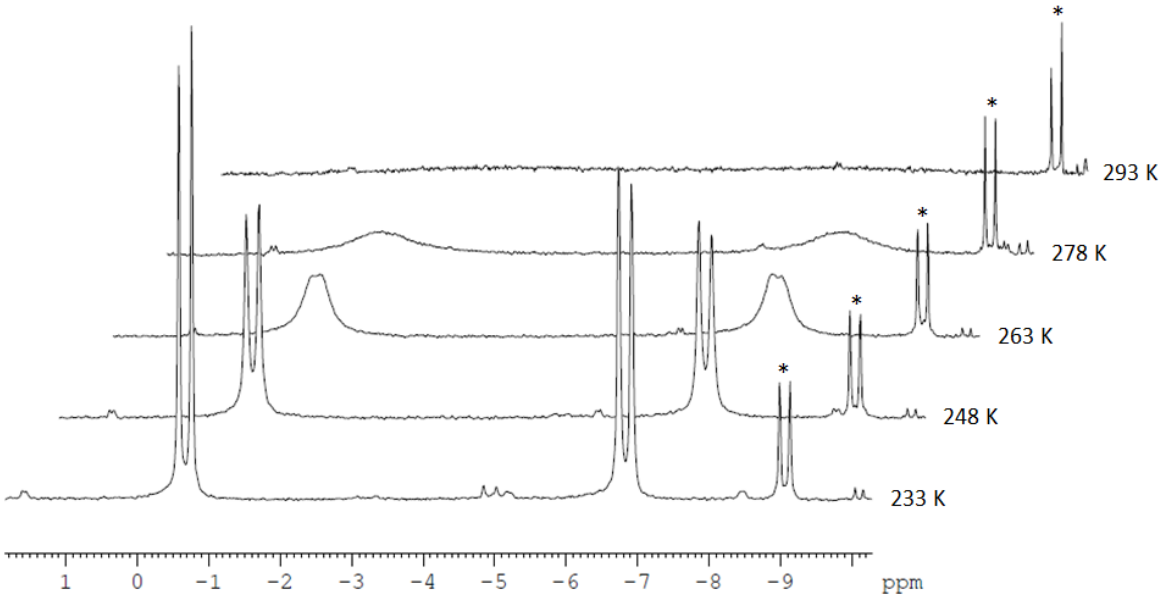
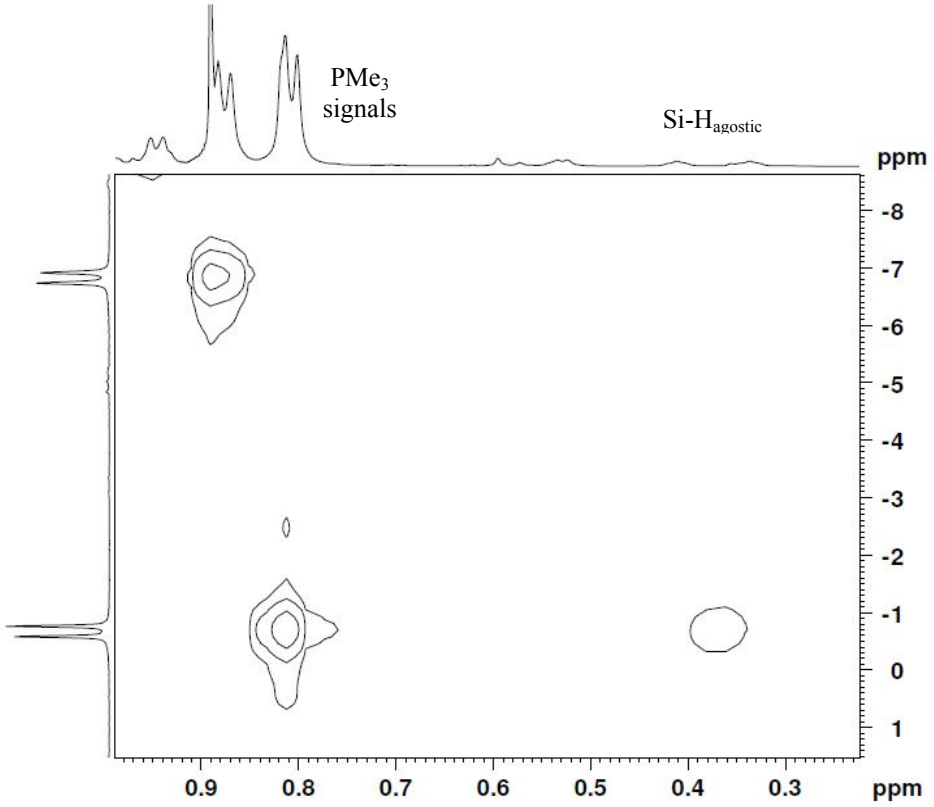
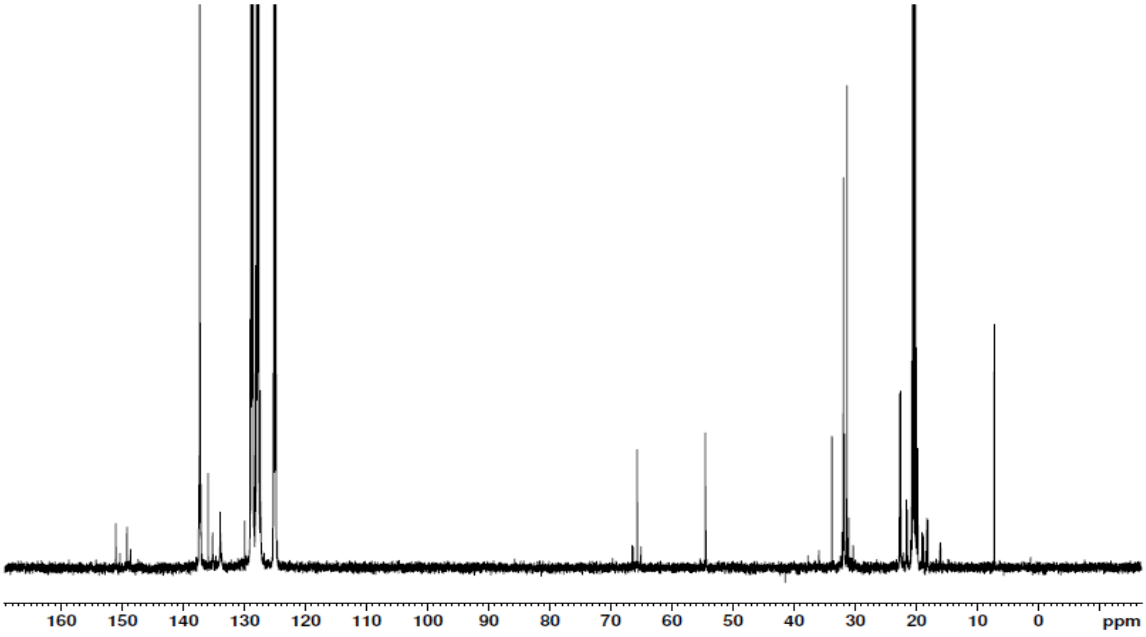


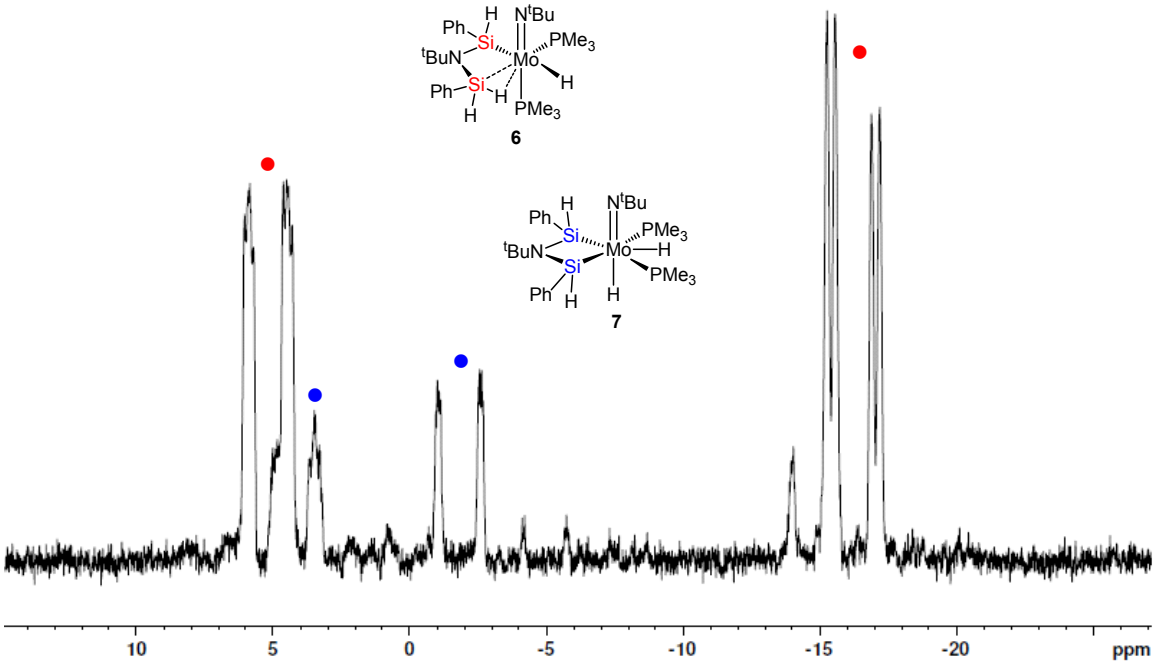
Figure S2–Variable temperature $^{31}P\{^{1}H\}$-NMR showing de-coalescence at room temperature for complex **6**(* - PMe_3 signal for complex **7**).



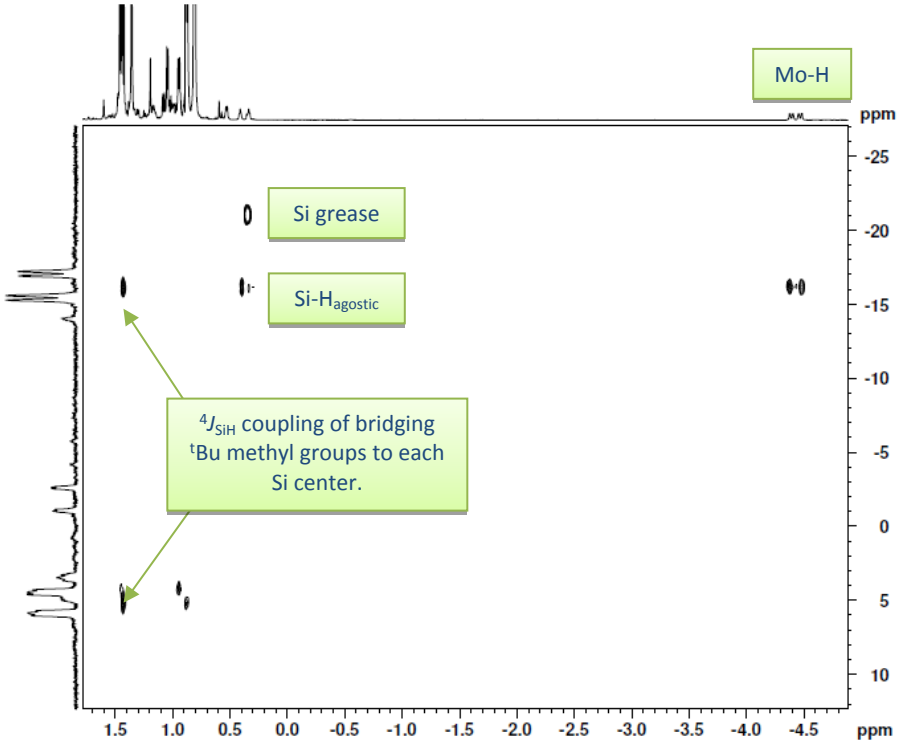
^{1}H-^{31}P HSQC (600 MHz / 243.0 MHz, Toluene-d_8, -40 °C, J = 15 Hz)



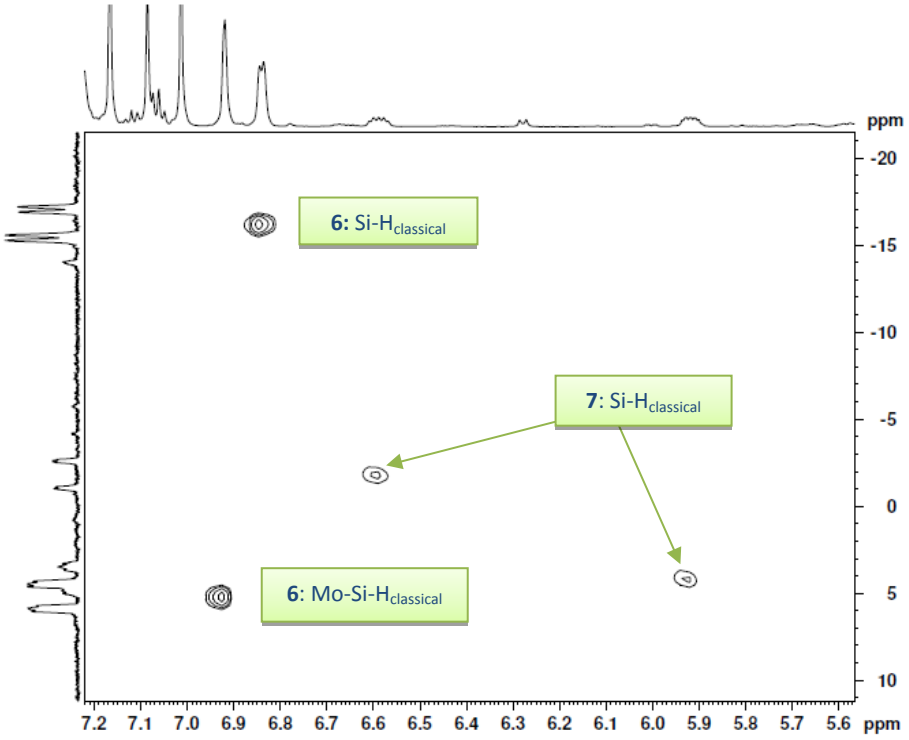
$^{13}C\{^{1}H\}$ NMR (151 MHz, Toluene-d_8, -40 °C)



^{29}Si INEPT+ NMR (119.2 MHz, Toluene-d_8, -40 °C)



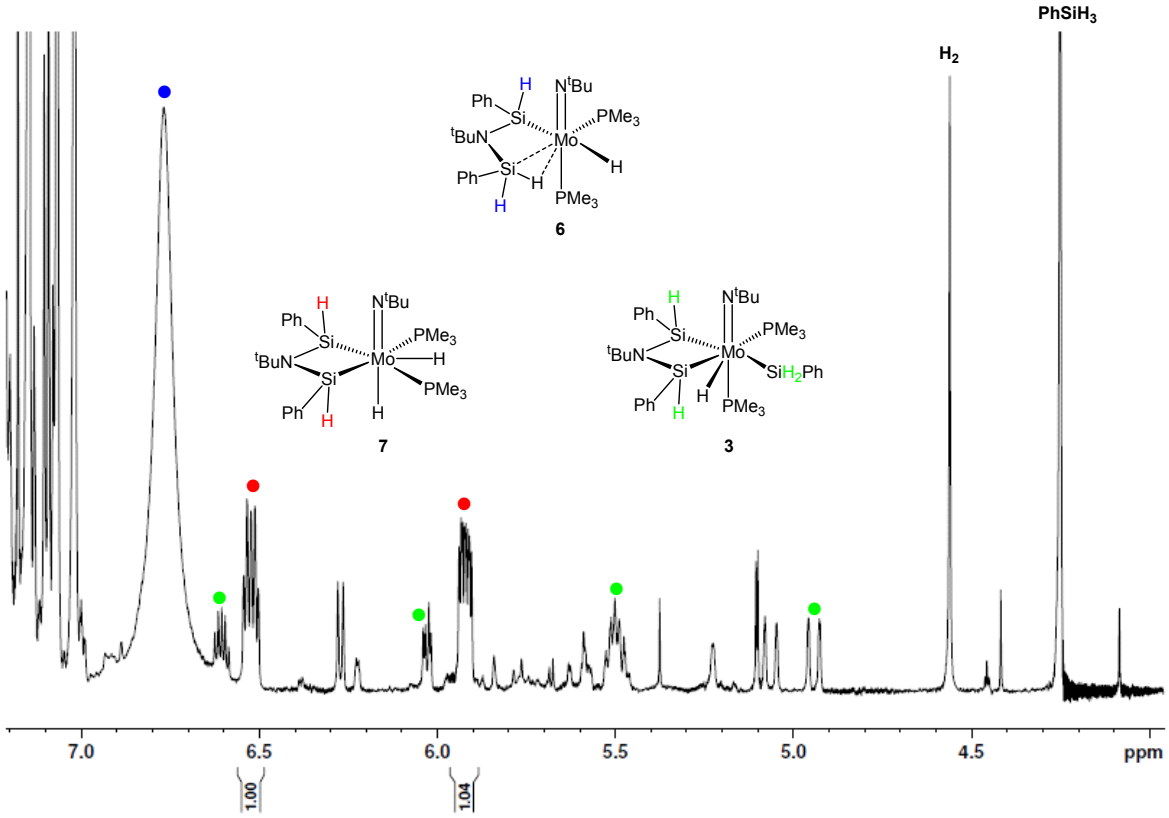
^{1}H-^{29}Si HSQC (600 MHz / 119.2 MHz, Toluene-d_8, -40 °C, J = 7 Hz)



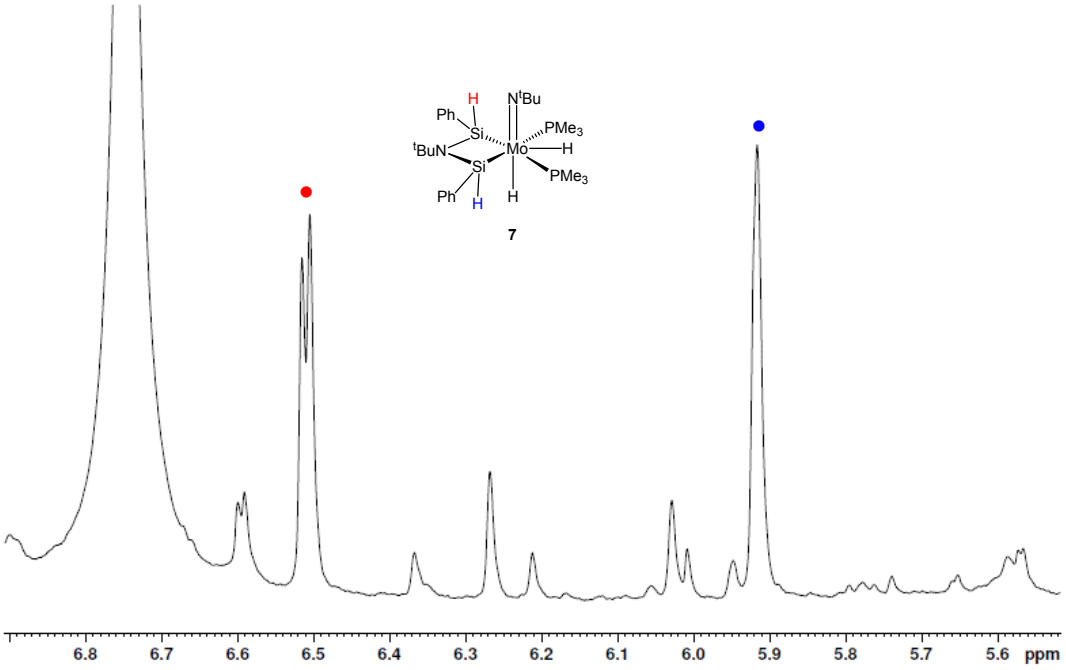
^{1}H-^{29}Si HSQC (600 MHz / 119.2 MHz, Toluene-d_8, -40 °C, J = 150 Hz)

(^{t}BuN=)Mo{(SiHPh)$_2$(μ-N^{t}Bu)}(PMe$_3$)$_2$H$_2$ (7)

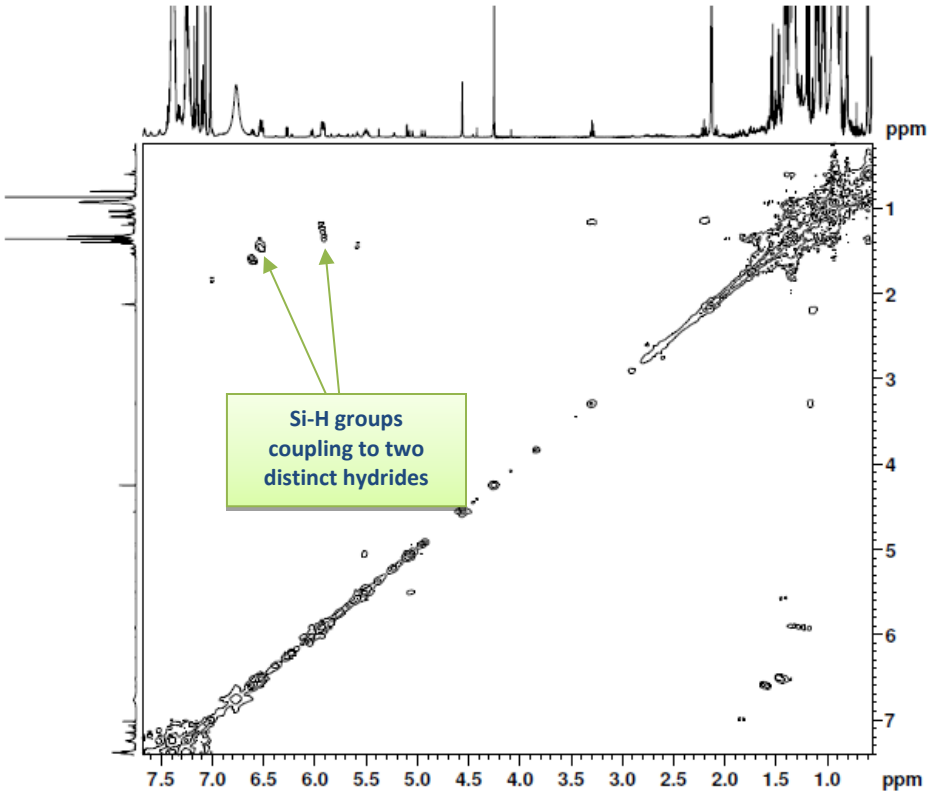
^{1}H-NMR (600 MHz, Toluene-d_8, 0 °C, δ, ppm): 0.80 (s, 9H, 3 CH_3, Mo=N^t*Bu*), 1.05 (d, 9H, PMe_3, $^2J_{H-P}$ = 7.7 Hz), 1.10 (d, 9H, PMe_3, $^2J_{H-P}$ = 6.7 Hz), 1.25 (Mo-H, found by ^{1}H-^{1}H COSY and ^{1}H-^{29}Si HSQC (J = 7 Hz), partially obscured by complex **3**) 1.39 (s, 9H, 3 CH_3, Si-N^t*Bu*-Si), 1.48 (Mo-H, found by ^{1}H-^{1}H COSY and ^{1}H-^{29}Si HSQC (J = 7 Hz), partially obscured by complex **3**), 5.92 (ddd, 1H, Si-*H*, $^3J_{H-H}$ = 3.8 Hz, $^3J_{H-P}$ = 5.93 Hz, $^2J_{H-P}$ = 11.57 Hz, $^1J_{Si-H}$ = 169.2 Hz {found by ^{1}H-^{29}Si HSQC 1D JC}), 6.51 (dt, 1H, Si-*H*, $^3J_{H-H}$ = 6.1 Hz, $^2J_{H-P}$ = 6.1 Hz, $^2J_{H-P}$ = 12.2 Hz, $^1J_{Si-H}$ = 187.1 Hz {found by ^{1}H-^{29}Si HSQC 1D JC}), 8.33 (d, 2H, *o*-Ph, $^3J_{H-H}$ = 6.9 Hz).**^{1}H{^{31}P}-NMR** (600 MHz, Toluene-d_8, 0 °C, δ, ppm, selected signals): 6.51 (d, 1H, Si-*H*, $^3J_{H-H}$ = 6.12 Hz), 5.92 (bd, 1H, Si-*H*, $^3J_{H-H}$ = 3.7 Hz), 1.10 (s, P*Me$_3$*), 1.05 (s, P*Me$_3$*).**^{31}P{^{1}H}-NMR** (243.0 MHz, Toluene-d_8, 0 °C, δ, ppm): -9.65 (d, 1P, PMe_3, $^2J_{P-P}$ = 31.3 Hz), -34.60 (d, 1P, PMe_3, $^2J_{P-P}$ = 31.1 Hz).**^{31}P{^{1}H}-NMR** (selectively decoupled from methyl group at 1.10 ppm in ^{1}H-NMR, 243.0 MHz, Toluene-d_8, 0 °C, δ, ppm): -9.63 (bt, 1P, PMe_3, $^2J_{P-P}$ = 33.4 Hz), -34.49 (m, 1P, PMe_3, $^3J_{P-H}$ = 13.0 Hz, $^2J_{P-P}$ = 27.6 Hz, $^2J_{P-H}$ = 51.7 Hz).**^{31}P{^{1}H}-NMR** (selectively decoupled from methyl group at 1.05 ppm in ^{1}H-NMR, 243.0 MHz, Toluene-d_8, 0 °C, δ, ppm): -9.63 (dd, 1P, PMe_3, $^2J_{P-P}$ = 33.4 Hz, $^2J_{P-H}$ = 33.4 Hz), -34.70 (m, 1P, PMe_3).**^{31}P{^{1}H}-NMR** (selectively decoupled from hydride at 1.25 ppm in ^{1}H-NMR, 243.0 MHz, Toluene-d_8, 0 °C, δ, ppm): -9.63 (d, 1P, PMe_3, $^2J_{P-P}$ = 33.4 Hz), -34.60 (m, 1P, PMe_3).**^{29}Si INEPT +** (119 MHz, Toluene-d_8, 0 °C, J = 150 Hz, δ, ppm): 4.05 (d, $^1J_{Si-H}$ = 170.0 Hz), -2.17 (d, $^1J_{Si-H}$ = 185.3 Hz).



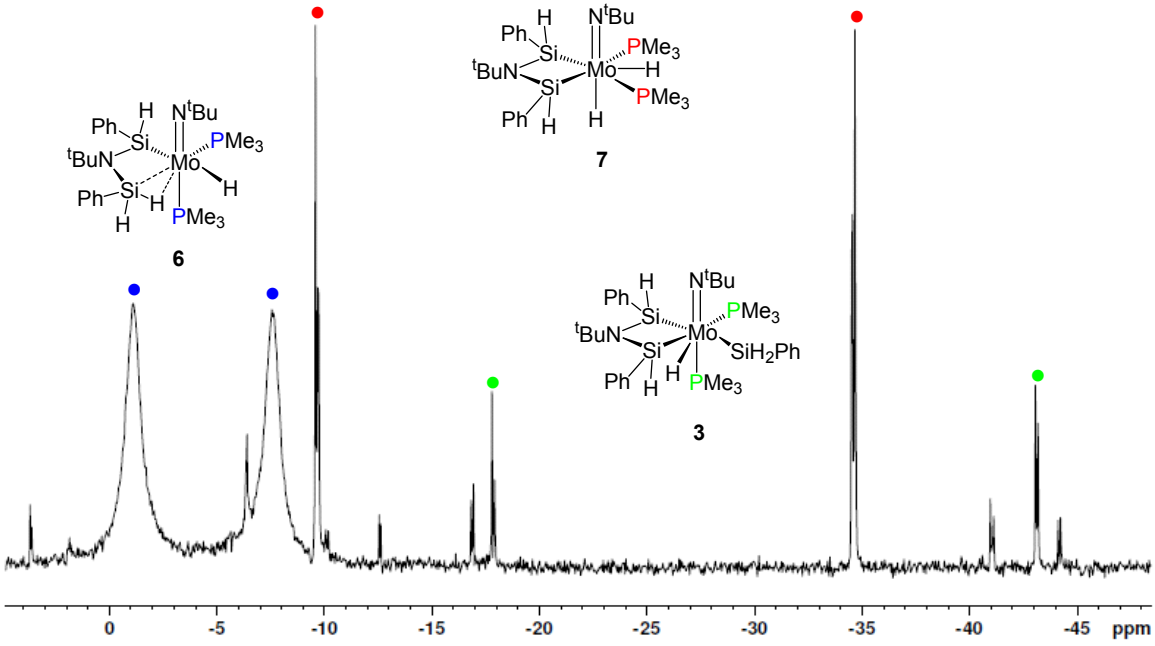
^{1}H-NMR (600 MHz, Toluene-$d_{8,}$ 0 °C, reacted at -20 °C for 3 hours)



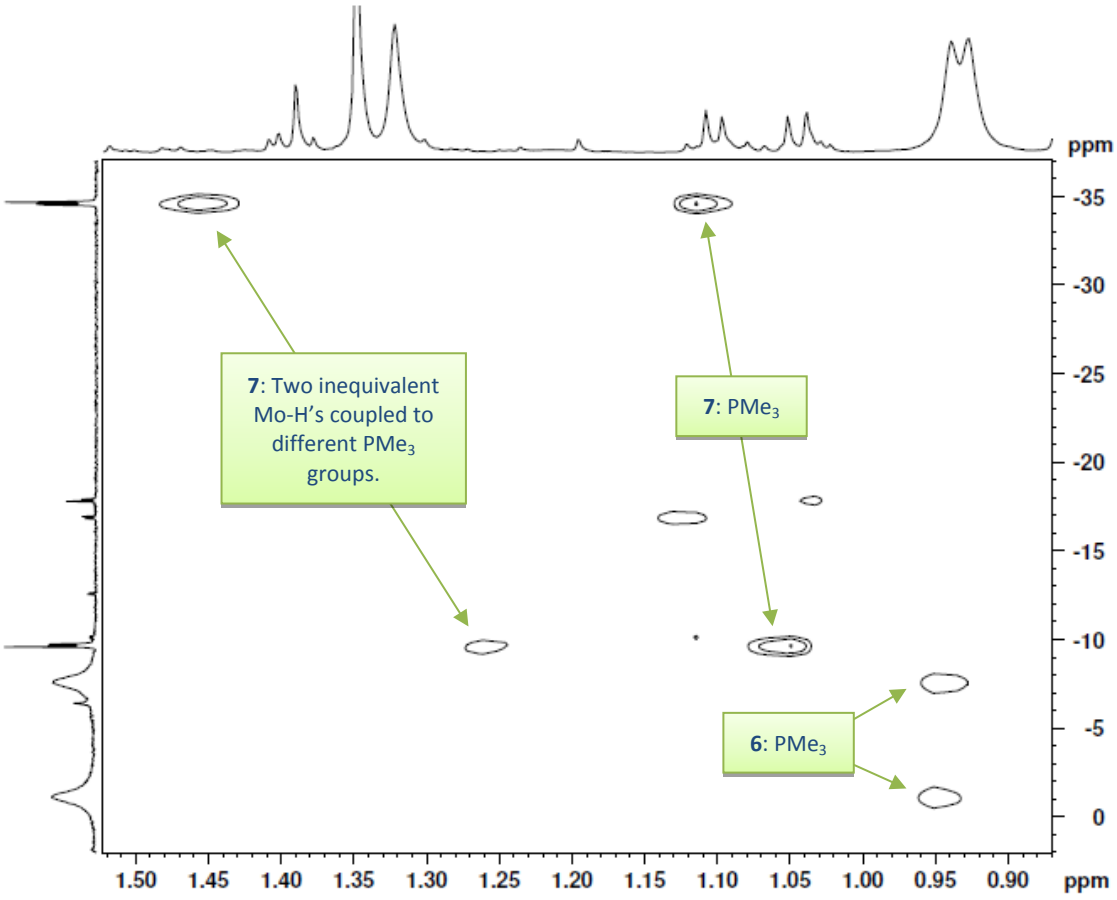
^{1}H{^{31}P} NMR(600 MHz, Toluene-$d_{8,}$ 0 °C, reacted at -20 °C for 3 hours)



^{1}H-^{1}H COSY(600 MHz, Toluene-d_8, 0 °C, reacted at -20 °C for 3 hours)



^{31}P{^{1}H} NMR (243.0 MHz, Toluene-d_8, 0 °C, reacted at -20 °C for 3 hours)

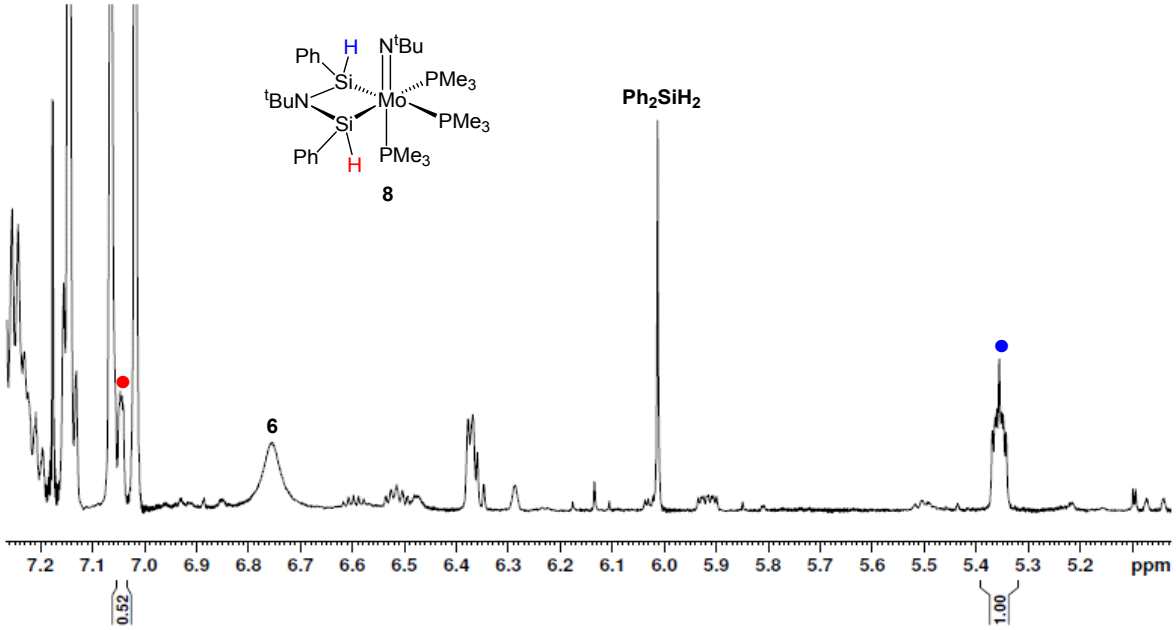


^{1}H-^{31}P HSQC (600 MHz / 243.0 MHz, Toluene-d$_8$, 0 °C, J = 15 Hz)

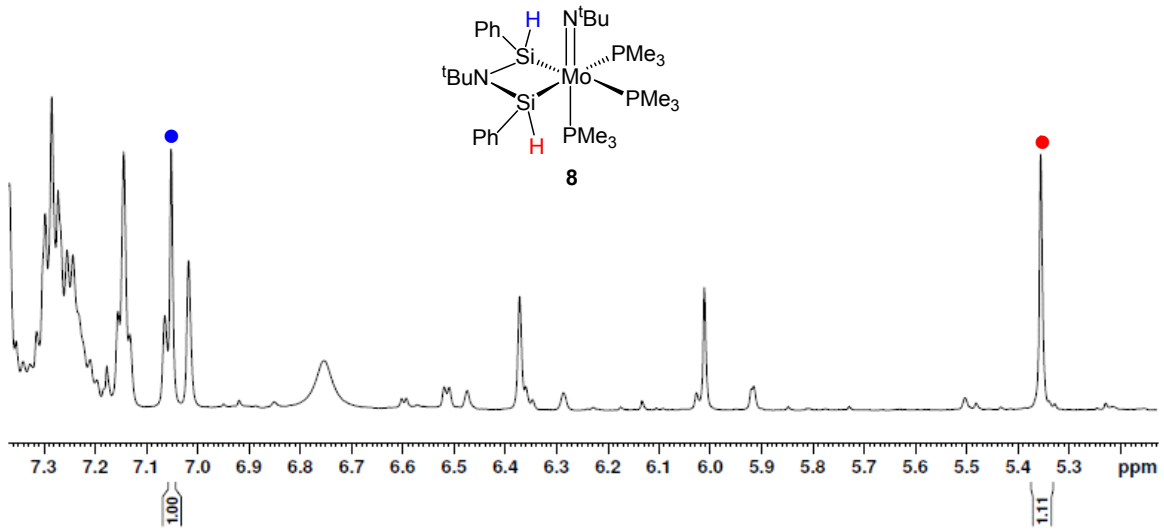
(^{t}BuN=){μ-^{t}BuN(SiHPh)$_2$}Mo(PMe$_3$)$_3$(8)

^{1}H-NMR (600 MHz, Toluene-d_8, 0 °C, δ, ppm): 0.90 (d, 9H, PMe$_3$, $^{2}J_{H-P}$ = 6.78 Hz), 1.06 (s, 9H, 3 CH$_3$, ^{t}*Bu*N=Mo), 1.26 (d, 9H, PMe$_3$, $^{2}J_{H-P}$ = 6.12 Hz), 1.45 (s, 9H, 3 CH$_3$, μ-N^{t}*Bu*), 1.74 (d, 9H, PMe$_3$, $^{2}J_{H-P}$ = 6.90 Hz), 5.36 (ddd, 1H, MoSi*H*Ph, $^{1}J_{Si-H}$ = 226.1 Hz, found by ^{1}H-^{29}Si HSQC 1D JC, $^{2}J_{H-P}$ = 3.00 Hz, $^{2}J_{H-P}$ = 4.98 Hz, $^{2}J_{H-P}$ = 7.80 Hz), 7.05 (bd, 1H, MoSi*H*Ph, $^{1}J_{Si-H}$ = 226.1 Hz, found by ^{1}H-^{29}Si HSQC 1D JC, partially obscured by solvent peaks), 7.29 (t, 2H, *m*-Ph,$^{3}J_{H-H}$ = 7.56 Hz), 7.47 (t, 2H, *m*-Ph, $^{3}J_{H-H}$ = 7.47 Hz), 7.96 (d, 2H, *o*-Ph, $^{3}J_{H-H}$ = 7.08Hz), 8.27 (d, 2H, *o*-Ph, $^{3}J_{H-H}$ = 6.96 Hz).**^{1}H{^{31}P}-NMR** (600 MHz, Toluene-d_8, 0 °C, δ, ppm; selected signals): 0.90 (s, 9H, PMe$_3$), 1.26 (s, 9H, PMe$_3$), 1.74 (s, 9H, PMe$_3$), 5.36 (s, 1H, Mo-Si*H*Ph), 7.05 (s, 1H, Mo-Si*H*Ph).**^{31}P{^{1}H}-NMR** (243.0 MHz, Toluene-d_8, 0 °C, δ, ppm): 5.66 (t, 1P, PMe$_3$, $^{2}J_{P-P}$ = 22.6 Hz), -7.48 (dd, 1P, PMe$_3$, $^{2}J_{P-Pcis}$ = 18.2 Hz, $^{2}J_{P-Ptrans}$ =

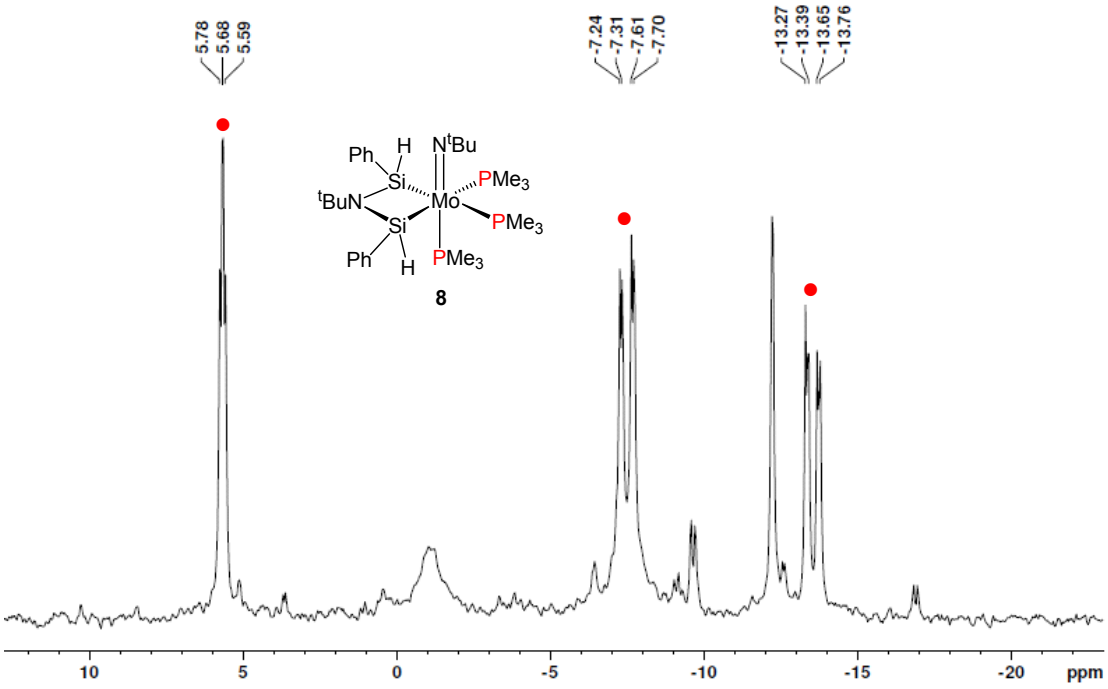
91.1 Hz), -13.54 (dd, 1P, PMe_3, $^2J_{P\text{-}Pcis}$ = 27.4 Hz, $^2J_{P\text{-}Ptrans}$ = 91.2 Hz).**^{29}Si INEPT+** (119 MHz, Toluene-d_8, 0 °C, J = 150 Hz, δ, ppm): 41.70 (bd, $^1J_{Si\text{-}H}$ = 169.3 Hz), -10.42 (dddd, Mo-*Si*HPh, $^1J_{Si\text{-}H}$ = 152.0 Hz, $^2J_{Si\text{-}P}$ = 19.3 Hz, $^2J_{Si\text{-}P}$ = 19.3 Hz, $^2J_{Si\text{-}P}$ = 38.3 Hz).



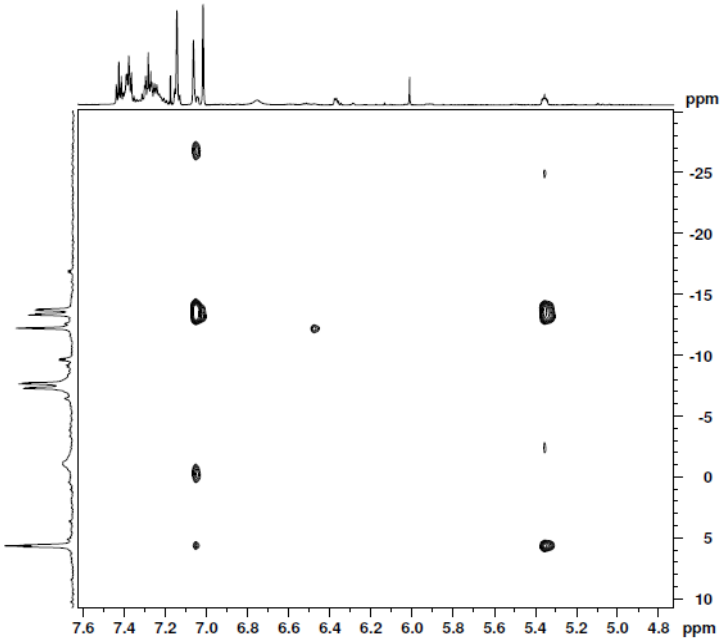
^{1}H-NMR (600 MHz, Toluene-d_8, 0 °C; after 3 days at -30 °C. *Note*: Si-H peak at 7.053 ppm (bd) is partially obscured by solvent peaks)



^{1}H{^{31}P}-NMR(600 MHz, Toluene-d_8, 0 °C; after 3 days at -30 °C)

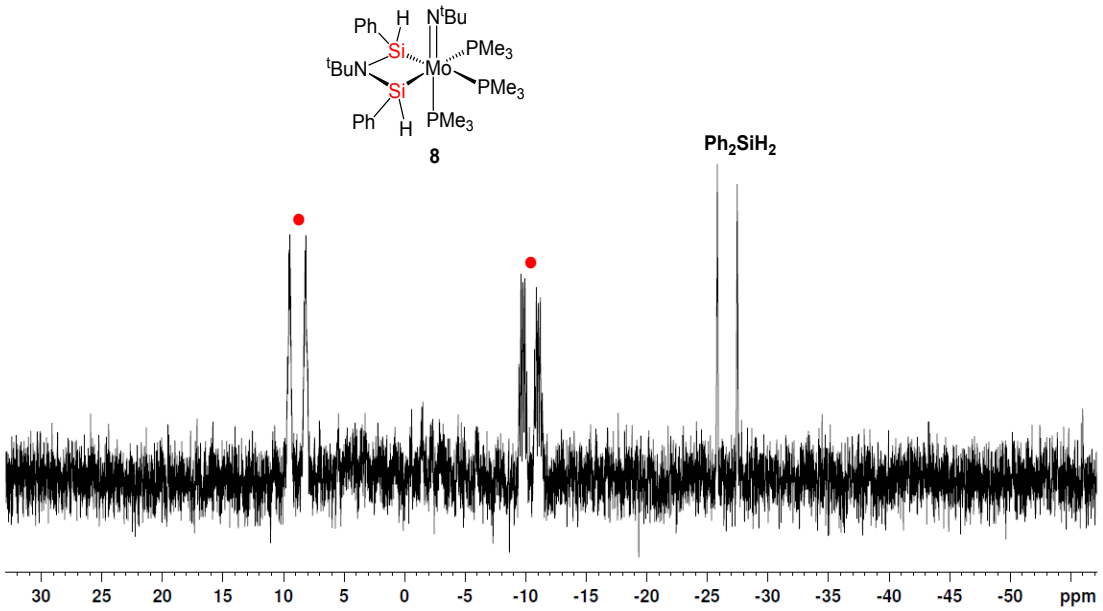


^{31}P{^{1}H}-NMR(243.0 MHz, Toluene-d_8, 0 °C; after 3 days at -30 °C)

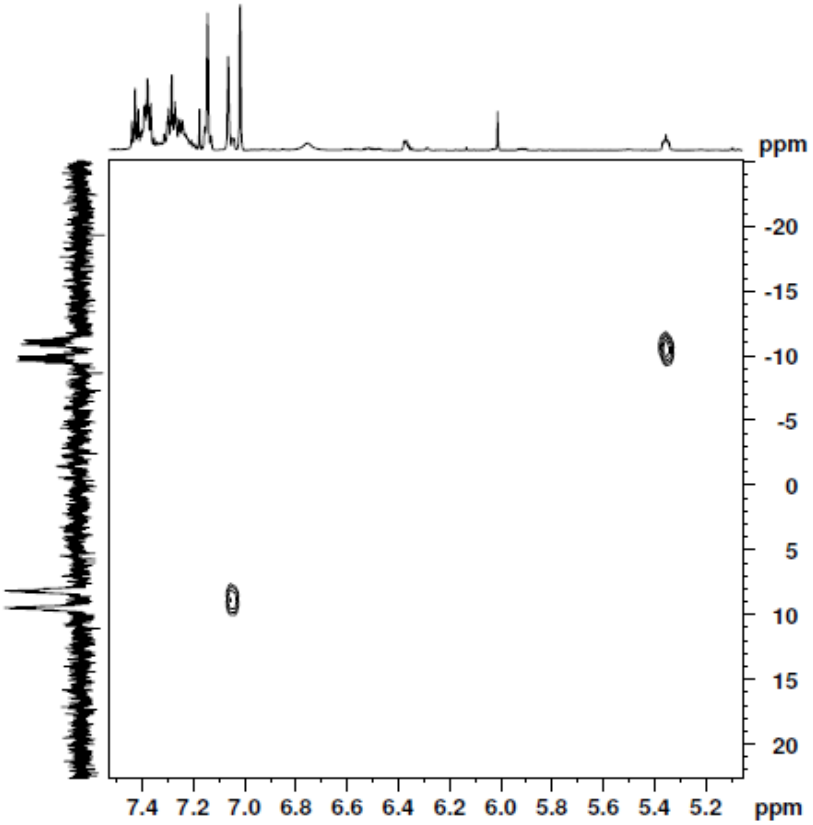


^{1}H-^{31}P HSQC(600 MHz / 243.0 MHz, Toluene-d_8, 0 °C, J = 15 Hz,after 3 days at -30 °C.

Note: Artifacts shown for cross peaks @ -14 ppm on vertical scale)



^{29}Si INEPT+ NMR (119.2 MHz, Toluene-d_8, 0 °C, J = 200 Hz, after 3 days at -30 °C)



^{1}H-^{29}Si HSQC (600 MHz / 119.2 MHz, Toluene-d_8, 0 °C, J = 150 Hz, after 3 days at -30 °C)

II. Cartesian coordinates of various compounds and stationary points in the reaction of (^{t}BuN)$_2$Mo(PMe$_3$)$_2$ (1) with PhSiH$_3$ with *B3PW91/6-31G**, Hay-Wadt DZ* calculation

Structure 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	-0.000001	0.165013	0.000001
2	15	0	-0.101047	-1.403536	1.833922
3	15	0	0.101234	-1.403896	-1.833611
4	7	0	1.65236	0.874875	0.050258
5	7	0	-1.65261	0.874498	-0.050431
6	6	0	2.840679	1.68113	0.087896
7	6	0	3.550047	1.589579	-1.275139
8	1	0	3.817697	0.551276	-1.496214
9	1	0	4.466307	2.191477	-1.282426
10	1	0	2.89	1.952353	-2.068902
11	6	0	3.777176	1.154519	1.191009
12	1	0	3.27998	1.204777	2.164964
13	1	0	4.697025	1.74864	1.24387
14	1	0	4.04889	0.112559	0.99462
15	6	0	2.47449	3.147133	0.382146
16	1	0	1.95091	3.218979	1.340412
17	1	0	1.812486	3.536508	-0.39698
18	1	0	3.370818	3.777521	0.426685
19	6	0	-2.840787	1.680953	-0.088183
20	6	0	-3.776965	1.154912	-1.191837
21	1	0	-4.048629	0.112813	-0.99613
22	1	0	-3.279551	1.205803	-2.165655
23	1	0	-4.69685	1.748983	-1.244561
24	6	0	-2.474299	3.14702	-0.381745
25	1	0	-1.812678	3.536075	0.397866
26	1	0	-3.370539	3.777511	-0.426557
27	1	0	-1.950204	3.219109	-1.339707
28	6	0	-3.550658	1.58897	1.274566
29	1	0	-4.466744	2.191132	1.281855

30	1	0	-2.890747	1.951158	2.068711
31	6	0	-0.60349	-0.670111	3.456687
32	1	0	-0.597863	-1.408636	4.266502
33	1	0	-1.606285	-0.247241	3.356579
34	1	0	0.081983	0.145651	3.70105
35	6	0	1.514582	-2.172079	2.273953
36	1	0	1.42522	-2.798085	3.168342
37	1	0	2.243307	-1.378574	2.451554
38	1	0	1.871153	-2.778325	1.438569
39	6	0	-1.224688	-2.872553	1.788494
40	1	0	-1.195588	-3.4342	2.729077
41	1	0	-0.932215	-3.532262	0.967421
42	1	0	-2.247654	-2.532539	1.605921
43	6	0	1.224082	-2.873538	-1.788045
44	1	0	1.194213	-3.4355	-2.728415
45	1	0	0.93165	-3.5328	-0.966602
46	1	0	2.247336	-2.534036	-1.606101
47	6	0	0.604395	-0.670826	-3.456329
48	1	0	0.599015	-1.409568	-4.265948
49	1	0	1.607162	-0.247965	-3.355987
50	1	0	-0.080977	0.144881	-3.701149
51	6	0	-1.514692	-2.171688	-2.273926
52	1	0	-1.4255	-2.797684	-3.168336
53	1	0	-2.243034	-1.377829	-2.451524
54	1	0	-1.871652	-2.777821	-1.438628
55	1	0	-3.818692	0.550642	1.495065

E	-1414.729977
Sigma	2
Nneg	0
E+ZPE	-1414.24565
U	-1414.214903
H	-1414.213958
G	-1414.307117

Structure 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	-0.351847	-0.704273	-0.136451
2	15	0	-0.87908	-1.515448	2.445062
3	15	0	0.496696	-3.077997	-0.643518
4	14	0	-2.731619	-1.691938	-0.368059
5	14	0	2.110045	-0.422989	0.768775
6	14	0	0.251537	1.437479	1.156953
7	7	0	1.96568	1.191928	1.460746
8	7	0	-0.411188	-0.024706	-1.747173
9	6	0	2.953105	2.001053	2.213653
10	6	0	3.860148	1.076084	3.035832
11	1	0	3.273813	0.468847	3.732644
12	1	0	4.581455	1.663317	3.614714
13	1	0	4.427091	0.399342	2.38775
14	6	0	2.221452	2.956133	3.164389
15	1	0	1.558799	3.632954	2.614449
16	1	0	2.941316	3.57101	3.715405
17	1	0	1.617702	2.404952	3.892663
18	6	0	3.821251	2.819606	1.244222
19	1	0	3.209228	3.537724	0.691369
20	1	0	4.319167	2.163539	0.524363
21	1	0	4.591469	3.380071	1.787657
22	6	0	-0.72212	0.553355	-3.037699
23	6	0	0.54251	1.192153	-3.629991
24	1	0	1.338344	0.449877	-3.73676
25	1	0	0.895799	2.005767	-2.992213
26	1	0	0.319673	1.604184	-4.619995
27	6	0	-1.816296	1.616282	-2.850574
28	1	0	-2.727499	1.163889	-2.451201
29	1	0	-2.05067	2.075751	-3.817004
30	1	0	-1.482855	2.397251	-2.163947
31	6	0	-1.231651	-0.555119	-3.974431
32	1	0	-0.443979	-1.283258	-4.188021
33	1	0	-1.547427	-0.113458	-4.925535
34	1	0	-2.0832	-1.077245	-3.531728
35	6	0	-4.294279	-0.606478	-0.182825

36	6	0	-5.55349	-1.233331	-0.212389
37	1	0	-5.61131	-2.314943	-0.321986
38	6	0	-6.735128	-0.503223	-0.102622
39	1	0	-7.693905	-1.015692	-0.127162
40	6	0	-6.687658	0.883973	0.040243
41	1	0	-7.607493	1.456888	0.126227
42	6	0	-5.453113	1.527805	0.073957
43	1	0	-5.404889	2.608422	0.184722
44	6	0	-4.274029	0.787602	-0.033584
45	1	0	-3.318164	1.305239	0.000297
46	6	0	3.580419	-0.569202	-0.440772
47	6	0	4.66842	-1.409015	-0.148038
48	1	0	4.675151	-1.966142	0.787901
49	6	0	5.752961	-1.533096	-1.018595
50	1	0	6.581434	-2.189908	-0.764389
51	6	0	5.777601	-0.80646	-2.207103
52	1	0	6.621087	-0.896951	-2.886599
53	6	0	4.714518	0.043651	-2.516542
54	1	0	4.730226	0.619633	-3.43878
55	6	0	3.63282	0.153993	-1.644484
56	1	0	2.809807	0.815615	-1.900081
57	6	0	-0.128907	3.073196	0.271747
58	6	0	0.728178	3.625038	-0.693323
59	1	0	1.653563	3.109713	-0.940059
60	6	0	0.425143	4.826267	-1.333943
61	1	0	1.109972	5.236154	-2.072449
62	6	0	-0.755333	5.50263	-1.025952
63	1	0	-0.995692	6.43815	-1.524299
64	6	0	-1.62107	4.975357	-0.06834
65	1	0	-2.538355	5.501614	0.18424
66	6	0	-1.304548	3.7785	0.574572
67	1	0	-1.980805	3.390102	1.334381
68	6	0	-2.430358	-0.756973	3.083153
69	1	0	-2.616834	-1.069339	4.115864
70	1	0	-3.278398	-1.045452	2.457737
71	1	0	-2.33153	0.330152	3.044212
72	6	0	0.290334	-1.121789	3.81804
73	1	0	-0.141511	-1.413483	4.781065
74	1	0	0.501824	-0.050638	3.825455
75	1	0	1.232841	-1.652424	3.666379
76	6	0	-1.192292	-3.300047	2.813592

77	1	0	-1.489417	-3.418723	3.860633
78	1	0	-0.290631	-3.892299	2.642077
79	1	0	-1.993416	-3.673706	2.172528
80	6	0	1.795925	-3.916949	0.361138
81	1	0	1.980509	-4.9195	-0.038439
82	1	0	1.499165	-3.998915	1.40828
83	1	0	2.720201	-3.338523	0.313846
84	6	0	1.319315	-3.043528	-2.289627
85	1	0	1.750233	-4.022495	-2.525092
86	1	0	2.106971	-2.286605	-2.285332
87	1	0	0.582278	-2.780081	-3.049944
88	6	0	-0.693847	-4.468353	-0.867165
89	1	0	-0.181947	-5.345633	-1.276183
90	1	0	-1.49526	-4.164843	-1.54469
91	1	0	-1.14503	-4.734587	0.091146
92	1	0	-3.078564	-2.870732	0.506618
93	1	0	-2.903775	-2.308438	-1.732823
94	1	0	2.54564	-1.408027	1.824737
95	1	0	-0.495422	1.615177	2.452459
96	1	0	-1.574226	0.286884	0.519074

E	-2980.838033
Sigma	1
Nneg	0
E+ZPE	-2980.031468
U	-2979.979482
H	-2979.978538
G	-2980.117882

TS(1-4H)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	0.609028	0.094666	0.000632
2	15	0	2.133560 29	0.568195	-1.836375

3	15	0	0.394268	-2.402353	-0.372731
4	14	0	-2.031164	0.362737	-1.659943
5	7	0	-0.656147	1.455858	-0.032649
6	7	0	1.716110	-0.067670	1.366649
7	6	0	-0.950347	2.771754	0.521548
8	6	0	-0.428237	3.823865	-0.477329
9	1	0	0.652914	3.716241	-0.607938
10	1	0	-0.633107	4.837735	-0.113718
11	1	0	-0.909787	3.703795	-1.452190
12	6	0	-0.251825	2.978505	1.874191
13	1	0	-0.588599	2.225001	2.593559
14	1	0	-0.470468	3.972041	2.285090
15	1	0	0.830601	2.875487	1.760189
16	6	0	-2.462746	2.989778	0.710930
17	1	0	-2.878361	2.280431	1.430173
18	1	0	-3.003858	2.871855	-0.231664
19	1	0	-2.649157	4.003064	1.085072
20	6	0	2.711910	-0.185343	2.402794
21	6	0	2.901870	1.177156	3.090180
22	1	0	1.962198	1.517290	3.532615
23	1	0	3.229819	1.928567	2.365647
24	1	0	3.655757	1.107223	3.882594
25	6	0	4.050856	-0.645517	1.800531
26	1	0	3.940903	-1.612589	1.301884
27	1	0	4.814503	-0.744007	2.580415
28	1	0	4.408680	0.081168	1.064878
29	6	0	2.222112	-1.215328	3.435594
30	1	0	1.258565	-0.906422	3.850601
31	1	0	2.942338	-1.311761	4.255769
32	1	0	2.095002	-2.198402	2.972271
33	6	0	-3.349908	-0.145477	-0.391620
34	6	0	-4.639672	-0.385520	-0.896485
35	1	0	-4.825722	-0.270017	-1.962196
36	6	0	-5.687058	-0.779105	-0.063870
37	1	0	-6.676921	-0.947096	-0.481040
38	6	0	-5.460083	-0.970121	1.297779
39	1	0	-6.270588	-1.288048	1.948829
40	6	0	-4.184094	-0.755478	1.817915
41	1	0	-3.996471	-0.906524	2.878409
42	6	0	-3.146500	-0.340478	0.982903
43	1	0	-2.157378	-0.159931	1.395590

44	6	0	3.300123	1.964202	-1.503584
45	1	0	3.935788	2.178907	-2.369782
46	1	0	3.930294	1.712813	-0.647021
47	1	0	2.723530	2.855716	-1.246558
48	6	0	1.324001	1.140934	-3.388287
49	1	0	2.069556	1.470716	-4.119495
50	1	0	0.730026	0.329411	-3.815187
51	6	0	3.324835	-0.690782	-2.481435
52	1	0	3.991018	-0.261219	-3.237956
53	1	0	2.771913	-1.523456	-2.923877
54	1	0	3.927007	-1.075339	-1.654032
55	6	0	-0.699030	-3.228151	0.866502
56	1	0	-0.762302	-4.310128	0.704060
57	1	0	-1.699172	-2.790985	0.806539
58	1	0	-0.307010	-3.032763	1.868305
59	6	0	1.906333	-3.456941	-0.218972
60	1	0	1.654628	-4.519657	-0.303548
61	1	0	2.372262	-3.279401	0.752739
62	1	0	2.626466	-3.196228	-0.997630
63	6	0	-0.323477	-3.052261	-1.945441
64	1	0	-0.393515	-4.144463	-1.913142
65	1	0	0.305874	-2.757136	-2.789221
66	1	0	-1.320464	-2.636177	-2.107570
67	1	0	-2.001857	1.746573	-2.205201
68	1	0	-2.657210	-0.363220	-2.856489
69	1	0	0.649745	1.967935	-3.154889
70	1	0	-0.711871	-0.380409	-1.716679

E	-1937.506125
Sigma	-153
Nneg	0
E+ZPE	-1936.905075
U	-1936.866883
H	-1936.865939
G	-1936.976713

Structure 4Ha

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	-0.918413	0.048663	-0.375083
2	15	0	0.061505	2.344177	-0.674976
3	15	0	-1.791432	-2.271871	-0.857249
4	14	0	1.894406	-1.222103	-0.284513
5	7	0	0.753126	-0.648200	0.832910
6	7	0	-2.528221	0.665663	-0.096408
7	6	0	0.767604	-0.765789	2.293420
8	6	0	-0.544246	-1.403492	2.779013
9	1	0	-1.405328	-0.835280	2.408419
10	1	0	-0.593248	-1.429910	3.874100
11	1	0	-0.634528	-2.426996	2.406228
12	6	0	0.886785	0.629325	2.931673
13	1	0	1.844223	1.091623	2.672185
14	1	0	0.822484	0.576373	4.025081
15	1	0	0.084288	1.278056	2.566756
16	6	0	1.937506	-1.636471	2.778957
17	1	0	2.900840	-1.204874	2.485355
18	1	0	1.871004	-2.646779	2.359804
19	1	0	1.934853	-1.727566	3.871123
20	6	0	-3.760592	1.132847	0.488438
21	6	0	-4.672892	1.667576	-0.628812
22	1	0	-4.877184	0.884051	-1.363935
23	1	0	-4.195480	2.501243	-1.150932
24	1	0	-5.626186	2.015914	-0.215920
25	6	0	-3.454436	2.249448	1.502200
26	1	0	-2.823016	1.869335	2.310404
27	1	0	-4.382597	2.636057	1.937843
28	1	0	-2.931574	3.080084	1.020287
29	6	0	-4.457539	-0.027349	1.220890
30	1	0	-4.704021	-0.835726	0.527429
31	1	0	-5.388324	0.319721	1.683001
32	1	0	-3.810490	-0.430649	2.004924
33	6	0	3.660437	-0.532122	-0.294568
34	6	0	4.663283	-1.233705	-0.982841
35	1	0	4.419234	-2.172569	-1.477712

36	6	0	5.972387	-0.758030	-1.039152
37	1	0	6.731321	-1.317062	-1.580854
38	6	0	6.309746	0.431037	-0.392795
39	1	0	7.330955	0.801385	-0.429839
40	6	0	5.333397	1.138334	0.307336
41	1	0	5.592821	2.060975	0.820651
42	6	0	4.024321	0.658734	0.351504
43	1	0	3.269010	1.213342	0.903216
44	6	0	1.490904	2.356494	-1.841629
45	1	0	1.788357	3.382541	-2.083538
46	1	0	1.198483	1.834585	-2.756124
47	1	0	2.346401	1.832854	-1.408858
48	6	0	0.671496	3.519883	0.624620
49	1	0	1.027300	4.457431	0.183400
50	1	0	-0.137753	3.740813	1.326342
51	6	0	-1.116202	3.433534	-1.582701
52	1	0	-0.638948	4.372121	-1.884230
53	1	0	-1.976961	3.657929	-0.948725
54	1	0	-1.474717	2.899213	-2.465264
55	6	0	-3.273518	-2.166666	-1.950036
56	1	0	-3.596304	-3.160441	-2.278910
57	1	0	-3.019948	-1.552421	-2.816805
58	1	0	-4.094369	-1.678536	-1.421146
59	6	0	-2.353318	-3.565822	0.349402
60	1	0	-2.797219	-4.425574	-0.164559
61	1	0	-3.091350	-3.138666	1.033606
62	1	0	-1.502099	-3.911912	0.941170
63	6	0	-0.680249	-3.287764	-1.925850
64	1	0	-1.192513	-4.194099	-2.265730
65	1	0	0.221255	-3.570001	-1.377463
66	1	0	-0.380478	-2.691890	-2.791511
67	1	0	2.123222	-2.706155	-0.395965
68	1	0	1.200166	-0.825193	-1.572650
69	1	0	1.486632	3.059495	1.187559
70	1	0	-0.921238	0.135875	-2.068089

E	-1937.541093
Sigma	1

Nneg	0
E+ZPE	-1936.939877
U	-1936.901250
H	-1936.900306
G	-1937.011138

Structure 4Hb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	-0.618197	0.056738	0.2761
2	15	0	-2.462728	0.919222	-1.113701
3	15	0	-1.979047	-1.201534	1.887671
4	14	0	1.733946	0.731223	1.24526
5	7	0	0.793858	1.678392	0.207868
6	7	0	-0.240526	-1.254774	-0.884571
7	6	0	0.891377	3.131084	0.034174
8	6	0	0.050098	3.857678	1.095391
9	1	0	-0.976011	3.480571	1.086272
10	1	0	0.039563	4.942521	0.932635
11	1	0	0.454739	3.666132	2.09523
12	6	0	0.416214	3.518877	-1.369762
13	1	0	0.997917	2.983367	-2.127226
14	1	0	0.524302	4.595896	-1.542213
15	1	0	-0.635028	3.260486	-1.504751
16	6	0	2.359139	3.575421	0.172008
17	1	0	2.990832	3.063267	-0.561213
18	1	0	2.744425	3.349929	1.174325
19	1	0	2.463765	4.655897	0.019687
20	6	0	-0.138942	-2.385838	-1.769573
21	6	0	0.659191	-3.480215	-1.035761
22	1	0	0.112605	-3.839475	-0.160218
23	1	0	1.623457	-3.085025	-0.705214
24	1	0	0.838355	-4.329196	-1.704979
25	6	0	0.640204	-1.959511	-3.028799
26	1	0	0.130059	-1.138968	-3.541838

27	1	0	0.734996	-2.798425	-3.727856
28	1	0	1.641932	-1.61925	-2.754602
29	6	0	-1.520254	-2.924061	-2.173488
30	1	0	-2.113108	-3.169629	-1.287963
31	1	0	-1.421779	-3.827322	-2.786089
32	1	0	-2.069282	-2.180782	-2.759805
33	6	0	3.285712	-0.089504	0.580069
34	6	0	4.248775	-0.640094	1.438014
35	1	0	4.10323	-0.59304	2.516156
36	6	0	5.400985	-1.241912	0.932198
37	1	0	6.137452	-1.664282	1.61119
38	6	0	5.61054	-1.293597	-0.445335
39	1	0	6.510029	-1.757741	-0.841722
40	6	0	4.667443	-0.741903	-1.313778
41	1	0	4.833807	-0.774286	-2.387744
42	6	0	3.514871	-0.147747	-0.803223
43	1	0	2.775282	0.285054	-1.472745
44	6	0	-2.060333	1.180506	-2.899871
45	1	0	-2.888992	1.662815	-3.429582
46	1	0	-1.866088	0.207163	-3.357474
47	1	0	-1.158623	1.785735	-3.001752
48	6	0	-3.25127	2.518047	-0.643816
49	1	0	-4.059736	2.770127	-1.338272
50	1	0	-3.652481	2.418748	0.367534
51	6	0	-4.000853	-0.093455	-1.319678
52	1	0	-4.603609	0.289123	-2.150446
53	1	0	-4.597889	-0.043495	-0.407601
54	1	0	-3.741813	-1.136433	-1.510955
55	6	0	-1.440761	-0.84232	3.617348
56	1	0	-2.021749	-1.420874	4.34372
57	1	0	-1.564782	0.225731	3.809628
58	1	0	-0.380557	-1.085627	3.726407
59	6	0	-1.866154	-3.050394	1.906717
60	1	0	-2.411456	-3.480642	2.753513
61	1	0	-0.813807	-3.337562	1.976278
62	1	0	-2.269947	-3.461017	0.977938
63	6	0	-3.80573	-0.991192	2.082877
64	1	0	-4.154719	-1.457775	3.010081
65	1	0	-4.326847	-1.455032	1.242511
66	1	0	-4.044958	0.074965	2.107896
67	1	0	2.042929	1.185594	2.638246

68	1	0	0.667173	-0.401924	1.616573
69	1	0	-2.519498	3.326572	-0.633394
70	1	0	-1.593289	1.078127	1.453097

E	-1937.537683
Sigma	1
Nneg	0
E+ZPE	-1936.935398
U	-1936.897828
H	-1936.896884
G	-1937.003631

TS (4-9)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	0.602617	0.011821	-0.256807
2	15	0	2.746321	1.14898	0.066033
3	15	0	1.42627	-2.127294	-1.360313
4	14	0	-1.577289	0.785578	-1.236419
5	7	0	-0.648708	1.787253	-0.249287
6	7	0	0.338355	-0.893177	1.257468
7	6	0	-0.76746	3.211536	0.049371
8	6	0	-0.398441	4.066624	-1.17596
9	1	0	0.609554	3.830365	-1.526188
10	1	0	-0.448987	5.139797	-0.953805
11	1	0	-1.087912	3.860201	-2.001833
12	6	0	0.11594	3.582439	1.243971
13	1	0	-0.123012	2.941371	2.098369
14	1	0	-0.030723	4.628605	1.535519
15	1	0	1.172393	3.446984	1.007921
16	6	0	-2.226577	3.524007	0.432181
17	1	0	-2.530134	2.93794	1.304974
18	1	0	-2.906042	3.277856	-0.392107

19	1	0	-2.357912	4.587316	0.6667
20	6	0	0.260062	-1.676039	2.461775
21	6	0	-1.023302	-2.525376	2.445383
22	1	0	-1.011173	-3.239739	1.617997
23	1	0	-1.903191	-1.889981	2.321988
24	1	0	-1.122476	-3.085844	3.381989
25	6	0	0.199425	-0.696169	3.65059
26	1	0	1.109565	-0.09153	3.697784
27	1	0	0.093648	-1.239984	4.596495
28	1	0	-0.651409	-0.018568	3.538811
29	6	0	1.486311	-2.590629	2.615566
30	1	0	1.510115	-3.341155	1.820086
31	1	0	1.461585	-3.118589	3.575649
32	1	0	2.41044	-2.005566	2.567709
33	6	0	-3.181658	-0.001205	-0.647851
34	6	0	-4.104695	-0.492427	-1.583925
35	1	0	-3.884292	-0.41655	-2.647699
36	6	0	-5.310403	-1.064783	-1.177671
37	1	0	-6.01104	-1.440381	-1.919426
38	6	0	-5.620189	-1.143736	0.17886
39	1	0	-6.561782	-1.58235	0.499105
40	6	0	-4.719451	-0.650039	1.124819
41	1	0	-4.962402	-0.701126	2.183488
42	6	0	-3.511957	-0.091193	0.713802
43	1	0	-2.809934	0.290126	1.451274
44	6	0	3.180644	1.572449	1.813521
45	1	0	4.160121	2.059272	1.874419
46	1	0	3.205809	0.646675	2.394042
47	1	0	2.421488	2.223227	2.249038
48	6	0	3.173574	2.69752	-0.84321
49	1	0	4.208721	2.988211	-0.634856
50	1	0	3.056292	2.515587	-1.914466
51	6	0	4.255352	0.167433	-0.359793
52	1	0	5.169344	0.722761	-0.120606
53	1	0	4.247729	-0.064705	-1.427917
54	1	0	4.250286	-0.769869	0.200874
55	6	0	1.611436	-2.028788	-3.194574
56	1	0	1.84605	-3.010281	-3.618621
57	1	0	2.407032	-1.32444	-3.449839
58	1	0	0.681656	-1.660969	-3.635831
59	6	0	0.174496	-3.478685	-1.22386

60	1	0	0.43354	-4.337139	-1.853253
61	1	0	-0.803019	-3.08764	-1.516479
62	1	0	0.105426	-3.80686	-0.184467
63	6	0	2.961952	-3.081121	-0.944831
64	1	0	2.952489	-4.063567	-1.429252
65	1	0	3.038609	-3.219405	0.135792
66	1	0	3.84311	-2.532749	-1.284774
67	1	0	-1.845303	1.172536	-2.663574
68	1	0	0.051549	-0.015879	-1.986446
69	1	0	2.511564	3.516833	-0.563259
70	1	0	1.117995	0.3899	-2.011618

E	-1937.512266
Sigma	1
Nneg	-975
E+ZPE	-1936.912314
U	-1936.874795
H	-1936.873851
G	-1936.980224

Structure 9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	-0.648183	-0.129963	0.04377
2	15	0	-2.690113	0.571319	-1.25472
3	15	0	-1.668056	-0.541881	2.197296
4	14	0	1.477386	0.613481	1.006834
5	7	0	0.491668	1.58955	-0.04082
6	7	0	-0.458697	-1.780384	-0.54645
7	6	0	0.589865	2.994185	-0.441258
8	6	0	0.084094	3.878682	0.712832

9	1	0	-0.966459	3.657837	0.929938
10	1	0	0.171116	4.944081	0.467596
11	1	0	0.665819	3.688683	1.620653
12	6	0	-0.246679	3.267166	-1.691928
13	1	0	0.071207	2.613999	-2.510771
14	1	0	-0.141697	4.308826	-2.015425
15	1	0	-1.305803	3.083844	-1.494282
16	6	0	2.051789	3.361205	-0.744082
17	1	0	2.44763	2.742069	-1.554619
18	1	0	2.683653	3.201503	0.135642
19	1	0	2.138645	4.4135	-1.039276
20	6	0	0.081034	-2.967694	-1.164918
21	6	0	1.283287	-3.453004	-0.338599
22	1	0	0.974619	-3.679419	0.686039
23	1	0	2.053897	-2.679293	-0.297397
24	1	0	1.712158	-4.359118	-0.781761
25	6	0	0.525572	-2.64132	-2.600018
26	1	0	-0.316518	-2.260762	-3.186502
27	1	0	0.91678	-3.536269	-3.096706
28	1	0	1.310694	-1.880566	-2.588523
29	6	0	-1.012488	-4.049737	-1.186935
30	1	0	-1.358936	-4.265935	-0.171876
31	1	0	-0.625891	-4.976203	-1.62549
32	1	0	-1.872175	-3.722994	-1.780211
33	6	0	3.223888	0.189105	0.417759
34	6	0	4.274175	0.071632	1.342281
35	1	0	4.084706	0.271842	2.395852
36	6	0	5.561338	-0.284758	0.939894
37	1	0	6.3572	-0.366639	1.676538
38	6	0	5.829468	-0.527491	-0.406387
39	1	0	6.832294	-0.801297	-0.724125
40	6	0	4.801878	-0.413679	-1.344108
41	1	0	5.004722	-0.597213	-2.396755
42	6	0	3.516956	-0.065577	-0.933018
43	1	0	2.7232	0.023341	-1.672221
44	6	0	-2.608492	0.970548	-3.066357
45	1	0	-3.610133	1.064498	-3.500567
46	1	0	-2.075378	0.162649	-3.575836
47	1	0	-2.056905	1.89636	-3.235415
48	6	0	-3.828984	1.90292	-0.655916
49	1	0	-4.706675	1.998701	-1.304466

50	1	0	-3.308512	2.863006	-0.621774
51	1	0	-4.162021	1.663494	0.357802
52	6	0	-3.866618	-0.851833	-1.352649
53	1	0	-4.736688	-0.603807	-1.970731
54	1	0	-4.20116	-1.13166	-0.352285
55	1	0	-3.345079	-1.708312	-1.78538
56	6	0	-1.610607	0.951634	3.275724
57	1	0	-1.968637	0.716255	4.283469
58	1	0	-2.232998	1.742135	2.849774
59	1	0	-0.581125	1.313399	3.327812
60	6	0	-0.797718	-1.804741	3.220553
61	1	0	-1.272318	-1.929889	4.200077
62	1	0	0.242475	-1.497002	3.345111
63	1	0	-0.806339	-2.758617	2.687427
64	6	0	-3.420831	-1.094565	2.438973
65	1	0	-3.65781	-1.225633	3.500715
66	1	0	-3.575898	-2.046635	1.923579
67	1	0	-4.104329	-0.355952	2.011882
68	1	0	1.695105	1.181097	2.389631

E	-1936.360867
Sigma	1
Nneg	0
E+ZPE	-1935.774487
U	-1935.737089
H	-1935.736145
G	-1935.843996

Structure 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	-1.047159	-0.62973	0.032887
2	15	0	-1.772625	-1.209362	2.325629
3	15	0	-0.817273	-2.849448	-1.040935
4	14	0	1.99384	-0.628751	1.010538

5	14	0	0.041905	1.500993	0.862458
6	7	0	1.750608	1.059775	1.231623
7	7	0	-2.491289	0.055738	-0.666786
8	6	0	2.845198	1.9919	1.632001
9	6	0	3.924521	1.238853	2.422709
10	1	0	3.512288	0.78835	3.331132
11	1	0	4.722838	1.928933	2.715417
12	1	0	4.391416	0.44639	1.824463
13	6	0	2.286843	3.104341	2.526857
14	1	0	1.547722	3.710562	1.996475
15	1	0	3.097484	3.769648	2.843854
16	1	0	1.810522	2.688604	3.42012
17	6	0	3.486206	2.614961	0.381548
18	1	0	2.73819	3.152988	-0.205858
19	1	0	3.927491	1.840026	-0.253246
20	1	0	4.27872	3.319864	0.660251
21	6	0	-3.627296	0.682862	-1.292858
22	6	0	-3.276105	0.972465	-2.762184
23	1	0	-3.040648	0.043351	-3.290165
24	1	0	-2.405944	1.6311	-2.818398
25	1	0	-4.119271	1.456027	-3.268261
26	6	0	-3.934143	1.999379	-0.560199
27	1	0	-4.184923	1.807636	0.486929
28	1	0	-4.782635	2.50674	-1.032831
29	1	0	-3.06595	2.662367	-0.590854
30	6	0	-4.839288	-0.260254	-1.21508
31	1	0	-4.633021	-1.19975	-1.73649
32	1	0	-5.71434	0.205997	-1.681118
33	1	0	-5.085667	-0.491038	-0.174284
34	6	0	3.129949	-1.240796	-0.364369
35	6	0	4.059772	-2.25207	-0.071732
36	1	0	4.107503	-2.662752	0.935438
37	6	0	4.933556	-2.737672	-1.045674
38	1	0	5.643684	-3.522078	-0.796681
39	6	0	4.90001	-2.207106	-2.333397
40	1	0	5.582713	-2.577437	-3.093809
41	6	0	3.992002	-1.192721	-2.642451
42	1	0	3.96865	-0.771141	-3.644136
43	6	0	3.11618	-0.717697	-1.668467
44	1	0	2.406966	0.066606	-1.918289
45	6	0	-0.053871	2.97536	-0.347954

46	6	0	0.269556	2.848755	-1.710471
47	1	0	0.592688	1.880371	-2.08615
48	6	0	0.167758	3.927164	-2.587795
49	1	0	0.431929	3.802462	-3.635526
50	6	0	-0.281547	5.165492	-2.12547
51	1	0	-0.366651	6.006681	-2.808897
52	6	0	-0.624126	5.314152	-0.783106
53	1	0	-0.978989	6.273825	-0.414436
54	6	0	-0.50668	4.230915	0.090218
55	1	0	-0.774244	4.362929	1.137578
56	6	0	-3.139575	-0.107376	2.889364
57	1	0	-3.439177	-0.33595	3.917988
58	1	0	-3.999468	-0.229485	2.226803
59	1	0	-2.798542	0.928359	2.825064
60	6	0	-0.542096	-0.985367	3.681762
61	1	0	-1.00829	-1.135116	4.661174
62	1	0	-0.125905	0.024088	3.62529
63	1	0	0.276455	-1.700378	3.564819
64	6	0	-2.468841	-2.867086	2.792564
65	1	0	-2.791076	-2.901024	3.839829
66	1	0	-1.709452	-3.638208	2.631612
67	1	0	-3.324866	-3.094557	2.150399
68	6	0	0.373933	-4.105241	-0.400485
69	1	0	0.34529	-5.019709	-1.002678
70	1	0	0.129434	-4.350458	0.636152
71	1	0	1.386112	-3.69306	-0.429515
72	6	0	-0.338878	-2.806327	-2.82371
73	1	0	-0.359451	-3.800028	-3.285338
74	1	0	0.666339	-2.384684	-2.901576
75	1	0	-1.023198	-2.140612	-3.356192
76	6	0	-2.37761	-3.834155	-1.121219
77	1	0	-2.250323	-4.744555	-1.717491
78	1	0	-3.164643	-3.21901	-1.563984
79	1	0	-2.686915	-4.103055	-0.108704
80	1	0	2.519608	-1.334952	2.223096
81	1	0	-0.475469	2.166227	2.120871
82	1	0	0.245123	-0.268234	-1.078666
83	1	0	0.640821	-1.358419	0.928937

E	-2459.201376

Sigma	1
Nneg	0
E+ZPE	-2458.497529
U	-2458.452275
H	-2458.451331
G	-2458.577693

TS(6-7)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	-1.045268	-0.773009	-0.216061
2	15	0	-1.429341	-1.539361	2.16126
3	15	0	-0.456654	-3.110442	-1.04859
4	14	0	1.659722	-0.532759	0.581878
5	14	0	-0.278966	1.418963	0.821834
6	7	0	1.408672	1.040125	1.277733
7	7	0	-2.589278	-0.069107	-0.693989
8	6	0	2.393206	1.88239	1.998456
9	6	0	3.352015	0.983713	2.791755
10	1	0	2.806586	0.380177	3.524747
11	1	0	4.09141	1.588357	3.328291
12	1	0	3.902255	0.30665	2.128458
13	6	0	1.673116	2.815945	2.979042
14	1	0	1.004046	3.504618	2.454135
15	1	0	2.404278	3.418069	3.52939
16	1	0	1.079575	2.250478	3.704432
17	6	0	3.196941	2.730257	0.998802
18	1	0	2.525784	3.358645	0.406591
19	1	0	3.758873	2.088968	0.313592
20	1	0	3.909618	3.381042	1.519966
21	6	0	-3.718769	0.655042	-1.222251
22	6	0	-3.325189	1.249489	-2.583961
23	1	0	-3.032008	0.45417	-3.275646
24	1	0	-2.479239	1.931057	-2.467297
25	1	0	-4.168006	1.799742	-3.017477
26	6	0	-4.113249	1.77838	-0.250128

27	1	0	-4.379457	1.36807	0.728375
28	1	0	-4.978312	2.326546	-0.639398
29	1	0	-3.287048	2.48186	-0.120803
30	6	0	-4.888685	-0.329961	-1.391461
31	1	0	-4.610027	-1.142264	-2.06936
32	1	0	-5.764991	0.182043	-1.804096
33	1	0	-5.168044	-0.76814	-0.428095
34	6	0	3.180202	-0.734719	-0.533693
35	6	0	4.137751	-1.725628	-0.262127
36	1	0	4.014403	-2.360882	0.613497
37	6	0	5.248471	-1.910131	-1.087099
38	1	0	5.977288	-2.682328	-0.853378
39	6	0	5.425475	-1.098281	-2.205719
40	1	0	6.29088	-1.235715	-2.848831
41	6	0	4.487331	-0.106236	-2.496058
42	1	0	4.62124	0.53021	-3.367171
43	6	0	3.378806	0.06815	-1.671011
44	1	0	2.65745	0.846231	-1.911034
45	6	0	-0.366178	2.999392	-0.239456
46	6	0	0.053271	3.007378	-1.580792
47	1	0	0.403521	2.079632	-2.029376
48	6	0	0.0055	4.167232	-2.352092
49	1	0	0.339271	4.146598	-3.386911
50	6	0	-0.480821	5.35357	-1.799929
51	1	0	-0.524055	6.25859	-2.400593
52	6	0	-0.916466	5.369019	-0.476493
53	1	0	-1.301979	6.287785	-0.040725
54	6	0	-0.855745	4.204167	0.290846
55	1	0	-1.198852	4.232208	1.324037
56	6	0	-2.967075	-0.676752	2.705779
57	1	0	-3.220441	-0.946806	3.736829
58	1	0	-3.785247	-0.954475	2.038119
59	1	0	-2.81193	0.401385	2.634726
60	6	0	-0.300614	-1.151228	3.568294
61	1	0	-0.789481	-1.361339	4.525223
62	1	0	-0.015539	-0.09795	3.520619
63	1	0	0.610064	-1.750183	3.492923
64	6	0	-1.872839	-3.280748	2.604505
65	1	0	-2.282671	-3.325348	3.619207
66	1	0	-0.98723	-3.918339	2.560727
67	1	0	-2.618797	-3.661329	1.901779

68	6	0	-0.031304	-4.606658	-0.044838
69	1	0	0.225693	-5.44731	-0.697748
70	1	0	-0.875579	-4.896961	0.582489
71	1	0	0.824494	-4.386578	0.599793
72	6	0	0.885013	-3.201338	-2.31092
73	1	0	0.942322	-4.20183	-2.752875
74	1	0	1.846555	-2.954136	-1.853585
75	1	0	0.686273	-2.46464	-3.092296
76	6	0	-1.900959	-3.723199	-2.018216
77	1	0	-1.667051	-4.663788	-2.528564
78	1	0	-2.170969	-2.963338	-2.755099
79	1	0	-2.755163	-3.872006	-1.352952
80	1	0	1.875946	-1.653614	1.562665
81	1	0	-1.002499	1.864392	2.070078
82	1	0	-0.464082	-0.797765	-1.841928
83	1	0	0.590488	-0.266484	-0.706492

E	-2459.182143
Sigma	1
Nneg	-267
E+ZPE	-2458.479478
U	-2458.435025
H	-2458.434081
G	-2458.557289

Structure 7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	-0.331047	-1.119554	-0.175782
2	15	0	-0.689194	-1.883534	2.247913
3	15	0	1.602429	-2.721411	-0.447162
4	14	0	1.665676	0.524609	0.639331
5	14	0	-0.960333	1.152083	0.867782
6	7	0	0.623383	1.87687	1.097645

7	7	0	-1.816604	-1.660501	-0.98199
8	6	0	0.975894	3.218161	1.615127
9	6	0	2.326534	3.160731	2.338654
10	1	0	2.291255	2.461708	3.180546
11	1	0	2.59437	4.150707	2.724047
12	1	0	3.124916	2.840422	1.661371
13	6	0	-0.092768	3.69953	2.605391
14	1	0	-1.076358	3.770216	2.129007
15	1	0	0.161652	4.694539	2.987168
16	1	0	-0.173975	3.016852	3.457658
17	6	0	1.067692	4.210367	0.443786
18	1	0	0.110237	4.268088	-0.082518
19	1	0	1.831251	3.886582	-0.269697
20	1	0	1.328396	5.21644	0.794767
21	6	0	-2.997094	-1.824255	-1.794408
22	6	0	-2.801448	-1.036623	-3.100203
23	1	0	-1.909446	-1.388609	-3.626402
24	1	0	-2.677227	0.027321	-2.883533
25	1	0	-3.670942	-1.164225	-3.754708
26	6	0	-4.217661	-1.286305	-1.030752
27	1	0	-4.366931	-1.84128	-0.099283
28	1	0	-5.123077	-1.389747	-1.638968
29	1	0	-4.078493	-0.230063	-0.786699
30	6	0	-3.175564	-3.321518	-2.098463
31	1	0	-2.308182	-3.708532	-2.641974
32	1	0	-4.068207	-3.483831	-2.71229
33	1	0	-3.285687	-3.893792	-1.171838
34	6	0	3.019591	1.012673	-0.613067
35	6	0	4.380521	0.862765	-0.296931
36	1	0	4.660158	0.507617	0.69403
37	6	0	5.385601	1.173073	-1.21536
38	1	0	6.430543	1.047588	-0.941233
39	6	0	5.048315	1.655333	-2.478253
40	1	0	5.826457	1.904177	-3.195365
41	6	0	3.703492	1.819886	-2.815831
42	1	0	3.432845	2.197311	-3.79915
43	6	0	2.707586	1.495393	-1.89693
44	1	0	1.664323	1.613647	-2.181361
45	6	0	-2.199169	2.224761	-0.105118
46	6	0	-1.985975	2.603163	-1.441829
47	1	0	-1.082188	2.275089	-1.95219

48	6	0	-2.906511	3.389096	-2.132452
49	1	0	-2.713171	3.67275	-3.164245
50	6	0	-4.078773	3.808937	-1.501467
51	1	0	-4.800708	4.418072	-2.039431
52	6	0	-4.316745	3.443435	-0.17824
53	1	0	-5.226367	3.768115	0.321407
54	6	0	-3.382948	2.665002	0.508181
55	1	0	-3.575905	2.396504	1.54562
56	6	0	-2.453636	-1.732119	2.758255
57	1	0	-2.595909	-2.11019	3.776375
58	1	0	-3.069807	-2.309546	2.065406
59	1	0	-2.760847	-0.686444	2.710884
60	6	0	0.207323	-1.069746	3.628494
61	1	0	-0.13136	-1.456315	4.595043
62	1	0	0.031798	0.007257	3.580593
63	1	0	1.280772	-1.240098	3.518553
64	6	0	-0.437623	-3.673378	2.649503
65	1	0	-0.742673	-3.88449	3.679958
66	1	0	0.608342	-3.96413	2.530853
67	1	0	-1.044496	-4.280259	1.971724
68	6	0	2.912534	-2.981153	0.827269
69	1	0	3.600888	-3.775999	0.520988
70	1	0	2.475239	-3.241247	1.793443
71	1	0	3.471548	-2.050613	0.953736
72	6	0	2.637328	-2.440697	-1.938974
73	1	0	3.410458	-3.210851	-2.031708
74	1	0	3.102274	-1.454159	-1.875849
75	1	0	1.99211	-2.457036	-2.820605
76	6	0	1.015391	-4.447128	-0.753402
77	1	0	1.848882	-5.111078	-1.007005
78	1	0	0.301549	-4.427204	-1.580654
79	1	0	0.501287	-4.836677	0.127859
80	1	0	2.530967	0.108324	1.810158
81	1	0	-1.680942	1.091226	2.197232
82	1	0	0.557737	-0.787388	-1.583026
83	1	0	-0.375462	0.374115	-0.924154

E -2459.197662

Sigma	1
Nneg	0
E+ZPE	-2458.493774
U	-2458.448884
H	-2458.44794
G	-2458.572227

TS (7-10)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	-0.502035	-1.077889	-0.166925
2	15	0	-0.930814	-1.857061	2.232034
3	15	0	1.184087	-2.89451	-0.584912
4	14	0	1.710767	0.26605	0.65686
5	14	0	-0.796801	1.244923	0.886345
6	7	0	0.86935	1.728648	1.176233
7	7	0	-2.083576	-1.360178	-0.920795
8	6	0	1.406701	2.982665	1.750724
9	6	0	2.68694	2.68532	2.541342
10	1	0	2.487945	1.98465	3.358852
11	1	0	3.094211	3.607515	2.970296
12	1	0	3.458328	2.248802	1.89819
13	6	0	0.376088	3.60862	2.698818
14	1	0	-0.555502	3.844682	2.173832
15	1	0	0.764347	4.541674	3.122009
16	1	0	0.140316	2.930491	3.525623
17	6	0	1.726298	3.976153	0.621155
18	1	0	0.821858	4.211389	0.05217
19	1	0	2.462114	3.549443	-0.066965
20	1	0	2.133296	4.912597	1.021906
21	6	0	-3.279551	-1.309207	-1.725942
22	6	0	-2.997011	-0.435466	-2.959089
23	1	0	-2.166925	-0.851952	-3.537468
24	1	0	-2.730337	0.578983	-2.651629
25	1	0	-3.883507	-0.388384	-3.60137

26	6	0	-4.423076	-0.699261	-0.898904
27	1	0	-4.626971	-1.306863	-0.011819
28	1	0	-5.339531	-0.650539	-1.497258
29	1	0	-4.163602	0.312262	-0.57577
30	6	0	-3.639957	-2.740756	-2.158041
31	1	0	-2.830196	-3.177021	-2.750943
32	1	0	-4.551979	-2.741489	-2.764783
33	1	0	-3.807393	-3.377014	-1.283171
34	6	0	3.114065	0.610325	-0.592756
35	6	0	4.443026	0.266701	-0.291041
36	1	0	4.673917	-0.152655	0.687249
37	6	0	5.478576	0.462599	-1.20696
38	1	0	6.49718	0.187864	-0.942805
39	6	0	5.207591	1.020419	-2.454625
40	1	0	6.010557	1.179878	-3.169749
41	6	0	3.897081	1.376203	-2.778884
42	1	0	3.677544	1.814229	-3.74972
43	6	0	2.869358	1.166532	-1.861504
44	1	0	1.852783	1.439649	-2.137249
45	6	0	-1.804452	2.513849	-0.117269
46	6	0	-1.408981	2.947331	-1.394153
47	1	0	-0.49351	2.553891	-1.832423
48	6	0	-2.15859	3.874876	-2.115111
49	1	0	-1.82397	4.198221	-3.09796
50	6	0	-3.339972	4.387704	-1.576623
51	1	0	-3.928424	5.10913	-2.137736
52	6	0	-3.757392	3.971066	-0.314291
53	1	0	-4.674072	4.368657	0.114922
54	6	0	-2.992812	3.049818	0.404251
55	1	0	-3.322618	2.746706	1.396742
56	6	0	-2.676906	-1.514259	2.701394
57	1	0	-2.868955	-1.793903	3.742605
58	1	0	-3.332937	-2.086531	2.041535
59	1	0	-2.879958	-0.451729	2.558648
60	6	0	0.0212	-1.139633	3.629343
61	1	0	-0.334974	-1.537951	4.58485
62	1	0	-0.093203	-0.053355	3.620561
63	1	0	1.082735	-1.367024	3.506649
64	6	0	-0.861441	-3.663773	2.626434
65	1	0	-1.227707	-3.857372	3.64042
66	1	0	0.16015	-4.041862	2.548569

67	1	0	-1.487517	-4.208575	1.914407
68	6	0	2.495653	-3.379973	0.619754
69	1	0	3.065085	-4.237495	0.246158
70	1	0	2.061508	-3.634725	1.588968
71	1	0	3.171518	-2.533962	0.765663
72	6	0	2.194269	-2.686195	-2.107464
73	1	0	2.855607	-3.544479	-2.267778
74	1	0	2.788571	-1.773539	-2.020068
75	1	0	1.522632	-2.576059	-2.962709
76	6	0	0.37302	-4.521089	-0.926798
77	1	0	1.106979	-5.275682	-1.230022
78	1	0	-0.360884	-4.387607	-1.725326
79	1	0	-0.154325	-4.871711	-0.036769
80	1	0	2.525946	-0.304822	1.800518
81	1	0	-1.570612	1.274868	2.187964
82	1	0	0.293713	-0.730976	-1.647068
83	1	0	-0.207151	0.268284	-1.14225

E	-2459.196158
Sigma	1
Nneg	-559
E+ZPE	-2458.494154
U	-2458.449279
H	-2458.448335
G	-2458.573166

Structure 10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	-0.602791	-1.02835	-0.147511
2	15	0	-1.154217	-1.804823	2.18174
3	15	0	0.911284	-2.952099	-0.630786
4	14	0	1.730289	0.1239	0.676798

5	14	0	-0.671448	1.319499	0.878664
6	7	0	1.030382	1.65845	1.189089
7	7	0	-2.217013	-1.168824	-0.871704
8	6	0	1.671199	2.857874	1.772066
9	6	0	2.929325	2.449519	2.548037
10	1	0	2.680977	1.759025	3.36065
11	1	0	3.414149	3.331194	2.981771
12	1	0	3.656772	1.958181	1.893361
13	6	0	0.701451	3.554905	2.735069
14	1	0	-0.21185	3.871343	2.220312
15	1	0	1.167335	4.448749	3.164648
16	1	0	0.416494	2.888915	3.556185
17	6	0	2.060249	3.834689	0.649668
18	1	0	1.173938	4.143001	0.08703
19	1	0	2.758513	3.358593	-0.045138
20	1	0	2.539274	4.734097	1.05566
21	6	0	-3.405651	-1.007162	-1.67307
22	6	0	-3.018087	-0.276338	-2.96962
23	1	0	-2.265249	-0.84831	-3.520828
24	1	0	-2.608081	0.71075	-2.739702
25	1	0	-3.898049	-0.150861	-3.60994
26	6	0	-4.434338	-0.17545	-0.890795
27	1	0	-4.719818	-0.684147	0.034941
28	1	0	-5.338589	-0.025397	-1.490897
29	1	0	-4.015538	0.801178	-0.635314
30	6	0	-3.974917	-2.398831	-1.996011
31	1	0	-3.245995	-2.990114	-2.558532
32	1	0	-4.887389	-2.311597	-2.595737
33	1	0	-4.217878	-2.938989	-1.075546
34	6	0	3.185525	0.330664	-0.544096
35	6	0	4.443467	-0.226989	-0.256668
36	1	0	4.598695	-0.720968	0.701373
37	6	0	5.506266	-0.147873	-1.158468
38	1	0	6.468007	-0.587739	-0.904797
39	6	0	5.33837	0.506942	-2.376918
40	1	0	6.164058	0.576765	-3.080357
41	6	0	4.102819	1.079261	-2.684577
42	1	0	3.964951	1.598476	-3.630109
43	6	0	3.045489	0.98497	-1.781773
44	1	0	2.090629	1.437439	-2.042913
45	6	0	-1.537844	2.676555	-0.148608

46	6	0	-1.107893	3.046822	-1.434331
47	1	0	-0.234898	2.560824	-1.86727
48	6	0	-1.766249	4.02953	-2.171519
49	1	0	-1.405383	4.300706	-3.160897
50	6	0	-2.889981	4.66502	-1.640441
51	1	0	-3.407856	5.429465	-2.214035
52	6	0	-3.339941	4.315162	-0.369099
53	1	0	-4.211189	4.808876	0.055007
54	6	0	-2.666158	3.33679	0.364568
55	1	0	-3.020283	3.084705	1.362897
56	6	0	-2.839159	-1.266829	2.688236
57	1	0	-3.056519	-1.56395	3.719532
58	1	0	-3.567741	-1.722955	2.01414
59	1	0	-2.90671	-0.181936	2.591595
60	6	0	-0.105891	-1.232318	3.57738
61	1	0	-0.481667	-1.61885	4.530275
62	1	0	-0.106915	-0.139917	3.59859
63	1	0	0.92379	-1.563421	3.423549
64	6	0	-1.286676	-3.617045	2.534967
65	1	0	-1.654423	-3.79436	3.551293
66	1	0	-0.315225	-4.105202	2.425466
67	1	0	-1.981882	-4.069319	1.821974
68	6	0	2.160365	-3.580084	0.575849
69	1	0	2.637563	-4.493115	0.203986
70	1	0	1.692419	-3.788923	1.540586
71	1	0	2.924226	-2.814782	0.732473
72	6	0	1.953255	-2.8244	-2.145525
73	1	0	2.525487	-3.742971	-2.314728
74	1	0	2.639685	-1.980582	-2.043556
75	1	0	1.305482	-2.639398	-3.006911
76	6	0	-0.037481	-4.495385	-1.005875
77	1	0	0.631151	-5.311699	-1.300569
78	1	0	-0.739551	-4.292848	-1.818498
79	1	0	-0.613254	-4.800118	-0.1292
80	1	0	2.453255	-0.553031	1.822458
81	1	0	-1.449801	1.450101	2.171299
82	1	0	0.163654	-0.606218	-1.72848
83	1	0	-0.109984	0.178916	-1.364764

E	-2459.197798

Sigma	1
Nneg	0
E+ZPE	-2458.493745
U	-2458.44869
H	-2458.447746
G	-2458.57288

Structure 11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	42	0	1.163014	-0.284152	-0.170761
2	15	0	2.976585	1.138717	-1.049533
3	15	0	2.035249	-2.54989	-0.586157
4	14	0	-1.141573	-1.136493	-0.965328
5	14	0	-0.504924	1.480152	-1.053107
6	7	0	-1.834754	0.402633	-1.489785
7	7	0	1.19035	-0.152078	1.55326
8	6	0	-3.132071	0.695823	-2.136886
9	6	0	-3.558744	-0.490879	-3.010235
10	1	0	-2.812359	-0.693702	-3.784945
11	1	0	-4.51632	-0.280564	-3.499544
12	1	0	-3.684368	-1.399056	-2.411241
13	6	0	-3.002923	1.94102	-3.023159
14	1	0	-2.710523	2.818002	-2.435784
15	1	0	-3.960807	2.16727	-3.504708
16	1	0	-2.251758	1.789562	-3.805009
17	6	0	-4.202951	0.947575	-1.061941
18	1	0	-3.922625	1.799373	-0.43524
19	1	0	-4.313502	0.070448	-0.417284
20	1	0	-5.176563	1.163073	-1.519095
21	6	0	1.402599	0.032192	2.970327
22	6	0	0.063832	-0.114269	3.708416
23	1	0	-0.376898	-1.095997	3.517213
24	1	0	-0.637684	0.654804	3.375751
25	1	0	0.21504	-0.001197	4.787597
26	6	0	1.976424	1.439462	3.198675

27	1	0	2.948385	1.539767	2.705459
28	1	0	2.112052	1.62725	4.269495
29	1	0	1.297991	2.193459	2.791238
30	6	0	2.393144	-1.034803	3.463638
31	1	0	1.991111	-2.038069	3.29418
32	1	0	2.579023	-0.915112	4.536629
33	1	0	3.346091	-0.946163	2.933188
34	6	0	-2.277152	-2.135685	0.195014
35	6	0	-2.79798	-3.376975	-0.207346
36	1	0	-2.561194	-3.756585	-1.200074
37	6	0	-3.621591	-4.131042	0.6306
38	1	0	-4.011797	-5.087881	0.291606
39	6	0	-3.95247	-3.651556	1.896201
40	1	0	-4.598408	-4.231955	2.550115
41	6	0	-3.451946	-2.418478	2.317972
42	1	0	-3.708167	-2.036672	3.303555
43	6	0	-2.622664	-1.678517	1.477548
44	1	0	-2.226531	-0.726524	1.821671
45	6	0	-1.020439	2.891202	0.123262
46	6	0	-1.717075	2.646687	1.318951
47	1	0	-2.002889	1.626517	1.565488
48	6	0	-2.068053	3.680815	2.184934
49	1	0	-2.615177	3.462614	3.099211
50	6	0	-1.72138	4.997601	1.877681
51	1	0	-1.99233	5.806244	2.551694
52	6	0	-1.037439	5.268846	0.694262
53	1	0	-0.777369	6.293372	0.438292
54	6	0	-0.700682	4.226685	-0.171167
55	1	0	-0.194154	4.459035	-1.106949
56	6	0	3.001068	2.905113	-0.516951
57	1	0	3.792643	3.464876	-1.027082
58	1	0	3.167339	2.955593	0.562144
59	1	0	2.031495	3.361263	-0.726101
60	6	0	2.915305	1.294761	-2.888291
61	1	0	3.712316	1.955829	-3.244133
62	1	0	1.945456	1.705132	-3.17976
63	1	0	3.036628	0.313606	-3.355516
64	6	0	4.761144	0.710285	-0.789609
65	1	0	5.42634	1.485487	-1.18652
66	1	0	4.983802	-0.237208	-1.286342
67	1	0	4.956646	0.587441	0.27931

68	6	0	2.005703	-3.083552	-2.353232
69	1	0	2.322523	-4.127622	-2.444651
70	1	0	2.678028	-2.457967	-2.946952
71	1	0	0.990289	-2.977494	-2.743777
72	6	0	1.115464	-3.917545	0.242498
73	1	0	1.572522	-4.893429	0.044461
74	1	0	0.077048	-3.920509	-0.096085
75	1	0	1.106681	-3.733137	1.319911
76	6	0	3.766035	-3.002827	-0.101184
77	1	0	3.968723	-4.063227	-0.289116
78	1	0	3.908947	-2.797664	0.963225
79	1	0	4.481734	-2.397099	-0.661709
80	1	0	-1.073652	-2.088116	-2.147729
81	1	0	-0.077057	2.288163	-2.2649

E	-2458.009923
Sigma	1
Nneg	0
E+ZPE	-2457.322134
U	-2457.277415
H	-2457.276471
G	-2457.401072

$PhSiH_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	2.344439	0.000001	0.005629
2	6	0	0.466737	0.000011	-0.011433
3	6	0	-0.256036	1.203912	-0.009184
4	1	0	0.273534	2.154253	-0.022288
5	6	0	-1.649718	1.206168	0.003145
6	1	0	-2.190168	2.149051	0.003063
7	6	0	-2.348717	-0.000009	0.010145
8	1	0	-3.435425	-0.000016	0.016737
9	6	0	-1.649702	-1.206178	0.003148

10	1	0	-2.190139	-2.149068	0.003068
11	6	0	-0.256022	-1.203903	-0.009186
12	1	0	0.273558	-2.15424	-0.022292
13	1	0	2.859176	1.215319	-0.685163
14	1	0	2.888868	-0.000496	1.394275
15	1	0	2.859195	-1.214822	-0.686022

E	-522.8075772
Sigma	1
Nneg	0
E+ZPE	-522.691954
U	-522.684935
H	-522.683991
G	-522.723868

H_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0	0	0.371682
2	1	0	0	0	-0.371682

E	-1.17751651
Sigma	2
Nneg	0
E+ZPE	-1.17751651
U	-1.17515599
H	-1.17421178
G	-1.18900554

III. DFT calculations

The unconstrained geometry optimization was carried out for all the considered structures with the Gaussian03 program package[2] using DFT and applying Becke three parameter hybrid exchange functional in conjunction with gradient-corrected nonlocal correlation functional of Perdew and Wang (B3PW91)[3].The 6-31G(d,p) basis set was used for the H, C, N, O, Si, P and Cl atoms. The Hay-Wadt effective core potentials (ECP) and the corresponding VDZ basis sets were used for the Mo atoms[4]. The same level of theory was used in the frequency calculations performed at all the located stationary points. The thermodynamic parameters were calculated in the rigid rotor-harmonic oscillator approximation. For all the located transition state structures, the minimum energy reaction paths were investigated using the Gonzales-Schlegel method[5].

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