Examination of Pt_2dba_3 as a "cocktail"-type catalytic system for alkene and alkyne hydrosilylation reactions

Authors: Evgeniia E. Ondar, Alexander Yu. Kostyukovich, Julia V. Burykina, Alexey S. Galushko, Valentine P. Ananikov*

N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Leninsky prospekt 47, Moscow, 119991, Russia.

E-mail: val@ioc.ac.ru; Web: http://AnanikovLab.ru

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Model reaction scalability

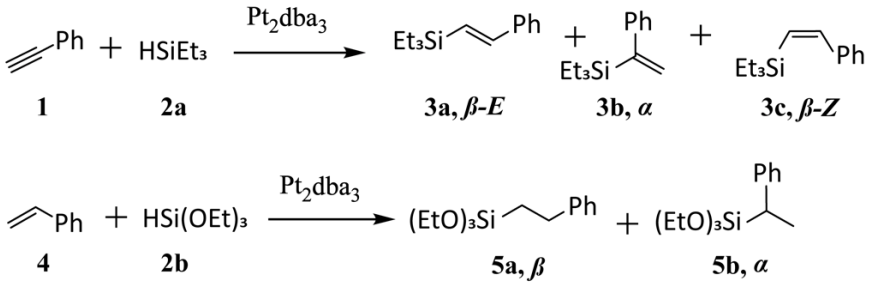
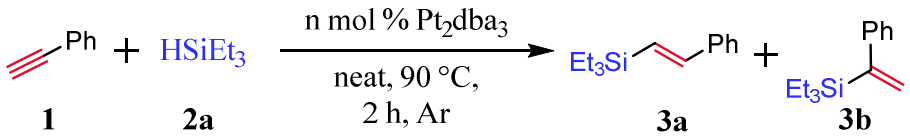


Table S1. Catalytic reaction with increased substrate scale (0.05 mol % of Pt_2dba_3 was used).

Model reaction	Amount, mmol Substrate / Silane	Conditions	Yield of **n a** + **n b**, % (**n a** / **n b**)
Phenylacetylene, $HSiEt_3$	5 / 5	90 °C, Ar, neat, 4 h	95 (4.6)
Styrene, $HSi(OEt)_3$	4 / 4		86 (1.9)

Catalyst loading variation in the alkyne model reaction

Table S2. Catalyst loading variation of the phenylacetylene hydrosilylation reaction. The average and standard deviation values of 3 runs are presented.

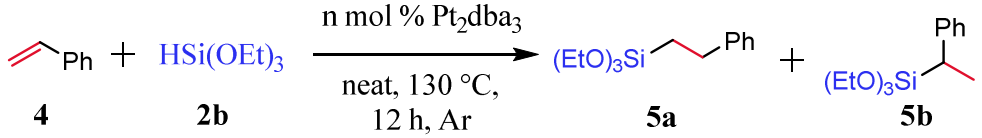


Entry	Catalyst amount, mol %	Yield of **3a**, % [a]	Yield of **3b**, % [a]	Ratio of **3a / 3b**	Sum of isomers yield , %
1	0.25	68.7 ± 2.2	11.3 ± 3.4	6.1	80
2	0.1	71.3 ± 9.0	15.3 ± 1.1	4.7	86
3	0.05	71.4 ± 4.8	16.2 ± 1.2	4.4	87
4	0.01	74.3 ± 2.8	20.1 ± 0.2	3.7	94
5	0.005	41.4 ± 3.9	13.4 ± 1.1	3.1	54
6	0.0025	-[b]	-[b]	-[b]	-[b]

Full conversion of reagents was achieved if otherwise not stated. [a] Yield was measured by ^{1}H NMR with dimethyl terephthalate as an internal standard. [b] No product was detected.

Catalyst loading variation in the alkene model reaction

Table S3. Catalyst loading variation in the styrene hydrosilylation reaction. The average and standard deviation values of 3 runs are presented.



4 **2b** **5a** **5b**

Entry	Catalyst amount, mol %	Yield of **5a**, % [a]	Yield of **5b**, % [a]	Ratio of **5a / 5b**	Sum of isomers yield , %
1	0.25	52.3 ± 18.2	23.1 ± 13.5	2.3	75
2	0.1	55.7 ± 4.9	31.5 ± 4.4	1.8	87
3	0.05	61.7 ± 1.2	25.4 ± 0.9	2.4	87
4	0.01	58.6 ± 6.1	21.8 ± 2.2	2.7	80
5	0.005	58.5 ± 5.2	20.7 ± 2.5	2.8	79
6	0.0025	60.1 ± 2.5	21.0 ± 0.6	2.9	81

Full conversion of reagents was achieved if otherwise not stated. [a] Yield was measured by ^{1}H NMR with dimethyl terephthalate as an internal standard.

Pt_2dba_3 purity estimation

The ratio of the Pt_2dba_3 complex and noncoordinated dba ligands was evaluated using the following procedure. The $^1H\{^{195}Pt\}$ NMR spectrum of Pt_2dba_3 in $CDCl_3$ was registered, and the integral intensities of free dba protons (7.77, d, J = 16.0 Hz, 2H) and coordinated dba protons (4.03, d, J = 11.3 Hz, 1H) were measured (Figure S1). According to formula (**1**), the ratio of the Pt_2dba_3 complex to noncoordinated dba ligands in the solution was calculated.

$$Ratio\ of\ Pt_2dba_3 \text{ complex to noncoordinated dba ligands} = \frac{I_2}{\frac{I_1}{2}+I_2} = \frac{2.17}{\frac{1.00}{2}+2.17} = 0.81 \qquad (\mathbf{1})$$

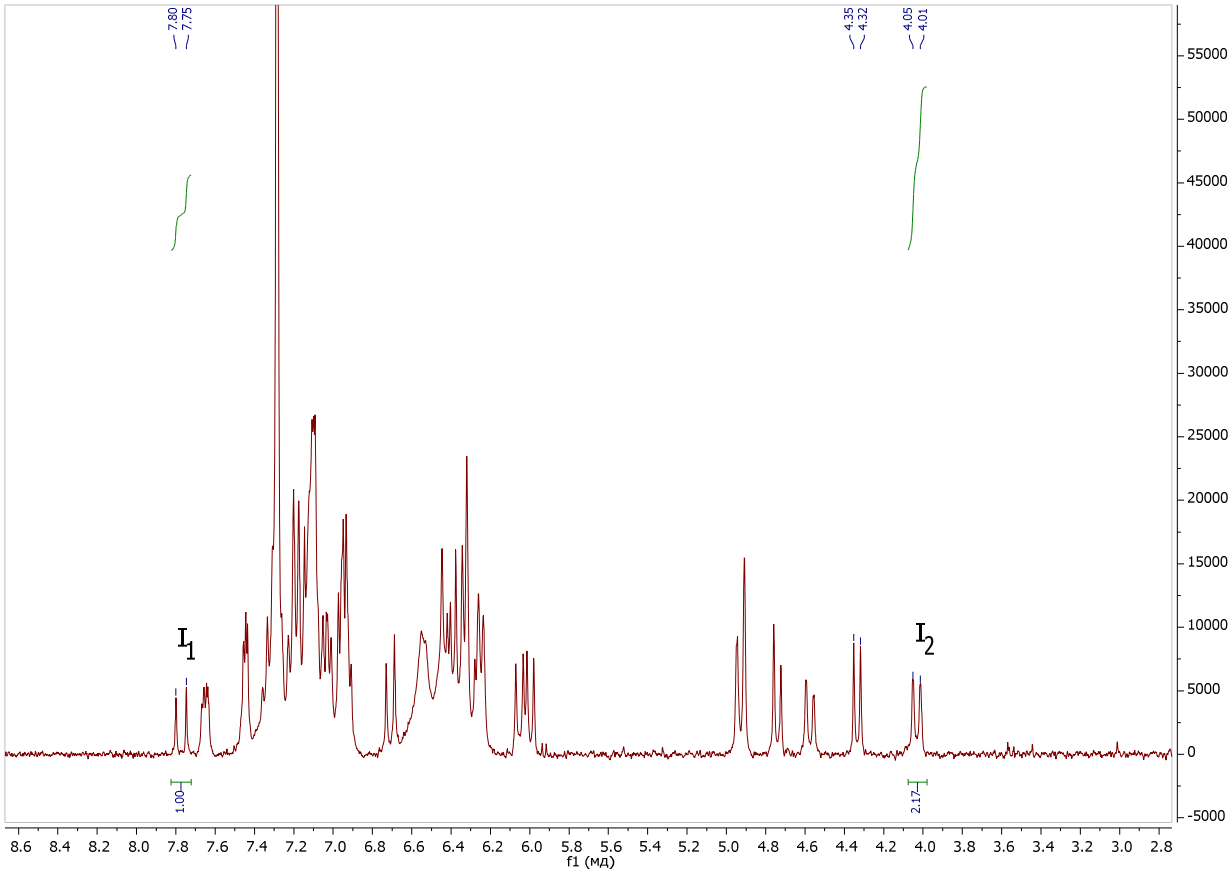
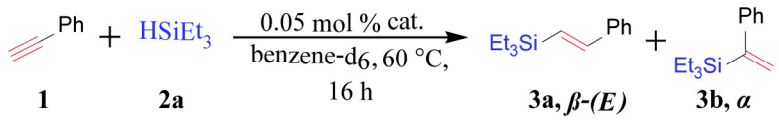


Figure S1. $^1H\{^{195}Pt\}$ NMR spectrum of Pt_2dba_3 in $CDCl_3$.

Kinetic curves



1 **2a** **3a, *β-(E)*** **3b, *α***

Scheme S1. In-tube ^{1}H NMR monitoring of model reactions with respect to the catalyst used.

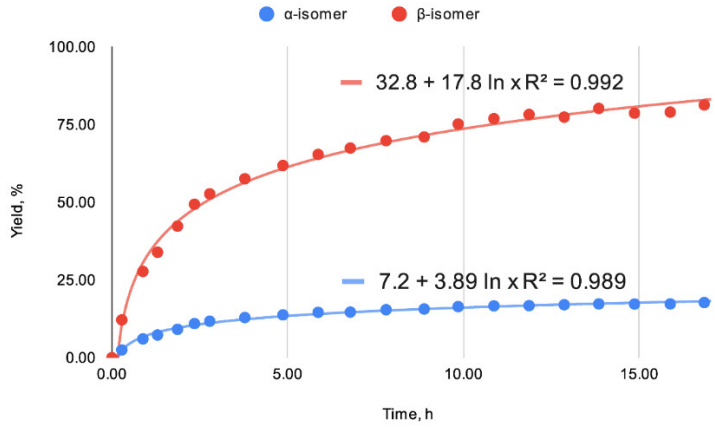


Figure S2. Isomer yield vs. time plot with a linear trendline (equation and R^2 are given) for the phenylacetylene hydrosilylation reaction in the presence of Pt_2dba_3. Dimethyl terephthalate was used as an internal standard.

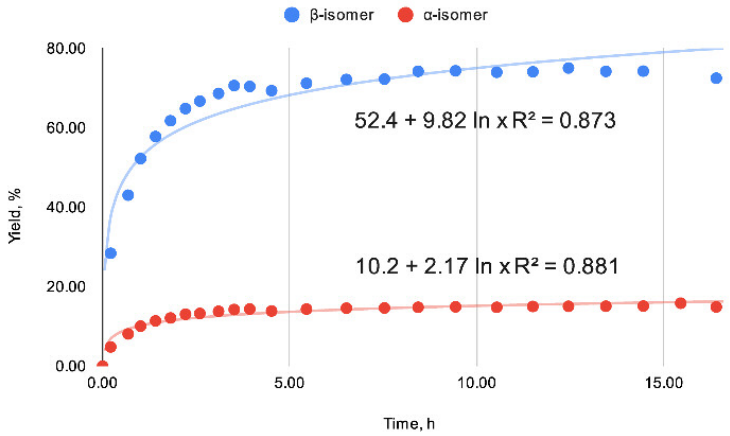


Figure S3. Isomer yield vs. time plot with a linear trendline (equation and R^2 are given) for the phenylacetylene hydrosilylation reaction in the presence of Karstedt's catalyst. Dimethyl terephthalate was used as an internal standard.

Mass spectra of Pt species after heating of Pt_2dba_3 solution

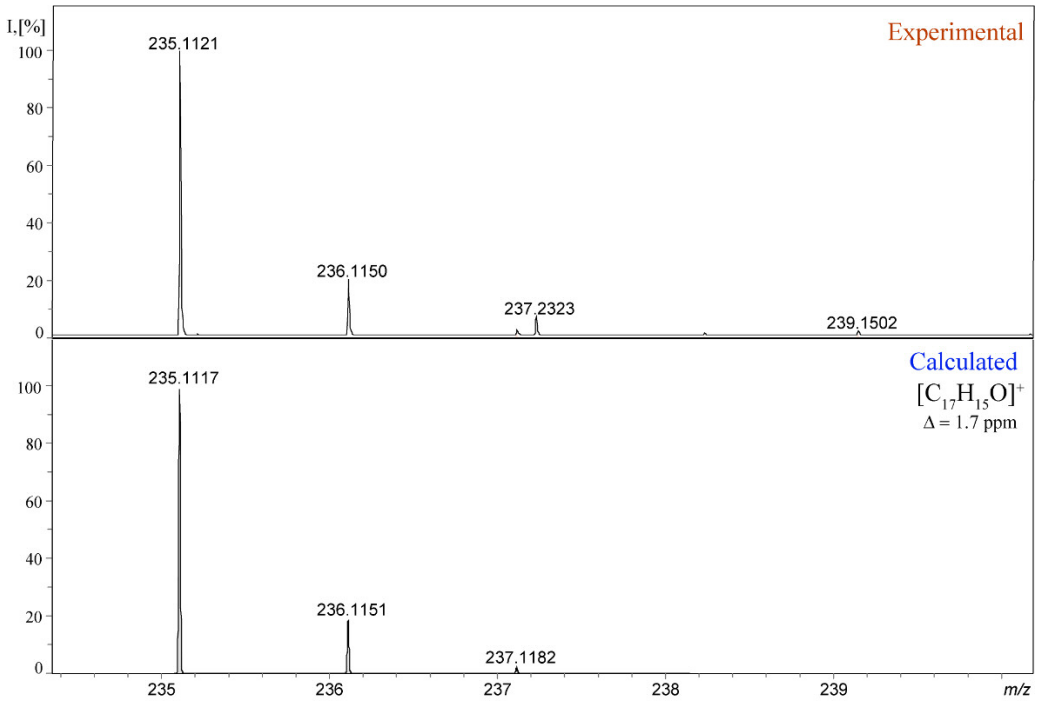


Figure S4. Experimentally detected and theoretical ESI-(+)MS spectrum of Pt_2dba_3; main experimental peak $[M+H]^+$ = 235.1121 Da, calculated for $C_{17}H_{15}O$ = 235.1117 Da, Δ = 1.7 ppm.

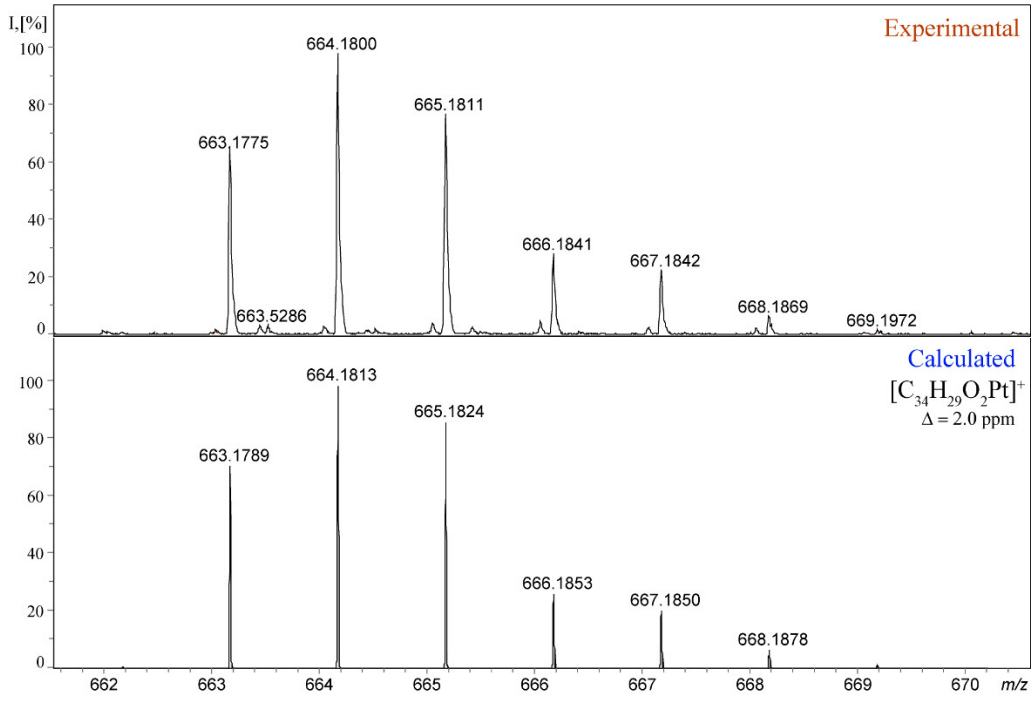


Figure S5. Experimentally detected and theoretical ESI-(+)MS spectrum of Pt_2dba_2; main experimental peak $[M+H]^+$ = 664.1800 Da, calculated for $C_{34}H_{29}O_2Pt$ = 664.1813 Da, Δ = 2.0 ppm.

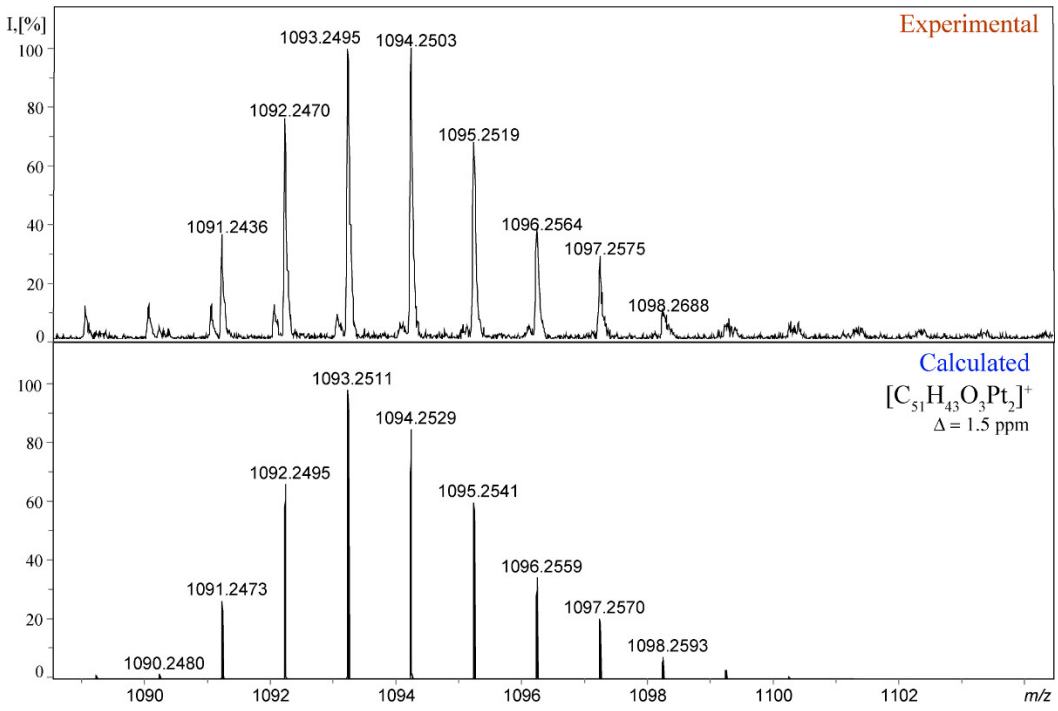


Figure S6. Experimentally detected and theoretical ESI-(+)MS spectrum of Pt_2dba_3; main experimental peak $[M+H]^+$ = 1093.2495 Da, calculated for $C_{51}H_{43}O_3Pt_2$ = 1093.2511 Da, Δ = 1.5 ppm.

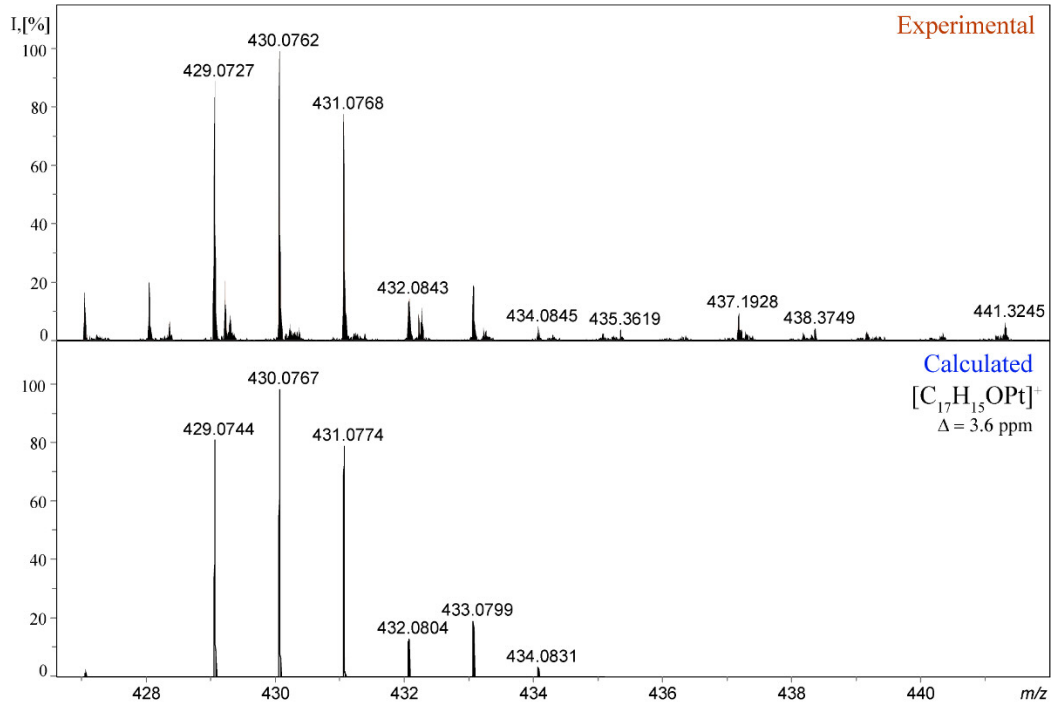


Figure S7. Experimentally detected and theoretical ESI-(+)MS spectrum of Ptdba; main experimental peak $[M+H]^+$ = 430.0762 Da, calculated for $C_{17}H_{15}OPt$ = 430.0767 Da, Δ = 3.6 ppm.

Microscopy images of Pt nanoparticles after Pt_2dba_3 decomposition in toluene-d_6

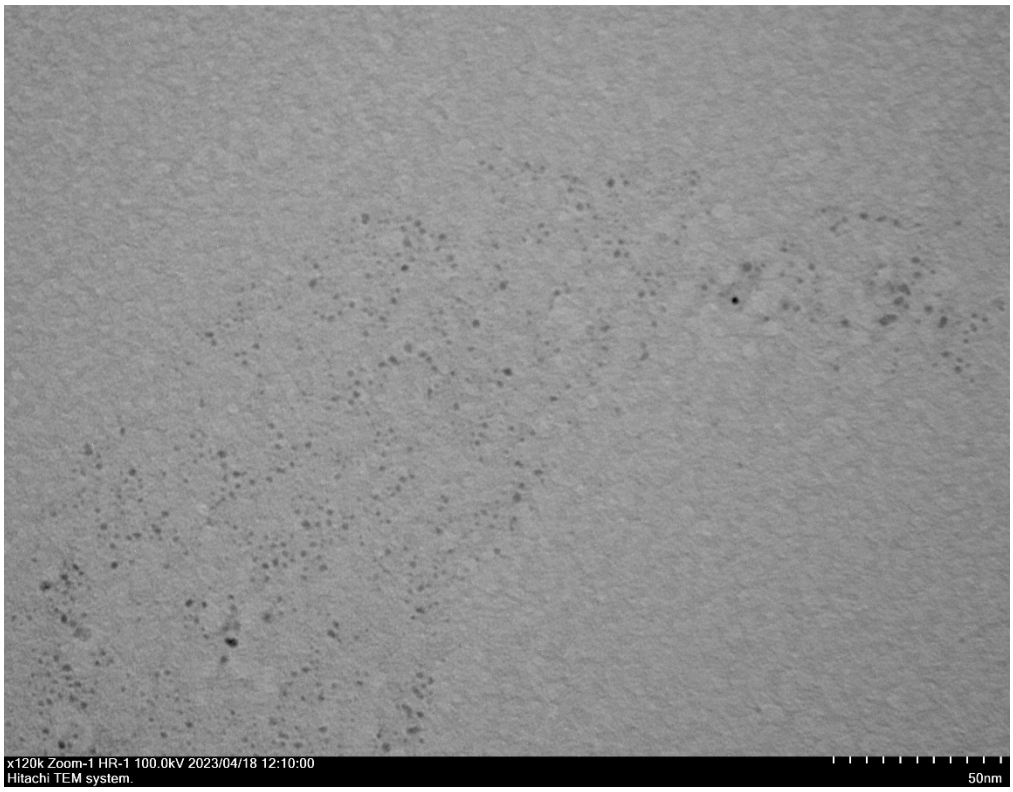


Figure S8. Pt particles captured from Pt_2dba_3 in benzene-d6 after heating for 18 h at 70 °C.

Figure S9. Pt particles captured from Pt_2dba_3 in benzene-d6 after heating for 18 h at 70 °C.

Experiment on reusability of catalytic system

Table S6. Conversion of substrates in each cycle (determined by NMR spectroscopy).

Model reaction	Cycle 1 conversion, %	Cycle 2 conversion, %	Cycle 3 conversion, %
Phenylacetylene, $HSiEt_3$	99	98	99
Styrene, $HSi(OEt)_3$	99	97	96

XAFS analysis of the phenylacetylene hydrosilylation reaction

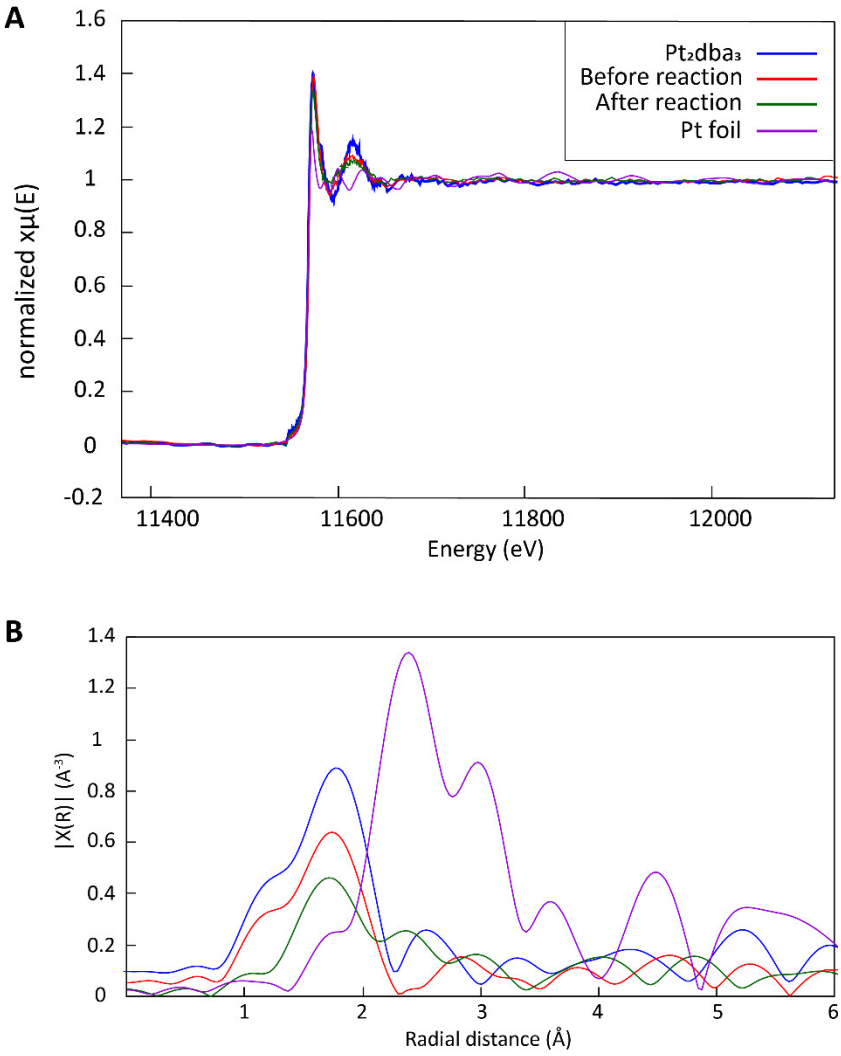


Figure S10. A. K-edge XAFS spectrum of Pt before and after reaction with respect to Pt foil and Pt_2dba_3 in toluene. **B.** Forward Fourier transforms of the XAFS spectrum of the Pt K-edge before and after reaction comparison with Pt foil and Pt_2dba_3 in toluene. The initial scale of the signals is given.

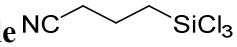
Product characterization data

General hydrosilylation procedure. Reactions were carried out under an Ar atmosphere using the Shlenk technique. 1 mmol of substrate, 1 mmol of silane and 0.05 mol % of Pt_2dba_3 were added into a Schlenk tube. The reaction was carried out at temperature t °C (Table S7) overnight. The product was purified by column chromatography (ethyl acetate – petroleum ether) or vacuum distillation.

The products 4-(trichlorosilyl)butanenitrile and 4-(triethoxysilyl)butanenitrile are novel, and their characterization data are presented below. Other product characterization is in agreement with literature data (references are given in Table S7).

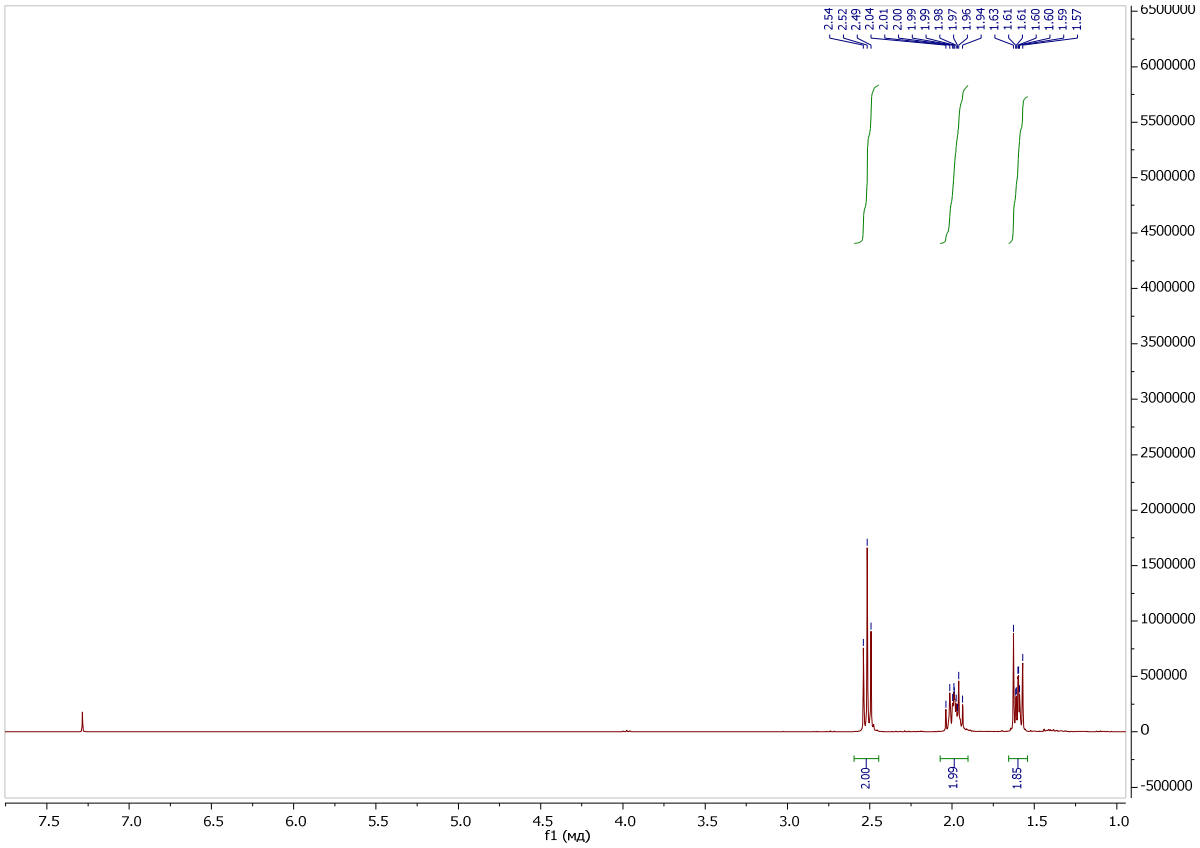
Table S7. Scope reaction conditions and literature data.

Reagents	Temperature, °C	Reference
Trimethylsilylacetylene, $HSiEt_3$	50	***β-(E)***[1], ***α***[2]
Trimethylsilylacetylene, $HSi(OEt)_3$	50	[1]
Diphenylacetylene, $HSiEt_3$	90	[1]
Diphenylacetylene, $HSi(OEt)_3$	120	[1]
Allylbenzene, $HSiCl_3$	50	[3]
Allylbenzene, $HSi(OEt)_3$	130	[4]
Allylcianide, $HSiCl_3$	50	See below
Allylcianide, $HSi(OEt)_3$	110	See below
Allylphenyl ether, $HSiEt_3$	95	[5]
Vinyltrimethoxysilane, $HSi(OEt)_3$	110	[6]
Phenylacetylene, $HSiEt_3$	90	[1]
Styrene, $HSi(OEt)_3$	100	[7]

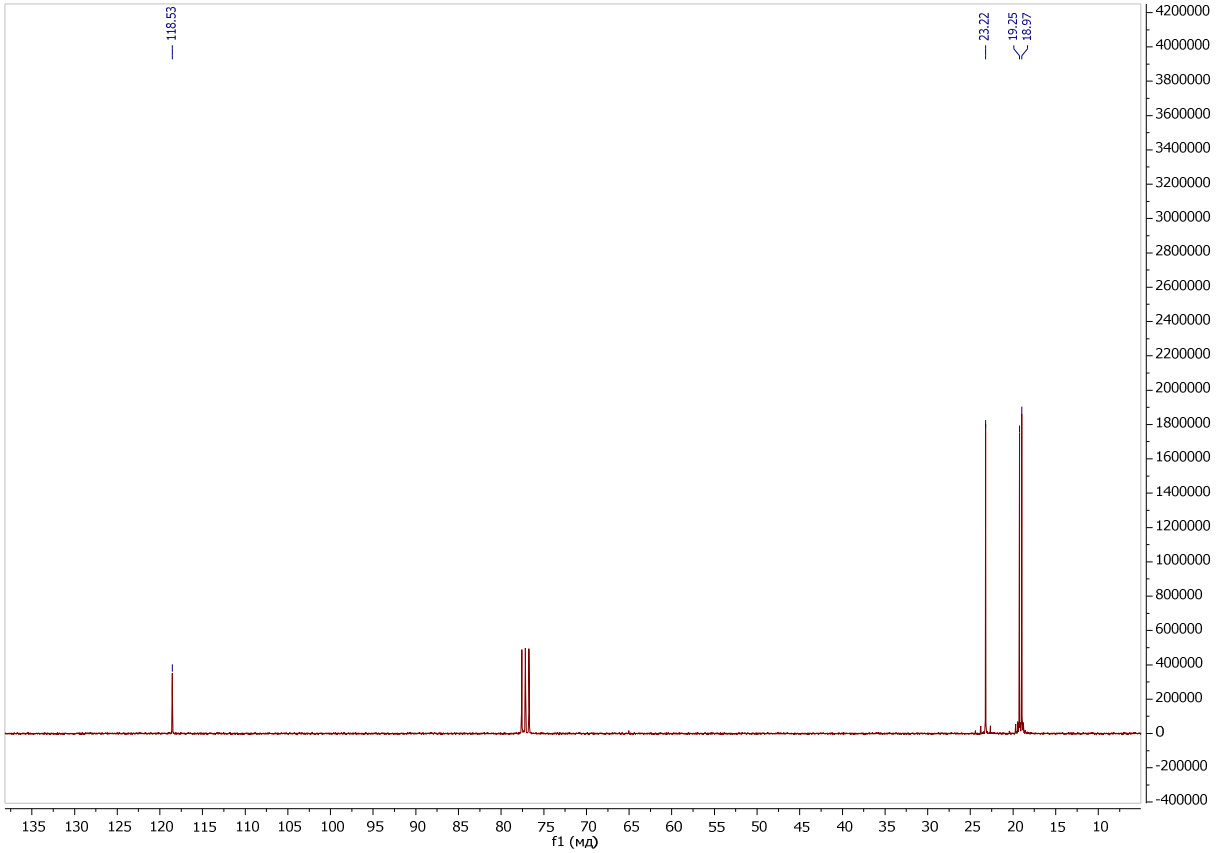
4-(Trichlorosilyl)butanenitrile 

Purified by vacuum distillation. The yield was 98 %.

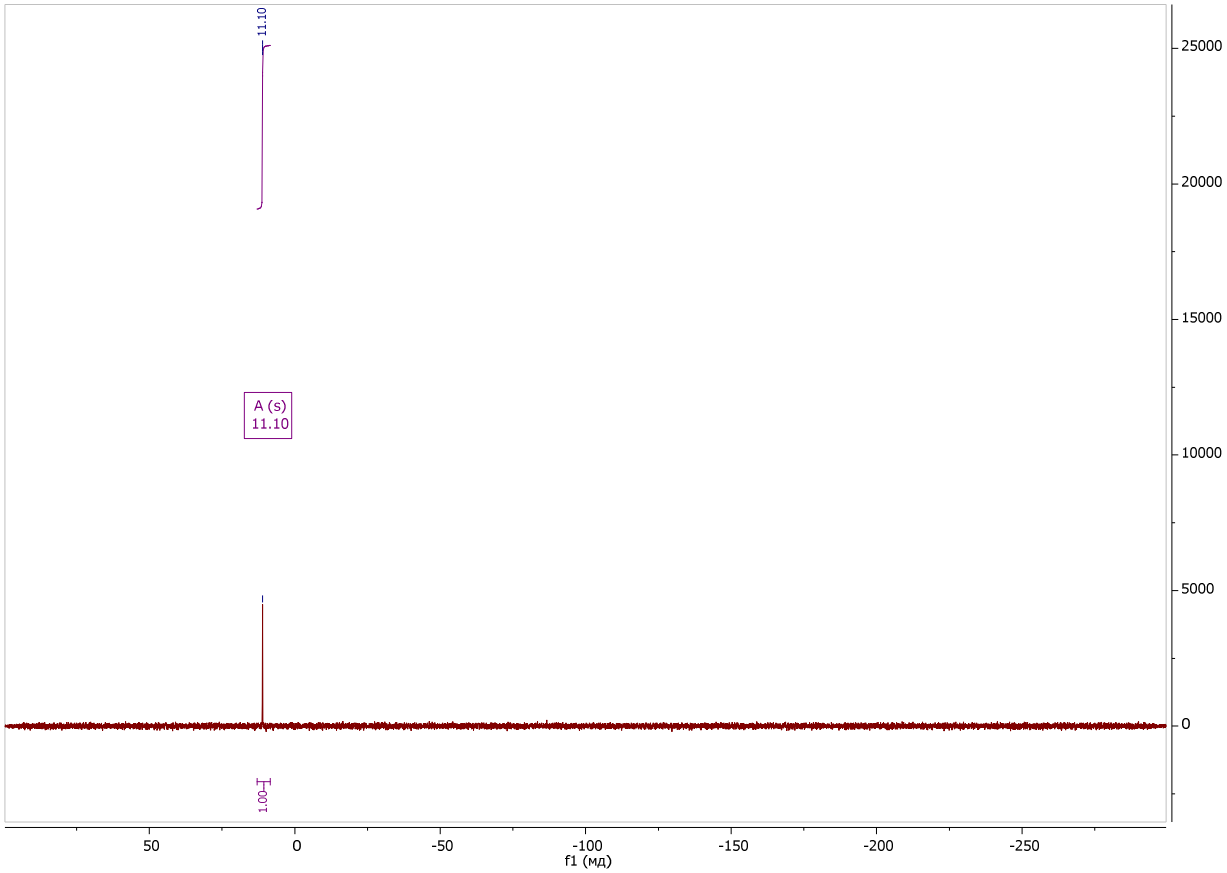
^{1}H NMR (300 MHz, Chloroform-*d*) δ 2.52 (t, *J* = 6.9 Hz, 2H, NC-*CH*$_2$-), 2.08 – 1.90 (m, 2H, CH_2-*CH*$_2$-CH_2-), 1.66 – 1.54 (m, 2H, -*CH*$_2$-$SiCl_3$).

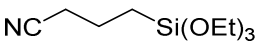


^{13}C NMR (76 MHz, Chloroform-*d*) δ 118.53 (*NC*-), 23.22 (-*CH*$_2$-SiCl$_3$), 19.25 (NC-*CH*$_2$-), 18.97 (CH$_2$-*CH*$_2$-CH$_2$-).



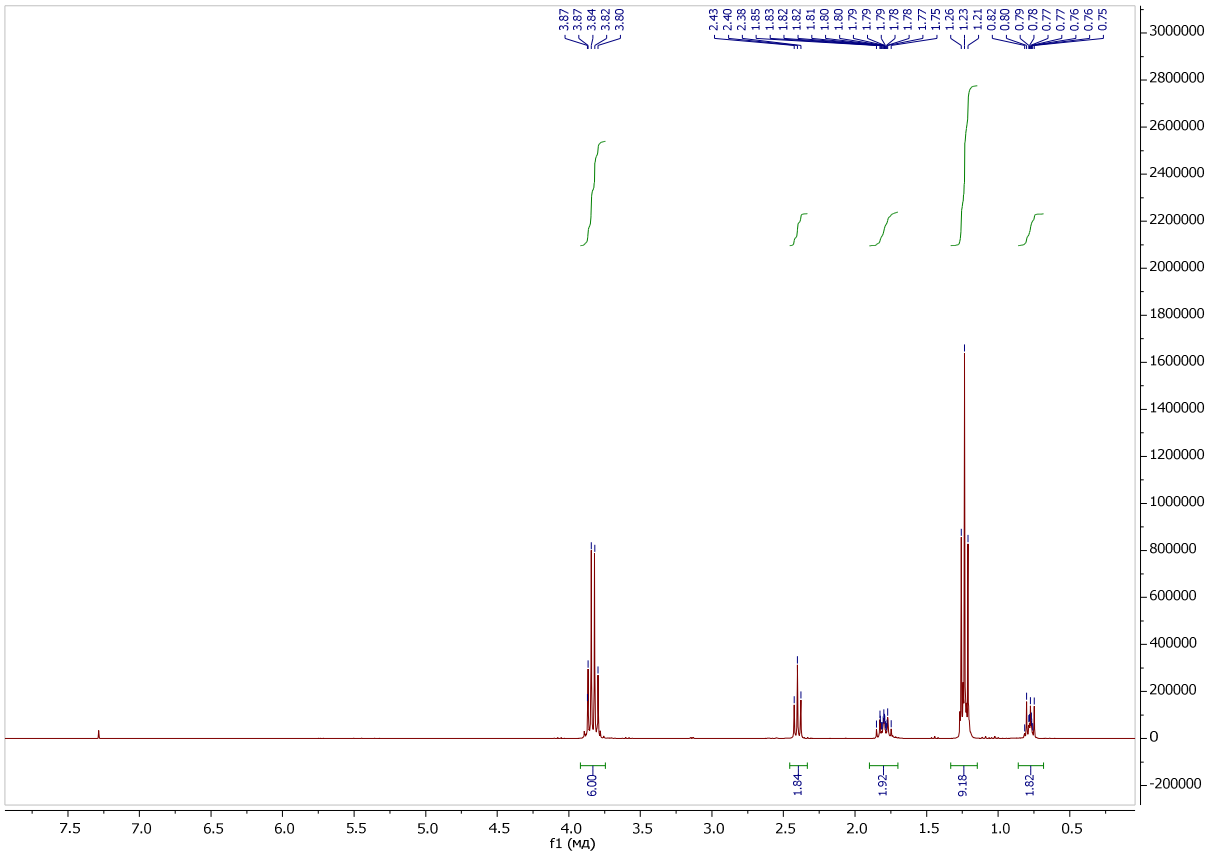
^{29}Si NMR (60 MHz, Chloroform-*d*) δ 11.10 (-$SiCl_3$).



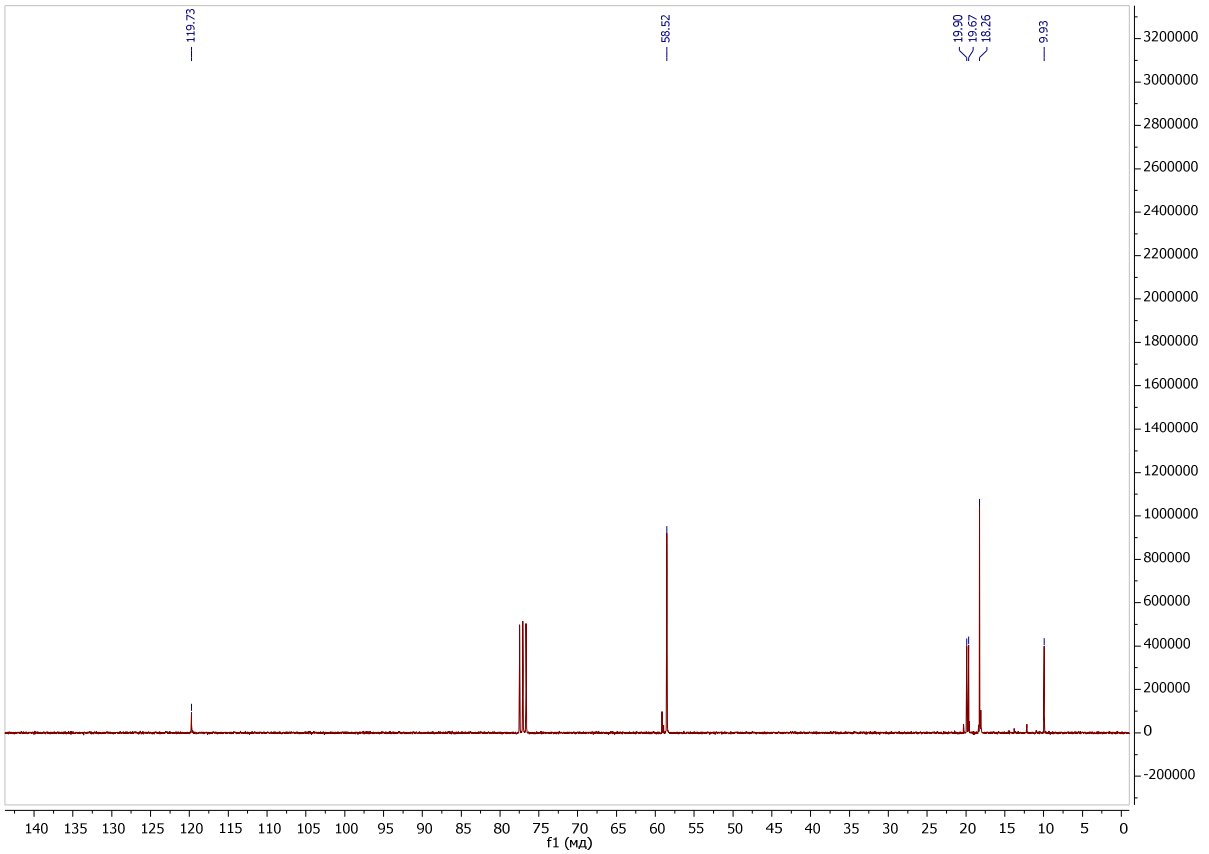
4-(triethoxysilyl)butanenitrile 

Purified by column chromatography (ethyl acetate – petroleum ether). The yield was 77 %.

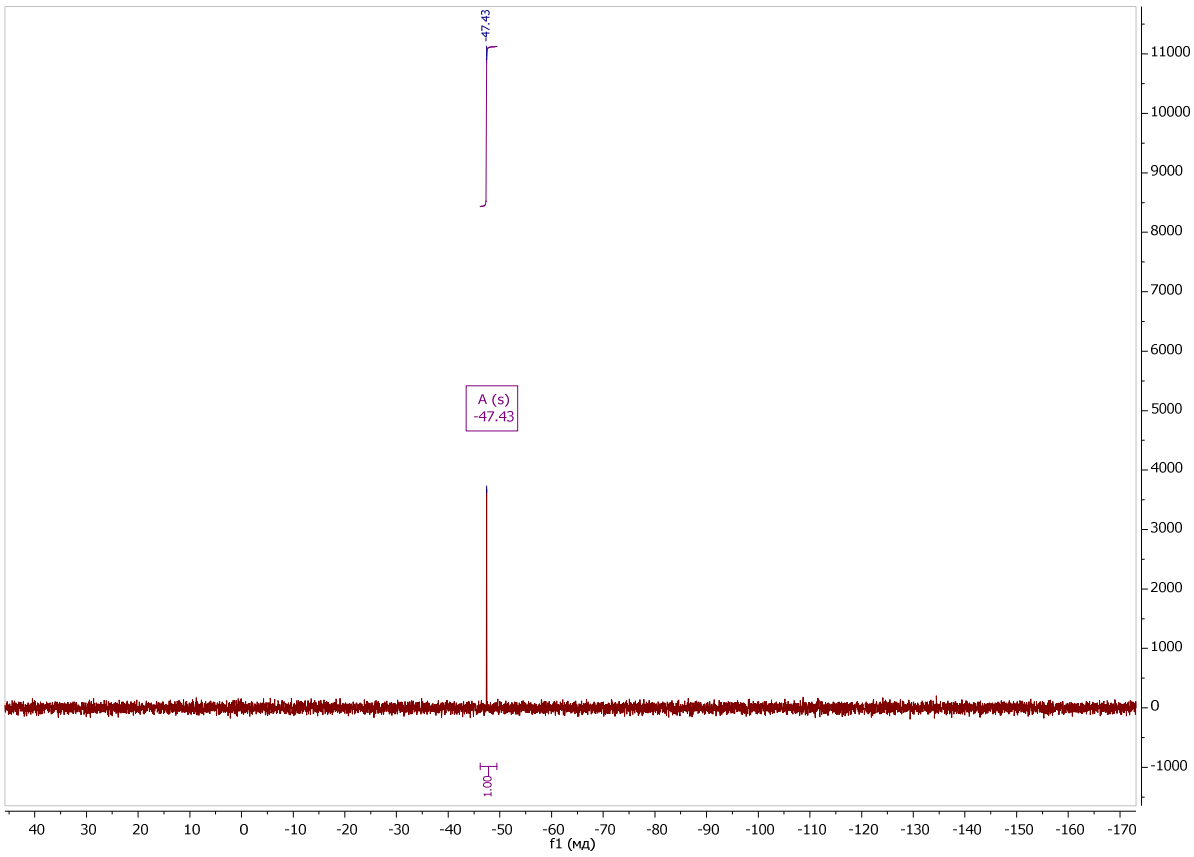
^{1}H NMR (300 MHz, Chloroform-*d*) δ 3.83 (q, *J* = 7.0 Hz, 6H), 2.40 (t, *J* = 7.1 Hz, 2H), 1.87 – 1.68 (m, 2H), 1.23 (t, *J* = 7.0 Hz, 9H), 0.83 – 0.72 (m, 2H).



^{13}C NMR (76 MHz, Chloroform-*d*) δ 119.73, 59.14, 58.52, 19.79, 18.26, 9.93.

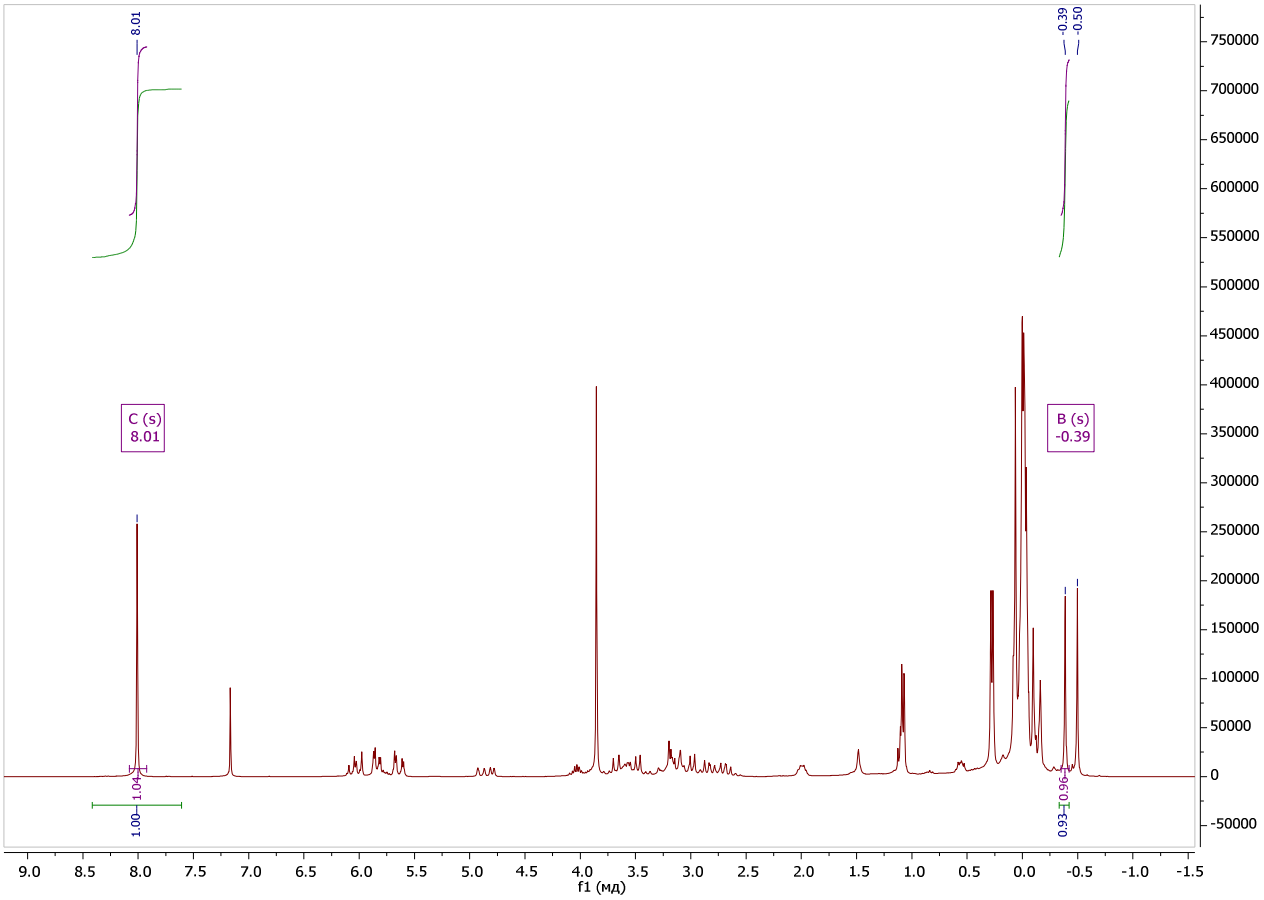


^{29}Si NMR (60 MHz, Chloroform-*d*) δ -47.43.



Pt_2dvtms_3 content estimation

Having an $^{1}H\{^{195}Pt\}$ NMR spectrum of the Pt_2dvtms_3 sample with an internal standard (dimethyl terephthalate), the content of complex as the number of moles was calculated.



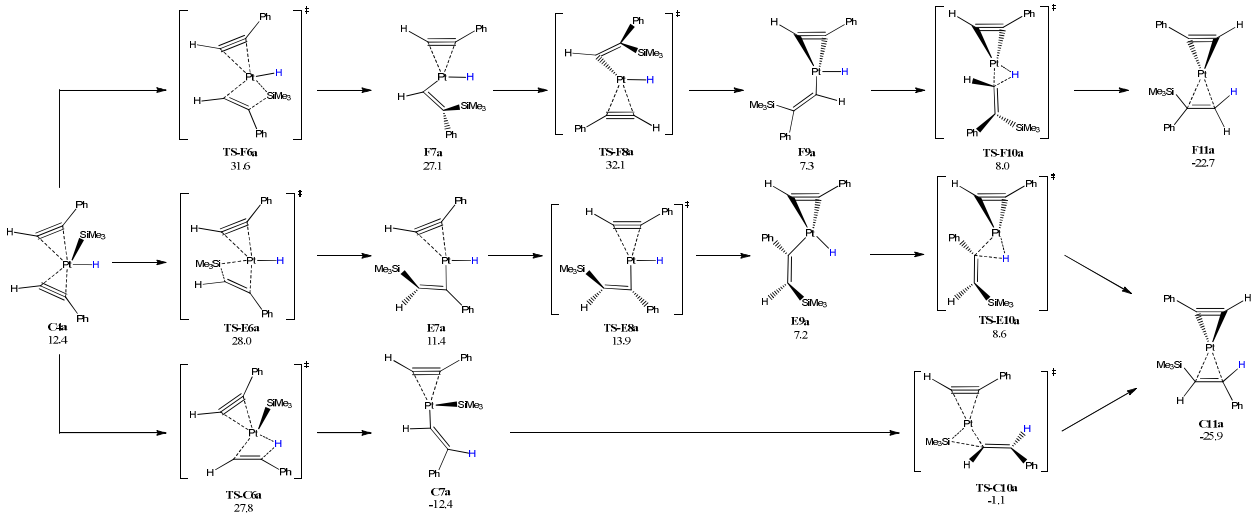
The peak at -0.39 ppm (s, 6H) was taken as a complex peak.[8] The peak at 8.01 ppm (s, 4H) of dimethyl terephthalate was integrated as well. The number of moles of Pt_2dvtms_3 was calculated as follows:

$$n_{Pt2dvtms3} = \frac{I_{Pt2dvtms3}}{1.5} \cdot n_{standard}$$

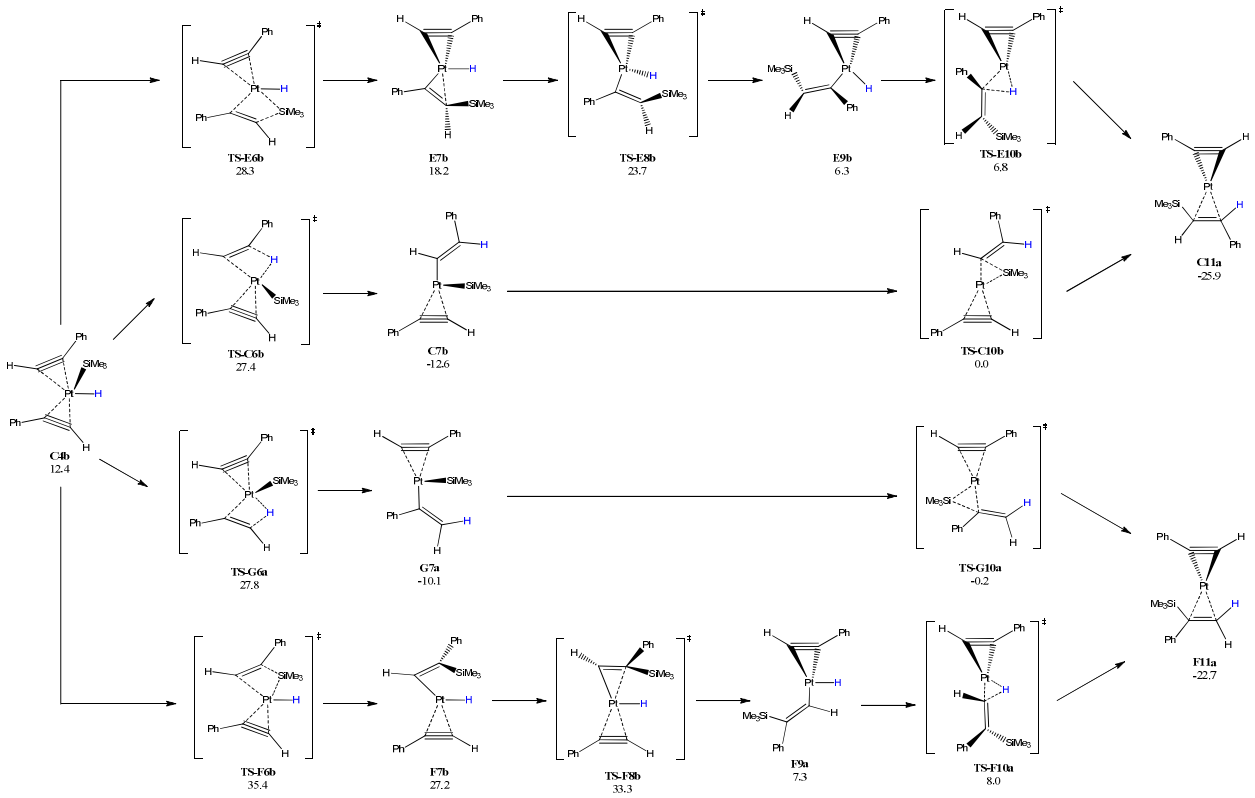
The calculated amount of complex before heating was used as the initial amount. The decomposition level of the complex was calculated as follows:

$$x_{Pt2dvtms3} = \frac{n_{Pt2dvtms3}^{after}}{n_{Pt2dvtms3}^{before}} \cdot 100\%$$

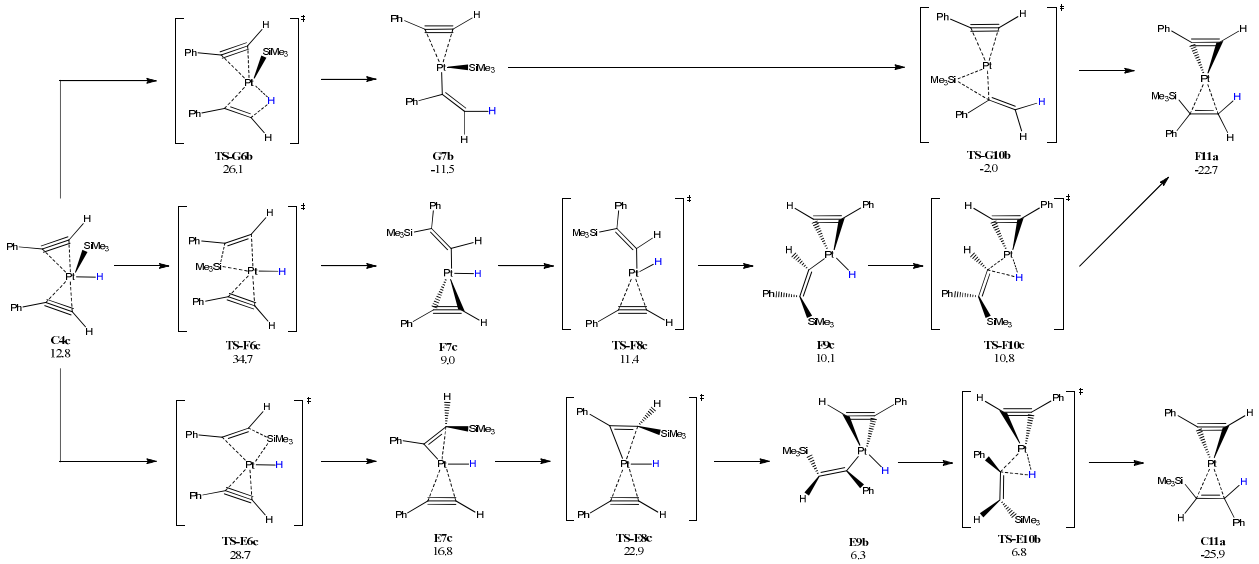
Theoretical calculations



Scheme S2. Alternative pathways of phenylacetylene insertion, isomerization, and reductive elimination steps for intermediate **C4a**.



Scheme S3. Alternative pathways of phenylacetylene insertion, isomerization, and reductive elimination steps for intermediate **C4b**.

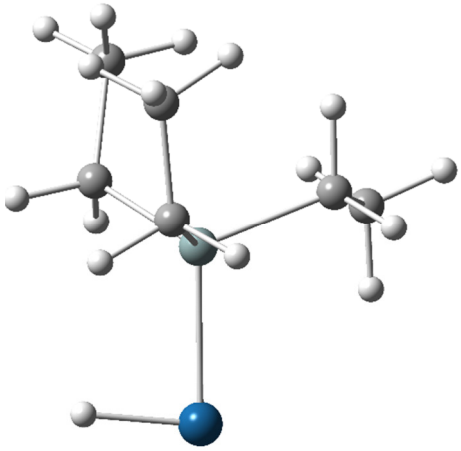


Scheme S4. Alternative pathways of phenylacetylene insertion, isomerization, and reductive elimination steps for intermediate **C4c**.

Structures, thermodynamic parameters and XYZ coordinates of calculated compounds

A3

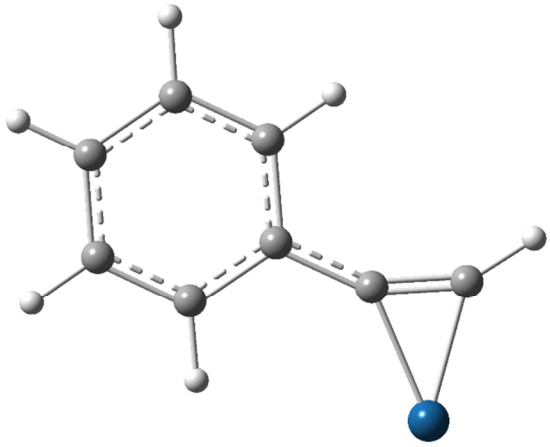
E = -646.764368; (E+ZPE) = -646.557906; H = -646.543289; G = -646.599570



Pt	-1.41620	-0.10440	0.08020
Si	0.84860	-0.11450	-0.08560
C	1.35350	1.17630	-1.39150
C	0.96230	2.61650	-1.05760
C	1.45110	-1.82280	-0.66420
C	2.96960	-2.00800	-0.73760
C	1.63160	0.36360	1.58290
C	3.08430	0.84580	1.52930
H	-1.14410	-1.06000	1.22290
H	2.44530	1.10130	-1.50580
H	0.93440	0.87930	-2.36210
H	1.30500	3.32330	-1.82220
H	-0.12470	2.72670	-0.97030
H	1.38880	2.93680	-0.10060
H	1.01380	-2.57790	0.00130
H	1.00070	-2.00290	-1.64980
H	3.23420	-2.98250	-1.16490
H	3.44710	-1.24110	-1.35800
H	3.42660	-1.95670	0.25590
H	0.99880	1.14310	2.02610
H	1.54050	-0.50250	2.25280
H	3.45090	1.11930	2.52580
H	3.75820	0.08000	1.13360
H	3.19130	1.72990	0.89140

B1

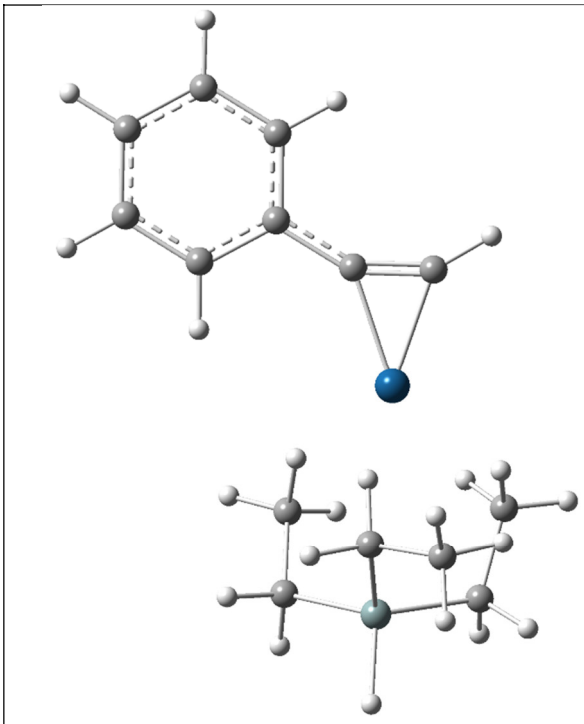
E = -427.414735; (E+ZPE) = -427.303424; H = -427.294500; G = -427.339079



C	-4.32340	-0.46130	-0.00020
C	-3.32360	-1.43400	0.00020
C	-3.97360	0.89040	-0.00040
C	-2.63630	1.26920	-0.00020
C	-1.62340	0.29430	0.00020
C	-1.98360	-1.06090	0.00040
C	-0.23930	0.69390	0.00040
C	0.68650	1.59740	0.00070
H	-5.36940	-0.75370	-0.00030
H	-3.58930	-2.48730	0.00040
H	-4.74780	1.65260	-0.00070
H	-2.36320	2.32040	-0.00040
H	-1.19790	-1.81100	0.00070
H	0.99160	2.63210	0.00100
Pt	1.54840	-0.15750	-0.00010

B2

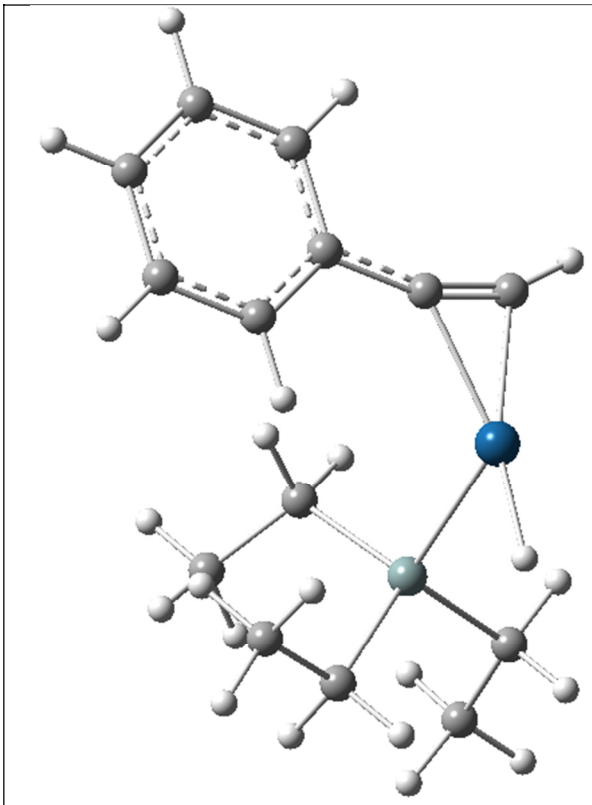
E = -954.823248; (E+ZPE) = -954.504680; H = -954.483470; G = -954.556544



C	5.39960	1.46590	0.37290
C	4.21250	2.03330	-0.08990
C	5.41770	0.12690	0.76870
C	4.25980	-0.63930	0.70330
C	3.05910	-0.07530	0.23840
C	3.05140	1.26980	-0.15720
C	1.85900	-0.87360	0.17400
C	1.25060	-2.00230	0.35090
H	6.30600	2.06210	0.42520
H	4.19190	3.07440	-0.39970
H	6.33930	-0.32080	1.13020
H	4.27210	-1.68070	1.01160
H	2.12330	1.70330	-0.51800
H	1.29260	-3.03670	0.65420
Pt	-0.06450	-0.68670	-0.33160
Si	-3.50170	1.21660	0.04810
C	-2.84670	1.06910	1.81140
C	-3.73960	0.23730	2.73490
C	-2.32390	2.25260	-1.01140
C	-1.00440	1.56900	-1.36720
C	-3.77320	-0.50910	-0.68620
C	-2.60610	-1.47810	-0.50260
H	-4.82580	1.91510	0.07320
H	-1.83700	0.63560	1.76900
H	-2.72320	2.08340	2.21390
H	-3.33490	0.18940	3.75180
H	-4.74980	0.65680	2.80200
H	-3.83920	-0.79410	2.37790
H	-2.84330	2.54510	-1.93290
H	-2.12640	3.18470	-0.46560
H	-0.27140	2.25040	-1.80960
H	-0.49970	1.21340	-0.41800
H	-1.14610	0.75960	-2.09220
H	-4.66290	-0.93130	-0.20030
H	-4.03170	-0.41420	-1.74870
H	-2.84380	-2.49810	-0.82130
H	-1.75320	-1.20900	-1.19280
H	-2.27930	-1.53910	0.54150

B4

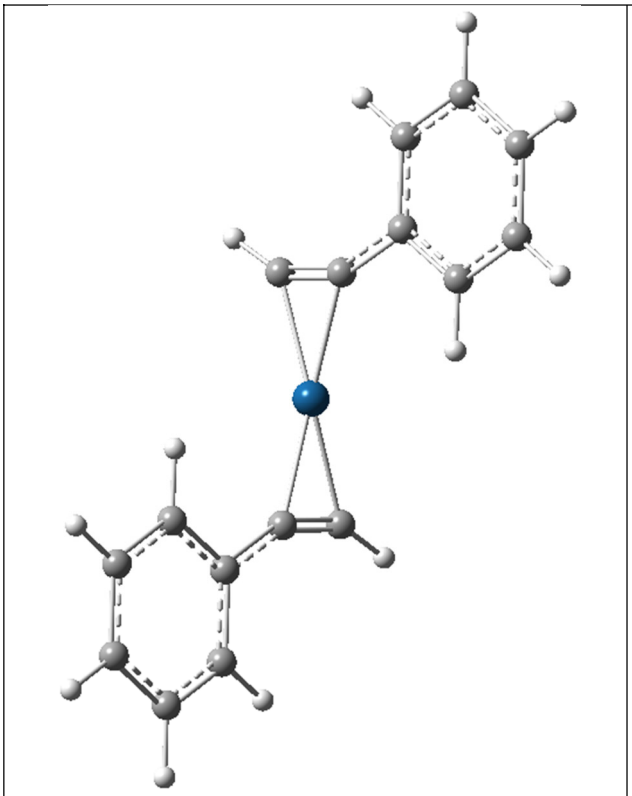
E = -954.870729; (E+ZPE) = -954.552292; H = -954.530260; G = -954.605776



C	4.73480	1.55990	0.11110
C	3.59920	1.62100	0.91860
C	4.79790	0.63690	-0.93410
C	3.73090	-0.22130	-1.17490
C	2.58590	-0.16200	-0.36440
C	2.52910	0.76400	0.68530
C	1.47950	-1.04340	-0.63680
C	0.79530	-1.90650	-1.25360
H	5.56980	2.22970	0.29490
H	3.54680	2.33790	1.73270
H	5.68090	0.58740	-1.56440
H	3.77200	-0.93950	-1.98820
H	1.63870	0.79980	1.30510
H	0.55200	-2.61670	-2.02280
Pt	-0.36060	-1.23610	0.34620
Si	-1.77620	0.54530	-0.04200
C	-2.13020	1.63320	1.46860
C	-0.88430	2.10270	2.21930
C	-3.41720	-0.14140	-0.70580
C	-4.37630	0.91060	-1.27080
C	-0.88280	1.60080	-1.35500
C	-1.38150	3.04320	-1.48400
H	-1.40110	-1.15810	1.57240
H	-2.71360	2.50040	1.12730
H	-2.78570	1.06670	2.14260
H	-1.13480	2.75890	3.06080
H	-0.32980	1.24680	2.62100
H	-0.20260	2.65720	1.56330
H	-3.19270	-0.89360	-1.47280
H	-3.89450	-0.68720	0.11860
H	-5.33050	0.46180	-1.57050
H	-4.60100	1.69290	-0.53720
H	-3.95730	1.40090	-2.15580
H	0.18830	1.60470	-1.11780
H	-0.96890	1.07430	-2.31530
H	-0.84140	3.58210	-2.27140
H	-2.44770	3.09300	-1.72700
H	-1.23610	3.59980	-0.55200

C1

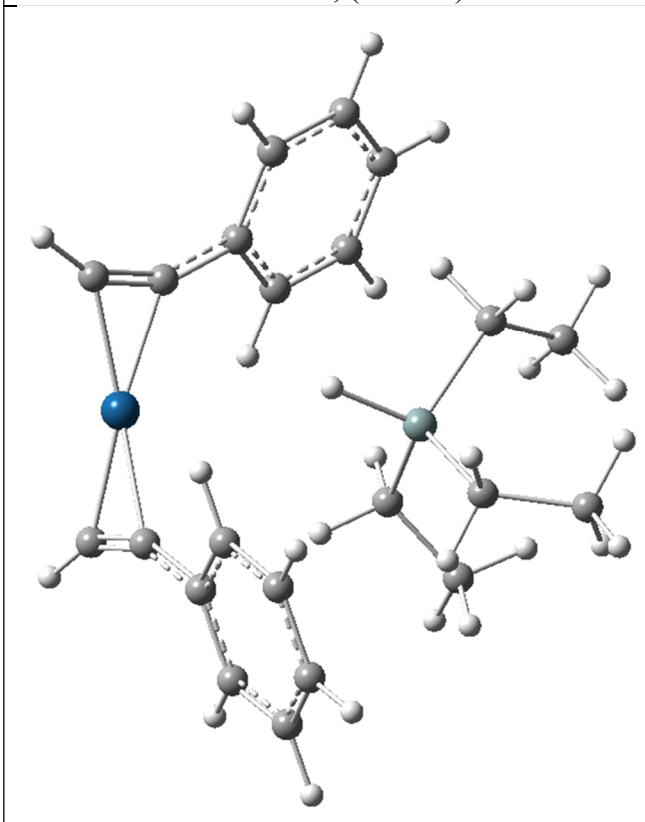
E = -735.558785; (E+ZPE) = -735.334513; H = -735.318281; G = -735.381411



C	-4.89290	-2.16650	0.59790
C	-3.68060	-2.12410	1.28690
C	-5.10700	-1.31670	-0.48840
C	-4.11420	-0.42790	-0.88610
C	-2.89260	-0.38080	-0.19620
C	-2.68470	-1.23640	0.89330
C	-1.86240	0.54200	-0.61410
C	-1.38790	1.45600	-1.38070
H	-5.66990	-2.86010	0.90620
H	-3.51160	-2.78460	2.13240
H	-6.05010	-1.34780	-1.02640
H	-4.27450	0.23590	-1.73060
H	-1.73560	-1.19200	1.41960
H	-1.46610	2.12730	-2.22000
Pt	-0.00000	1.01920	-0.00000
C	4.89320	-2.16590	-0.59830
C	3.68090	-2.12370	-1.28720
C	5.10720	-1.31640	0.48830
C	4.11420	-0.42790	0.88620
C	2.89250	-0.38090	0.19640
C	2.68490	-1.23640	-0.89340
C	1.86220	0.54160	0.61450
C	1.38730	1.45500	1.38140
H	5.67040	-2.85930	-0.90670
H	3.51210	-2.78400	-2.13290
H	6.05030	-1.34740	1.02620
H	4.27440	0.23570	1.73080
H	1.73570	-1.19200	-1.41960
H	1.46500	2.12570	2.22130

C2a

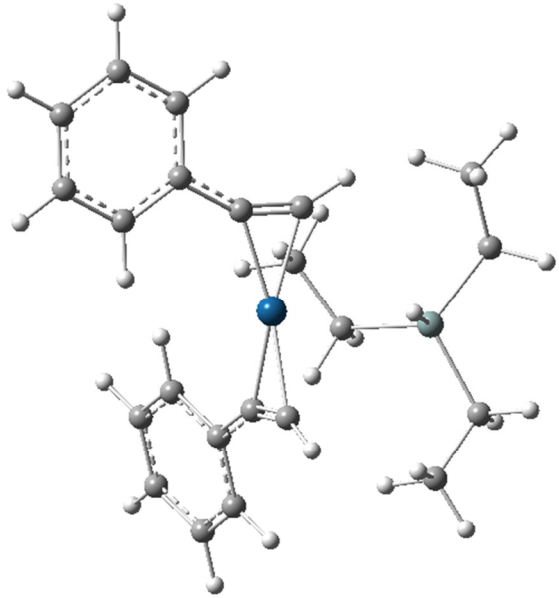
E = -1262.958504; (E+ZPE) = -1262.526271; H = -1262.496910; G = -1262.590500



C	-4.84570	0.80790	-0.84080
C	-4.78550	0.50080	0.51920
C	-3.88230	0.30030	-1.71240
C	-2.85960	-0.50810	-1.22880
C	-2.80220	-0.83380	0.13290
C	-3.77340	-0.31970	1.00610
C	-1.74650	-1.67870	0.64030
C	-1.21050	-2.46020	1.50560
H	-5.63840	1.44720	-1.21870
H	-5.53040	0.90030	1.20140
H	-3.92180	0.54510	-2.76980
H	-2.09260	-0.89600	-1.89220
H	-3.72100	-0.56300	2.06330
H	-1.25940	-3.04550	2.40910
Pt	0.12960	-2.12310	0.04820
C	4.75570	1.42930	0.33350
C	4.74170	0.87610	-0.94770
C	3.84800	0.98260	1.29370
C	2.92650	-0.00880	0.97460
C	2.90950	-0.57190	-0.30820
C	3.82720	-0.12170	-1.26960
C	1.95310	-1.60140	-0.64110
C	1.51600	-2.59140	-1.32930
H	5.46940	2.20970	0.58070
H	5.44450	1.22510	-1.69870
H	3.85460	1.41260	2.29110
H	2.20950	-0.36330	1.70920
H	3.80900	-0.55270	-2.26610

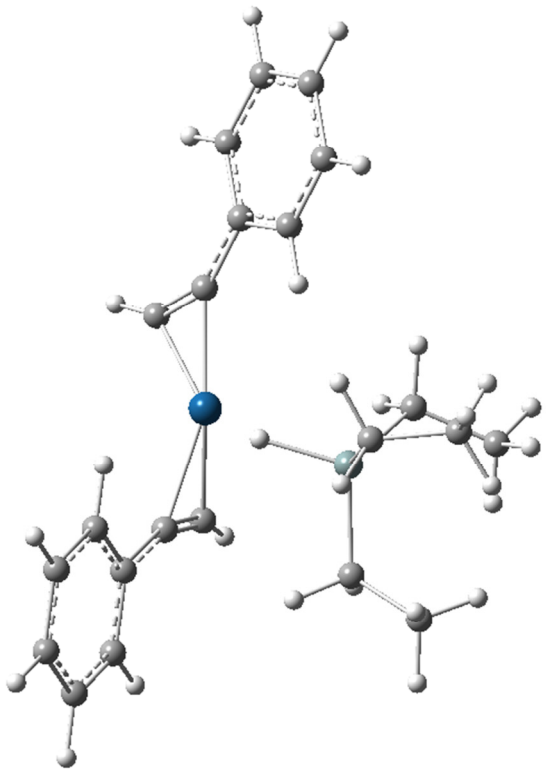
	H 1.63750 -3.33500 -2.09970 Si -0.15710 2.18810 -0.38290 C 1.45070 3.13140 -0.72740 C 1.85570 4.16120 0.32950 C -1.66920 3.15300 -0.99880 C -1.65370 4.65980 -0.72910 C -0.32050 1.76010 1.45740 C -0.99980 2.81820 2.32950 H 2.24620 2.38240 -0.82730 H 1.36540 3.61060 -1.71280 H 2.80980 4.64050 0.07980 H 1.10910 4.95520 0.43870 H 1.97840 3.69050 1.31130 H -1.74930 2.97420 -2.07980 H -2.56590 2.69420 -0.56180 H -2.55230 5.14920 -1.12300 H -1.60550 4.88240 0.34190 H -0.78920 5.14100 -1.19990 H -0.87420 0.81610 1.52410 H 0.68370 1.54100 1.84200 H -1.06960 2.49260 3.37430 H -0.45480 3.76840 2.32070 H -2.01940 3.02250 1.98460 H -0.09360 0.91050 -1.15710

C2b

E = -1262.956043; (E+ZPE) = -1262.524479; H = -1262.494709; G = -1262.591153	
	C 2.76770 3.80700 1.82720 C 1.62630 3.11610 2.23450 C 3.16890 3.76360 0.49100 C 2.43440 3.03160 -0.43560 C 1.29130 2.32630 -0.02870 C 0.89300 2.37620 1.31360 C 0.55090 1.53550 -0.98290 C 0.22220 1.17030 -2.16760 H 3.34430 4.37840 2.54890 H 1.31170 3.14860 3.27360 H 4.05750 4.30040 0.17150 H 2.74490 2.98730 -1.47520 H 0.01190 1.81930 1.61870 H 0.27100 1.27180 -3.23920 Pt -0.76540 0.01100 -0.85510 C -6.38150 0.24350 0.85040 C -5.50400 1.17640 0.29720 C -5.94700 -1.05920 1.09980 C -4.64100 -1.42960 0.79830 C -3.75360 -0.49510 0.24170 C -4.19670 0.81060 -0.00630 C -2.39640 -0.88260 -0.06670 C -1.42880 -1.72500 -0.10130 H -7.40210 0.53020 1.08690 H -5.83990 2.19060 0.10200 H -6.62840 -1.78750 1.53010 H -4.29660 -2.44170 0.98960 H -3.50190 1.52530 -0.43800 H -0.99690 -2.69470 0.08550 Si 3.07590 -1.90870 0.09490 C 4.54210 -1.40570 -0.98890 C 4.42920 0.01430 -1.54990 C 3.27400 -3.69470 0.69950

	C 1.95470 -4.40410 1.01880 C 2.90420 -0.69160 1.52940 C 1.69820 -0.91580 2.44270 H 1.83580 -1.85090 -0.74220 H 5.46700 -1.51040 -0.40460 H 4.62020 -2.13130 -1.80980 H 5.26350 0.25630 -2.21880 H 3.50060 0.14410 -2.11790 H 4.42290 0.76220 -0.75010 H 3.81530 -4.25560 -0.07460 H 3.92870 -3.69520 1.58210 H 2.11700 -5.43310 1.36000 H 1.39330 -3.88500 1.80300 H 1.30940 -4.44880 0.13430 H 3.83510 -0.72930 2.11350 H 2.85810 0.31890 1.10400 H 1.63210 -0.14240 3.21680 H 0.76220 -0.89010 1.87320 H 1.75010 -1.88400 2.95260

TS-C3a

E = -1262.936975; (E+ZPE) = -1262.505769; H = -1262.477030; G = -1262.568672	
	C -5.56010 -0.25200 1.59610 C -4.37060 0.44870 1.79530 C -5.56950 -1.37990 0.77320 C -4.39970 -1.80420 0.15230 C -3.19710 -1.10300 0.34250 C -3.20040 0.02600 1.17300 C -1.97740 -1.53440 -0.30470 C -1.38730 -2.42670 -1.04030 H -6.47540 0.07740 2.07940 H -4.35540 1.32540 2.43690 H -6.49330 -1.92970 0.61550 H -4.40570 -2.68030 -0.48990 H -2.26810 0.56120 1.32400 H -1.45200 -3.35810 -1.58390 Pt -0.06500 -0.98180 -0.69320 C 4.99940 -1.34210 2.21110 C 5.38300 -1.07050 0.89580 C 3.65120 -1.52310 2.51740 C 2.68750 -1.43230 1.51780 C 3.06540 -1.16110 0.19500 C 4.42630 -0.97980 -0.10800 C 2.07890 -1.03740 -0.84150 C 1.60680 -0.82940 -1.99000 H 5.75020 -1.41160 2.99290 H 6.43230 -0.92820 0.65340 H 3.34860 -1.73520 3.53890 H 1.63320 -1.56870 1.74090 H 4.71850 -0.76520 -1.13170 H 1.63410 -0.72800 -3.05950 Si 0.26480 1.96080 -0.01240 C 1.97180 2.39980 -0.68830 C 2.39510 3.85570 -0.47140 C -1.12540 2.33120 -1.23610 C -1.01680 3.69470 -1.92670 C -0.04240 2.74830 1.68500 C -0.58880 4.17870 1.66860 H 2.69680 1.72730 -0.21260 H 1.99350 2.14680 -1.75580

	H 3.39470 4.04210 -0.87980 H 1.70970 4.56030 -0.95400 H 2.42810 4.10870 0.59380 H -1.12070 1.53160 -1.98660 H -2.08520 2.23860 -0.71170 H -1.84880 3.85060 -2.62250 H -1.02980 4.52390 -1.21200 H -0.09040 3.77540 -2.50560 H -0.73660 2.09810 2.23330 H 0.90200 2.70470 2.24450 H -0.73170 4.56150 2.68540 H 0.08550 4.86950 1.15200 H -1.55900 4.22780 1.16290 H 0.30760 0.46080 0.39820

TS-C3b

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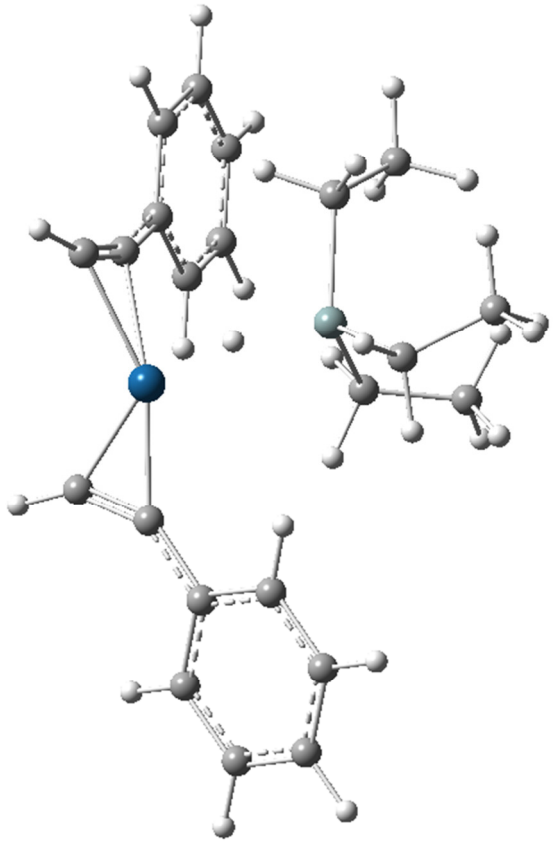	C 4.79150 -0.79000 2.23550 C 3.46060 -1.08700 2.52780 C 5.19550 -0.65010 0.90660 C 4.27620 -0.80140 -0.12480 C 2.93220 -1.09260 0.16400 C 2.53360 -1.23340 1.50090 C 1.98340 -1.21650 -0.90830 C 1.52920 -1.37730 -2.06740 H 5.51180 -0.66670 3.03900 H 3.14140 -1.19930 3.56000 H 6.23100 -0.41870 0.67400 H 4.58470 -0.68730 -1.15980 H 1.49200 -1.45550 1.71350 H 1.54800 -1.61960 -3.11370 Pt -0.17590 -1.02120 -0.81960 C -5.64690 0.31140 1.21170 C -5.31110 -0.97260 1.64560 C -4.77870 1.00650 0.36990 C -3.58070 0.42340 -0.03030 C -3.23190 -0.86470 0.39910 C -4.11590 -1.55830 1.24260 C -1.97660 -1.45480 -0.01190 C -1.23430 -2.52390 -0.06020 H -6.58110 0.76630 1.52830 H -5.98470 -1.51780 2.30100 H -5.03590 2.00440 0.02540 H -2.89870 0.95180 -0.68990 H -3.85120 -2.55580 1.58170 H -1.15690 -3.58170 0.14960 Si 0.27830 1.80920 -0.48320 C -0.01260 1.51410 1.36330 C -0.13720 2.78700 2.20680 C 2.07780 2.18590 -0.93330 C 2.94390 2.72090 0.20940 C -0.86470 3.18620 -1.11930 C -0.33710 4.60730 -0.89560 H -0.92600 0.91590 1.46140 H 0.80180 0.88510 1.74030 H -0.29130 2.53910 3.26290 H 0.75880 3.41330 2.14710 H -0.99050 3.39560 1.88970 H 2.52190 1.26730 -1.33160 H 2.06620 2.89860 -1.76880

	H 3.97640 2.88480 -0.11880 H 2.56850 3.67520 0.59450 H 2.97890 2.01440 1.04550 H -1.02940 3.01970 -2.19170 H -1.84690 3.07050 -0.64170 H -1.03000 5.35660 -1.29480 H -0.19340 4.82920 0.16630 H 0.62690 4.75950 -1.39280 H -0.14720 0.66230 -1.47360

TS-C3c

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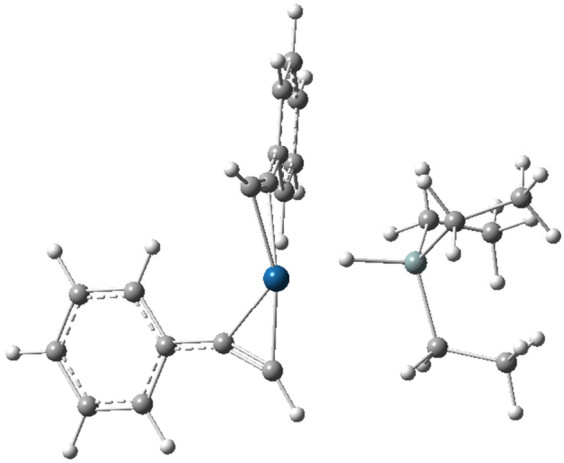
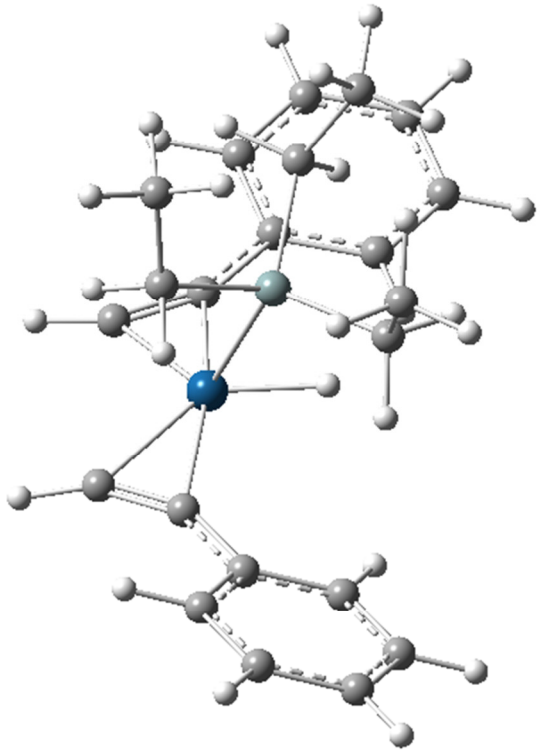
	C 5.91350 -0.76770 0.48320 C 5.07480 0.09960 -0.21700 C 5.38460 -1.91020 1.08690 C 4.02450 -2.18380 0.99410 C 3.17430 -1.31410 0.29200 C 3.71390 -0.17190 -0.31480 C 1.75680 -1.58780 0.20650 C 0.72070 -2.29350 0.54720 H 6.97620 -0.55550 0.55870 H 5.48250 0.98960 -0.68800 H 6.03540 -2.58820 1.63200 H 3.60750 -3.07050 1.46310 H 3.04820 0.49350 -0.85730 H 0.36960 -3.12720 1.13590 Pt 0.15460 -0.74700 -0.62020 C 0.80260 4.79530 1.12600 C 0.31330 4.89570 -0.17760 C 1.09080 3.54090 1.66370 C 0.88490 2.39120 0.90860 C 0.39900 2.48510 -0.40330 C 0.11440 3.75100 -0.94150 C 0.19570 1.30330 -1.19880 C 0.06350 0.60880 -2.24350 H 0.95680 5.69170 1.71960 H 0.08660 5.87040 -0.60030 H 1.47310 3.45730 2.67700 H 1.09650 1.40710 1.31730 H -0.26490 3.82370 -1.95660 H -0.00230 0.43120 -3.30180 Si -2.86290 -0.66150 -0.02960 C -4.35050 -0.59780 -1.20340 C -5.62870 0.03100 -0.64140 C -2.91660 -2.16140 1.11750 C -4.29140 -2.49060 1.70570 C -2.62940 0.95910 0.90980 C -3.53340 1.13110 2.13450 H -4.03010 -0.04150 -2.09450 H -4.54790 -1.62190 -1.54890 H -6.43750 0.01770 -1.38090 H -5.99020 -0.49710 0.24700 H -5.46540 1.07600 -0.35770 H -2.53890 -3.01990 0.54730 H -2.18350 -1.99330 1.91730 H -4.24540 -3.36860 2.35980 H -4.69240 -1.66280 2.30000 H -5.02050 -2.71020 0.91830 H -1.57970 1.00940 1.22070 H -2.76660 1.79220 0.20750

	H -3.34320 2.08910 2.63100 H -4.59660 1.10230 1.87540 H -3.35470 0.34230 2.87320 H -1.71410 -0.88960 -1.03050

C4a

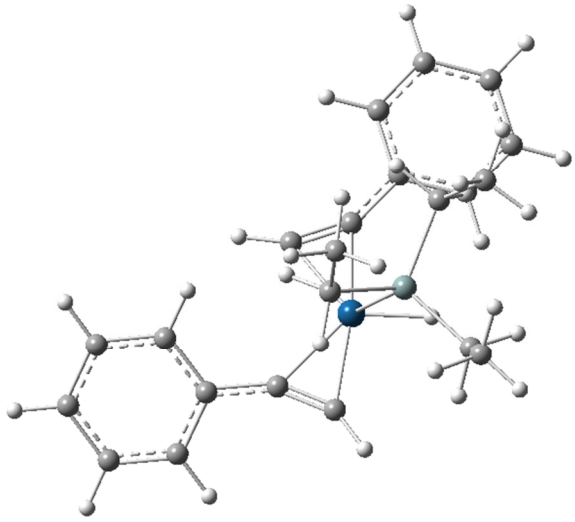
E = -1262.949699; (E+ZPE) = -1262.518390; H = -1262.489341; G = -1262.579677



C	-5.37710	-0.62490	1.81800
C	-4.14900	-0.91900	2.41070
C	-5.47450	-0.54160	0.42850
C	-4.35240	-0.75450	-0.36590
C	-3.11230	-1.04540	0.22410
C	-3.02180	-1.11950	1.62070
C	-1.95160	-1.26670	-0.60680
C	-1.43030	-1.65360	-1.70580
H	-6.25480	-0.45920	2.43610
H	-4.06790	-0.98450	3.49200
H	-6.42800	-0.30930	-0.03740
H	-4.42150	-0.68940	-1.44780
H	-2.05630	-1.33410	2.07010
H	-1.52200	-2.11600	-2.67290
Pt	0.12020	-0.91910	-0.48640
C	5.58980	-0.15700	1.78360
C	5.73330	-0.37510	0.41230
C	4.32760	-0.24400	2.37050
C	3.21350	-0.54140	1.59210
C	3.34770	-0.76230	0.21530
C	4.62280	-0.67800	-0.36760
C	2.20320	-1.07180	-0.61060
C	1.72010	-1.51060	-1.70940
H	6.45850	0.08020	2.39100
H	6.71400	-0.30640	-0.05000
H	4.21060	-0.07670	3.43740
H	2.22370	-0.60530	2.03500
H	4.72840	-0.84350	-1.43580
H	1.84340	-1.95270	-2.68230
Si	-0.19530	1.40890	-0.19670
C	1.51010	2.23470	-0.16340
C	1.51900	3.70440	0.26750
C	-1.12240	1.83430	-1.80490
C	-0.98220	3.28150	-2.28470
C	-1.21060	1.95500	1.30870
C	-1.96470	3.27950	1.16710
H	2.14870	1.65730	0.51350
H	1.95950	2.12030	-1.15910
H	2.53860	4.10700	0.26740
H	0.91860	4.33740	-0.39320
H	1.12400	3.82310	1.28220
H	-0.76000	1.15230	-2.58300
H	-2.17900	1.57460	-1.65320
H	-1.54620	3.44540	-3.21060
H	-1.35100	4.00130	-1.54750
H	0.06340	3.53150	-2.49380
H	-1.92730	1.15770	1.53260
H	-0.52610	1.99040	2.16840
H	-2.52220	3.51600	2.08090
H	-1.29460	4.12160	0.96660
H	-2.69080	3.23420	0.34850
H	0.14950	-0.35180	1.03540

C4b

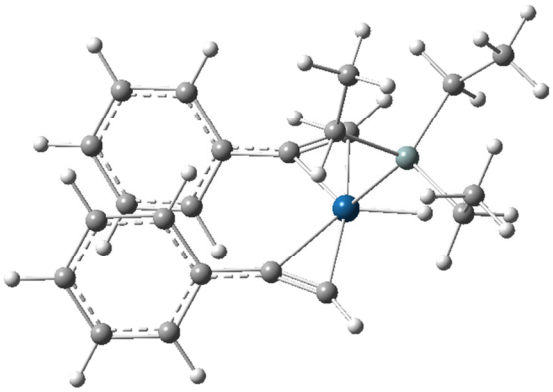
E = -1262.948435; (E+ZPE) = -1262.517596; H = -1262.488371; G = -1262.579645



C	5.78010	-1.61290	1.07650
C	4.59180	-1.50620	1.79870
C	5.82090	-1.19350	-0.25410
C	4.68450	-0.66780	-0.85920
C	3.48230	-0.56180	-0.13940
C	3.44840	-0.99390	1.19400
C	2.31530	0.00570	-0.76750
C	1.75580	0.80460	-1.58930
H	6.66970	-2.02200	1.54650
H	4.55430	-1.82760	2.83580
H	6.74310	-1.27560	-0.82240
H	4.71320	-0.33950	-1.89390
H	2.51860	-0.90750	1.74770
H	1.83470	1.61770	-2.29050
Pt	0.19840	-0.22050	-0.66130
C	-5.18040	-2.67950	0.12210
C	-4.35040	-3.14630	1.14260
C	-4.65080	-1.88060	-0.89110
C	-3.30120	-1.54310	-0.88170
C	-2.46020	-2.00840	0.13750
C	-2.99930	-2.81760	1.15070
C	-1.05440	-1.67550	0.15780
C	0.13470	-1.91800	0.56160
H	-6.23540	-2.93800	0.11740
H	-4.75850	-3.76780	1.93470
H	-5.29180	-1.51700	-1.68910
H	-2.87740	-0.91740	-1.66200
H	-2.34960	-3.17580	1.94400
H	0.83820	-2.53840	1.08990
Si	-0.74870	1.81030	0.10010
C	-2.40280	1.46980	0.95750
C	-3.24360	2.70680	1.28700
C	0.57730	2.30860	1.37310
C	0.10430	3.23680	2.49510
C	-0.94610	3.16940	-1.21170
C	-0.85990	4.61070	-0.70410
H	-2.98320	0.79690	0.31700
H	-2.19280	0.89250	1.86830
H	-4.18010	2.42480	1.78200
H	-2.72040	3.40170	1.95110
H	-3.51100	3.25940	0.37980
H	0.98000	1.38500	1.80660
H	1.41270	2.75800	0.81970
H	0.92620	3.47600	3.18010
H	-0.28680	4.18450	2.11190
H	-0.68850	2.77070	3.08980
H	-0.17930	3.00490	-1.97870
H	-1.90670	2.99770	-1.71780
H	-0.98420	5.32950	-1.52240
H	-1.63040	4.83080	0.04160
H	0.11170	4.81140	-0.24000
H	-0.99580	0.49400	-1.50430

C4c

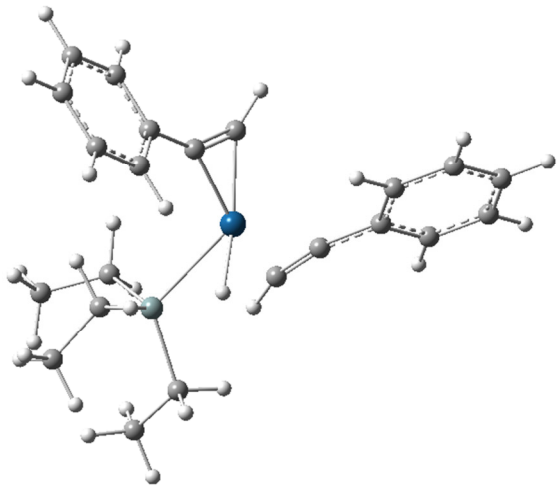
E = -1262.948240; (E+ZPE) = -1262.517254; H = -1262.488099; G = -1262.578889



C	-4.83550	-1.95290	-0.58890
C	-4.48900	-1.18270	0.52120
C	-3.84310	-2.62460	-1.30220
C	-2.51130	-2.53270	-0.90740
C	-2.15610	-1.75650	0.20610
C	-3.15950	-1.07490	0.91010
C	-0.77450	-1.64700	0.60760
C	0.36370	-2.12520	0.92960
H	-5.87370	-2.02420	-0.90070
H	-5.25510	-0.64730	1.07430
H	-4.10640	-3.22470	-2.16880
H	-1.73500	-3.05340	-1.46050
H	-2.88100	-0.45330	1.75540
H	0.96560	-2.99320	1.13950
Pt	0.62850	-0.07500	0.93920
C	-4.46340	2.11190	-1.24630
C	-4.16140	2.74150	-0.03890
C	-3.50460	1.31340	-1.86970
C	-2.25660	1.13560	-1.28630
C	-1.94030	1.77470	-0.07850
C	-2.90720	2.58000	0.54240
C	-0.64070	1.60420	0.52010
C	0.43530	2.00110	1.06820
H	-5.44420	2.23780	-1.69580
H	-4.90520	3.36260	0.45260
H	-3.73730	0.80990	-2.80350
H	-1.51560	0.49200	-1.75000
H	-2.66830	3.06740	1.48310
H	1.07270	2.81360	1.37100
Si	2.71470	0.00740	-0.21340
C	3.94040	1.34050	0.35950
C	4.86270	1.92250	-0.71400
C	3.55240	-1.69570	-0.24240
C	4.99970	-1.71600	-0.74130
C	2.02840	0.44210	-1.93680
C	2.93050	0.07590	-3.11920
H	3.35530	2.14990	0.81390
H	4.53170	0.91160	1.18080
H	5.53330	2.68120	-0.29430
H	5.49030	1.15460	-1.17750
H	4.28860	2.40320	-1.51340
H	3.51030	-2.10160	0.77630
H	2.92830	-2.36180	-0.85370
H	5.41090	-2.73210	-0.72860
H	5.08750	-1.34260	-1.76640
H	5.64680	-1.09640	-0.11120
H	1.06220	-0.06580	-2.04380
H	1.79800	1.51600	-1.93750
H	2.46590	0.35980	-4.07080
H	3.90310	0.57490	-3.06950
H	3.11620	-1.00280	-3.15850
H	2.10630	-0.09750	1.63020

TS-C5a

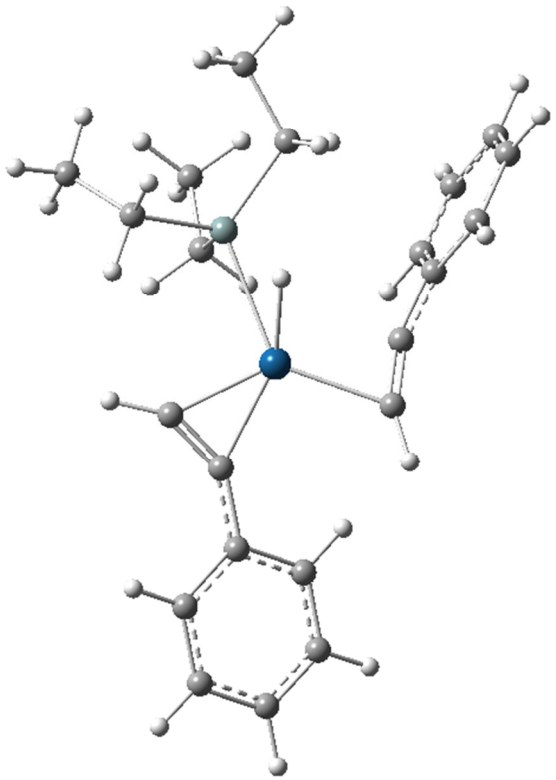
E = -1262.936138; (E+ZPE) = -1262.504728; H = -1262.476317; G = -1262.565647



C	6.06550	-1.28120	-0.65550
C	4.83590	-1.85810	-0.97070
C	6.10790	-0.02920	-0.03950
C	4.92930	0.64310	0.26080
C	3.68720	0.06460	-0.05320
C	3.65150	-1.19110	-0.67410
C	2.48520	0.78440	0.26550
C	1.73540	1.69570	0.67380
H	6.98850	-1.80410	-0.88840
H	4.79790	-2.83160	-1.45080
H	7.06330	0.42390	0.20890
H	4.95670	1.61610	0.74190
H	2.68770	-1.62970	-0.91260
H	1.44560	2.66080	1.04170
Pt	0.40500	0.01660	0.16730
C	-4.09100	-3.91300	-0.45300
C	-3.51640	-4.02730	0.81370
C	-3.50600	-3.07740	-1.40470
C	-2.36150	-2.35220	-1.08960
C	-1.77260	-2.46530	0.17700
C	-2.36310	-3.31490	1.12660
C	-0.56960	-1.72750	0.50340
C	0.55140	-1.73880	1.16490
H	-4.99040	-4.47150	-0.69610
H	-3.96830	-4.67530	1.55960
H	-3.94690	-2.98580	-2.39350
H	-1.90290	-1.69410	-1.82120
H	-1.91310	-3.40070	2.11160
H	1.21810	-2.35390	1.75220
Si	-1.34200	1.75950	-0.24480
C	-2.86380	1.10180	-1.16220
C	-3.92170	2.14290	-1.53830
C	-1.72210	2.00080	1.61110
C	-3.11740	2.55540	1.91560
C	-0.79070	3.40650	-1.02110
C	-1.47440	4.67050	-0.49570
H	-2.50300	0.61050	-2.07480
H	-3.30860	0.30090	-0.55720
H	-4.75880	1.68040	-2.07400
H	-4.33710	2.64670	-0.66030
H	-3.50570	2.91660	-2.19270
H	-1.59590	1.03470	2.11220
H	-0.95100	2.65820	2.03410
H	-3.26140	2.67690	2.99550
H	-3.28730	3.53160	1.45110
H	-3.90000	1.87800	1.55860
H	0.29590	3.49640	-0.89410
H	-0.94460	3.31640	-2.10580
H	-1.08880	5.56930	-0.99070
H	-2.55660	4.64820	-0.65970
H	-1.31150	4.79640	0.58040
H	-0.09890	0.92110	-1.13020

TS-C5b

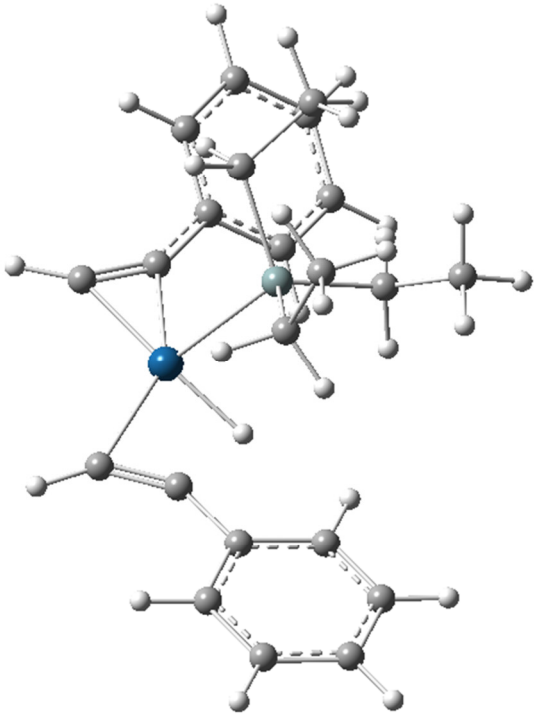
E = -1262.938721; (E+ZPE) = -1262.507360; H = -1262.478968; G = -1262.566734



C	-4.19930	-3.15400	0.59080
C	-3.82110	-3.18290	-0.75140
C	-3.28550	-2.74130	1.56150
C	-2.00420	-2.34740	1.19310
C	-1.62120	-2.37120	-0.15650
C	-2.53920	-2.79580	-1.12780
C	-0.30180	-1.95260	-0.53950
C	0.87410	-1.93400	-0.95650
H	-5.20250	-3.45300	0.88000
H	-4.52900	-3.50490	-1.50960
H	-3.57400	-2.72080	2.60840
H	-1.29140	-2.01450	1.94100
H	-2.24160	-2.80720	-2.17170
H	1.81060	-2.35210	-1.27500
Pt	0.51630	0.15500	-0.54100
C	6.28490	-0.97000	0.72400
C	5.14010	-1.73120	0.95910
C	6.16130	0.33490	0.24360
C	4.90360	0.87630	0.00090
C	3.74400	0.11630	0.23080
C	3.88020	-1.19570	0.70880
C	2.43590	0.68170	-0.00690
C	1.69830	1.73810	-0.12370
H	7.26850	-1.39050	0.91300
H	5.22930	-2.74570	1.33760
H	7.04970	0.93220	0.05770
H	4.80450	1.89040	-0.37550
H	2.98410	-1.78010	0.89630
H	1.65430	2.81370	-0.03820
Si	-1.64130	1.37760	-0.06620
C	-1.53980	3.13110	-0.78490
C	-2.10200	4.24210	0.10550
C	-3.33900	0.63040	-0.49720
C	-4.52380	1.59510	-0.39750
C	-1.39530	1.37760	1.82300
C	-2.65400	1.65500	2.64840
H	-0.48950	3.33990	-1.01850
H	-2.05950	3.12060	-1.75330
H	-1.99530	5.22570	-0.36650
H	-3.16600	4.09800	0.31930
H	-1.57970	4.28460	1.06760
H	-3.28340	0.23230	-1.51830
H	-3.50980	-0.24170	0.14550
H	-5.46160	1.09620	-0.66880
H	-4.64910	1.99150	0.61500
H	-4.40490	2.45050	-1.07120
H	-0.97230	0.40780	2.10780
H	-0.60970	2.11160	2.04600
H	-2.43340	1.63160	3.72210
H	-3.08470	2.63650	2.42550
H	-3.42790	0.90370	2.45760
H	-0.90450	0.45260	-1.33840

TS-C6a

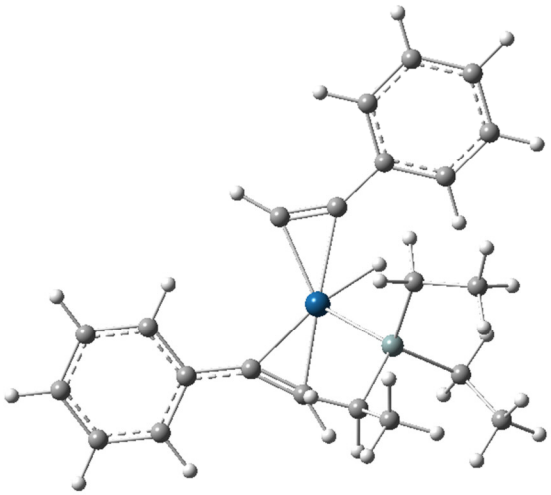
E = -1262.924266; (E+ZPE) = -1262.494047; H = -1262.465420; G = -1262.555070



C	-5.64890	0.80450	1.47240
C	-4.38680	1.09560	1.98730
C	-5.78350	-0.16390	0.47590
C	-4.66570	-0.83430	-0.00610
C	-3.39140	-0.54340	0.50610
C	-3.26610	0.42440	1.50890
C	-2.24900	-1.27260	-0.02120
C	-1.85730	-2.22740	-0.79310
H	-6.52410	1.32880	1.84460
H	-4.27360	1.84580	2.76430
H	-6.76400	-0.39390	0.06920
H	-4.76600	-1.58200	-0.78720
H	-2.28190	0.65110	1.91340
H	-2.24700	-3.00730	-1.42600
Pt	-0.08720	-1.18830	-0.32670
C	5.31570	0.24130	1.86640
C	5.45800	-0.21020	0.55340
C	4.07020	0.17550	2.49160
C	2.97060	-0.32990	1.80600
C	3.10370	-0.78760	0.48850
C	4.36200	-0.72430	-0.13160
C	1.96860	-1.33700	-0.22090
C	1.54200	-2.15360	-1.12470
H	6.17250	0.64370	2.39930
H	6.42530	-0.15810	0.06170
H	3.95540	0.52310	3.51440
H	1.99400	-0.38000	2.27840
H	4.46570	-1.07360	-1.15510
H	1.79970	-2.96460	-1.78750
Si	0.31740	1.15290	-0.55540
C	0.69720	2.08760	1.05940
C	0.25160	3.55210	1.09630
C	1.68920	1.45070	-1.84070
C	2.30620	2.85180	-1.80780
C	-1.32810	1.77420	-1.29460
C	-1.24780	3.06170	-2.11950
H	0.21890	1.53930	1.88100
H	1.77500	2.01680	1.24940
H	0.48740	4.01390	2.06240
H	0.74510	4.14910	0.32300
H	-0.82900	3.64800	0.94390
H	2.47950	0.70800	-1.70200
H	1.25640	1.24440	-2.82930
H	3.08160	2.96000	-2.57540
H	1.56510	3.63830	-1.98190
H	2.77850	3.05330	-0.84020
H	-1.72570	0.96660	-1.92230
H	-2.05270	1.89360	-0.47950
H	-2.23110	3.33130	-2.52280
H	-0.89600	3.91120	-1.52590
H	-0.56750	2.95160	-2.97060
H	-1.14740	-0.51990	0.75100

TS-C6b

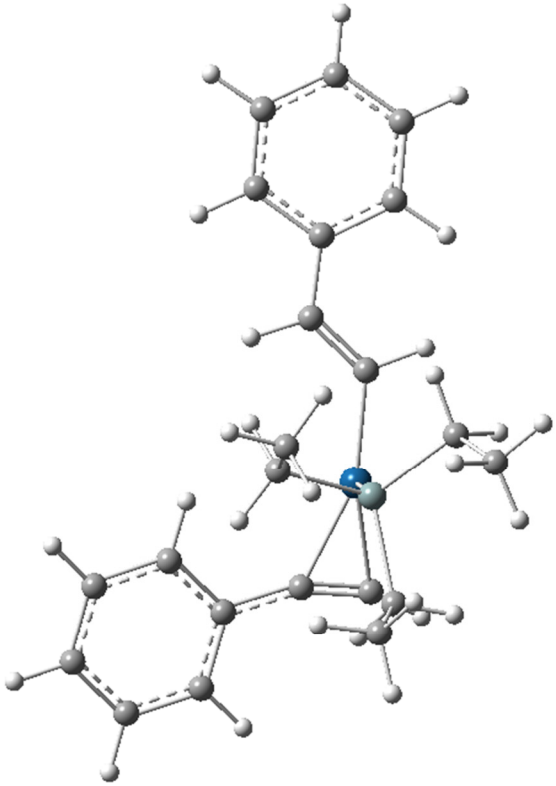
E = -1262.924766; (E+ZPE) = -1262.494505; H = -1262.465903; G = -1262.555636



C	6.09930	-1.56910	0.67040
C	4.90940	-2.15970	1.09440
C	6.05800	-0.42550	-0.13040
C	4.83710	0.12340	-0.50420
C	3.63210	-0.46660	-0.08350
C	3.68520	-1.61340	0.72020
C	2.36670	0.10990	-0.47070
C	1.74220	1.05950	-1.08020
H	7.05480	-1.99610	0.96120
H	4.93570	-3.04830	1.71890
H	6.98220	0.03830	-0.46400
H	4.80260	1.01210	-1.12800
H	2.75090	-2.06070	1.04500
H	1.80650	2.00940	-1.58980
Pt	0.32840	-0.27200	-0.42600
C	-5.37890	-2.52860	0.11490
C	-4.46600	-3.37680	0.74450
C	-4.91710	-1.42840	-0.60510
C	-3.55200	-1.17600	-0.69500
C	-2.63020	-2.01760	-0.06230
C	-3.10210	-3.12600	0.65970
C	-1.19540	-1.79630	-0.12830
C	-0.02710	-2.26180	0.14770
H	-6.44450	-2.72550	0.18640
H	-4.81980	-4.23500	1.30850
H	-5.62030	-0.76470	-1.09960
H	-3.19270	-0.31910	-1.26090
H	-2.39000	-3.77850	1.15600
H	0.45440	-3.13130	0.56320
Si	-0.70410	1.81100	0.13880
C	-2.04080	1.36700	1.42510
C	-3.21860	2.34230	1.50520
C	0.54910	2.95660	1.00130
C	-0.05760	3.99370	1.95030
C	-1.45940	2.66400	-1.38270
C	-1.74280	4.16290	-1.26220
H	-2.42270	0.36200	1.22190
H	-1.53760	1.29730	2.39910
H	-3.94350	2.02520	2.26420
H	-2.89950	3.35730	1.76230
H	-3.75300	2.39970	0.55050
H	1.24820	2.31480	1.55250
H	1.15580	3.45980	0.23750
H	0.72340	4.60170	2.42180
H	-0.73520	4.67970	1.43200
H	-0.62670	3.51760	2.75570
H	-0.77600	2.48310	-2.22250
H	-2.38060	2.12170	-1.63960
H	-2.15630	4.56850	-2.19300
H	-2.45980	4.38140	-0.46450
H	-0.82810	4.72380	-1.04150
H	-1.22990	-0.43210	-0.92350

C7a

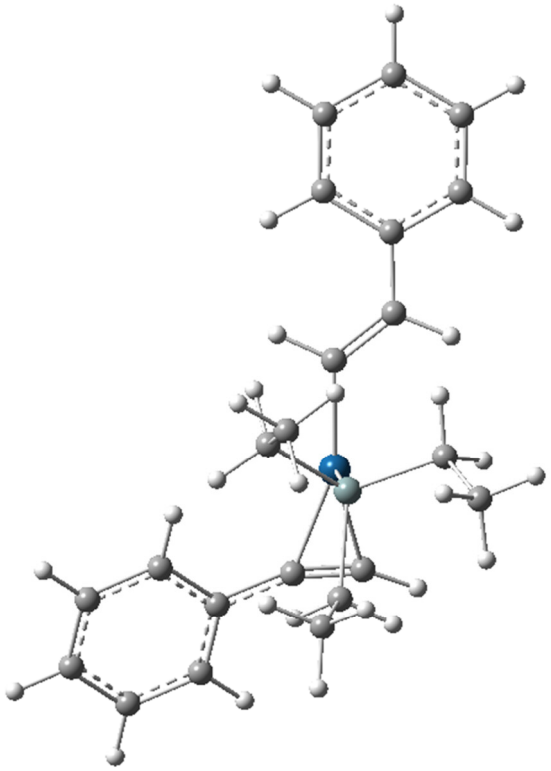
E = -1262.991998; (E+ZPE) = -1262.556240; H = -1262.527238; G = -1262.619181



C	-6.45160	-1.48290	0.57850
C	-5.54870	-2.26680	1.29450
C	-5.96460	-0.52720	-0.31620
C	-4.59650	-0.35940	-0.49510
C	-3.67150	-1.14830	0.21050
C	-4.17860	-2.09780	1.11250
C	-2.21700	-1.01310	0.06110
C	-1.56270	-0.27240	-0.85830
H	-7.52140	-1.60910	0.71810
H	-5.91130	-3.01190	1.99760
H	-6.65850	0.09700	-0.87320
H	-4.24040	0.40000	-1.18560
H	-3.48000	-2.71390	1.67480
H	-2.18450	0.29190	-1.56390
Pt	0.40810	-0.13250	-1.21930
C	4.59460	-2.55830	1.96780
C	5.27330	-2.00270	0.88190
C	3.20270	-2.49110	2.02760
C	2.48870	-1.87100	1.00820
C	3.16520	-1.30940	-0.08290
C	4.56650	-1.38000	-0.14050
C	2.44620	-0.64440	-1.13780
C	2.25280	-0.00490	-2.20670
H	5.15070	-3.04240	2.76530
H	6.35710	-2.05310	0.83340
H	2.67200	-2.92280	2.87110
H	1.40520	-1.80900	1.04170
H	5.08830	-0.94180	-0.98590
H	2.50000	0.47770	-3.13450
Si	0.23210	1.60350	0.31950
C	0.11340	0.86610	2.06730
C	-0.52600	1.78510	3.11280
C	1.85980	2.58440	0.17030
C	2.20620	3.45520	1.38220
C	-1.24650	2.73080	-0.07500
C	-1.15190	4.17320	0.42820
H	-0.46090	-0.06440	2.00550
H	1.12780	0.58020	2.37630
H	-0.56870	1.29930	4.09470
H	0.03090	2.71960	3.23580
H	-1.55230	2.04750	2.83510
H	2.66810	1.86400	0.00170
H	1.80930	3.19530	-0.74150
H	3.15330	3.98630	1.22980
H	1.43990	4.20900	1.58680
H	2.31840	2.84800	2.28690
H	-1.36820	2.73310	-1.16640
H	-2.14710	2.24300	0.31950
H	-2.04290	4.74800	0.14970
H	-1.06170	4.22180	1.51810
H	-0.28540	4.69080	0.00300
H	-1.64350	-1.58750	0.79060

C7b

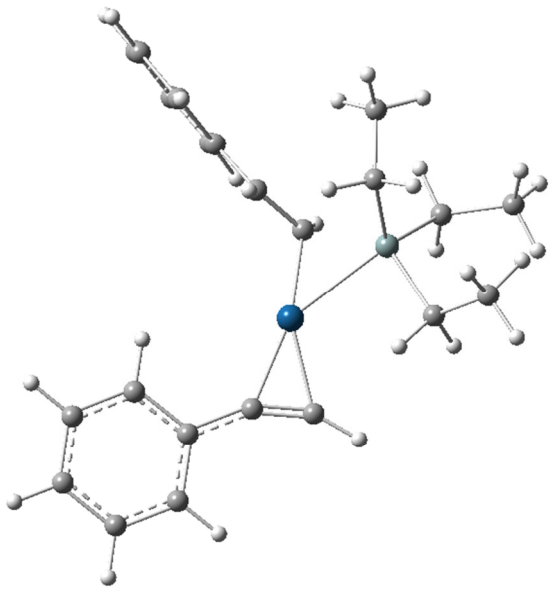
E = -1262.991320; (E+ZPE) = -1262.555686; H = -1262.526592; G = -1262.619405



C	5.45280	-1.55640	1.85760
C	4.13900	-1.32840	2.26660
C	5.76820	-1.56320	0.49790
C	4.77730	-1.34150	-0.45140
C	3.45320	-1.11160	-0.04390
C	3.14150	-1.10940	1.32290
C	2.43760	-0.86580	-1.03340
C	1.92410	-0.62780	-2.15980
H	6.23030	-1.72900	2.59610
H	3.89080	-1.32260	3.32380
H	6.79050	-1.74080	0.17680
H	5.01620	-1.34300	-1.51060
H	2.11380	-0.93260	1.62690
H	1.89130	-0.43140	-3.21600
Pt	0.36220	-0.60010	-0.77980
C	-6.58270	-1.41570	1.01360
C	-5.45670	-1.71300	1.78510
C	-6.41260	-0.84320	-0.24550
C	-5.13280	-0.57430	-0.72390
C	-3.98970	-0.87000	0.03640
C	-4.18050	-1.44380	1.30520
C	-2.66780	-0.55310	-0.51960
C	-1.46490	-0.82330	0.03130
H	-7.57860	-1.62710	1.39220
H	-5.57650	-2.15650	2.77010
H	-7.27830	-0.60410	-0.85750
H	-5.00790	-0.12660	-1.70750
H	-3.32000	-1.68060	1.92470
H	-1.46840	-1.31980	1.00870
Si	0.14490	1.55960	0.05390
C	-0.21670	1.55870	1.92110
C	-0.85850	2.84620	2.44870
C	1.84340	2.37430	-0.24100
C	2.12540	3.63570	0.58060
C	-1.20700	2.47710	-0.91680
C	-1.03020	3.99290	-1.03460
H	-0.87440	0.71110	2.14280
H	0.72750	1.36050	2.44740
H	-1.04400	2.78400	3.52740
H	-0.22700	3.72340	2.27650
H	-1.82220	3.03450	1.96390
H	2.61260	1.62590	-0.01820
H	1.93770	2.58330	-1.31540
H	3.12020	4.03800	0.35540
H	1.40060	4.43200	0.38600
H	2.09930	3.42330	1.65480
H	-1.24770	2.03410	-1.92060
H	-2.16990	2.23670	-0.45050
H	-1.84010	4.44030	-1.62270
H	-1.03250	4.48170	-0.05490
H	-0.08780	4.25240	-1.52870
H	-2.70760	-0.04380	-1.48340

TS-C10a

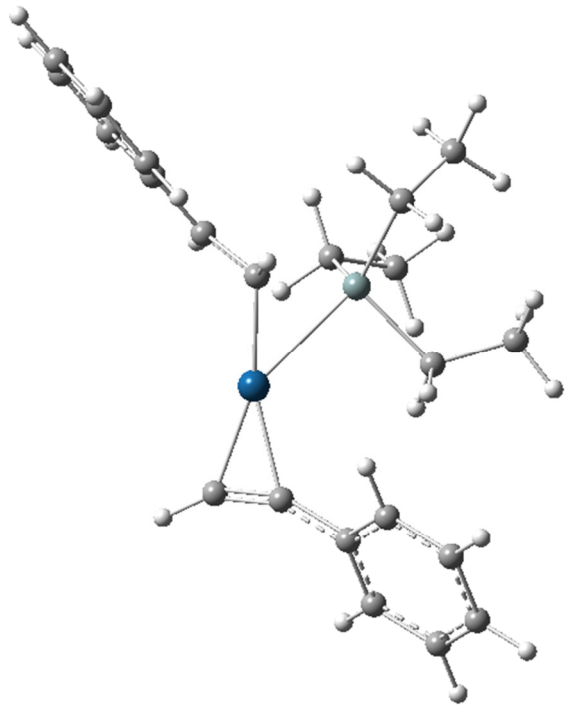
E = -1262.976194; (E+ZPE) = -1262.539722; H = -1262.511849; G = -1262.601166



C	-2.99710	-5.19600	-0.30710
C	-2.77820	-4.70920	0.98100
C	-2.67420	-4.40270	-1.41020
C	-2.14030	-3.13260	-1.22940
C	-1.92950	-2.62240	0.06240
C	-2.24680	-3.43620	1.16190
C	-1.40910	-1.27810	0.30820
C	-1.26730	-0.27910	-0.61420
H	-3.40860	-6.19060	-0.45270
H	-3.02140	-5.32160	1.84450
H	-2.82960	-4.78290	-2.41590
H	-1.86840	-2.53590	-2.09510
H	-2.08000	-3.05530	2.16680
H	-1.67190	-0.42070	-1.61750
Pt	0.55410	0.51240	-0.34610
C	5.92460	-1.67740	0.67150
C	6.12350	-0.42110	0.09610
C	4.62820	-2.13290	0.91130
C	3.53570	-1.33880	0.57880
C	3.72640	-0.07490	0.00200
C	5.03500	0.37700	-0.23740
C	2.59710	0.75110	-0.34580
C	2.04060	1.82250	-0.76030
H	6.77730	-2.29840	0.93070
H	7.13150	-0.06300	-0.09320
H	4.46820	-3.11020	1.35780
H	2.52190	-1.68490	0.76030
H	5.18560	1.35400	-0.68690
H	2.04680	2.85300	-1.07390
Si	-1.60900	1.71470	0.17170
C	-2.42440	1.31510	1.84250
C	-3.75930	0.57210	1.77870
C	-0.69490	3.39860	0.36700
C	-1.43500	4.45920	1.18950
C	-2.93300	1.96810	-1.17740
C	-3.77590	3.24060	-1.09400
H	-1.70400	0.76420	2.46210
H	-2.56990	2.27330	2.35660
H	-4.15410	0.37090	2.78150
H	-4.51380	1.15870	1.24350
H	-3.66990	-0.38870	1.26160
H	0.28570	3.21980	0.81710
H	-0.49900	3.76920	-0.64860
H	-0.91870	5.42490	1.12990
H	-2.46390	4.61940	0.85590
H	-1.47440	4.18270	2.24790
H	-2.40950	1.93490	-2.14350
H	-3.58840	1.08740	-1.16730
H	-4.54390	3.25930	-1.87620
H	-4.29220	3.32700	-0.13100
H	-3.16290	4.13860	-1.22000
H	-1.14570	-1.07740	1.34620

TS-C10b

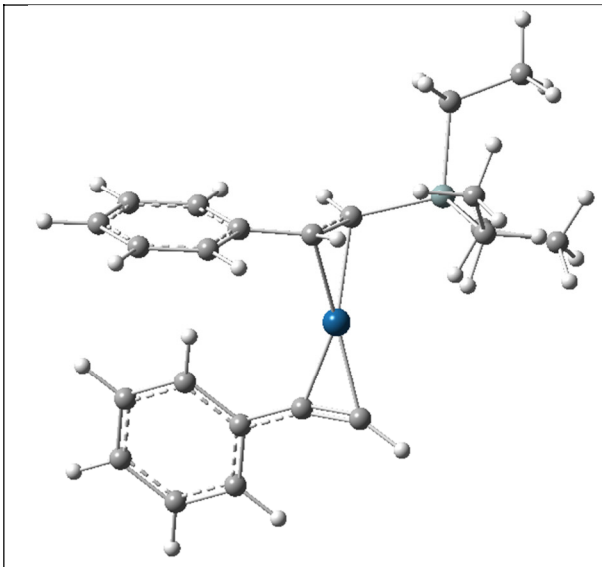
E = -1262.975947; (E+ZPE) = -1262.539214; H = -1262.511469; G = -1262.599287



C	5.82310	-0.50550	1.37560
C	4.63480	-0.59120	2.10160
C	5.82030	-0.77080	0.00600
C	4.63740	-1.12010	-0.63800
C	3.43860	-1.20290	0.08630
C	3.44820	-0.93310	1.46200
C	2.21200	-1.56230	-0.58360
C	1.50160	-2.18790	-1.43870
H	6.74820	-0.23280	1.87520
H	4.63270	-0.38840	3.16870
H	6.74300	-0.70410	-0.56340
H	4.62840	-1.32220	-1.70480
H	2.51600	-1.00090	2.01550
H	1.37690	-2.93510	-2.20380
Pt	0.28280	-0.89470	-0.46430
C	-6.40190	-1.34470	0.90350
C	-5.34400	-1.50830	1.80060
C	-6.15230	-0.83570	-0.37030
C	-4.85670	-0.48840	-0.73900
C	-3.78380	-0.63640	0.15600
C	-4.04960	-1.16420	1.43120
C	-2.45000	-0.22460	-0.27280
C	-1.33070	-0.13860	0.51100
H	-7.41160	-1.61960	1.19450
H	-5.53030	-1.91600	2.79020
H	-6.96780	-0.70960	-1.07690
H	-4.66430	-0.08940	-1.73230
H	-3.23490	-1.31870	2.13220
H	-1.44460	-0.31000	1.58300
Si	-0.23000	1.58380	0.00940
C	-1.07750	2.56190	1.42680
C	-1.32280	4.04330	1.12360
C	1.64090	1.91110	0.21530
C	2.05630	3.33090	0.61030
C	-0.88320	2.20560	-1.66520
C	-0.11370	3.39400	-2.24740
H	-2.03690	2.08840	1.66340
H	-0.45590	2.45710	2.32750
H	-1.80900	4.54320	1.96980
H	-0.39710	4.58620	0.91310
H	-1.97940	4.16660	0.25550
H	2.01460	1.21120	0.97020
H	2.13650	1.61150	-0.71620
H	3.14620	3.39660	0.71080
H	1.75240	4.07600	-0.13140
H	1.62430	3.62550	1.57230
H	-0.84540	1.37070	-2.37630
H	-1.94380	2.46530	-1.55010
H	-0.51280	3.68240	-3.22670
H	-0.17190	4.27470	-1.60020
H	0.94640	3.15600	-2.38430
H	-2.38180	0.05370	-1.32350

C11a

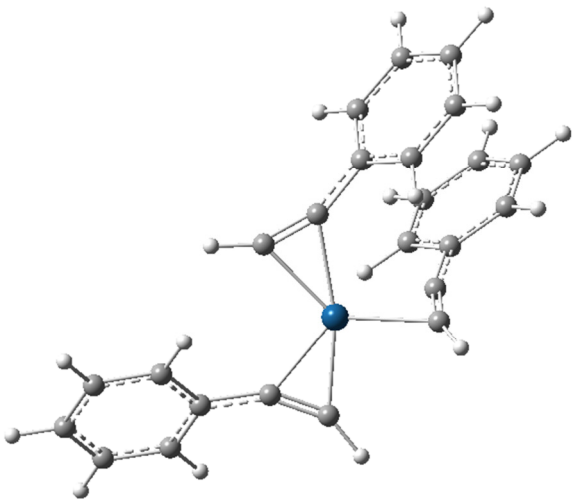
E = -1263.014238; (E+ZPE) = -1262.577638; H = -1262.549037; G = -1262.640591



C	2.48630	4.21260	0.28150
C	1.90360	4.04870	-0.97470
C	2.00540	3.47000	1.36070
C	0.96010	2.56850	1.18570
C	0.37000	2.38860	-0.07400
C	0.85590	3.14900	-1.14740
C	-0.72130	1.41820	-0.32160
C	-1.31050	0.57150	0.64820
H	3.30420	4.91370	0.41980
H	2.26640	4.62260	-1.82290
H	2.44700	3.59370	2.34600
H	0.60400	1.99610	2.03720
H	0.41030	3.01850	-2.13080
H	-0.94420	0.64420	1.67620
Pt	0.11010	-0.53900	-0.47020
C	5.64690	-1.25500	1.06990
C	5.26990	-2.45280	0.46070
C	4.75300	-0.18460	1.11330
C	3.48550	-0.30830	0.55520
C	3.10290	-1.50850	-0.06020
C	4.00570	-2.58230	-0.10440
C	1.79640	-1.63940	-0.65710
C	0.89140	-2.15570	-1.39350
H	6.63550	-1.15710	1.50910
H	5.96350	-3.28790	0.42550
H	5.04400	0.75070	1.58280
H	2.78240	0.51960	0.58180
H	3.70650	-3.51150	-0.58010
H	0.52450	-2.86430	-2.11580
Si	-3.02460	-0.19720	0.49630
C	-3.56910	-0.29400	-1.31620
C	-4.08430	1.01580	-1.91970
C	-2.95510	-1.92060	1.28440
C	-4.01580	-2.91900	0.81400
C	-4.22060	0.91410	1.45890
C	-5.65620	0.39100	1.54770
H	-2.72640	-0.68310	-1.90440
H	-4.35510	-1.05780	-1.38570
H	-4.36740	0.89050	-2.97100
H	-4.96790	1.38030	-1.38500
H	-3.33650	1.81480	-1.87820
H	-1.95350	-2.32640	1.09180
H	-3.02030	-1.78740	2.37370
H	-3.93740	-3.87080	1.35180
H	-5.03360	-2.54300	0.96470
H	-3.90730	-3.14000	-0.25320
H	-3.80990	1.05540	2.46820
H	-4.20590	1.90810	0.99150
H	-6.31530	1.09660	2.06640
H	-6.08570	0.21450	0.55460
H	-5.70210	-0.55730	2.09380
H	-1.26190	1.60340	-1.25020

D1

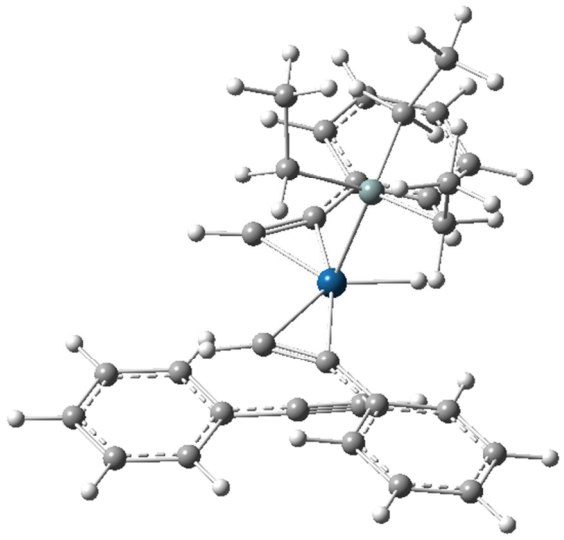
E = -1043.609103; (E+ZPE) = -1043.274317; H = -1043.250039; G = -1043.330491



C	-6.14080	0.62990	-1.45660
C	-5.86260	-0.72980	-1.31220
C	-5.25640	1.57430	-0.93530
C	-4.09730	1.16470	-0.28360
C	-3.81270	-0.20020	-0.12780
C	-4.71080	-1.14470	-0.65150
C	-2.62730	-0.63800	0.57030
C	-2.01980	-1.43060	1.36930
H	-7.04090	0.95100	-1.97280
H	-6.54670	-1.47090	-1.71620
H	-5.46930	2.63470	-1.03840
H	-3.40880	1.89550	0.13040
H	-4.49080	-2.20230	-0.53910
H	-2.07200	-2.23970	2.07950
C	4.65640	2.26040	-0.35630
C	3.91060	2.38490	0.81580
C	4.02710	1.87450	-1.53980
C	2.66060	1.61670	-1.55550
C	1.90550	1.73740	-0.37890
C	2.54640	2.11430	0.81050
C	0.50300	1.41460	-0.38170
C	-0.70370	1.42660	-0.76080
H	5.72410	2.46000	-0.34700
H	4.39560	2.68510	1.74050
H	4.60380	1.76950	-2.45430
H	2.16820	1.30300	-2.47070
H	1.96350	2.18740	1.72330
H	-1.51590	1.82800	-1.34150
Pt	-0.60510	-0.10410	0.66840
C	4.19760	-2.29620	-1.69390
C	4.61760	-1.82100	-0.45110
C	2.83620	-2.35880	-1.99120
C	1.89590	-1.94360	-1.05520
C	2.31390	-1.46760	0.19550
C	3.68460	-1.40920	0.49280
C	1.36330	-1.00170	1.16340
C	0.82400	-0.60990	2.21930
H	4.93060	-2.61310	-2.43030
H	5.67730	-1.76110	-0.22010
H	2.50610	-2.72550	-2.95870
H	0.83390	-1.96690	-1.27980
H	4.00480	-1.01890	1.45350
H	0.66730	-0.47470	3.27180

D4

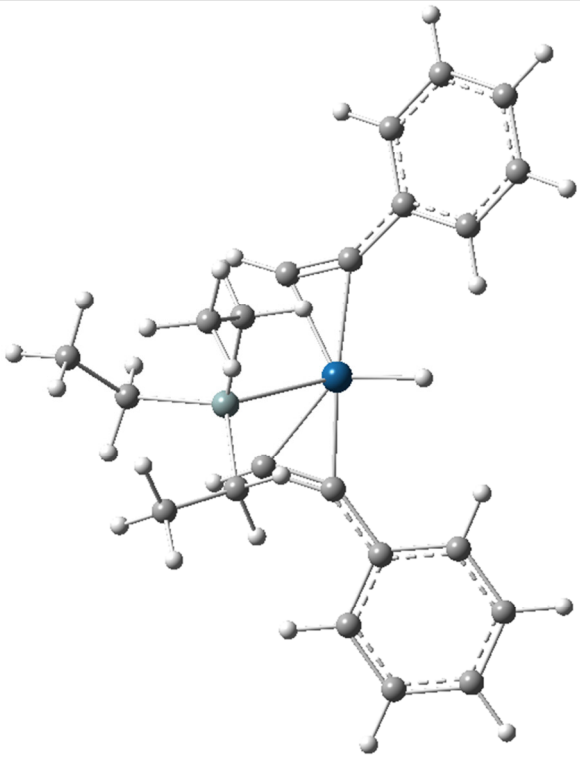
E = -1571.008225; (E+ZPE) = -1570.466227; H = -1570.428540; G = -1570.541826



C	-5.47550	-0.89310	-2.13220
C	-4.19720	-1.07730	-2.65870
C	-5.62890	-0.31120	-0.87240
C	-4.51240	0.08450	-0.14440
C	-3.22150	-0.09870	-0.66750
C	-3.07780	-0.68470	-1.93170
C	-2.07100	0.32570	0.09510
C	-1.57600	0.99580	1.06340
H	-6.34890	-1.20310	-2.69880
H	-4.07220	-1.53120	-3.63770
H	-6.62230	-0.16870	-0.45620
H	-4.62570	0.53320	0.83850
H	-2.07460	-0.83190	-2.32140
H	-1.67470	1.67210	1.89410
Pt	0.00820	0.05250	0.04420
C	5.48600	-0.95120	-2.11080
C	5.64250	-0.37050	-0.85090
C	4.20710	-1.11940	-2.64130
C	3.09050	-0.71270	-1.91780
C	3.23750	-0.12870	-0.65340
C	4.52860	0.03950	-0.12670
C	2.09050	0.30710	0.10770
C	1.59660	0.97660	1.07620
H	6.35720	-1.27220	-2.67450
H	6.63620	-0.23980	-0.43160
H	4.07970	-1.57120	-3.62110
H	2.08680	-0.84510	-2.31200
H	4.64430	0.48690	0.85650
H	1.69300	1.65190	1.90790
Si	-0.01750	-2.14290	0.85770
C	1.67520	-2.95770	0.60970
C	1.70570	-4.47860	0.78690
C	-0.37130	-1.87550	2.70730
C	0.04080	-3.01750	3.64010
C	-1.37250	-3.19810	0.05740
C	-1.90970	-4.34780	0.91420
H	2.02100	-2.70240	-0.39800
H	2.38800	-2.47540	1.29200
H	2.71570	-4.87270	0.62410
H	1.39320	-4.78830	1.78910
H	1.04440	-4.97650	0.06960
H	0.14760	-0.95440	2.99960
H	-1.44280	-1.65590	2.80840
H	-0.19750	-2.78150	4.68410
H	-0.46600	-3.95610	3.39500
H	1.11900	-3.20330	3.58800
H	-2.19960	-2.53500	-0.21610
H	-0.97350	-3.57800	-0.89360
H	-2.68600	-4.90820	0.38010
H	-1.12730	-5.06030	1.19430
H	-2.35990	-3.97440	1.84030
H	0.01800	-0.94090	-1.24660
C	0.00300	5.50410	1.90470
C	1.21460	5.07540	1.36160
C	-1.20090	5.08080	1.34050
C	-1.19820	4.22890	0.24120
C	0.01850	3.79200	-0.30660
C	1.22740	4.22350	0.26230
C	0.02610	2.89290	-1.41170
C	0.03180	2.09840	-2.32850
H	-0.00310	6.16960	2.76310
H	2.15350	5.40590	1.79670

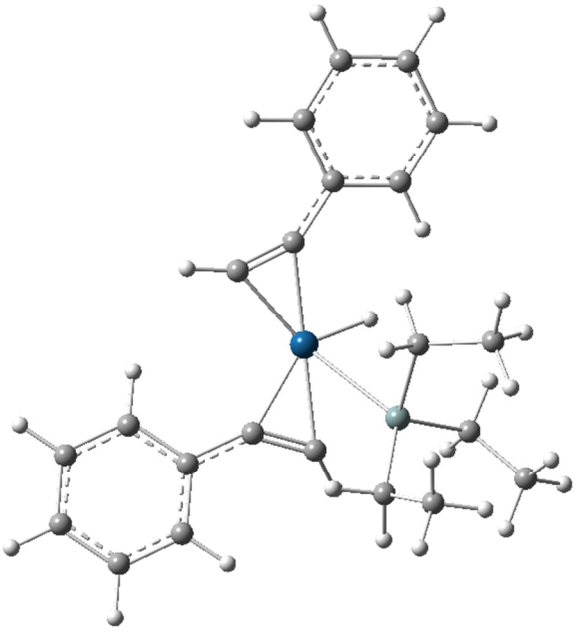
	H -2.14580 5.41520 1.75910 H -2.12960 3.88780 -0.19940 H 2.16490 3.87870 -0.16210 H 0.03740 1.41480 -3.14780

TS-E6a

E = -1262.925993; (E+ZPE) = -1262.494721; H = -1262.466661; G = -1262.554810	
	C -5.00210 -3.19210 0.69470 C -3.66700 -3.54080 0.90080 C -5.32110 -1.97250 0.09310 C -4.30910 -1.10740 -0.30360 C -2.96040 -1.45390 -0.10590 C -2.65170 -2.67510 0.50900 C -1.91880 -0.55360 -0.53230 C -1.70770 0.56250 -1.19290 H -5.79450 -3.86640 1.00690 H -3.41870 -4.48660 1.37340 H -6.36040 -1.69790 -0.06280 H -4.54850 -0.15560 -0.76970 H -1.60630 -2.92150 0.67140 H -2.16950 1.16080 -1.96850 Pt 0.09330 -0.36050 -0.59290 C 5.57290 -2.19480 1.05680 C 5.72640 -1.35950 -0.05170 C 4.29860 -2.44050 1.56580 C 3.18170 -1.85860 0.97290 C 3.32570 -1.01900 -0.13790 C 4.61430 -0.77390 -0.64430 C 2.19440 -0.38050 -0.76890 C 1.73350 0.44160 -1.62500 H 6.44330 -2.65070 1.52000 H 6.71660 -1.16450 -0.45390 H 4.17280 -3.08850 2.42850 H 2.18380 -2.04250 1.35890 H 4.72930 -0.12280 -1.50610 H 1.84230 1.19500 -2.38500 Si -0.49760 1.94870 0.15030 C 1.17910 2.18340 1.05080 C 1.17000 3.23300 2.16510 C -0.67120 3.32460 -1.15620 C -0.04470 4.67740 -0.81600 C -1.84770 2.02850 1.49020 C -2.33400 3.44690 1.80360 H 1.48100 1.21600 1.46600 H 1.93670 2.42460 0.29500 H 2.16100 3.30790 2.62830 H 0.90550 4.23050 1.80180 H 0.46280 2.97160 2.95910 H -0.22350 2.93370 -2.08020 H -1.73880 3.45430 -1.37720 H -0.15960 5.38470 -1.64560 H -0.51030 5.13220 0.06410 H 1.02690 4.58580 -0.61130 H -2.69880 1.41020 1.19130 H -1.43530 1.55910 2.39380 H -3.10690 3.43420 2.58090 H -1.52720 4.09460 2.15930 H -2.77020 3.92380 0.91910 H 0.32790 -1.63500 0.37680

TS-E6b

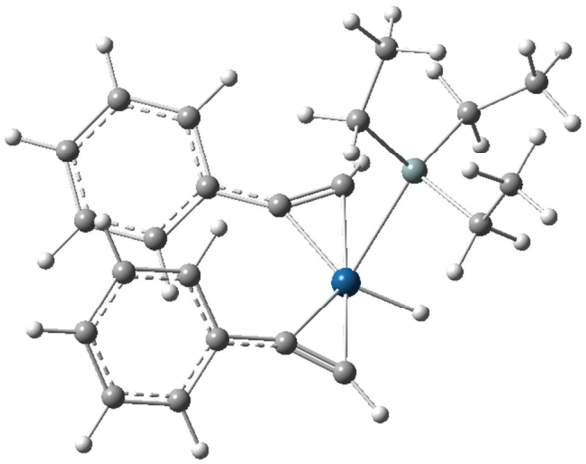
E = -1262.925702; (E+ZPE) = -1262.493964; H = -1262.466000; G = -1262.554199



C	5.53460	-2.56870	0.46060
C	4.30610	-3.22950	0.41120
C	5.59540	-1.18800	0.25840
C	4.43390	-0.47110	-0.00020
C	3.18980	-1.12740	-0.05180
C	3.13990	-2.51280	0.17020
C	1.98870	-0.38470	-0.32190
C	1.61410	0.73740	-0.92300
H	6.44400	-3.12780	0.66120
H	4.25960	-4.30310	0.56890
H	6.55120	-0.67390	0.30180
H	4.47030	0.60340	-0.15670
H	2.17560	-3.00990	0.13430
H	2.04310	1.29820	-1.75050
Pt	-0.04810	-0.46950	-0.46940
C	-5.91060	-1.53560	0.17980
C	-5.21620	-2.55330	0.83710
C	-5.20350	-0.53320	-0.48250
C	-3.81170	-0.54440	-0.48940
C	-3.10600	-1.55940	0.16770
C	-3.82670	-2.56710	0.83270
C	-1.66110	-1.59110	0.20380
C	-0.58850	-2.16230	0.60280
H	-6.99670	-1.52620	0.18410
H	-5.76090	-3.33850	1.35380
H	-5.73740	0.26070	-0.99690
H	-3.25070	0.22920	-1.00540
H	-3.28350	-3.35650	1.34420
H	-0.08540	-2.93380	1.15860
Si	0.27280	2.05170	0.02250
C	-1.12580	1.93410	1.33070
C	-1.93280	3.23140	1.45870
C	1.75010	2.84560	0.94050
C	1.45380	4.01130	1.88540
C	-0.30290	3.08510	-1.46100
C	-0.06250	4.59290	-1.36020
H	-1.80500	1.11340	1.08940
H	-0.66040	1.67390	2.29030
H	-2.69690	3.13440	2.23880
H	-1.31130	4.09370	1.71680
H	-2.45310	3.46920	0.52470
H	2.21650	2.02600	1.50430
H	2.49460	3.14450	0.19020
H	2.37340	4.36840	2.36410
H	1.00760	4.86330	1.36320
H	0.76750	3.71580	2.68520
H	0.18680	2.69080	-2.35990
H	-1.37230	2.87840	-1.60020
H	-0.39540	5.11080	-2.26700
H	-0.60170	5.03620	-0.51700
H	1.00020	4.82210	-1.22510
H	-1.19630	0.17910	-1.39070

TS-E6c

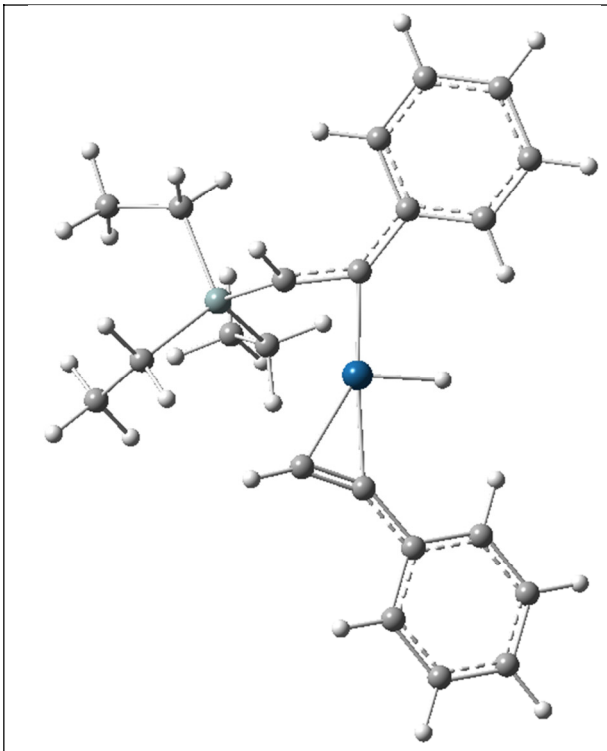
E = -1262.926220; (E+ZPE) = -1262.494073; H = -1262.466281; G = -1262.553581



C	-3.55440	3.65320	-0.25980
C	-3.71420	2.34320	-0.71330
C	-2.27870	4.14480	0.02770
C	-1.16540	3.33230	-0.14590
C	-1.31700	2.00640	-0.59470
C	-2.60650	1.51790	-0.86370
C	-0.16600	1.16400	-0.75490
C	1.11860	1.24280	-1.07790
H	-4.42350	4.29120	-0.12650
H	-4.70600	1.95970	-0.93360
H	-2.15530	5.16400	0.38260
H	-0.16820	3.70470	0.07180
H	-2.71950	0.49170	-1.19730
H	1.66000	1.90510	-1.74640
Pt	0.46310	-0.76640	-1.00190
C	-4.69680	-1.31400	1.92430
C	-4.62520	-2.32030	0.95960
C	-3.58550	-0.50730	2.16740
C	-2.41230	-0.69690	1.44560
C	-2.32720	-1.71310	0.48310
C	-3.44890	-2.52450	0.24550
C	-1.10340	-1.93700	-0.24760
C	-0.24110	-2.69620	-0.80510
H	-5.61670	-1.15750	2.48050
H	-5.48880	-2.94990	0.76460
H	-3.63640	0.28200	2.91190
H	-1.54830	-0.06020	1.60990
H	-3.38840	-3.30730	-0.50490
H	0.09970	-3.68410	-1.05880
Si	2.41930	0.27130	0.27800
C	3.17830	-1.46910	0.57640
C	3.93520	-1.59730	1.90220
C	3.84870	1.36870	-0.35780
C	5.23890	1.15410	0.23910
C	1.69530	0.86540	1.93570
C	2.67670	1.62450	2.83300
H	2.37970	-2.21520	0.54600
H	3.83470	-1.69700	-0.27380
H	4.36690	-2.60000	2.00510
H	4.75560	-0.88040	1.99500
H	3.26770	-1.44590	2.75710
H	3.89090	1.19510	-1.44280
H	3.54470	2.41710	-0.23750
H	5.97190	1.82260	-0.22780
H	5.25880	1.35240	1.31530
H	5.59050	0.12920	0.08380
H	0.82360	1.49640	1.73080
H	1.31050	-0.01990	2.45980
H	2.19400	1.95110	3.76150
H	3.53700	1.00910	3.11380
H	3.06420	2.51960	2.33420
H	1.60990	-1.54380	-1.82950

E7a

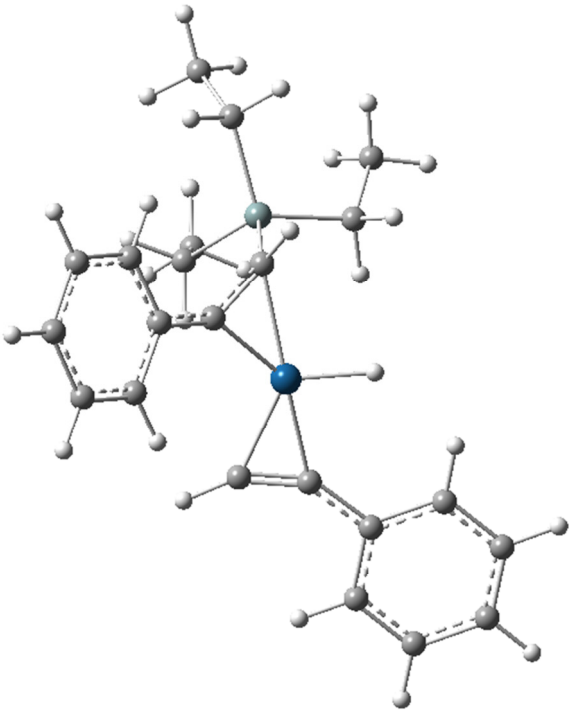
E = -1262.951345; (E+ZPE) = -1262.519191; H = -1262.490519; G = -1262.581183



C	3.39420	4.64480	0.41160
C	2.00280	4.62360	0.53600
C	4.09020	3.48390	0.06720
C	3.39490	2.30310	-0.15730
C	1.99160	2.27180	-0.04520
C	1.30570	3.44320	0.31810
C	1.28440	1.04610	-0.29790
C	1.62750	-0.16170	-0.89190
H	3.93890	5.56730	0.59210
H	1.46830	5.52800	0.81070
H	5.17250	3.50390	-0.02040
H	3.92160	1.38920	-0.41790
H	0.22550	3.39710	0.42200
H	2.19700	-0.11170	-1.82940
Pt	-0.48370	0.34270	-0.52980
C	-6.25420	0.40050	1.09400
C	-6.09950	-0.55950	0.09230
C	-5.14860	1.13020	1.52970
C	-3.89500	0.90490	0.96900
C	-3.72940	-0.05510	-0.03640
C	-4.84840	-0.78770	-0.46860
C	-2.44030	-0.32150	-0.63540
C	-1.74020	-0.98690	-1.47890
H	-7.23240	0.57820	1.53190
H	-6.95710	-1.13080	-0.25190
H	-5.26320	1.87810	2.30920
H	-3.02710	1.46720	1.29970
H	-4.72310	-1.53390	-1.24800
H	-1.67240	-1.72310	-2.26190
Si	1.91520	-1.79400	0.03130
C	1.04210	-1.79080	1.70910
C	1.65730	-2.70640	2.77120
C	1.34250	-3.21960	-1.07360
C	1.10590	-4.55410	-0.36150
C	3.80360	-1.86070	0.25290
C	4.41720	-3.24340	0.48850
H	1.03220	-0.75570	2.07420
H	-0.01240	-2.04860	1.54610
H	1.09860	-2.65080	3.71240
H	1.66190	-3.75580	2.45810
H	2.69300	-2.42580	2.99150
H	0.41420	-2.89170	-1.55660
H	2.07650	-3.34440	-1.88200
H	0.76710	-5.32700	-1.06090
H	2.01310	-4.92960	0.12300
H	0.33770	-4.45800	0.41340
H	4.24670	-1.41740	-0.65030
H	4.06730	-1.18060	1.07530
H	5.50640	-3.18620	0.59870
H	4.02310	-3.71810	1.39260
H	4.21080	-3.91710	-0.35010
H	-1.09480	1.55250	0.30980

E7b

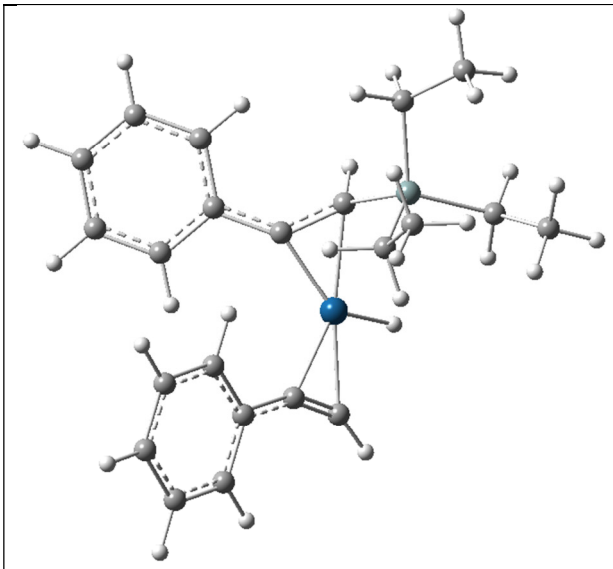
E = -1262.940132; (E+ZPE) = ; -1262.507922 H = -1262.479249; G = -1262.570297



C	3.85630	-4.39380	0.06250
C	2.49860	-4.46630	0.38520
C	4.42200	-3.18640	-0.35350
C	3.62870	-2.05100	-0.45520
C	2.25930	-2.11120	-0.13330
C	1.70660	-3.32980	0.29980
C	1.43880	-0.93690	-0.22140
C	1.54160	0.27050	-0.90070
H	4.47750	-5.28170	0.14000
H	2.06690	-5.40850	0.70910
H	5.47880	-3.13680	-0.59840
H	4.05280	-1.10410	-0.77770
H	0.65070	-3.35580	0.55340
H	1.93510	0.23230	-1.92500
Pt	-0.42490	-0.39640	-0.27240
C	-6.44060	0.06060	-0.24950
C	-6.04450	-0.67530	0.86900
C	-5.47740	0.54580	-1.13310
C	-4.12690	0.29930	-0.90360
C	-3.71900	-0.43780	0.21420
C	-4.69680	-0.92360	1.10010
C	-2.32490	-0.71130	0.49130
C	-1.46820	-1.27160	1.26640
H	-7.49430	0.25380	-0.42990
H	-6.78930	-1.05650	1.56200
H	-5.77860	1.11920	-2.00530
H	-3.36820	0.67250	-1.58500
H	-4.38570	-1.49610	1.96940
H	-1.23270	-1.83090	2.15640
Si	1.72210	1.97920	-0.08860
C	1.55000	1.81210	1.78730
C	1.17700	3.10170	2.52270
C	3.48390	2.52950	-0.54550
C	4.08800	3.63040	0.33060
C	0.44460	3.15400	-0.84170
C	0.78110	4.64560	-0.79360
H	0.78970	1.04470	1.97900
H	2.49340	1.40680	2.17950
H	1.08670	2.93420	3.60200
H	1.92230	3.89080	2.37690
H	0.21490	3.49180	2.17330
H	4.12370	1.63700	-0.49990
H	3.48250	2.84000	-1.60000
H	5.10440	3.88740	0.01030
H	3.49450	4.54960	0.29970
H	4.14710	3.31610	1.37830
H	0.30370	2.83550	-1.88340
H	-0.51600	2.95600	-0.34860
H	-0.01070	5.24810	-1.25340
H	0.90700	5.00500	0.23320
H	1.70930	4.86490	-1.33260
H	-1.30100	0.36750	-1.38640

E7c

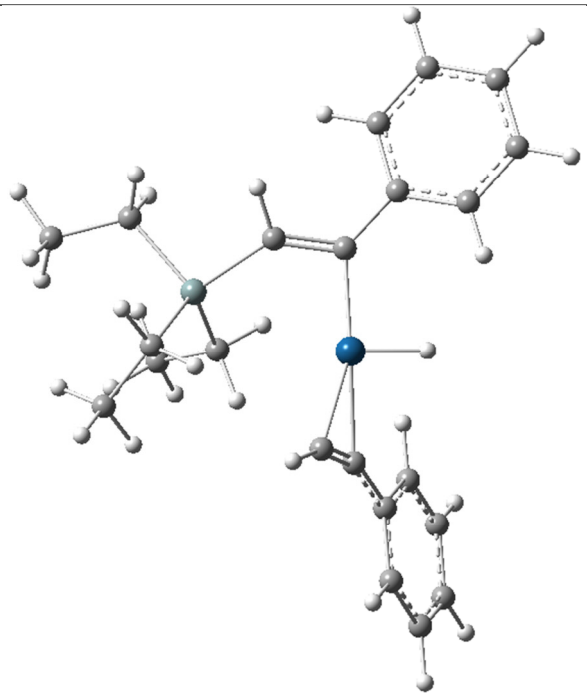
E = -1262.943569; (E+ZPE) = -1262.511143; H = -1262.482544; G = -1262.572626



C	-2.16850	4.68170	0.06960
C	-2.80440	3.49740	-0.31310
C	-0.78620	4.71040	0.26630
C	-0.03640	3.55690	0.07270
C	-0.66570	2.35770	-0.31200
C	-2.06120	2.33900	-0.49040
C	0.10490	1.15720	-0.48260
C	1.44760	0.90560	-0.75340
H	-2.75390	5.58440	0.22080
H	-3.88010	3.48100	-0.46070
H	-0.29870	5.63270	0.56810
H	1.03990	3.56140	0.22200
H	-2.53670	1.40330	-0.77000
H	1.94230	1.58190	-1.46340
Pt	-0.03040	-0.59840	-1.28680
C	-4.55450	-1.36680	2.49340
C	-4.71380	-2.30320	1.47020
C	-3.44430	-0.52280	2.49360
C	-2.49870	-0.61100	1.47700
C	-2.65040	-1.54640	0.44520
C	-3.77020	-2.39600	0.45340
C	-1.68280	-1.65520	-0.62140
C	-1.20890	-2.25040	-1.65260
H	-5.29310	-1.29700	3.28680
H	-5.57680	-2.96310	1.46560
H	-3.31420	0.20700	3.28760
H	-1.63030	0.04060	1.46100
H	-3.89150	-3.12200	-0.34520
H	-1.26520	-3.04730	-2.37240
Si	2.64630	0.01560	0.41640
C	3.73060	-1.16020	-0.59550
C	4.45170	-2.24970	0.20240
C	3.69630	1.41690	1.15900
C	5.05970	1.01820	1.72990
C	1.67750	-0.88060	1.77290
C	2.44600	-1.13880	3.07160
H	3.07620	-1.62070	-1.34570
H	4.45710	-0.55670	-1.15770
H	5.05310	-2.89180	-0.45120
H	5.12560	-1.83190	0.95750
H	3.73740	-2.89640	0.72350
H	3.83970	2.16510	0.36660
H	3.09160	1.91580	1.92990
H	5.59830	1.88570	2.12890
H	4.96660	0.29070	2.54250
H	5.69520	0.56730	0.96010
H	0.78530	-0.27800	1.98760
H	1.29580	-1.82320	1.35970
H	1.81940	-1.65680	3.80650
H	3.33380	-1.75820	2.90750
H	2.78100	-0.20300	3.53210
H	0.71500	-1.27600	-2.54110

TS-E8a

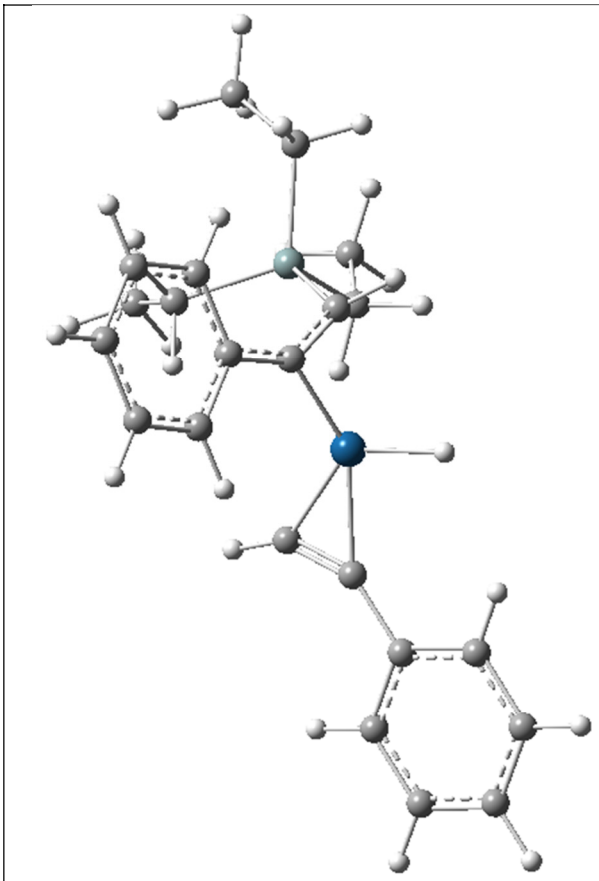
E = -1262.947619; (E+ZPE) = -1262.516234; H = -1262.487864; G = -1262.577203



C	4.40230	3.87870	0.63680
C	3.18320	4.12120	0.00120
C	4.71290	2.58780	1.06350
C	3.81530	1.54680	0.84660
C	2.58950	1.77400	0.19830
C	2.28210	3.08230	-0.20320
C	1.66890	0.65750	-0.03640
C	2.05360	-0.63230	-0.25980
H	5.09970	4.69360	0.80920
H	2.93250	5.12560	-0.32850
H	5.65270	2.39380	1.57330
H	4.04930	0.54430	1.19520
H	1.32720	3.26970	-0.68630
H	3.09720	-0.79180	-0.57090
Pt	-0.17440	0.54570	-0.71660
C	-5.45370	1.55350	1.64160
C	-5.71240	1.12330	0.33910
C	-4.14210	1.59110	2.11410
C	-3.09010	1.20310	1.29070
C	-3.34320	0.77180	-0.01780
C	-4.66610	0.73250	-0.48850
C	-2.27380	0.34820	-0.88540
C	-1.76100	-0.16860	-1.91810
H	-6.27350	1.85830	2.28570
H	-6.73250	1.09430	-0.03280
H	-3.93780	1.92340	3.12770
H	-2.06430	1.22570	1.64570
H	-4.85990	0.39910	-1.50360
H	-1.77020	-0.67840	-2.86470
Si	1.17290	-2.27500	0.12050
C	-0.19650	-2.04190	1.41350
C	-0.43560	-3.23970	2.33760
C	0.51700	-3.10430	-1.45810
C	-0.56810	-4.16020	-1.23430
C	2.59290	-3.32200	0.82850
C	2.39240	-4.83930	0.81750
H	0.07070	-1.15980	2.00950
H	-1.12910	-1.77470	0.90080
H	-1.22560	-3.02330	3.06570
H	-0.74280	-4.13110	1.78080
H	0.46620	-3.49950	2.90220
H	0.13200	-2.31540	-2.11600
H	1.37200	-3.54180	-1.99250
H	-0.90810	-4.59450	-2.18150
H	-0.21410	-4.98500	-0.60720
H	-1.44470	-3.72720	-0.74010
H	3.49190	-3.07170	0.24810
H	2.79540	-2.97170	1.85030
H	3.26590	-5.36110	1.22530
H	1.52540	-5.14360	1.41200
H	2.23800	-5.21290	-0.20060
H	-0.43580	1.95880	-0.16130

TS-E8b

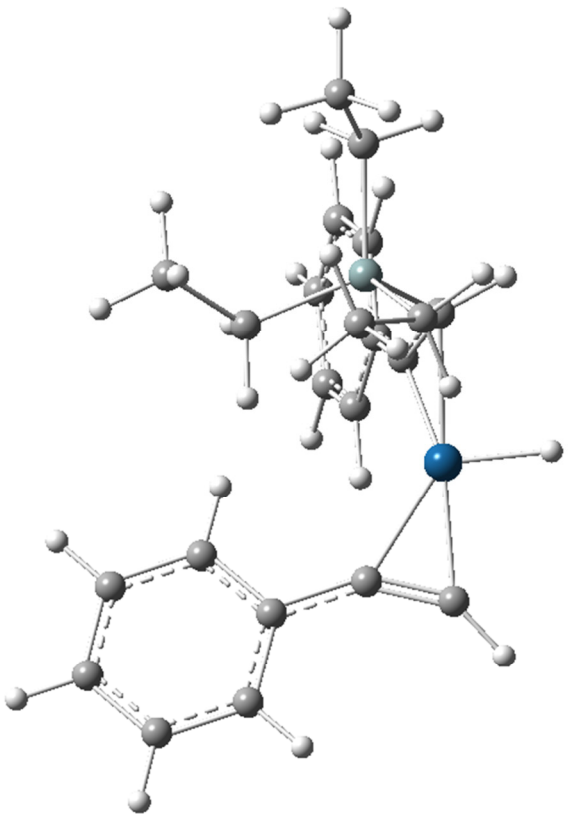
E = -1262.930829; (E+ZPE) = -1262.499787; H = -1262.471598; G = -1262.561663



C	-2.01670	4.96140	0.55510
C	-0.70880	4.51820	0.77870
C	-2.95050	4.11720	-0.04590
C	-2.58050	2.83320	-0.42870
C	-1.26890	2.37580	-0.19930
C	-0.33540	3.23530	0.41000
C	-0.92410	1.03860	-0.57660
C	-1.46010	-0.10690	-1.15490
H	-2.30510	5.96640	0.84910
H	0.01540	5.17900	1.24560
H	-3.96510	4.46270	-0.22040
H	-3.29410	2.16770	-0.90550
H	0.67380	2.87350	0.58420
H	-1.48280	-0.16520	-2.24550
Pt	0.63130	-0.01450	-0.41280
C	6.60020	-0.57100	-0.05670
C	6.06080	-0.81180	1.20830
C	5.75490	-0.27750	-1.12660
C	4.37750	-0.22390	-0.93550
C	3.82650	-0.46530	0.32900
C	4.68490	-0.75940	1.40160
C	2.39480	-0.41020	0.54330
C	1.42220	-0.56450	1.39080
H	7.67540	-0.61210	-0.20650
H	6.71520	-1.04100	2.04470
H	6.17040	-0.08960	-2.11260
H	3.70530	0.00350	-1.75810
H	4.26050	-0.94590	2.38420
H	1.15050	-0.82220	2.40540
Si	-2.57360	-1.31500	-0.21160
C	-2.76040	-0.66290	1.55360
C	-3.13770	-1.70400	2.61050
C	-4.23960	-1.34550	-1.11940
C	-5.42820	-1.85690	-0.30000
C	-1.73280	-3.00890	-0.26770
C	-2.63110	-4.22170	-0.01340
H	-1.80350	-0.19640	1.82400
H	-3.49730	0.15200	1.54190
H	-3.21790	-1.25290	3.60610
H	-4.09800	-2.18310	2.39220
H	-2.38450	-2.49690	2.67250
H	-4.44640	-0.32240	-1.46360
H	-4.12080	-1.94580	-2.03220
H	-6.35530	-1.84380	-0.88450
H	-5.27480	-2.88450	0.04470
H	-5.59440	-1.23740	0.58800
H	-1.26300	-3.09500	-1.25690
H	-0.89930	-2.98850	0.44710
H	-2.06230	-5.15720	-0.06410
H	-3.10500	-4.18230	0.97300
H	-3.43190	-4.28870	-0.75790
H	1.34390	-0.05080	-1.87290

TS-E8c

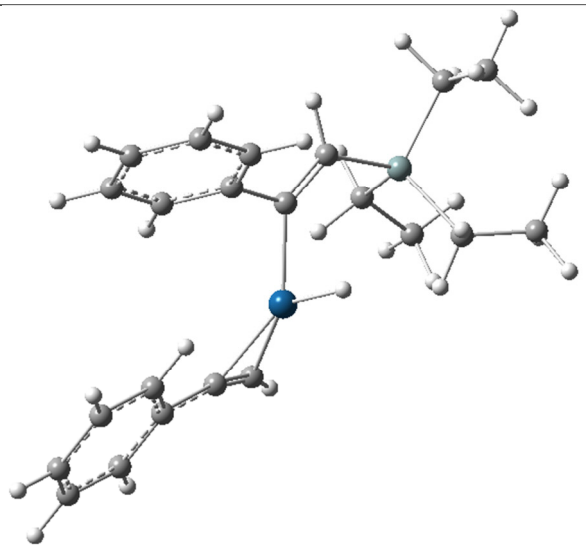
E = -1262.941786; (E+ZPE) = -1262.509567; H = -1262.481713; G = -1262.570189



C	0.11420	5.11210	1.29000
C	-0.98740	4.42720	0.76630
C	1.38590	4.53960	1.24350
C	1.56220	3.28740	0.66660
C	0.45930	2.58700	0.14120
C	-0.82060	3.17010	0.20580
C	0.64380	1.28020	-0.41570
C	1.69850	0.44930	-0.80610
H	-0.02200	6.09200	1.73870
H	-1.97560	4.87550	0.80870
H	2.23840	5.07340	1.65300
H	2.54710	2.83160	0.61660
H	-1.66670	2.61320	-0.18740
H	2.38980	0.83290	-1.56300
Pt	-0.33020	0.05030	-1.46110
C	-4.45680	-1.51850	2.57020
C	-4.82640	-2.07960	1.34620
C	-3.32260	-0.71010	2.64920
C	-2.55740	-0.46880	1.51280
C	-2.92480	-1.02040	0.27780
C	-4.07020	-1.83110	0.20600
C	-2.13600	-0.76170	-0.90690
C	-2.03610	-0.79330	-2.20020
H	-5.04980	-1.71430	3.45910
H	-5.70800	-2.71110	1.28160
H	-3.03020	-0.27300	3.59980
H	-1.66290	0.14650	1.55840
H	-4.35500	-2.26350	-0.74900
H	-2.54810	-1.00320	-3.12620
Si	2.34860	-0.96990	0.27070
C	2.43340	-2.52890	-0.79760
C	2.48250	-3.85580	-0.03580
C	4.07680	-0.42880	0.84050
C	5.01910	-1.55050	1.28630
C	1.17280	-1.17200	1.73700
C	1.75960	-1.86460	2.96950
H	1.54870	-2.50890	-1.44730
H	3.29980	-2.43940	-1.46780
H	2.52340	-4.70910	-0.72240
H	3.35640	-3.92340	0.62070
H	1.59250	-3.98550	0.58940
H	4.53640	0.12360	0.00880
H	3.95030	0.30500	1.64920
H	5.99390	-1.15730	1.59700
H	4.61110	-2.11540	2.13070
H	5.19940	-2.26290	0.47410
H	0.82560	-0.16570	2.01040
H	0.27620	-1.70170	1.39020
H	1.01810	-1.94130	3.77290
H	2.10160	-2.88040	2.74570
H	2.61710	-1.31240	3.36960
H	0.24770	0.21690	-2.91520

E9a

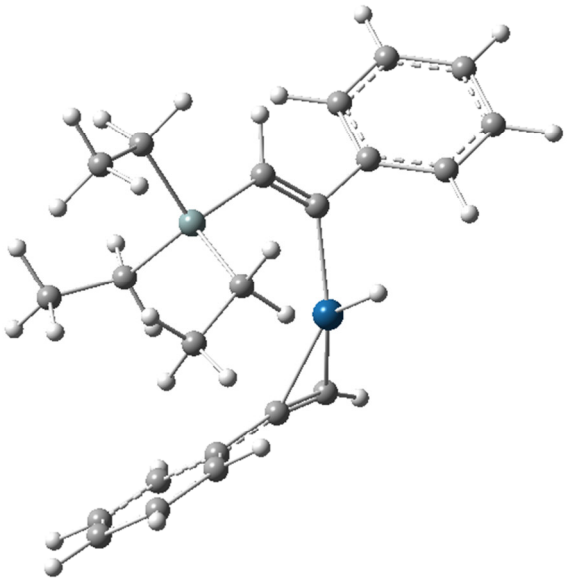
E = -1262.958027; (E+ZPE) = -1262.525571; H = -1262.496764; G = -1262.587962



C	-2.39960	4.27910	-0.33380
C	-2.51120	3.13620	-1.12630
C	-1.31440	4.41200	0.53180
C	-0.34900	3.41030	0.60630
C	-0.45180	2.25530	-0.18280
C	-1.55090	2.13190	-1.04730
C	0.58250	1.19780	-0.08780
C	1.88950	1.43800	-0.31710
H	-3.15280	5.05990	-0.39070
H	-3.34980	3.02510	-1.80840
H	-1.21990	5.29780	1.15420
H	0.49140	3.50680	1.28810
H	-1.64150	1.24400	-1.66730
H	2.12460	2.44080	-0.69390
Pt	-0.22500	-0.61960	0.24770
C	-6.00100	-0.92780	0.17630
C	-5.58080	-2.13030	-0.39440
C	-5.06050	-0.00240	0.62860
C	-3.70170	-0.27400	0.51380
C	-3.27580	-1.47920	-0.06030
C	-4.22430	-2.40910	-0.51500
C	-1.87220	-1.77430	-0.20550
C	-0.83360	-2.43030	-0.52340
H	-7.06180	-0.71300	0.26750
H	-6.31230	-2.85150	-0.74690
H	-5.38520	0.93460	1.07110
H	-2.95920	0.44050	0.85610
H	-3.88880	-3.34080	-0.96040
H	-0.27760	-3.27400	-0.89160
Si	3.31150	0.22480	-0.14860
C	3.27190	-0.58830	1.56760
C	4.61040	-1.12170	2.08500
C	3.16200	-1.09420	-1.50820
C	3.91070	-2.40600	-1.26540
C	4.89640	1.24340	-0.37590
C	6.14920	0.47130	-0.79610
H	2.87610	0.16000	2.26770
H	2.52470	-1.39310	1.55000
H	4.50560	-1.56880	3.08050
H	5.02710	-1.89030	1.42570
H	5.35540	-0.32250	2.16490
H	2.08830	-1.29790	-1.62360
H	3.48010	-0.64130	-2.45780
H	3.76160	-3.11510	-2.08850
H	4.98980	-2.24980	-1.16330
H	3.56540	-2.89510	-0.34760
H	4.67340	2.01220	-1.12920
H	5.08520	1.79330	0.55700
H	7.01240	1.13620	-0.91700
H	6.42630	-0.29080	-0.06050
H	5.99750	-0.04050	-1.75280
H	0.37780	-0.01570	1.55520

E9b

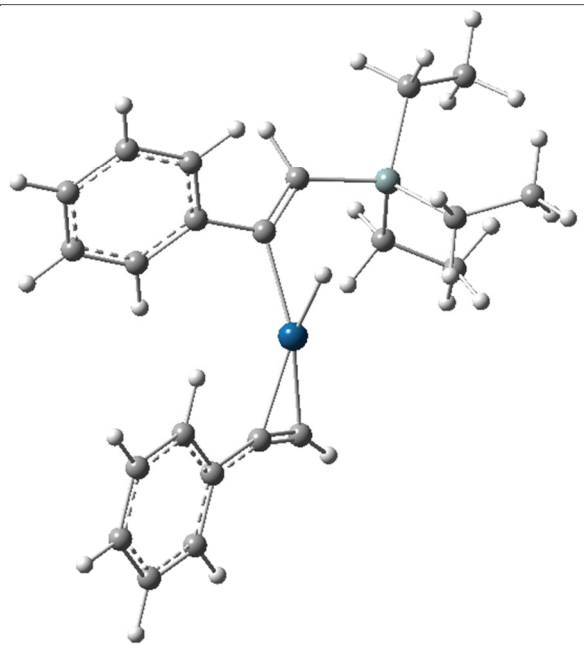
E = -1262.959726; (E+ZPE) = -1262.527410; H = -1262.498492; G = -1262.589371



C	-5.88350	-0.00460	0.58620
C	-5.28660	-0.38810	-0.61490
C	-5.10260	0.57400	1.58620
C	-3.73900	0.77210	1.38550
C	-3.12780	0.39880	0.17800
C	-3.92190	-0.19900	-0.81280
C	-1.67850	0.64290	-0.02000
C	-1.11010	1.83750	0.23900
H	-6.94680	-0.16160	0.74360
H	-5.88570	-0.84020	-1.40060
H	-5.55550	0.86680	2.52970
H	-3.12880	1.21080	2.17010
H	-3.46090	-0.50590	-1.74750
H	-1.79850	2.60710	0.61010
Pt	-0.70520	-1.07720	-0.40780
C	4.97780	-1.77090	0.41940
C	4.30400	-2.44310	1.43960
C	4.27660	-1.31110	-0.69500
C	2.90390	-1.51130	-0.78890
C	2.22590	-2.19440	0.22950
C	2.93390	-2.66130	1.34730
C	0.80320	-2.40210	0.15190
C	-0.31760	-2.97640	0.27580
H	6.04810	-1.60280	0.49490
H	4.84770	-2.79830	2.31000
H	4.79930	-0.78670	-1.48930
H	2.34280	-1.13910	-1.64050
H	2.40150	-3.18000	2.13850
H	-0.98320	-3.80220	0.45390
Si	0.68470	2.35750	0.07040
C	1.72720	1.41200	1.34330
C	3.09050	2.00690	1.70230
C	1.27410	2.02660	-1.70110
C	2.78390	2.06050	-1.94680
C	0.69880	4.21720	0.45440
C	1.89270	5.02120	-0.06470
H	1.11010	1.32970	2.24870
H	1.84810	0.38480	0.97800
H	3.61550	1.38680	2.43850
H	3.74340	2.09310	0.82780
H	2.98860	3.00920	2.13300
H	0.87730	1.04170	-1.98170
H	0.76380	2.74560	-2.35740
H	3.02610	1.84030	-2.99360
H	3.21780	3.03750	-1.71140
H	3.30150	1.32020	-1.32900
H	-0.22890	4.63570	0.03930
H	0.61140	4.33310	1.54440
H	1.82360	6.07760	0.22030
H	2.84340	4.64070	0.32320
H	1.94970	4.98400	-1.15800
H	-1.10030	-0.35930	-1.73520

TS-E10a

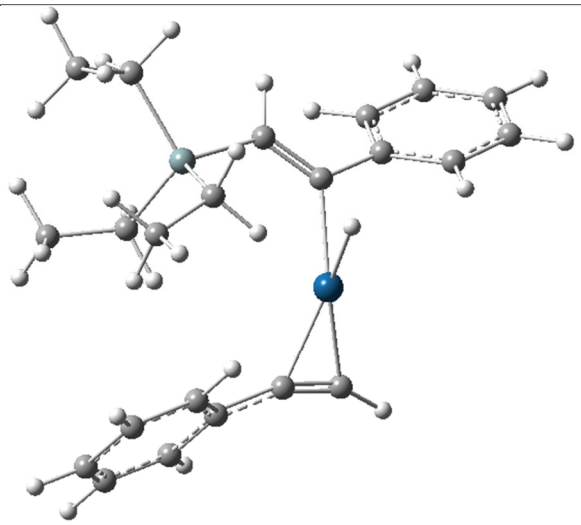
E = -1262.956035; (E+ZPE) = -1262.524292; H = -1262.495941; G = -1262.585644



C	-2.19520	4.46470	-0.32830
C	-2.42340	3.30100	-1.06330
C	-1.06340	4.55570	0.48060
C	-0.16710	3.49160	0.55340
C	-0.38650	2.31640	-0.17950
C	-1.53250	2.23450	-0.98420
C	0.59290	1.20260	-0.08900
C	1.91840	1.40590	-0.27880
H	-2.89570	5.29310	-0.38420
H	-3.30010	3.22150	-1.70040
H	-0.87900	5.45580	1.06090
H	0.70910	3.55640	1.19280
H	-1.71410	1.32990	-1.55770
H	2.18730	2.39860	-0.65660
Pt	-0.25830	-0.66080	0.01670
C	-6.00790	-0.87140	0.53980
C	-5.66370	-2.07590	-0.07620
C	-5.01360	0.04140	0.89090
C	-3.67790	-0.24520	0.63080
C	-3.32800	-1.45240	0.01150
C	-4.33100	-2.36880	-0.34240
C	-1.94950	-1.76330	-0.27720
C	-0.96290	-2.43970	-0.70740
H	-7.05040	-0.64580	0.74500
H	-6.43650	-2.78810	-0.35020
H	-5.27820	0.98010	1.36870
H	-2.89400	0.45810	0.89500
H	-4.05620	-3.30270	-0.82340
H	-0.48760	-3.30140	-1.14130
Si	3.31800	0.17340	-0.03650
C	3.14230	-0.64230	1.66940
C	4.43290	-1.20860	2.26780
C	3.24580	-1.13220	-1.41290
C	3.97480	-2.44870	-1.13630
C	4.91890	1.18400	-0.14820
C	6.19030	0.40510	-0.49390
H	2.72380	0.11420	2.34750
H	2.37860	-1.42870	1.60190
H	4.25490	-1.65370	3.25360
H	4.87110	-1.98650	1.63400
H	5.19010	-0.42740	2.39560
H	2.18050	-1.33330	-1.59280
H	3.61980	-0.67320	-2.33880
H	3.87350	-3.14820	-1.97450
H	5.04610	-2.29860	-0.96630
H	3.57020	-2.94560	-0.24760
H	4.75160	1.96130	-0.90700
H	5.05060	1.72330	0.80050
H	7.06420	1.06420	-0.55100
H	6.41280	-0.36670	0.25000
H	6.09740	-0.09540	-1.46400
H	0.42530	0.22640	1.15750

TS-E10b

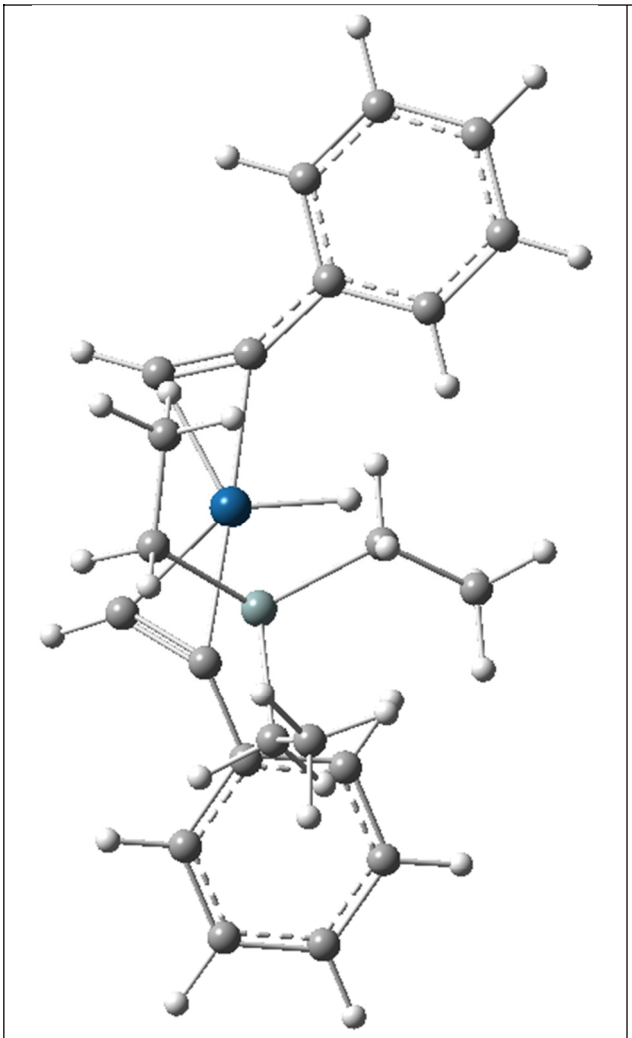
E = -1262.958016; (E+ZPE) = -1262.526679; H = -1262.498069; G = -1262.588516



C	-5.87000	0.00390	0.56320
C	-5.27340	-0.35040	-0.64650
C	-5.09070	0.56280	1.57600
C	-3.72840	0.77030	1.38020
C	-3.11910	0.42770	0.16330
C	-3.91000	-0.14890	-0.84190
C	-1.67090	0.68060	-0.03150
C	-1.09420	1.86570	0.26280
H	-6.93250	-0.16060	0.71800
H	-5.87120	-0.78740	-1.44150
H	-5.54410	0.83150	2.52630
H	-3.11870	1.18920	2.17570
H	-3.45050	-0.43050	-1.78560
H	-1.77290	2.61620	0.68440
Pt	-0.71600	-1.08850	-0.37210
C	4.96290	-1.79730	0.42880
C	4.27840	-2.52790	1.40030
C	4.27300	-1.27500	-0.66510
C	2.90200	-1.47190	-0.78610
C	2.21270	-2.21260	0.18330
C	2.90930	-2.74110	1.28020
C	0.79120	-2.42260	0.07280
C	-0.32020	-3.02780	0.13240
H	6.03210	-1.63290	0.52580
H	4.81260	-2.93230	2.25500
H	4.80390	-0.70600	-1.42260
H	2.34980	-1.05470	-1.62260
H	2.36880	-3.30450	2.03450
H	-0.95960	-3.88610	0.23840
Si	0.70280	2.37710	0.07780
C	1.74390	1.42360	1.34360
C	3.12070	1.99750	1.68440
C	1.26250	2.03760	-1.70160
C	2.76840	2.07910	-1.97010
C	0.72650	4.23630	0.46030
C	1.92310	5.03530	-0.06070
H	1.13540	1.35600	2.25600
H	1.84070	0.39250	0.98230
H	3.64250	1.37180	2.41800
H	3.76590	2.06750	0.80270
H	3.04110	3.00350	2.11100
H	0.86900	1.04860	-1.97370
H	0.73900	2.75180	-2.35250
H	2.99570	1.85510	-3.01930
H	3.19930	3.05990	-1.74600
H	3.29970	1.34550	-1.35640
H	-0.20020	4.66020	0.04880
H	0.64340	4.35070	1.55080
H	1.86180	6.09030	0.23100
H	2.87340	4.64670	0.32020
H	1.97400	5.00440	-1.15440
H	-1.17780	0.01000	-1.43640

TS-F6a

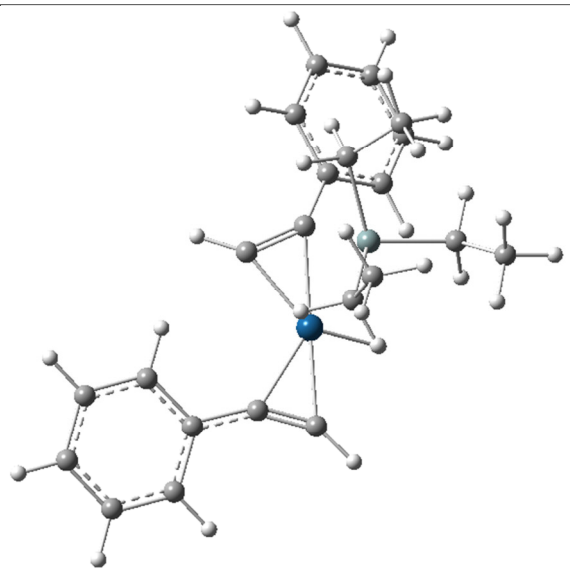
E = -1262.921569; (E+ZPE) = -1262.489912; H = -1262.462015; G = -1262.549047



C	-5.22040	-1.53610	1.68420
C	-3.97340	-1.40730	2.29530
C	-5.33820	-1.33510	0.30850
C	-4.21920	-1.00420	-0.45050
C	-2.96680	-0.87060	0.15990
C	-2.85400	-1.07190	1.53850
C	-1.77860	-0.52080	-0.63770
C	-1.27740	-1.04880	-1.75450
H	-6.09490	-1.79230	2.27530
H	-3.87120	-1.56750	3.36500
H	-6.30620	-1.43390	-0.17500
H	-4.31140	-0.83810	-1.52050
H	-1.87820	-0.97160	2.00650
H	-1.69540	-1.66210	-2.54660
Pt	0.34090	-0.77820	-0.56420
C	5.75750	0.15570	1.82950
C	5.93860	-0.30540	0.52400
C	4.46840	0.28630	2.34360
C	3.36500	-0.03840	1.56010
C	3.53600	-0.50320	0.25070
C	4.83930	-0.63290	-0.26040
C	2.41740	-0.83800	-0.60130
C	1.98310	-1.28420	-1.71710
H	6.61790	0.41130	2.44120
H	6.94040	-0.41020	0.11730
H	4.32020	0.64370	3.35860
H	2.35770	0.05940	1.95340
H	4.97670	-0.99130	-1.27640
H	2.12250	-1.66140	-2.71440
Si	-1.03090	1.43760	-0.34100
C	-0.45890	2.17260	-1.99420
C	1.03500	2.47130	-2.11760
C	-2.77040	2.14710	-0.00040
C	-2.75980	3.65690	0.24520
C	0.05100	2.11080	1.06870
C	-0.33090	1.68630	2.48300
H	-0.78050	1.50170	-2.79940
H	-1.03250	3.10140	-2.12470
H	1.27410	2.89970	-3.09760
H	1.36580	3.18800	-1.35830
H	1.63460	1.56430	-1.99480
H	-3.40360	1.90430	-0.86370
H	-3.22520	1.63480	0.85400
H	-3.78090	4.04740	0.32540
H	-2.24290	3.91040	1.17660
H	-2.26650	4.20860	-0.56330
H	1.10040	1.87450	0.86530
H	-0.03950	3.20370	0.97200
H	0.27780	2.20160	3.23480
H	-1.38210	1.90280	2.70520
H	-0.18160	0.60970	2.62310
H	0.68910	-0.70770	0.99290

TS-F6b

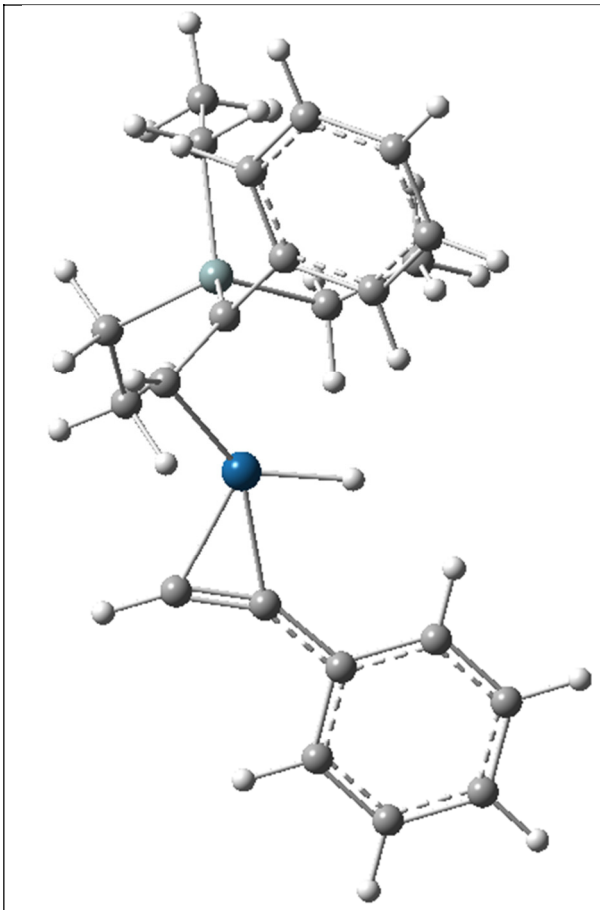
E = -1262.914926; (E+ZPE) = -1262.482932; H = -1262.454923; G = -1262.542999



C	5.97450	-0.86000	1.54940
C	4.69470	-0.97580	2.09010
C	6.13020	-0.48170	0.21440
C	5.01570	-0.21910	-0.57340
C	3.72160	-0.33650	-0.03580
C	3.57540	-0.72140	1.30310
C	2.58300	-0.04060	-0.87070
C	2.07290	0.45190	-1.93110
H	6.84720	-1.06460	2.16290
H	4.56710	-1.26870	3.12840
H	7.12470	-0.39080	-0.21330
H	5.13390	0.07580	-1.61200
H	2.57320	-0.80830	1.70880
H	2.17750	0.93160	-2.88720
Pt	0.49790	-0.26270	-0.79860
C	-4.87910	-2.87410	0.13950
C	-4.21160	-2.81070	1.36360
C	-4.31160	-2.28100	-0.98750
C	-3.09010	-1.61930	-0.89120
C	-2.41650	-1.55130	0.33260
C	-2.98890	-2.15440	1.46120
C	-1.11720	-0.87180	0.42570
C	0.05450	-1.17960	0.97120
H	-5.83460	-3.38510	0.06530
H	-4.64560	-3.27420	2.24530
H	-4.82050	-2.33360	-1.94580
H	-2.63590	-1.16450	-1.76710
H	-2.46810	-2.10400	2.41390
H	0.37660	-1.90830	1.70880
Si	-1.31340	1.27500	0.28310
C	-2.50990	1.71760	-1.12180
C	-2.66810	3.22280	-1.35830
C	-2.26000	1.31180	1.94410
C	-3.31750	2.41200	2.06710
C	0.11640	2.52880	0.47750
C	-0.22760	3.81480	1.23580
H	-2.15460	1.24030	-2.03990
H	-3.48390	1.26510	-0.89590
H	-3.35590	3.41730	-2.18910
H	-3.06620	3.74060	-0.48040
H	-1.71080	3.69070	-1.61160
H	-2.74510	0.34590	2.10990
H	-1.50210	1.41120	2.73390
H	-3.80830	2.37200	3.04670
H	-2.89780	3.41570	1.95480
H	-4.10000	2.29470	1.30980
H	0.94010	2.01640	0.98820
H	0.49620	2.76330	-0.52370
H	0.65200	4.46570	1.30020
H	-1.02020	4.38760	0.74490
H	-0.55240	3.60730	2.26020
H	-0.17990	0.00890	-2.21910

F7a

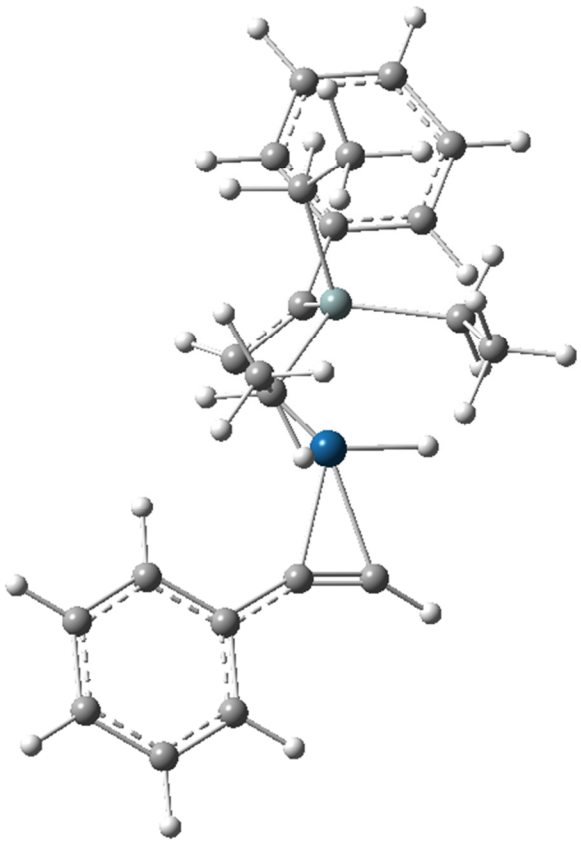
E = -1262.926253; (E+ZPE) = -1262.494333; H = -1262.465679; G = -1262.556173



C	-4.22470	-3.40910	0.43150
C	-2.86130	-3.44290	0.71910
C	-4.76040	-2.30420	-0.22990
C	-3.94180	-1.23530	-0.58750
C	-2.57350	-1.25790	-0.29230
C	-2.04200	-2.37710	0.35230
C	-1.69260	-0.10770	-0.68730
C	-1.08180	-0.17450	-1.92760
H	-4.86430	-4.24060	0.71320
H	-2.43070	-4.30400	1.22290
H	-5.82000	-2.27270	-0.46820
H	-4.36500	-0.37710	-1.10200
H	-0.97400	-2.40470	0.55870
H	-1.42960	-0.72310	-2.80360
Pt	0.54210	-0.15250	-0.88880
C	5.95080	-0.94890	1.69190
C	6.11540	-0.20020	0.52510
C	4.67530	-1.36220	2.07360
C	3.56950	-1.03150	1.29620
C	3.72350	-0.28000	0.12580
C	5.01310	0.13240	-0.25280
C	2.60400	0.10140	-0.70760
C	2.18180	0.73620	-1.73550
H	6.81320	-1.20860	2.29900
H	7.10640	0.12460	0.22120
H	4.54000	-1.94480	2.98020
H	2.57350	-1.35080	1.58870
H	5.13820	0.71460	-1.16110
H	2.32660	1.37690	-2.58830
Si	-1.78340	1.50340	0.36310
C	-1.10760	2.97120	-0.63190
C	0.19440	3.58720	-0.11670
C	-3.62170	1.81430	0.71530
C	-3.84930	3.00600	1.64940
C	-0.89920	1.34070	2.02590
C	-1.40830	0.21350	2.92420
H	-0.98030	2.64510	-1.67120
H	-1.89750	3.73500	-0.64660
H	0.51090	4.43110	-0.74060
H	0.08770	3.96030	0.90760
H	1.00750	2.85430	-0.11550
H	-4.13270	1.98450	-0.24250
H	-4.07400	0.91180	1.14360
H	-4.91680	3.21150	1.78790
H	-3.42220	2.82300	2.64140
H	-3.39040	3.92320	1.26200
H	0.17500	1.22360	1.84070
H	-1.01490	2.30810	2.53560
H	-0.90500	0.21740	3.89790
H	-2.48500	0.29700	3.11130
H	-1.23650	-0.76590	2.46790
H	0.95900	-0.92920	0.43680

F7b

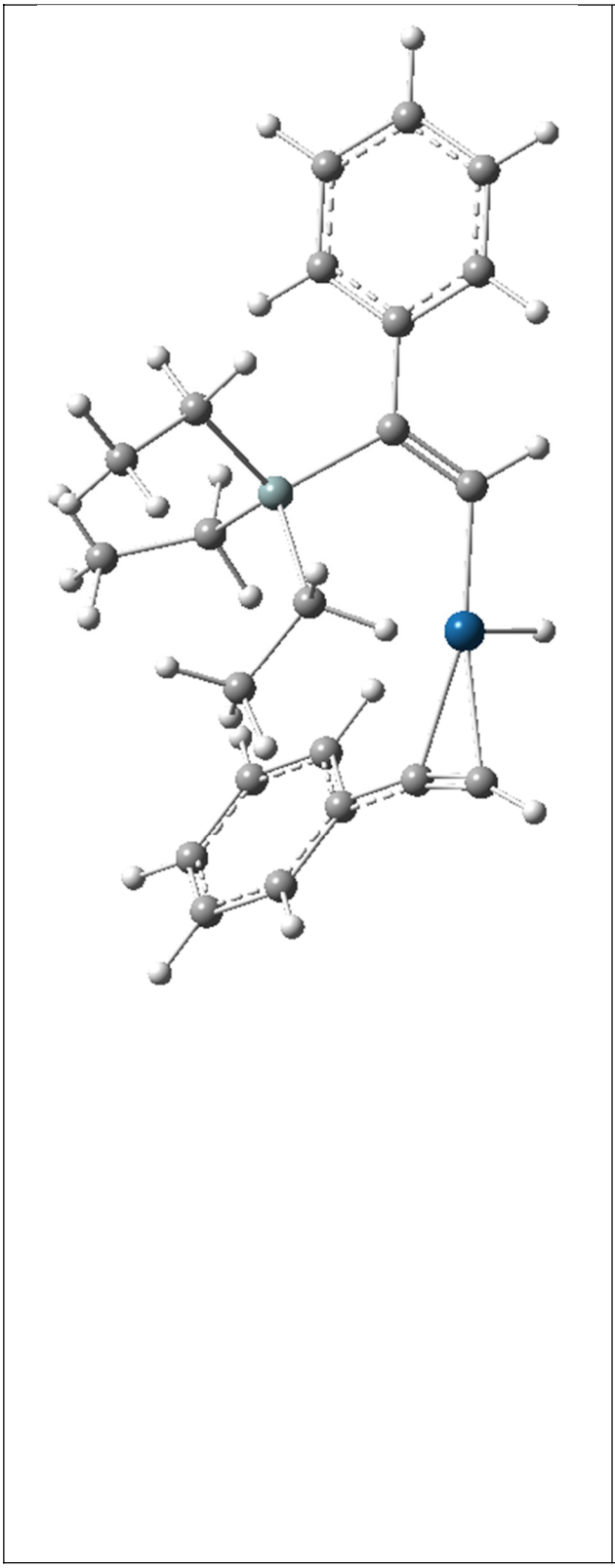
E = -1262.927352; (E+ZPE) = -1262.495039; H = -1262.466477; G = -1262.556023



C	-5.74550	0.68900	-1.45080
C	-4.48660	0.62600	-2.04730
C	-5.92790	0.19420	-0.15820
C	-4.85910	-0.36220	0.53450
C	-3.58790	-0.42680	-0.06150
C	-3.41170	0.07600	-1.35670
C	-2.49530	-1.01150	0.67760
C	-2.00860	-1.63900	1.67860
H	-6.58240	1.12470	-1.98910
H	-4.34030	1.01140	-3.05220
H	-6.90670	0.24200	0.31040
H	-4.99630	-0.74970	1.53970
H	-2.42070	0.02710	-1.79870
H	-2.13620	-2.16990	2.60420
Pt	-0.45210	-1.14660	0.39980
C	5.33740	-1.82260	-0.72310
C	4.73090	-1.36160	-1.89100
C	4.63030	-1.78870	0.47850
C	3.32880	-1.29260	0.51250
C	2.71480	-0.82620	-0.65290
C	3.42900	-0.86610	-1.85590
C	1.33110	-0.25360	-0.61380
C	0.31290	-0.85310	-1.34120
H	6.35200	-2.20960	-0.74990
H	5.27250	-1.38680	-2.83270
H	5.09100	-2.15400	1.39230
H	2.76940	-1.28230	1.44500
H	2.96100	-0.49860	-2.76600
H	0.41360	-1.49190	-2.22010
Si	1.22890	1.54460	0.05690
C	1.64260	1.55040	1.90640
C	1.16920	2.78860	2.67270
C	2.55170	2.50190	-0.91350
C	3.06000	3.78960	-0.25950
C	-0.48740	2.25630	-0.30310
C	-0.56360	3.78340	-0.38310
H	1.18750	0.65360	2.34380
H	2.72850	1.42560	2.01610
H	1.43870	2.72780	3.73340
H	1.60750	3.71100	2.27830
H	0.08030	2.89470	2.61960
H	3.39760	1.82190	-1.07580
H	2.14630	2.71650	-1.91260
H	3.82170	4.27750	-0.87870
H	2.25760	4.51650	-0.09740
H	3.51730	3.58490	0.71450
H	-0.81920	1.82160	-1.25460
H	-1.19350	1.87750	0.44650
H	-1.58390	4.11480	-0.60760
H	-0.26640	4.26090	0.55620
H	0.08760	4.17760	-1.17060
H	0.18190	-1.74370	1.73050

F7c

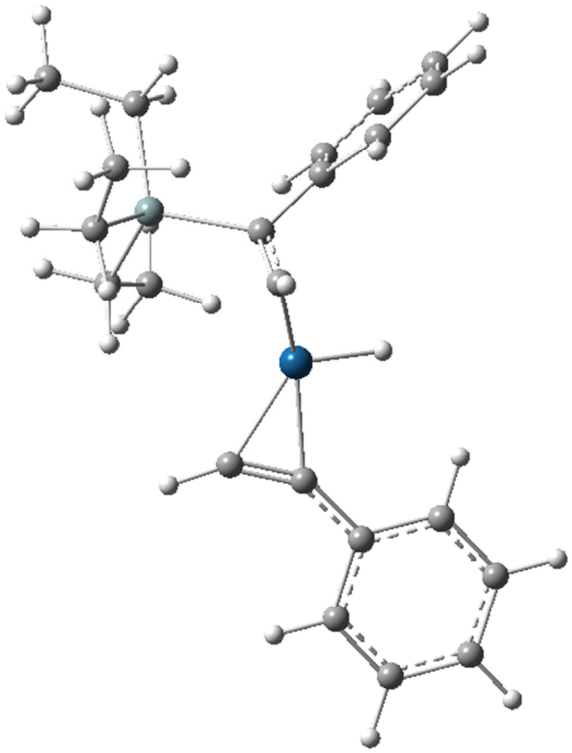
E = -1262.957243; (E+ZPE) = -1262.524578; H = -1262.495988; G = -1262.584989



C	6.11630	-0.11990	-1.34490
C	5.65090	-1.21390	-0.61530
C	5.23440	0.91050	-1.66950
C	3.90340	0.84680	-1.26580
C	3.41610	-0.25100	-0.53980
C	4.31810	-1.27730	-0.21750
C	1.99640	-0.32710	-0.12420
C	1.28800	-1.47880	-0.26100
H	7.15670	-0.06850	-1.65290
H	6.33120	-2.01810	-0.34750
H	5.58360	1.76680	-2.24030
H	3.22470	1.65180	-1.53660
H	3.96500	-2.12270	0.36700
H	1.80430	-2.33110	-0.71460
Pt	-0.65200	-1.57730	0.23540
C	-4.75390	1.81630	-1.96620
C	-5.17240	1.55140	-0.66150
C	-3.68860	1.10180	-2.51410
C	-3.03740	0.12990	-1.76260
C	-3.45530	-0.14070	-0.45160
C	-4.52990	0.57860	0.09610
C	-2.78630	-1.13180	0.34500
C	-2.52860	-2.00790	1.19820
H	-5.25630	2.57940	-2.55330
H	-6.00030	2.10750	-0.23140
H	-3.35950	1.30620	-3.52860
H	-2.19870	-0.42470	-2.17230
H	-4.84480	0.37280	1.11450
H	-2.69450	-2.76590	1.94020
Si	1.10510	1.19180	0.56550
C	-0.04620	0.59070	1.96960
C	-1.29320	1.42980	2.23690
C	2.35630	2.39920	1.32380
C	1.80670	3.35280	2.38820
C	0.10990	2.01900	-0.81900
C	-0.32730	3.46730	-0.59520
H	-0.34120	-0.48700	1.89830
H	0.58330	0.54060	2.87060
H	-1.90430	1.00060	3.03850
H	-1.02330	2.44710	2.53780
H	-1.92440	1.50690	1.34670
H	3.16950	1.79600	1.75000
H	2.81950	2.97640	0.51310
H	2.59210	4.00890	2.78040
H	1.01400	3.99600	1.99180
H	1.38800	2.80770	3.24130
H	0.72140	1.95260	-1.72950
H	-0.76390	1.38340	-1.01410
H	-0.88900	3.85130	-1.45470
H	-0.97210	3.56880	0.28340
H	0.53410	4.12790	-0.44660
H	-0.79300	-2.66360	-0.82440

TS-F8a

E = -1262.918078; (E+ZPE) = -1262.487554; H = -1262.459460; G = -1262.548279



C	-2.59760	-4.27230	0.48620
C	-2.30280	-3.36120	1.50040
C	-2.53140	-3.86290	-0.84520
C	-2.17160	-2.55490	-1.15820
C	-1.87780	-1.63030	-0.14740
C	-1.95260	-2.05160	1.18580
C	-1.52300	-0.22520	-0.49040
C	-0.78960	0.07970	-1.63400
H	-2.87530	-5.29330	0.73150
H	-2.34500	-3.67170	2.54080
H	-2.75900	-4.56450	-1.64300
H	-2.11900	-2.24080	-2.19740
H	-1.71110	-1.35190	1.98030
H	-0.85950	0.20570	-2.70810
Pt	0.70470	0.17600	-0.52070
C	6.56130	-0.64400	0.54700
C	6.29680	0.72580	0.59810
C	5.52440	-1.54150	0.29390
C	4.22900	-1.07530	0.09190
C	3.95330	0.29620	0.14430
C	5.00350	1.19460	0.39820
C	2.61410	0.80710	-0.05780
C	1.82470	1.82870	-0.05470
H	7.57230	-1.00920	0.70380
H	7.10110	1.42890	0.79500
H	5.72550	-2.60820	0.25300
H	3.41310	-1.76420	-0.10640
H	4.79280	2.25950	0.43740
H	1.70250	2.89110	0.09290
Si	-2.53750	1.20630	0.28970
C	-2.88890	2.44060	-1.09800
C	-3.80610	1.90650	-2.19960
C	-4.16640	0.52000	0.96130
C	-5.13630	1.61100	1.42260
C	-1.56980	2.09500	1.64560
C	-1.08430	1.22960	2.80730
H	-3.32730	3.33960	-0.64330
H	-1.92690	2.75950	-1.52110
H	-3.96400	2.64620	-2.99240
H	-3.39050	1.00780	-2.66940
H	-4.79130	1.63510	-1.80460
H	-4.62790	-0.09700	0.17870
H	-3.95370	-0.17030	1.78650
H	-6.07300	1.18490	1.79920
H	-4.70730	2.21600	2.22930
H	-5.39510	2.29460	0.60620
H	-0.71620	2.59200	1.16790
H	-2.22090	2.90020	2.01530
H	-0.57970	1.82880	3.57340
H	-1.91300	0.70610	3.29850
H	-0.36780	0.47660	2.46090
H	1.22140	-1.30740	-0.19050

TS-F8b

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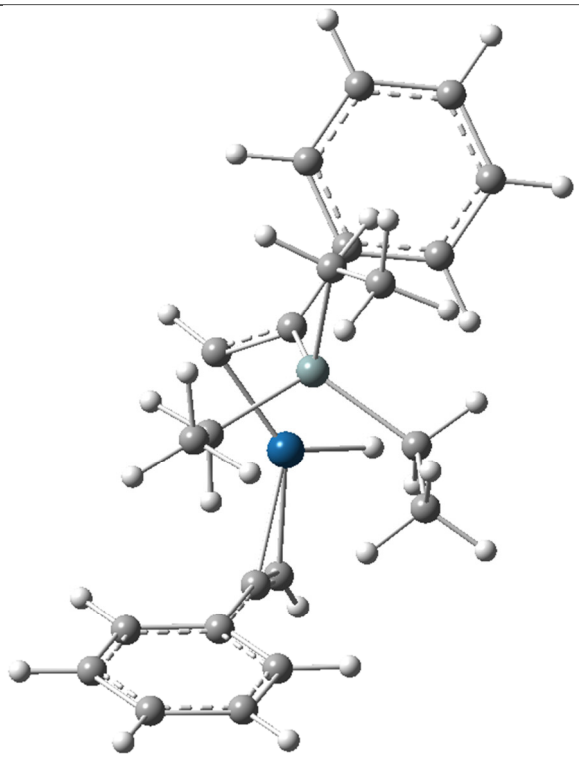
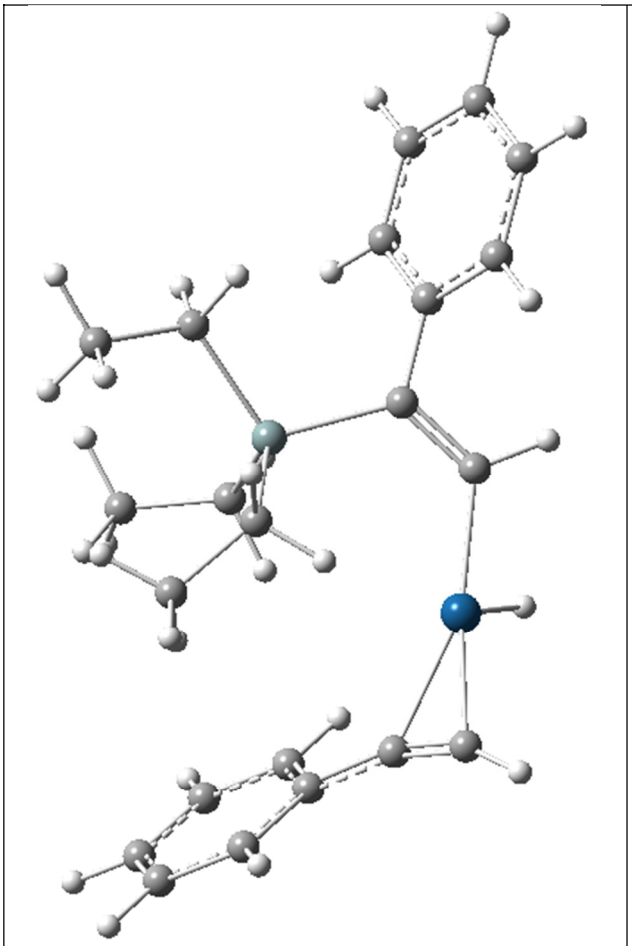


C	-5.06440	1.22860	-0.34740
C	-4.68700	0.34510	-1.35990
C	-4.48110	1.12680	0.91420
C	-3.51870	0.15390	1.16530
C	-3.13910	-0.73540	0.15030
C	-3.73000	-0.63230	-1.11750
C	-2.11800	-1.72000	0.40470
C	-1.63550	-2.86500	0.68340
H	-5.80730	1.99600	-0.54370
H	-5.13690	0.42290	-2.34540
H	-4.76870	1.81350	1.70510
H	-3.04640	0.08180	2.14010
H	-3.41340	-1.30720	-1.90650
H	-1.76760	-3.82850	1.14310
Pt	-0.06380	-1.68460	0.03280
C	5.58150	-0.21880	0.21270
C	5.12820	-0.04740	-1.09390
C	4.65740	-0.35280	1.24880
C	3.29210	-0.30940	0.98040
C	2.82820	-0.13610	-0.32700
C	3.76120	-0.00520	-1.36110
C	1.36250	-0.02470	-0.61570
C	0.74160	-0.91050	-1.48910
H	6.64680	-0.25170	0.42210
H	5.84010	0.05510	-1.90850
H	5.00150	-0.49590	2.26960
H	2.57050	-0.43530	1.78400
H	3.40910	0.14170	-2.37930
H	1.09120	-1.47760	-2.35090
Si	0.55800	1.63660	-0.10400
C	0.14460	1.58720	1.74590
C	-0.88060	2.62220	2.21660
C	1.85450	2.97470	-0.46440
C	1.67270	4.30440	0.27210
C	-0.98700	1.89350	-1.16250
C	-1.42780	3.34630	-1.35410
H	-0.22430	0.57520	1.96030
H	1.07980	1.69110	2.31280
H	-1.09400	2.51610	3.28690
H	-0.53330	3.64770	2.05550
H	-1.82950	2.51080	1.68150
H	2.83810	2.55560	-0.21800
H	1.87060	3.14180	-1.55090
H	2.45500	5.02200	-0.00090
H	0.70890	4.77390	0.04990
H	1.72670	4.16610	1.35740
H	-0.78560	1.43120	-2.13830
H	-1.80750	1.31120	-0.73170
H	-2.32750	3.40610	-1.97750
H	-1.66370	3.83130	-0.40100
H	-0.65130	3.94550	-1.84200
H	0.65030	-2.50320	1.21680

TS-F8c

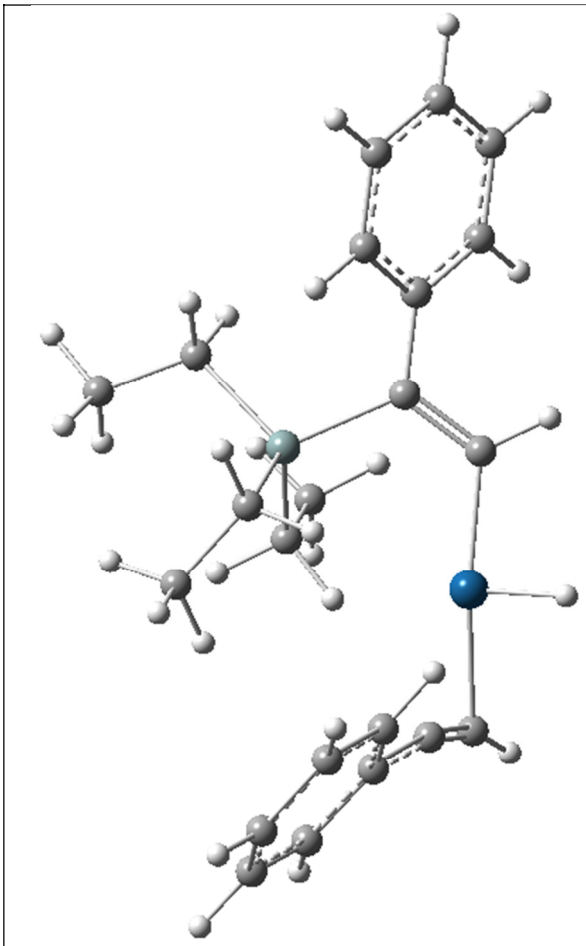
E = -1262.954395; (E+ZPE) = -1262.522046; H = -1262.493980; G = -1262.581258



C	6.25060	-0.27190	-0.61390
C	5.64870	-1.14920	0.28730
C	5.45550	0.61450	-1.34050
C	4.07470	0.62530	-1.16260
C	3.45290	-0.25510	-0.26460
C	4.26600	-1.13990	0.45910
C	1.97670	-0.26120	-0.09050
C	1.31310	-1.43650	-0.23920
H	7.32870	-0.27670	-0.74730
H	6.25820	-1.84040	0.86360
H	5.91220	1.29900	-2.05040
H	3.46430	1.31290	-1.74280
H	3.80040	-1.81600	1.17150
H	1.92570	-2.29950	-0.52310
Pt	-0.65750	-1.73640	0.01840
C	-4.97130	1.96820	-1.06440
C	-5.19800	1.46440	0.21720
C	-4.01250	1.37670	-1.88670
C	-3.27250	0.29230	-1.42890
C	-3.49300	-0.21350	-0.14020
C	-4.46650	0.37710	0.68100
C	-2.71580	-1.31450	0.36070
C	-2.39310	-2.34310	1.01350
H	-5.54140	2.82100	-1.42090
H	-5.94440	1.92330	0.85890
H	-3.83570	1.76520	-2.88520
H	-2.51820	-0.17260	-2.05610
H	-4.62870	-0.01300	1.68100
H	-2.55360	-3.22870	1.60160
Si	1.09210	1.37190	0.31610
C	-0.02120	1.09760	1.83600
C	-1.24770	2.00360	1.95140
C	2.37780	2.69630	0.76220
C	1.85210	3.85600	1.61300
C	0.09900	1.89500	-1.21070
C	-0.38260	3.34500	-1.27250
H	-0.34630	0.04750	1.85030
H	0.61590	1.20000	2.72600
H	-1.83980	1.76490	2.84270
H	-0.96690	3.05960	2.01980
H	-1.90720	1.89360	1.08490
H	3.20000	2.19450	1.28990
H	2.82350	3.08640	-0.16200
H	2.64590	4.57690	1.84050
H	1.04980	4.40440	1.10830
H	1.45230	3.50310	2.56970
H	0.73320	1.67630	-2.08110
H	-0.75140	1.20640	-1.29210
H	-0.93700	3.54360	-2.19760
H	-1.04670	3.59140	-0.43840
H	0.45770	4.04730	-1.24060
H	-0.40850	-2.40230	-1.32910

F9a

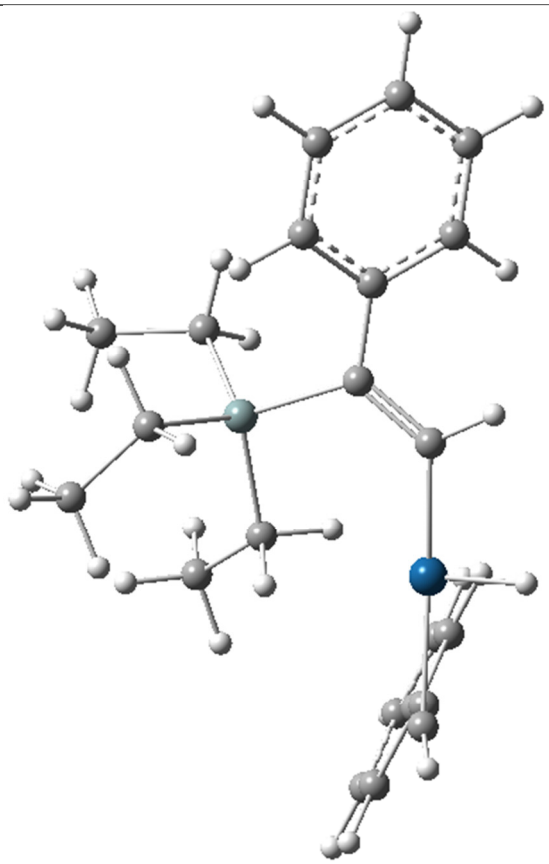
E = -1262.958752; (E+ZPE) = -1262.526566; H = -1262.497658; G = -1262.587767



C	-6.01880	0.03200	-1.55610
C	-5.58620	-1.07810	-0.83090
C	-5.11600	1.05520	-1.84470
C	-3.79700	0.96900	-1.40750
C	-3.34330	-0.14480	-0.68410
C	-4.26470	-1.16450	-0.40020
C	-1.93500	-0.23910	-0.23510
C	-1.22250	-1.38380	-0.40360
H	-7.05040	0.10110	-1.88960
H	-6.28330	-1.87720	-0.59250
H	-5.43980	1.92300	-2.41320
H	-3.09830	1.76660	-1.64990
H	-3.93590	-2.02310	0.17950
H	-1.73420	-2.21150	-0.90610
Pt	0.71500	-1.53690	0.10170
C	4.75850	2.09760	-1.70600
C	5.16590	1.71500	-0.42750
C	3.72620	1.40950	-2.34350
C	3.09730	0.34570	-1.70740
C	3.50620	-0.04530	-0.42390
C	4.54640	0.64870	0.21500
C	2.85530	-1.13130	0.25390
C	2.58580	-2.08610	1.01500
H	5.24350	2.93270	-2.20300
H	5.96750	2.25100	0.07200
H	3.40510	1.70690	-3.33740
H	2.28290	-0.19000	-2.18540
H	4.85410	0.34900	1.21210
H	2.74920	-2.92490	1.66510
Si	-1.09530	1.23150	0.60450
C	-0.02970	2.19650	-0.63140
C	1.13910	2.98650	-0.03770
C	-2.39960	2.33210	1.42470
C	-1.84700	3.42230	2.34550
C	0.00690	0.55250	1.99950
C	-0.75270	-0.19520	3.09410
H	0.35270	1.46460	-1.35490
H	-0.69070	2.86490	-1.20110
H	1.69080	3.52860	-0.81370
H	0.80600	3.72140	0.70300
H	1.85650	2.32250	0.45570
H	-3.01790	2.78400	0.63920
H	-3.07990	1.67410	1.98270
H	-2.65180	3.99780	2.81700
H	-1.23440	3.00290	3.15190
H	-1.21930	4.13310	1.79740
H	0.85450	-0.07050	1.63600
H	0.55070	1.40840	2.42520
H	-0.07810	-0.58440	3.86450
H	-1.47160	0.46690	3.58860
H	-1.31270	-1.03930	2.67980
H	0.80110	-2.60830	-0.97180

F9b

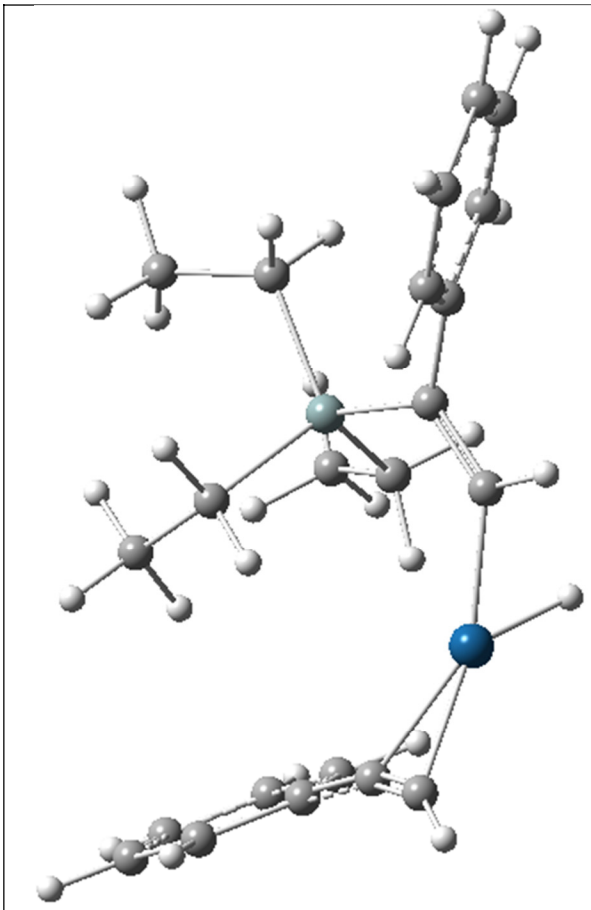
E = -1262.955552; (E+ZPE) = -1262.522472; H = -1262.493786; G = -1262.583822



C	5.10190	1.06710	2.41150
C	3.95260	0.33470	2.70780
C	5.55570	1.14880	1.09400
C	4.86410	0.50590	0.07410
C	3.70460	-0.23100	0.36810
C	3.25400	-0.31160	1.69360
C	2.97990	-0.86470	-0.69690
C	2.64700	-1.32190	-1.81030
H	5.64390	1.57350	3.20480
H	3.59810	0.26750	3.73210
H	6.45010	1.71900	0.86060
H	5.20680	0.57210	-0.95400
H	2.35660	-0.88420	1.90930
H	2.74010	-1.75210	-2.78920
Pt	0.82260	-1.28830	-0.66470
C	-5.98100	-1.21760	1.41880
C	-4.88970	-1.87950	1.98090
C	-5.76510	-0.28860	0.40170
C	-4.47300	-0.02510	-0.04610
C	-3.36380	-0.69210	0.49820
C	-3.59930	-1.61710	1.52860
C	-1.98450	-0.42170	0.02200
C	-1.11580	-1.45500	-0.15630
H	-6.98770	-1.41880	1.77380
H	-5.04270	-2.59630	2.78350
H	-6.60620	0.23290	-0.04740
H	-4.32530	0.69100	-0.84920
H	-2.75170	-2.11740	1.98890
H	-1.53450	-2.45220	0.01360
Si	-1.46770	1.37640	-0.26360
C	-2.22650	2.07300	-1.86190
C	-1.40130	3.15980	-2.55660
C	-1.96830	2.41470	1.23510
C	-1.95180	3.93110	1.02760
C	0.41830	1.30170	-0.44650
C	1.28130	2.54070	-0.20800
H	-2.37890	1.22980	-2.54830
H	-3.22770	2.46190	-1.63260
H	-1.89880	3.51940	-3.46450
H	-1.23950	4.02730	-1.90820
H	-0.41620	2.78490	-2.85430
H	-2.97500	2.09070	1.53100
H	-1.31140	2.13490	2.07040
H	-2.26050	4.46450	1.93380
H	-0.95550	4.29740	0.75790
H	-2.63620	4.23050	0.22620
H	0.72920	0.55180	0.32280
H	0.62000	0.91090	-1.46040
H	2.34670	2.31150	-0.31570
H	1.03650	3.33790	-0.91590
H	1.13020	2.93220	0.80270
H	0.83560	-2.81330	-0.70760

F9c

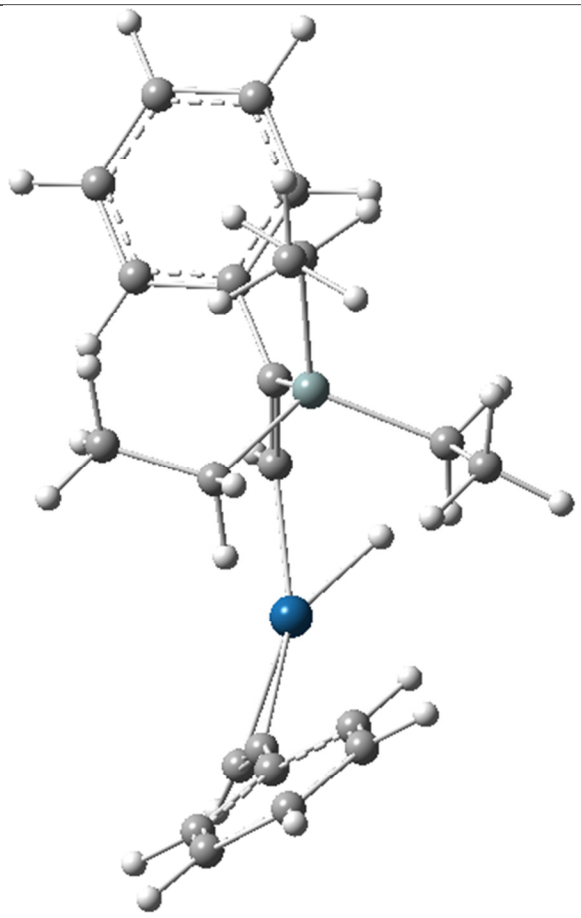
E = -1262.956185; (E+ZPE) = -1262.523411; H = -1262.494788; G = -1262.583347



C	6.19140	-0.37980	0.52310
C	5.31070	-1.02520	1.38930
C	5.68360	0.33030	-0.56550
C	4.30980	0.39720	-0.78110
C	3.41040	-0.25020	0.07910
C	3.93570	-0.95890	1.16920
C	1.94200	-0.19550	-0.15440
C	1.29120	-1.36980	-0.30710
H	7.26300	-0.42720	0.69470
H	5.69340	-1.57790	2.24340
H	6.36100	0.83310	-1.25070
H	3.92390	0.94730	-1.63540
H	3.24900	-1.45100	1.85320
H	1.89570	-2.28530	-0.34620
Pt	-0.65590	-1.80780	-0.31450
C	-4.93120	2.04900	0.18840
C	-4.84520	1.34360	1.38890
C	-4.24310	1.59720	-0.93800
C	-3.46280	0.44930	-0.86420
C	-3.37410	-0.26170	0.34050
C	-4.07320	0.19000	1.46940
C	-2.57080	-1.45380	0.42480
C	-2.22350	-2.63060	0.73680
H	-5.53320	2.95110	0.13110
H	-5.37900	1.69550	2.26660
H	-4.30900	2.14360	-1.87410
H	-2.91880	0.08940	-1.73160
H	-3.99610	-0.36050	2.40180
H	-2.37860	-3.62380	1.11950
Si	1.03760	1.47530	-0.10570
C	-0.04000	1.47130	1.45870
C	-1.19820	2.46950	1.51270
C	2.31210	2.87830	0.01530
C	1.79990	4.19160	0.61340
C	0.02580	1.65690	-1.69760
C	-0.52160	3.05020	-2.01210
H	-0.42920	0.45180	1.57780
H	0.63860	1.62760	2.30990
H	-1.74110	2.40070	2.46250
H	-0.85650	3.50380	1.40610
H	-1.92310	2.27870	0.71600
H	3.15550	2.51240	0.61460
H	2.72470	3.06110	-0.98670
H	2.58870	4.95250	0.63910
H	0.96360	4.60890	0.04280
H	1.45290	4.05030	1.64250
H	0.67850	1.31960	-2.51500
H	-0.79030	0.92590	-1.65800
H	-1.07970	3.05760	-2.95620
H	-1.19880	3.40900	-1.23060
H	0.28510	3.78510	-2.10870
H	-0.07860	-1.82130	-1.75910

TS-F10a

E = -1262.957723; (E+ZPE) = -1262.526646; H = -1262.497951; G = -1262.588810



C	-6.07180	-0.69980	0.77680
C	-5.08400	-1.28850	1.56450
C	-5.70070	0.05130	-0.33890
C	-4.35600	0.21460	-0.65930
C	-3.35000	-0.37690	0.11960
C	-3.73840	-1.12660	1.23950
C	-1.91640	-0.22340	-0.23630
C	-1.17690	-1.35020	-0.36680
H	-7.12100	-0.82200	1.03050
H	-5.36020	-1.87070	2.43970
H	-6.46210	0.51040	-0.96390
H	-4.07770	0.79320	-1.53600
H	-2.96920	-1.57180	1.86530
H	-1.70010	-2.31370	-0.32150
Pt	0.80910	-1.68650	-0.43350
C	4.88850	2.25440	0.74240
C	5.04290	1.20820	1.65270
C	4.02630	2.11140	-0.34460
C	3.31400	0.93080	-0.52040
C	3.47080	-0.12470	0.38780
C	4.34130	0.02020	1.47870
C	2.74070	-1.35580	0.21940
C	2.50100	-2.59900	0.26580
H	5.43850	3.18040	0.88180
H	5.71150	1.31850	2.50140
H	3.90440	2.92420	-1.05440
H	2.63020	0.81170	-1.35480
H	4.45310	-0.79680	2.18490
H	2.74420	-3.63730	0.40510
Si	-1.13480	1.50660	-0.32230
C	-0.26270	1.70070	-1.99170
C	0.54800	2.98510	-2.17690
C	-2.46950	2.83490	-0.08680
C	-1.93700	4.20090	0.35700
C	0.10050	1.64710	1.10300
C	-0.52560	1.37680	2.47190
H	0.38690	0.82400	-2.11720
H	-1.02420	1.61620	-2.77930
H	1.09940	2.98200	-3.12470
H	-0.09590	3.87050	-2.18160
H	1.27880	3.12070	-1.37200
H	-3.03540	2.94200	-1.02180
H	-3.19290	2.46450	0.65070
H	-2.74910	4.92730	0.47590
H	-1.41670	4.13460	1.31850
H	-1.22820	4.62120	-0.36390
H	0.91190	0.93370	0.91820
H	0.56240	2.64360	1.08020
H	0.21010	1.46480	3.27970
H	-1.34090	2.07560	2.69310
H	-0.94560	0.36580	2.51540
H	-0.14150	-1.40920	-1.66880

TS-=F10c

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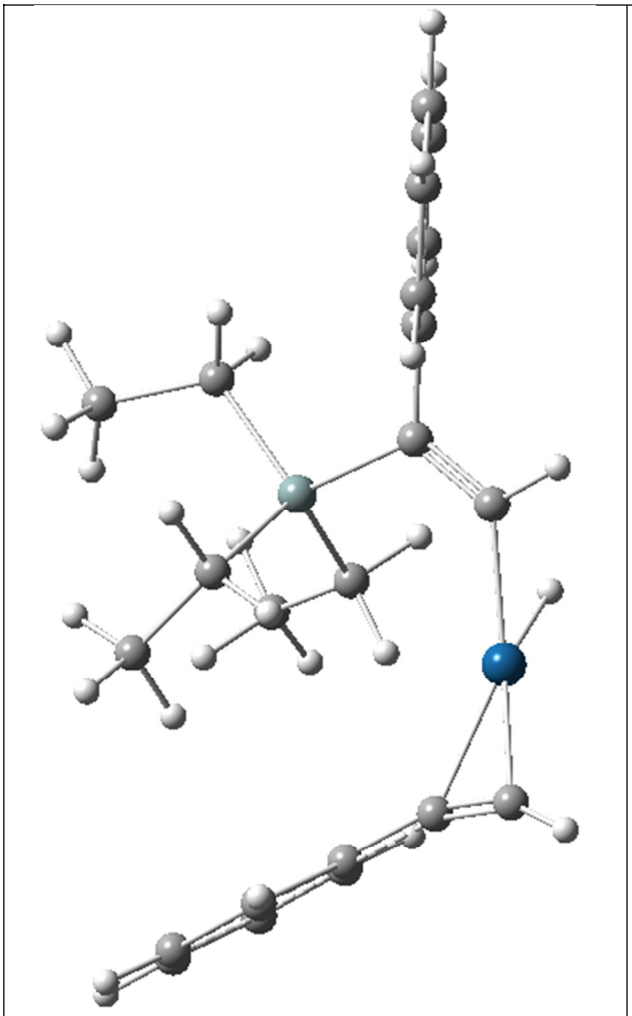
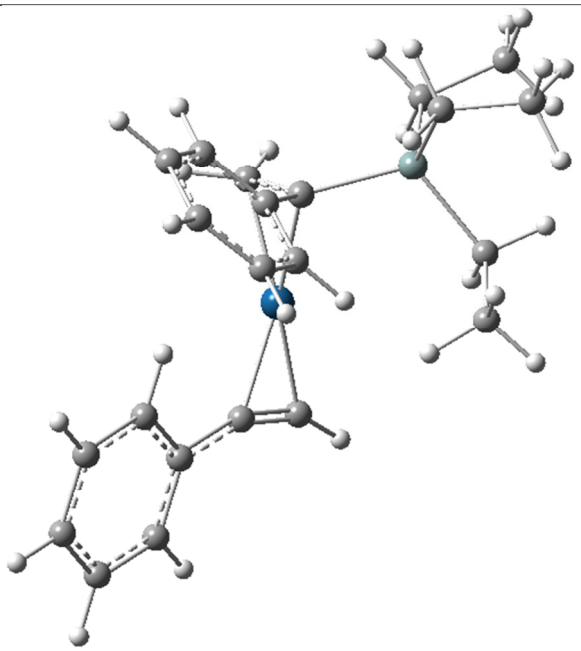


C	6.14780	-0.46540	0.73370
C	5.20350	-1.08220	1.55230
C	5.72120	0.24980	-0.38600
C	4.36410	0.35020	-0.67950
C	3.40160	-0.27040	0.13100
C	3.84540	-0.98390	1.25390
C	1.95380	-0.18840	-0.19360
C	1.28320	-1.35440	-0.34540
H	7.20650	-0.53880	0.96600
H	5.52310	-1.63790	2.42990
H	6.44890	0.73010	-1.03470
H	4.04170	0.90280	-1.55790
H	3.10900	-1.45370	1.90080
H	1.86480	-2.28500	-0.33960
Pt	-0.68010	-1.79990	-0.35270
C	-4.85330	2.09770	0.49040
C	-4.69910	1.31690	1.63580
C	-4.26280	1.69980	-0.70940
C	-3.51430	0.52970	-0.76450
C	-3.36180	-0.26010	0.38350
C	-3.95900	0.14020	1.58740
C	-2.60290	-1.48480	0.32860
C	-2.31720	-2.71030	0.47280
H	-5.43000	3.01690	0.53360
H	-5.15430	1.62710	2.57170
H	-4.37990	2.30570	-1.60290
H	-3.04610	0.21300	-1.69110
H	-3.83080	-0.46990	2.47610
H	-2.53870	-3.73580	0.71010
Si	1.05950	1.49030	-0.19430
C	0.03690	1.52970	1.40420
C	-1.10630	2.54310	1.48460
C	2.33800	2.89330	-0.18180
C	1.84480	4.23540	0.36680
C	-0.01300	1.60230	-1.75220
C	-0.56550	2.98530	-2.10230
H	-0.36290	0.51590	1.53900
H	0.74430	1.68300	2.23210
H	-1.61230	2.49660	2.45580
H	-0.75920	3.57190	1.34620
H	-1.86410	2.34490	0.72110
H	3.19920	2.55730	0.40910
H	2.71770	3.02530	-1.20480
H	2.63170	4.99730	0.32160
H	0.98510	4.62150	-0.19050
H	1.53990	4.14660	1.41490
H	0.60080	1.22560	-2.58260
H	-0.83280	0.88240	-1.64490
H	-1.17120	2.95390	-3.01590
H	-1.19960	3.38500	-1.30460
H	0.23970	3.70790	-2.27360
H	0.23610	-1.50210	-1.61490

F11a

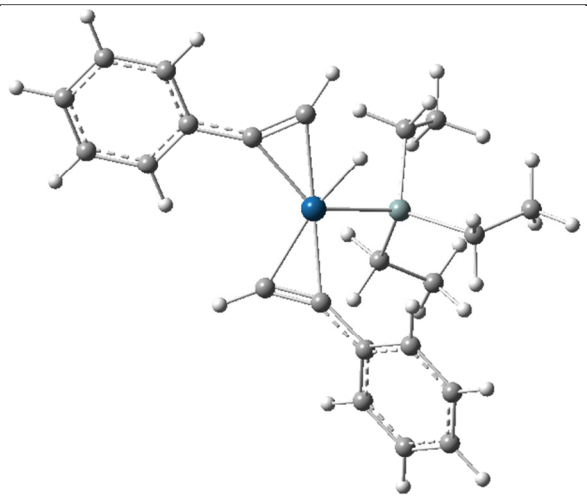
E = -1263.011705; (E+ZPE) = -1262.574670; H = -1262.546451; G = -1262.635563



C	-0.52940	4.26750	0.00240
C	-0.10170	3.92540	-1.27880
C	-0.39780	3.33840	1.03550
C	0.14750	2.08340	0.78610
C	0.56910	1.71830	-0.50170
C	0.44390	2.66660	-1.52630
C	1.15850	0.37210	-0.78350
C	0.82490	-0.26360	-2.00880
H	-0.95530	5.24780	0.19610
H	-0.18680	4.64220	-2.09130
H	-0.72790	3.58900	2.04000
H	0.22750	1.36290	1.59340
H	0.78890	2.41800	-2.52610
H	0.17450	0.22760	-2.73280
Pt	-0.34260	-1.10390	-0.46560
C	-5.70320	0.82830	0.43150
C	-5.74570	-0.52600	0.76660
C	-4.49630	1.41340	0.04780
C	-3.33490	0.65050	-0.00590
C	-3.37200	-0.70990	0.33190
C	-4.58760	-1.29450	0.72020
C	-2.16850	-1.50450	0.29490
C	-1.41540	-2.50940	0.52100
H	-6.60980	1.42560	0.46980
H	-6.68430	-0.98390	1.06540
H	-4.45800	2.46760	-0.21070
H	-2.38860	1.09660	-0.29840
H	-4.61390	-2.34860	0.98000
H	-1.20410	-3.48020	0.93450
Si	2.77200	-0.11280	0.13060
C	3.79260	-1.14940	-1.08440
C	5.19630	-1.53030	-0.60730
C	3.65970	1.49880	0.58660
C	4.75410	1.37230	1.64990
C	2.52370	-1.16840	1.68290
C	1.65860	-0.59660	2.80500
H	3.22060	-2.06170	-1.30490
H	3.85930	-0.59920	-2.03260
H	5.70070	-2.18410	-1.32800
H	5.82850	-0.64630	-0.47520
H	5.17160	-2.06180	0.35030
H	4.07270	1.92460	-0.33860
H	2.90250	2.21790	0.92340
H	5.22300	2.34090	1.85800
H	4.34920	0.99790	2.59640
H	5.54960	0.68470	1.34590
H	2.12100	-2.13800	1.36020
H	3.53470	-1.37580	2.06300
H	1.69240	-1.22770	3.70050
H	1.98180	0.40800	3.10160
H	0.61100	-0.53310	2.49280
H	1.47570	-1.02460	-2.43560

TS-G6a

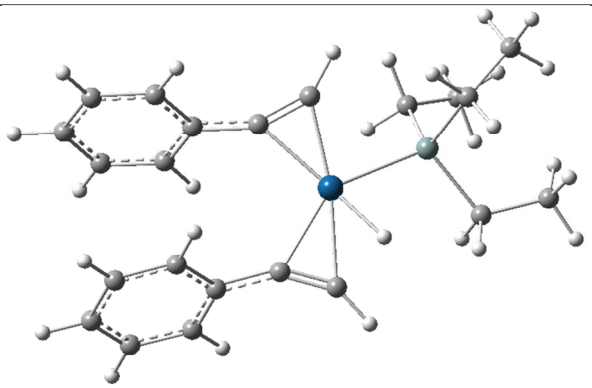
E = -1262.924239; (E+ZPE) = -1262.493922; H = -1262.465205; G = -1262.555124



C	6.34380	-1.00620	0.80010
C	5.17920	-1.36950	1.47590
C	6.26060	-0.23730	-0.36250
C	5.02250	0.17470	-0.84150
C	3.84340	-0.18970	-0.16790
C	3.93680	-0.97550	0.98940
C	2.55810	0.24170	-0.65960
C	1.93730	1.13100	-1.35110
H	7.31290	-1.32410	1.17380
H	5.23900	-1.96970	2.37930
H	7.16500	0.04490	-0.89400
H	4.95480	0.77560	-1.74390
H	3.02060	-1.26040	1.49690
H	1.99690	2.09240	-1.83630
Pt	0.48700	-0.12710	-0.38010
C	-4.90950	-2.76420	-0.31780
C	-4.32680	-2.82720	0.94810
C	-4.16330	-2.30300	-1.40320
C	-2.84650	-1.89490	-1.22220
C	-2.25060	-1.96080	0.04460
C	-3.00400	-2.43450	1.12970
C	-0.87050	-1.56540	0.22960
C	0.25960	-1.79870	0.80340
H	-5.94180	-3.07190	-0.45780
H	-4.90440	-3.18310	1.79650
H	-4.61250	-2.25310	-2.39100
H	-2.26150	-1.51780	-2.05590
H	-2.54460	-2.48240	2.11290
H	0.82160	-2.50910	1.38950
Si	-1.25290	1.42970	0.14430
C	-2.76270	1.43970	-1.01190
C	-3.52950	2.76220	-1.09710
C	-1.77790	1.10490	1.94560
C	-3.13520	1.69250	2.34070
C	-0.38210	3.12570	0.06540
C	-0.99670	4.23790	0.91940
H	-2.41100	1.15550	-2.01190
H	-3.43850	0.63470	-0.70050
H	-4.37400	2.68480	-1.79220
H	-3.93580	3.06300	-0.12620
H	-2.89030	3.57780	-1.45200
H	-1.78650	0.02400	2.11650
H	-0.98400	1.50100	2.59360
H	-3.37550	1.46730	3.38670
H	-3.16500	2.78100	2.22780
H	-3.94020	1.27590	1.72570
H	0.65950	2.97080	0.37360
H	-0.33910	3.43470	-0.98930
H	-0.42540	5.16950	0.82910
H	-2.02880	4.45910	0.63140
H	-1.00370	3.96490	1.98000
H	0.43080	0.89260	-1.67440

TS-G6b

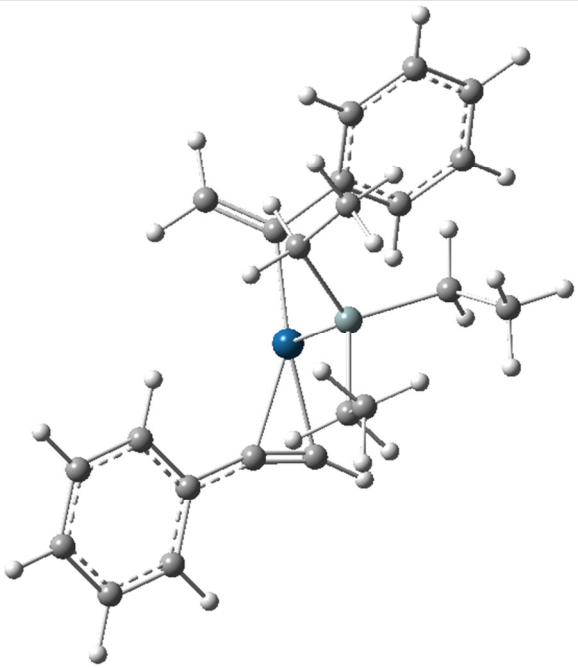
E = -1262.926008; (E+ZPE) = -1262.496226; H = -1262.467288; G = -1262.557704



C	5.20410	-1.70430	0.19020
C	4.62860	-1.00200	-0.86840
C	4.39220	-2.42260	1.06790
C	3.01280	-2.45050	0.88490
C	2.42900	-1.74240	-0.17650
C	3.25020	-1.00530	-1.04250
C	0.99920	-1.74570	-0.36460
C	-0.10010	-2.39070	-0.44980
H	6.28030	-1.68560	0.33590
H	5.25340	-0.42790	-1.54620
H	4.83470	-2.96840	1.89650
H	2.37750	-3.01020	1.56500
H	2.79300	-0.43070	-1.84180
H	-0.59870	-3.34650	-0.44140
Pt	-0.54690	-0.26140	-0.41660
C	4.63110	2.42680	0.69320
C	4.01300	2.98600	-0.42520
C	3.91480	1.56030	1.51890
C	2.59400	1.24580	1.22410
C	1.95990	1.81460	0.10920
C	2.68510	2.68720	-0.71660
C	0.58750	1.49140	-0.19090
C	-0.61930	1.78940	-0.49220
H	5.66810	2.66090	0.91670
H	4.56660	3.65960	-1.07360
H	4.39310	1.11150	2.38450
H	2.03920	0.55040	1.84640
H	2.20100	3.11890	-1.58780
H	-1.35410	2.57180	-0.60380
Si	-2.89010	0.02510	0.06900
C	-3.84860	0.88330	-1.33560
C	-5.09010	1.67400	-0.91400
C	-3.70440	-1.67160	0.40940
C	-5.23500	-1.69760	0.43840
C	-2.93990	1.06400	1.66890
C	-4.18770	0.94750	2.54650
H	-3.15510	1.54540	-1.86850
H	-4.12240	0.10590	-2.06290
H	-5.58060	2.14280	-1.77560
H	-5.83360	1.03880	-0.42200
H	-4.83250	2.47420	-0.21120
H	-3.35650	-2.37270	-0.36130
H	-3.29770	-2.05190	1.35750
H	-5.61400	-2.70530	0.64740
H	-5.64630	-1.03050	1.20160
H	-5.65330	-1.38800	-0.52540
H	-2.05430	0.78060	2.25260
H	-2.77300	2.11350	1.39030
H	-4.10830	1.58350	3.43630
H	-5.09590	1.24560	2.01280
H	-4.33490	-0.08000	2.89610
H	-1.33120	-1.59510	-0.93800

G7a

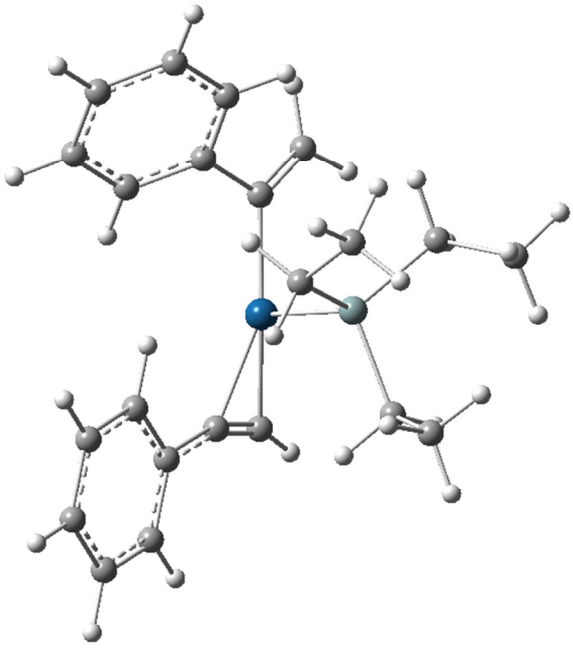
E = -1262.989962; (E+ZPE) = -1262.554415; H = -1262.525493; G = -1262.615454



C	5.39300	-0.80460	0.21930
C	4.47300	-1.38580	1.09350
C	4.97700	-0.41450	-1.05280
C	3.65410	-0.60480	-1.44810
C	2.71610	-1.18040	-0.57770
C	3.14990	-1.56020	0.70190
C	1.30050	-1.34300	-0.97730
C	1.00770	-1.86760	-2.18440
H	6.42310	-0.65340	0.52930
H	4.78700	-1.69420	2.08720
H	5.68300	0.04640	-1.73870
H	3.33030	-0.28220	-2.43400
H	2.42860	-1.99360	1.39090
H	1.79250	-2.21970	-2.85750
Pt	-0.19950	-0.88130	0.32070
C	-5.75600	-0.09620	-1.15110
C	-5.80670	-0.36910	0.21680
C	-4.52580	-0.04790	-1.80670
C	-3.34890	-0.27280	-1.10120
C	-3.39400	-0.54470	0.27330
C	-4.63430	-0.59160	0.93000
C	-2.18470	-0.75970	1.02290
C	-1.42460	-0.91150	2.01670
H	-6.67430	0.07860	-1.70420
H	-6.76330	-0.40650	0.72950
H	-4.48330	0.16520	-2.87080
H	-2.38280	-0.23750	-1.59700
H	-4.66630	-0.80130	1.99480
H	-1.14550	-0.98280	3.05220
Si	0.41350	1.35240	0.08580
C	-1.05770	2.37150	0.73930
C	-1.06630	3.84540	0.32350
C	1.94880	1.63140	1.17210
C	2.12650	3.05490	1.70800
C	0.74340	1.84510	-1.72050
C	1.67350	3.04890	-1.89830
H	-1.97960	1.89580	0.38480
H	-1.07920	2.27760	1.83350
H	-1.94630	4.36310	0.72300
H	-0.18230	4.38340	0.67930
H	-1.09670	3.95050	-0.76640
H	1.89130	0.92780	2.01210
H	2.83230	1.32520	0.59950
H	3.02410	3.12840	2.33340
H	2.23280	3.78690	0.90100
H	1.27490	3.36540	2.32300
H	1.16100	0.97560	-2.23660
H	-0.22850	2.03850	-2.19600
H	1.82630	3.27790	-2.95970
H	1.27930	3.95360	-1.42440
H	2.65910	2.85240	-1.46260
H	-0.01500	-1.97320	-2.53960

G7b

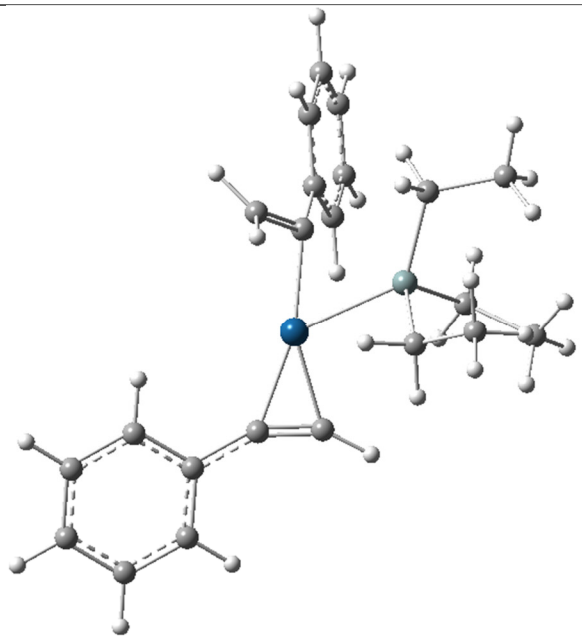
E = -1262.992028; (E+ZPE) = -1262.556347; H = -1262.527449; G = -1262.617685



C	-2.51280	-3.93010	1.24390
C	-1.40850	-3.84930	0.39390
C	-3.42090	-2.87340	1.28670
C	-3.22520	-1.74640	0.49080
C	-2.11790	-1.64760	-0.36580
C	-1.21130	-2.71960	-0.39450
C	-1.89720	-0.42250	-1.16840
C	-2.91670	0.09140	-1.88480
H	-2.66090	-4.80660	1.86840
H	-0.69670	-4.66930	0.34660
H	-4.28040	-2.92110	1.95020
H	-3.92030	-0.91290	0.54670
H	-0.34810	-2.66350	-1.05320
H	-3.87710	-0.42290	-1.95470
Pt	-0.00190	0.30650	-1.30480
C	4.48300	-1.91340	1.59170
C	5.06870	-1.01010	0.70300
C	3.10450	-2.12360	1.56380
C	2.31030	-1.43570	0.65280
C	2.89320	-0.52550	-0.23970
C	4.28170	-0.31690	-0.20950
C	2.08720	0.21280	-1.17670
C	1.79850	1.03300	-2.09060
H	5.10130	-2.45120	2.30450
H	6.14170	-0.84380	0.72340
H	2.64470	-2.82480	2.25410
H	1.23590	-1.59050	0.62440
H	4.72980	0.39090	-0.90040
H	1.96940	1.75760	-2.86550
Si	-0.52760	1.51850	0.61280
C	0.92340	2.72310	0.89130
C	1.04730	3.26080	2.32060
C	-2.14350	2.49410	0.39330
C	-2.30760	3.73310	1.27630
C	-0.61100	0.32110	2.08750
C	-1.49690	0.78420	3.24760
H	1.84890	2.20120	0.62410
H	0.82870	3.55010	0.17420
H	1.90450	3.93790	2.41550
H	0.15850	3.81490	2.63690
H	1.19780	2.44680	3.03790
H	-2.20350	2.78560	-0.66300
H	-2.97570	1.79600	0.54380
H	-3.26150	4.23570	1.07660
H	-2.28890	3.48400	2.34210
H	-1.51250	4.46430	1.09550
H	-0.96440	-0.65210	1.73040
H	0.41840	0.16140	2.43520
H	-1.50920	0.04290	4.05520
H	-1.15300	1.73070	3.67770
H	-2.53320	0.92830	2.92330
H	-2.82670	1.02330	-2.43800

TS-G10a

E = -1262.974955; (E+ZPE) = -1262.539576; H = -1262.511465; G = -1262.599693



C	-3.64240	-3.83140	-0.93010
C	-2.67090	-3.18090	-1.69260
C	-3.78680	-3.51560	0.42050
C	-2.96270	-2.55790	1.00520
C	-1.97350	-1.90760	0.25210
C	-1.85020	-2.22240	-1.10870
C	-1.11270	-0.88970	0.87550
C	-0.70040	-0.93930	2.17730
H	-4.28950	-4.57370	-1.38880
H	-2.55640	-3.41980	-2.74630
H	-4.54910	-4.00910	1.01700
H	-3.09020	-2.29530	2.05230
H	-1.09240	-1.70840	-1.69410
H	-0.78040	-1.85850	2.76070
Pt	0.49650	-0.02020	0.08450
C	6.38080	-0.75010	0.36730
C	6.11350	-0.09720	-0.83740
C	5.33370	-1.06050	1.23490
C	4.02630	-0.72140	0.90170
C	3.74850	-0.06260	-0.30450
C	4.80880	0.24550	-1.17350
C	2.39480	0.29240	-0.65340
C	1.53030	0.87510	-1.39750
H	7.40120	-1.01650	0.62720
H	6.92610	0.14530	-1.51660
H	5.53660	-1.56930	2.17290
H	3.20350	-0.95960	1.57000
H	4.59670	0.75220	-2.11040
H	1.26240	1.52670	-2.21390
Si	-1.55980	1.32620	0.13000
C	-0.67080	2.95190	0.60050
C	-1.54420	4.16710	0.91940
C	-2.11860	1.28600	-1.68990
C	-2.48350	2.65390	-2.27430
C	-3.11970	1.20310	1.22840
C	-4.31380	2.03470	0.75010
H	-0.03290	2.72270	1.46410
H	0.02880	3.18160	-0.21380
H	-0.92640	5.03340	1.18420
H	-2.16850	4.46030	0.06950
H	-2.20970	3.97270	1.76680
H	-1.32170	0.83280	-2.29010
H	-2.97230	0.59930	-1.76110
H	-2.77880	2.56980	-3.32680
H	-3.31590	3.12110	-1.73910
H	-1.63660	3.34730	-2.22710
H	-3.43200	0.15660	1.29760
H	-2.82850	1.49580	2.24710
H	-5.16230	1.93270	1.43700
H	-4.08340	3.10110	0.67440
H	-4.65630	1.70160	-0.23550
H	-0.28560	-0.07540	2.69020

TS-G10b

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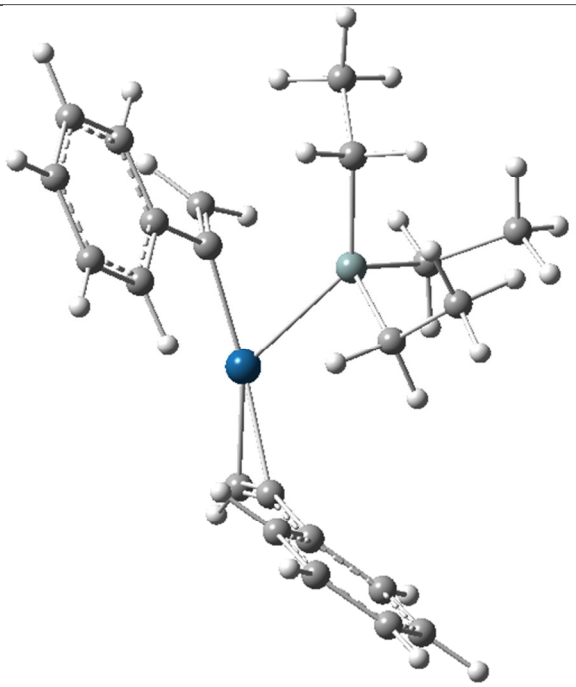

C	3.56670	3.41610	1.20820
C	2.18230	3.32830	1.06290
C	4.37580	2.38760	0.72480
C	3.80600	1.28300	0.09870
C	2.41640	1.18970	-0.06900
C	1.61570	2.22230	0.43750
C	1.79880	0.01260	-0.71420
C	2.46200	-0.76660	-1.61490
H	4.01160	4.27420	1.70380
H	1.54310	4.12100	1.44190
H	5.45420	2.44110	0.84610
H	4.44370	0.47530	-0.24900
H	0.53790	2.14110	0.32250
H	3.40920	-0.45310	-2.05530
Pt	-0.12620	-0.09610	-1.32360
C	-4.88420	1.40770	1.73490
C	-5.13870	0.32670	0.89110
C	-3.72320	2.16250	1.56490
C	-2.81600	1.83290	0.56410
C	-3.06680	0.74950	-0.28840
C	-4.23880	-0.00160	-0.11850
C	-2.12440	0.39410	-1.32390
C	-1.77280	0.08980	-2.51000
H	-5.58790	1.66090	2.52250
H	-6.04110	-0.26410	1.01980
H	-3.52170	3.00650	2.21810
H	-1.90560	2.40960	0.43070
H	-4.42870	-0.84560	-0.77480
H	-1.99100	-0.02640	-3.55800
Si	0.57590	-1.35150	0.68160
C	-0.78920	-0.70960	1.84660
C	-0.71170	-1.14630	3.31160
C	0.23660	-3.11270	0.05100
C	0.11600	-4.16120	1.16150
C	2.13040	-1.47880	1.78440
C	3.33630	-2.23300	1.23650
H	-0.78880	0.38520	1.79620
H	-1.74890	-1.01140	1.40970
H	-1.58340	-0.78350	3.86890
H	-0.68570	-2.23570	3.42080
H	0.17990	-0.74700	3.80520
H	-0.68070	-3.08850	-0.54880
H	1.04190	-3.39230	-0.64140
H	-0.03400	-5.16510	0.74750
H	1.01250	-4.19800	1.78980
H	-0.73500	-3.95080	1.81780
H	2.42180	-0.47530	2.11840
H	1.76780	-1.99520	2.68440
H	4.15040	-2.27220	1.96950
H	3.07970	-3.26630	0.97630
H	3.73090	-1.76310	0.32960
H	2.06490	-1.71860	-1.95700

Pt atom (triplet)

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PhCCH

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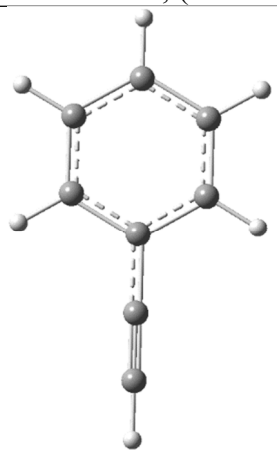
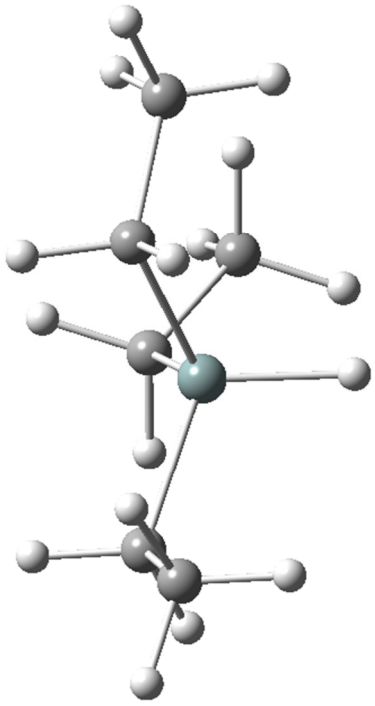
	C 2.20820 -0.00000 0.00000 C 1.50950 1.20690 0.00000 C 1.50950 -1.20690 0.00000 C 0.11900 -1.21170 0.00000 C -0.59030 -0.00000 0.00000 C 0.11900 1.21170 0.00000 C -2.01790 0.00000 0.00000 C -3.22980 0.00000 0.00000 H 3.29420 -0.00000 0.00000 H 2.04970 2.14900 0.00000 H 2.04970 -2.14900 0.00000 H -0.42940 -2.14830 0.00000 H -0.42940 2.14830 0.00000 H -4.29760 0.00000 0.00000

Et_3SiH

E = ; (E+ZPE) = ; H = ; G =	
	Si -0.16610 -0.21400 0.23450 C -1.86080 -0.85920 -0.29980 C -3.04300 -0.04240 0.22620 C 1.20140 -1.30060 -0.49800 C 2.51280 -1.31430 0.29200 C 0.01680 1.59830 -0.27450 C 1.38510 2.22190 0.00750 H -0.07380 -0.29390 1.73070 H -1.88350 -0.89270 -1.39810 H -1.94480 -1.90250 0.03310 H -4.00290 -0.47300 -0.08040 H -3.04000 0.00470 1.32110 H -3.01570 0.98800 -0.14420 H 0.80740 -2.32310 -0.57560 H 1.38350 -0.97340 -1.53130 H 3.25960 -1.96630 -0.17530 H 2.95360 -0.31510 0.36790 H 2.35380 -1.67460 1.31400 H -0.21440 1.66930 -1.34690 H -0.76780 2.17060 0.23810 H 1.40830 3.28450 -0.25980 H 1.65090 2.14490 1.06780 H 2.17650 1.72630 -0.56470

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