Supporting Information for

Olefin Hydrosilylation Catalyzed by Cationic Nickel(II) Allyl Complexes: Non-Innocent Allyl Ligand-Assisted Mechanism

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Experimental Details and Compound Characterization Data

General considerations.

Unless otherwise noted, all manipulations were performed under a nitrogen atmosphere using Schlenk techniques or a glove box. Benzene, hexane, and CH_2Cl_2 were purified by a solvent purification system (MBraun SPS-800). Other solvents (benzene-d_6) was dried over sodium benzophenone ketyl and distilled. CD_2Cl_2 was dried over CaH_2 and distilled prior to use. All reagents, unless otherwise stated, were purchased from commercial suppliers and used without further purification. ^{1}H, ^{13}C{^{1}H} and ^{29}Si{^{1}H} NMR spectra (^{1}H, 600 MHz; ^{13}C, 150 MHz; ^{29}Si, 119 MHz) were recorded using a Bruker AVANCE 600 spectrometer. Chemical shifts are reported in δ (ppm) and are referenced to the residual solvent signals for ^{1}H or to tetramethysilane (0.0 ppm) for ^{13}C and ^{29}Si. GLC analysis was performed on a Shimadzu GC-2014 instrument (FID; CBP-1, 25 m × 0.25 mm). Elemental analyses were carried out on a Thermo Scientific FLASH2000 CHNS analyzer. Complexes **1b**[1] and $NaBAr^F{}_4$[2] were prepared according to the literature procedures.

Synthesis of 1a. Complex **1a** was similarly prepared according to the literature procedure of **1b**.[1] To a Et_2O (5 mL) solution of [Ni(methallyl)Cl]$_2$ (83.6 mg, 0.028 mmol) was added a Et_2O solution (5 mL) of 2,6-di-*t*-butyl-4-methylphenol (12.3 mg, 0.056 mmol) and $NaBAr^F{}_4$ (49.6 mg, 0.056 mmol) at –80 °C. After stirring the mixture at room temperature for 2 h, volatiles were removed under vacuum. The residue was washed with hexane (2 mL × 3), extracted with CH_2Cl_2 (0.5 mL) and filtered using a glass wool filter paper. Cooling the solution at –30 °C gave **1a** as a dark red crystals (37.2 mg, 0.031 mmol, 56%). ^{1}H NMR (CD_2Cl_2, 25 °C) δ 1.50 (s, 18 H, *t*Bu), 2.21 (s, 3H, Me), 2.22 (s, 3H, Me), 2.40 (s, 2H, allyl-*syn*), 3.52 (s, 2H, allyl-*anti*), 5.89 (s, 1H, OH), 6.85 (s, 2H, Ar), 7.56 (s, 4H, $BAr^F{}_4$), 7.72 (s, 8H, $BAr^F{}_4$). ^{13}C{^{1}H} NMR (CD_2Cl_2, 25 °C) δ 20.1, 22.3, 29.8, 34.9, 58.7, 108.3, 117.4, 123.3, 124.5, 125.4 (q, $^1J_{FC}$ = 272 Hz), 125.5, 128.7 (q, $^1J_{FC}$ = 33 Hz), 134.8, 140.4, 161.7 (q, $^1J_{BC}$ = 50 Hz). Anal. Calcd. for $C_{51}H_{43}BF_{24}NiO$: C, 51.16; H, 3.62. Found: C, 51.81; H, 3.13.

Synthesis of 1c. Complex **1c** (64.0 g, 0.055 mmol, 18%) was prepared according to the above mentioned procedure using [Ni(methallyl)Cl]$_2$ (45.0 mg, 0.15 mmol), 2,6-di-*t*-butylbenzene (58.0 mg, 0.30 mmol), and NaBAr$^F_4$ (268.0 mg, 0.30 mmol). ^{1}H NMR (C_6D_6, 25 °C) δ 1.37 (s, 18 H, *t*Bu), 2.15 (s, 3H, Me), 2.39 (s, 2H, allyl-*syn*), 3.75 (s, 2H, allyl-*anti*), 6.92 (s, 4H, Ar), 7.56 (s, 4H, BAr$^F_4$), 7.72 (s, 8H, BAr$^F_4$). ^{13}C{^{1}H} NMR (C_6D_6, 25 °C) δ 24.7, 32.6, 37.1, 61.2, 106.9, 119.7, 125.7, 126.9 (q, $^1J_{FC}$ = 273 Hz), 131.1 (q, $^2J_{FC}$ = 30 Hz), 137.1, 142.4, 164.5 (q, $^1J_{BC}$ = 50 Hz). Anal. Calcd. for $C_{50}H_{41}BF_{24}Ni$: C, 51.45; H, 3.54. Found: C, 51.13; H, 3.22.

Synthesis of 1d. Complex **1d** (138.7 g, 0.11 mmol, 18%) was prepared according to the literature procedure of **1b** using [Ni(methallyl)Cl]$_2$ (95.5 mg, 0.32 mmol), 1,3,5-tri-*t*-butylbenzene (157 mg, 0.64 mmol), and NaBAr$^F_4$ 62.0 mg, 0.70 mmol). ^{1}H NMR (C_6D_6, 25 °C) δ 1.38 (s, 27 H, *t*Bu), 2.16 (s, 3H, Me), 2.32 (s, 2H, allyl-*syn*), 3.71 (s, 2H, allyl-*anti*), 6.99 (s, 3H, Ar), 7.56 (s, 4H, BAr$^F_4$), 7.72 (s, 8H, BAr$^F_4$). ^{13}C{^{1}H} NMR (C_6D_6, 25 °C) δ 22.6, 31.0, 35.8, 58.9, 102.7, 117.9, 122.3, 125.0 (q, $^1J_{FC}$ = 273 Hz), 129.3 (q, $^2J_{FC}$ = 31 Hz), 135.2, 138.0, 162.2 (q, $^1J_{BC}$ = 50 Hz). Anal. Calcd. for $C_{54}H_{49}BF_{24}Ni$: C, 53.01; H, 4.04. Found: C, 52.95; H, 3.85.

Catalytic hydrosilylations. A typical procedure (enrty 3 in Table 1) is as follows. To a stirred solution of 1-octene (94 mg, 0.84 mmol) and Et_2SiH_2 (74 mg, 0.84 mmol) in CH_2Cl_2 (4 mL) was added a CH_2Cl_2 solution of **1a** (5 mg, 0.0042 mmol) at room temperature. The solution was stirred at room temperature, and the progress of the reaction was monitored by GLC. After completion of the reaction, mesitylene (60 mg, 0.50 mmol) was added as an internal standard to the reaction mixture. The GLC analysis of the resulting solution revealed the formation of Et_2(*n*Oct)SiH (0.60 mmol, 75%), Et_2(*n*Oct)$_2$Si (0.09 mmol, 1%), and Et(*n*Oct)$_2$SiH (0.12 mmol, 2%). The solution was concentrated under vacuum, and the residue was purified by gel permeation chromatography (GPC) using toluene as an eluent to give Et_2(*n*Oct)SiH (113.4 mg, 0.57 mmol, 71%). The final products were characterized by ^{1}H, ^{13}C{^{1}H} and ^{29}Si{^{1}H} NMR.

Compound Characterization Data

The products in Table 1, (*n*Hex)(*n*Oct)SiH_2[3], (*n*Hex)(*n*Oct)$_2$SiH[3], (*n*Oct)$_2SiH_2$[3], (*n*Oct)$_3$SiH[4], Et_2(*n*Oct)SiH[3], Et_2(*n*Oct)$_2$Si[3], (*n*Hex)$_2$(*n*Oct)SiH [3], 1-(styryl)Et_2SiH[3], 2-(styryl)Et_2SiH[3] are reported compounds.

Et(*n*Oct)$_2$SiH: ^{1}H NMR (C_6D_6, 25 °C) δ 0.63-0.69 (m, 6H), 0.92 (t, 6H, J = 6.9 Hz), 1.05 (t, 3H, J = 8.1 Hz), 1.29-1.32 (16H), 1.38 (m, 4H), 1.47 (m, 4H), 4.04 (m, 1H). $^{13}C\{^1H\}$ NMR (C_6D_6, 25 °C) δ 3.7, 8.6, 11.4, 14.4, 23.1, 25.2, 29.8 (×2), 32.4, 33.9. $^{29}Si\{^1H\}$ NMR (C_6D_6, 25 °C) δ –3.82. Anal. Calcd. for $C_{20}H_{44}Si$: C, 76.83; H, 14.19. Found: C, 76.97; H, 14.49.

(*n*Hex)(*n*Oct)SiH_2: ^{1}H NMR (C_6D_6, 25 °C) δ 0.66 (m, 4H), 0.90 (m, 6H), 1.23-1.35 (m, 16H), 1.43 (m, 4H), 3.97 (m, 2H). $^{13}C\{^1H\}$ NMR (C_6D_6, 25 °C) δ 9.5 (×2), 14.3 (×2), 22.9, 23.1, 25.8, 25.9, 29.6, 29.7, 31.9, 32.3, 33.0, 33.3. $^{29}Si\{^1H\}$ NMR (C_6D_6, 25 °C) δ –28.18. Anal. Calcd. for $C_{14}H_{32}Si$: C, 73.59; H, 14.12. Found: C, 73.31; H, 13.92.

(*n*Pen)$_2$(*n*Oct)SiH: ^{1}H NMR (C_6D_6, 25 °C) δ 0.67 (m, 6H), 0.92 (m, 9H), 1.29-1.38 (m, 18H), 1.45 (m, 6H), 4.06 (m, 1H). $^{13}C\{^1H\}$ NMR (C_6D_6, 25 °C) δ 11.7, 11.8, 14.2, 14.3, 22.7, 23.1, 24.9, 25.2, 29.7, 29.8, 32.3, 33.9, 36.0. $^{29}Si\{1H\}$ NMR (C_6D_6, 25 °C) δ –6.09. Anal. Calcd. for $C_{20}H_{44}Si$: C, 76.83; H, 14.19. Found: C, 77.34; H, 14.52.

Monitoring the reaction of 1c with Et_2SiH_2 and 1-octene. A J-Young NMR tube was charged with a C_6D_6 solution (0.4 mL) of **1c** (2.2 mg, 0.018 mmol) and Et_2SiH_2 (1.1 μL, 0.086 mmol). After taking ^{1}H NMR, 1-octene (53 μL,0.36 mmol) and Et_2SiH_2 (34 μL, 0.27 mmol) were further added to the reaction mixture. The reaction was followed by ^{1}H NMR.

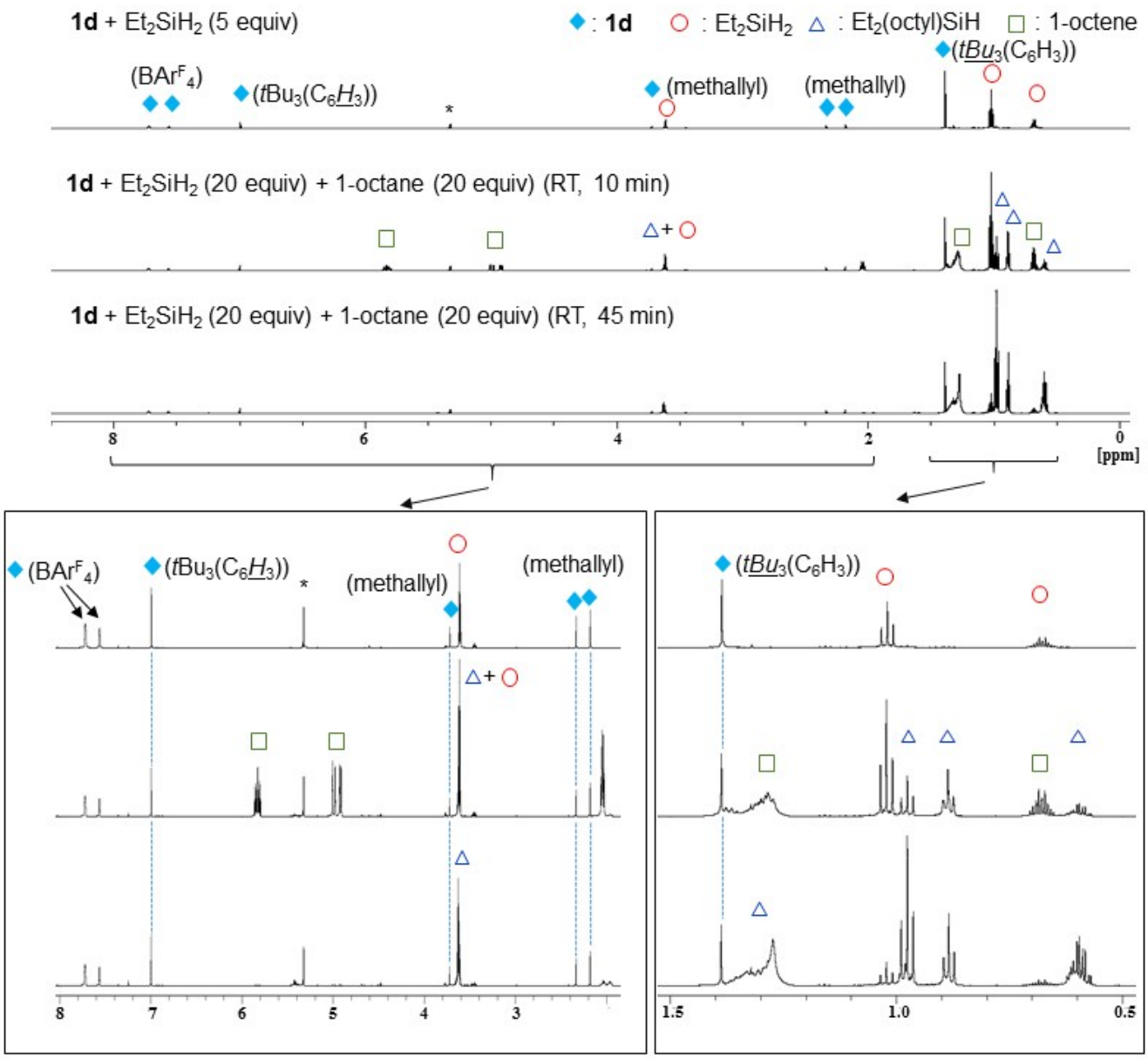


Figure S1. ^{1}H NMR time-course of the hydrosilylation reaction of 1-octene with Et_2SiH_2 in the presence of **1d** (5 mol%).

Computational Methods

All calculations of nickel species were carried out using M06 functional [5] with 6-311G(d,p) basis set for all atoms except for Ni which is treated with quasirelativistic SDD pseudopotential and corresponding basis set [6] with additional f function. Geometry optimization of $[Pt(SiH_4)(PH_3)_2]$ was performed following the slightly modified literature method[7] using LANL08(f) basis sets and ECP for Pt, LANL08(d) basis sets and ECP for Si and P and SVP basis sets for H.[8] Solvent effects (CH_2Cl_2) were treated with SMD solvation model.[9] Population analysis of $[Pt(SiH_4)(PH_3)_2]$ was carried out using M06 functional[5] with 6-311G(d,p) basis set for all atoms except for Pt which is treated with quasirelativistic SDD pseudopotential and corresponding basis set[6] with additional f function. All transition states were characterized by single imaginary frequency. Intrinsic reaction coordinate (IRC) calculations were performed to check that the transition states **TS_{4-5}** and **TS_{11-12}** are connected to the relevant reactant and product. Population analysis was carried out with the method of Weinhold *et. al.*[10] Bond order analysis is performed based on Mayer bond indices.[11] Gaussian 09 suite of programs [12] was used for all calculations. Free energy values calculated at M06/SDD-6-311G(d,p)/SMD is used for the discussion. Molecular orbitals were drawn using the Chemissian program [13].

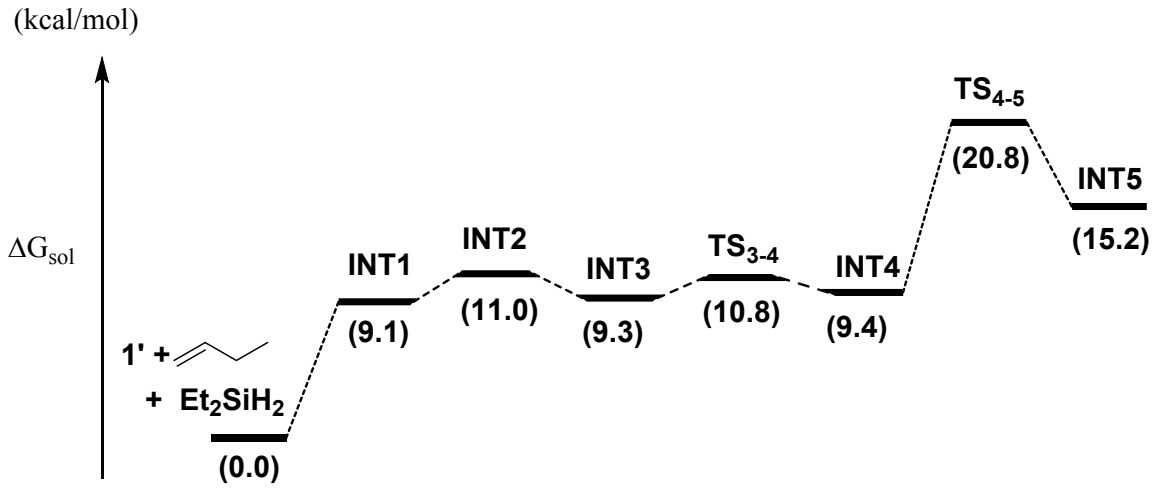


Figure S2. Free energy profile for hydrosilylation of 1-butene with Et_2SiH_2 from **1'** to **INT5**.

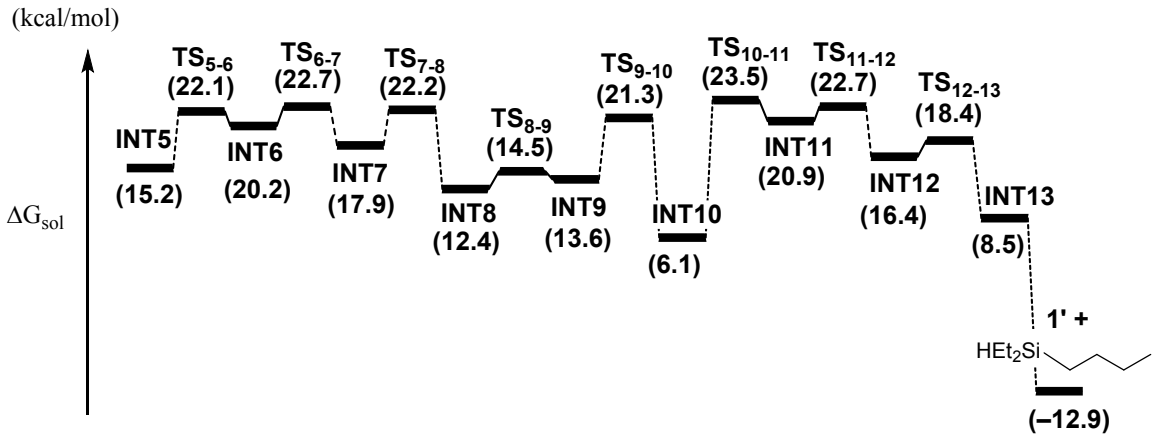


Figure S3. Free energy profile for hydrosilylation of 1-butene with Et_2SiH_2 from **INT5** to product.

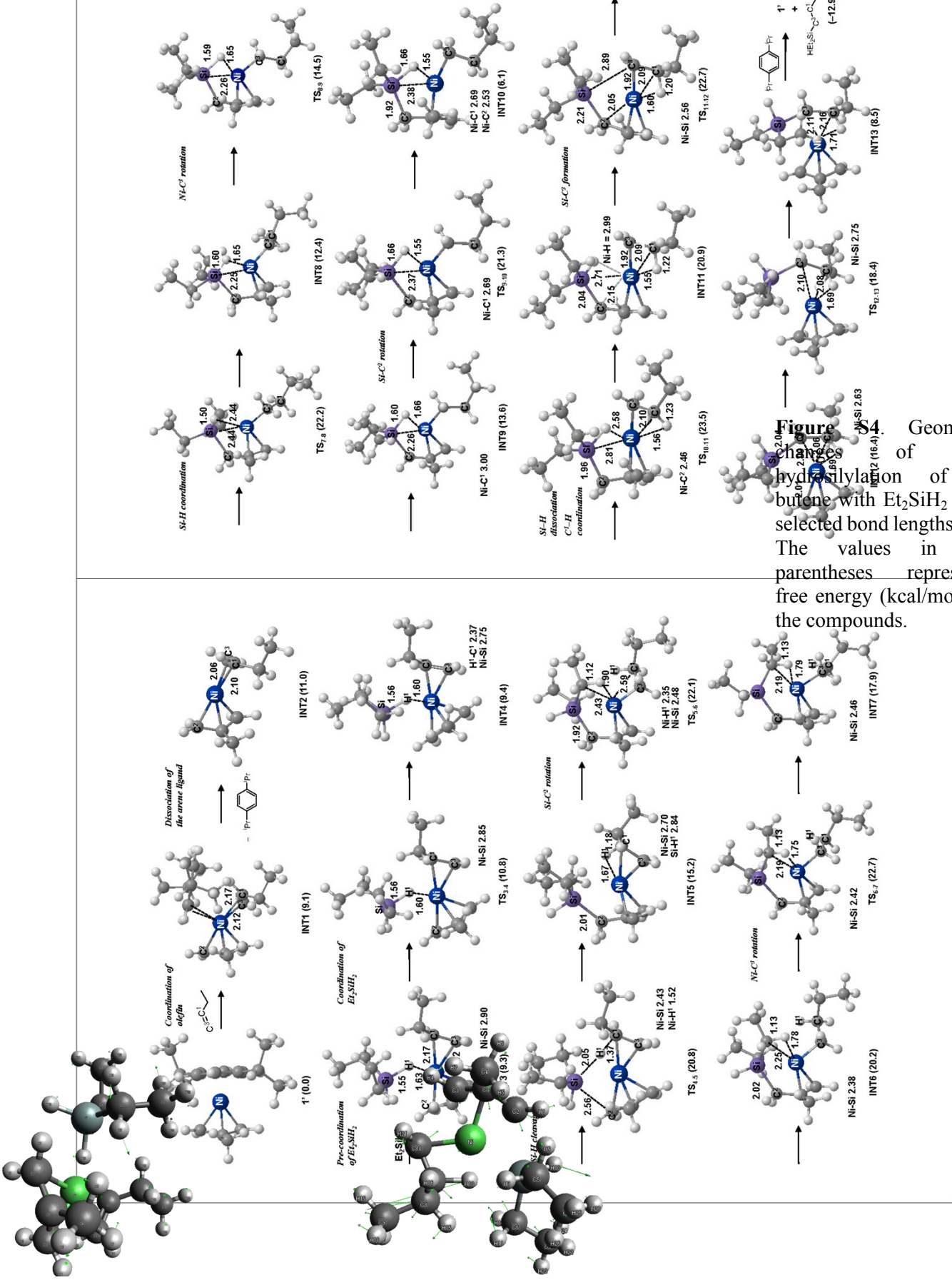
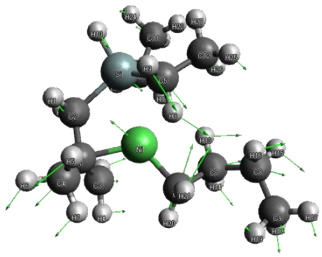


Figure S4. Geom changes of hydrosilylation of butene with Et_2SiH_2 selected bond lengths The values in parentheses repres free energy (kcal/mo the compounds.

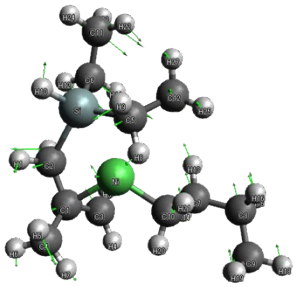
(a) TS_{3-4}: -92.17 cm^{-1}

(b) TS_{4-5}: -309.13 cm^{-1}

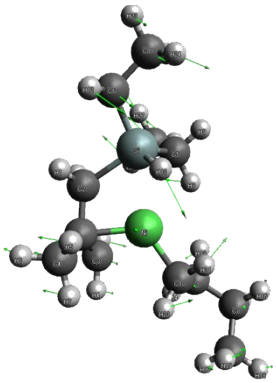
(c) TS_{5-6}: -75.75 cm^{-1}



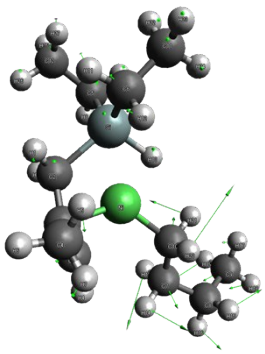
(d) TS_{6-7}: -29.87 cm^{-1}



(e) TS_{7-8}: -64.62 cm^{-1}

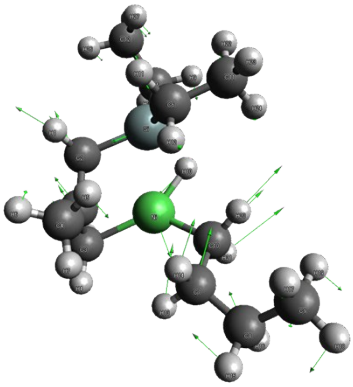


(f) TS_{8-9}: -70.64 cm^{-1}

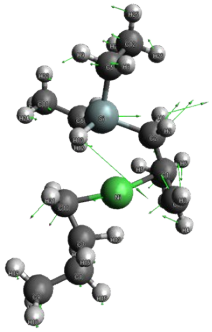


(g) TS_{9-10}: -161.25 cm^{-1}

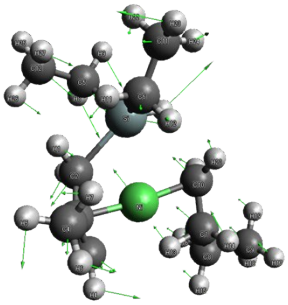
(h) TS_{10-11} -168.47 cm^{-1}



(i) $TS_{11\text{-}12}$: -65.09 cm^{-1}



(j) $TS_{12\text{-}13}$: -52.75 cm^{-1}



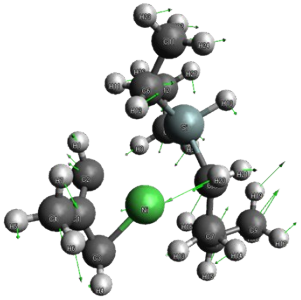


Figure S5. The displacement vectors (depicted by the arrows) associated with the imaginary modes of computed transition states. (a) **$TS_{3\text{-}4}$**, (b) **$TS_{4\text{-}5}$**, (c) **$TS_{5\text{-}6}$**, (d) **$TS_{6\text{-}7}$**, (e) **$TS_{7\text{-}8}$**, (f) **$TS_{8\text{-}9}$**, (g) **$TS_{9\text{-}10}$**, (h) **$TS_{10\text{-}11}$**, (i) **$TS_{11\text{-}12}$**, (j) **$TS_{12\text{-}13}$**.

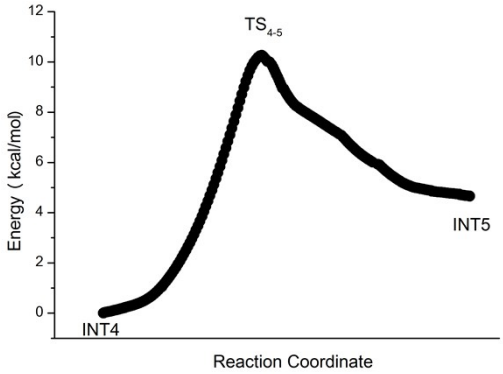


Figure S6. Energy change (zero point energy correction is not included) of the Si–H cleavage step from **INT4** to **INT5** via **$TS_{4\text{-}5}$**.

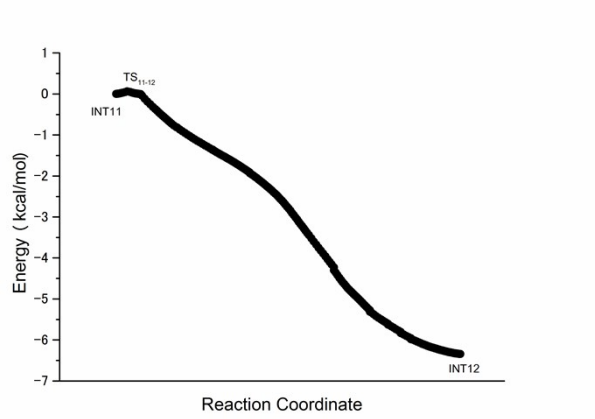


Figure S7. Energy change (zero point energy correction is not included) of the Si–C forming step from **INT11** to **INT12** via **TS_{11-12}**.

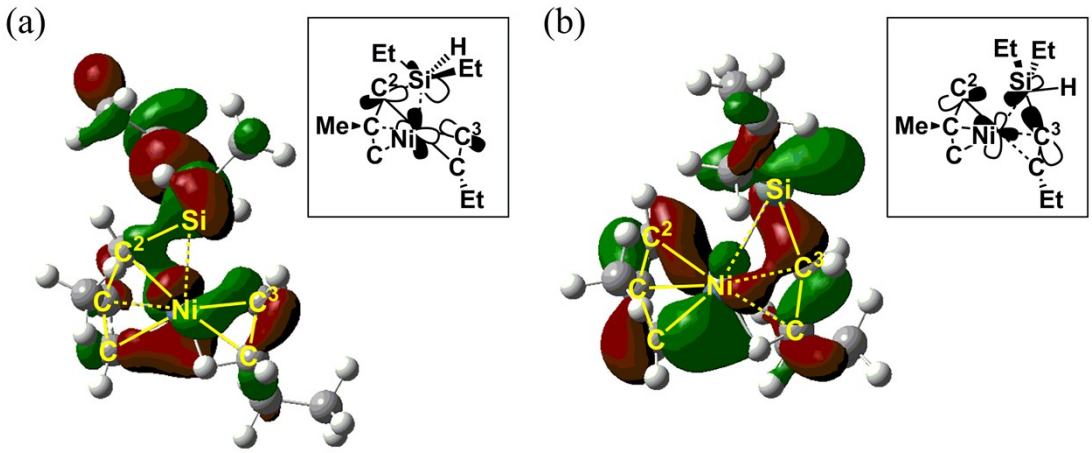


Figure S8. (a) 62th orbital of **INT11** (b) 60th orbital of **INT12**. Insets show schematic pictures of major orbital contributions.

Table S1. NBO charge of the Si–H bond activation and Si–C bond formation

	INT3	**TS_{3-4}**	**INT4**	**INT11**	**TS_{11-12}**	**INT12**
Ni	0.32	0.11	0.40	0.37	0.28	0.36
Si	1.31	1.31	1.37	1.41	1.38	1.41
H1	-0.14	0.20	0.22	0.26	0.27	0.25
C1	-0.19	-0.31	-0.40	-0.38	-0.38	-0.38
C2	-0.40	-0.50	-0.82	-0.80	-0.67	-0.41

C3	-0.41	-0.38	-0.40	-0.45	-0.46	-0.81

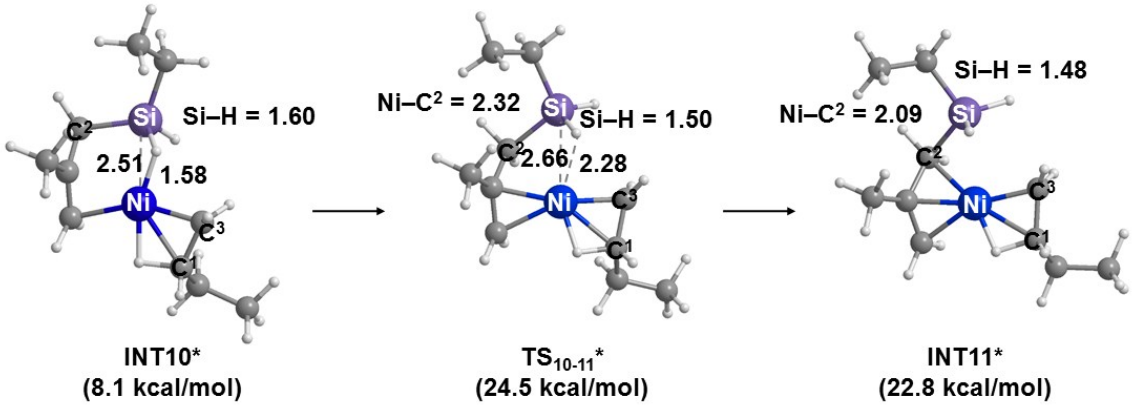


Figure S9. Geometry of the transition state **$TS_{10\text{-}11}$*** of the rate-limiting Si–H bond dissociation step with selected bond lengths (Å). The values in the parentheses represents free energy of the compounds.

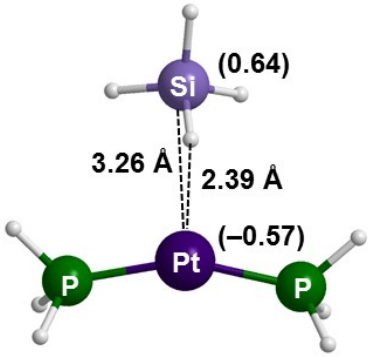


Figure S10. Geometry of [Pt(SiH_4)(PH_3)$_2$] with selected bond lengths (Å). The values in the parentheses represents Natural charges of the compounds.

Table S2. Total energies (Hartrees) of all molecules calculated at M06/SDD-6-311G(d) (SMD) level of theory

System	E_{sol} (a. u)	G_{sol} (a. u)
1-butene	-157.128415	-157.048993
Et_2SiH_2	-449.057290	-448.942979
1'	-795.267666	-794.948174
INT1	-952.404839	-951.982640
INT2	-484.496146	-484.327859
INT3	-933.582219	-933.273598
$TS_{3\text{-}4}$	-933.579475	-933.271189
INT4	-933.581048	-933.273415
$TS_{4\text{-}5}$	-933.563982	-933.255179
INT5	-933.573512	-933.264220
$TS_{5\text{-}6}$	-933.563964	-933.253201
INT6	-933.566163	-933.256251
$TS_{6\text{-}7}$	-933.565093	-933.252200

INT7	-933.571375	-933.259812
TS_{7-8}	-933.561874	-933.253023
INT8	-933.576340	-933.268678
TS_{8-9}	-933.573371	-933.265267
INT9	-933.575220	-933.266685
TS_{9-10}	-933.561285	-933.254442
INT10	-933.588927	-933.278658
TS_{10-11}	-933.559818	-933.250881
INT11	-933.562831	-933.254983
TS_{11-12}	-933.562236	-933.252251
INT12	-933.572958	-933.262291
TS_{12-13}	-933.570935	-933.259132
INT13	-933.584859	-933.274806
$Et_2(n\text{Bu})SiH$	-606.232515	-606.012619
$^{i}Pr_2C_6H_4$	-467.878445	-467.651748

Table 3. Cartesian coordinates of all compounds calculated at M06/SDD-6-311G(d) (SMD) level of theory

1'

Atomic Number	X	Y	Z
28	0.029322000	0.702407000	-0.092682000
6	-0.654332000	2.557880000	0.041537000
6	-0.795976000	2.083052000	-1.275744000
1	-0.000979000	2.245591000	-2.002309000
1	-1.787112000	1.895066000	-1.681632000
6	0.667223000	2.482297000	0.525833000
1	0.859943000	2.611179000	1.588836000
1	1.507036000	2.670599000	-0.142323000
6	-1.820352000	2.796213000	0.943450000
1	-2.075005000	3.862425000	0.934697000
1	-2.705944000	2.243177000	0.614826000
1	-1.586985000	2.521377000	1.976731000
6	-0.476530000	-1.161134000	-0.988328000
6	-1.213917000	-1.144775000	0.222309000
6	0.924413000	-1.032264000	-1.017562000
1	1.439192000	-1.080440000	-1.971097000
6	-0.506936000	-0.889446000	1.401181000
6	1.623018000	-0.718334000	0.156961000
1	-1.039038000	-0.819096000	2.345658000
6	0.868476000	-0.611338000	1.352699000
1	1.383691000	-0.312154000	2.261814000
1	-1.002560000	-1.303644000	-1.927355000
6	3.108727000	-0.474775000	0.196645000
1	3.280756000	0.258805000	0.998245000
6	3.811859000	-1.774860000	0.577803000
1	3.636989000	-2.541143000	-0.187860000
1	3.451546000	-2.163774000	1.536252000
1	4.892295000	-1.617258000	0.656952000
6	-2.698133000	-1.403456000	0.250930000

INT1

Atomic Number	X	Y	Z
28	-0.438323000	-1.299755000	-0.209080000
6	-1.958857000	-2.212495000	-1.214340000
6	-1.689607000	-2.823293000	0.026240000
1	-0.979778000	-3.649502000	0.073466000
1	-2.425270000	-2.781302000	0.825536000
6	-0.838459000	-2.117661000	-2.037695000
1	-0.858356000	-1.505472000	-2.935713000
1	-0.069946000	-2.890306000	-1.995179000
6	-3.206909000	-1.434498000	-1.465338000
1	-3.948676000	-2.088962000	-1.937903000
1	-3.645102000	-1.064072000	-0.533741000
1	-3.029851000	-0.595215000	-2.144649000
6	1.064195000	2.320940000	0.194904000
6	0.094505000	1.998820000	-0.741395000
6	2.118747000	1.451578000	0.493350000
1	2.856338000	1.761571000	1.228414000
6	0.213957000	0.761761000	-1.393926000
6	2.243702000	0.228939000	-0.141965000
1	-0.470740000	0.536778000	-2.208632000
6	1.264581000	-0.114350000	-1.097427000
1	1.450138000	-0.981447000	-1.733182000
1	1.020528000	3.276488000	0.710667000
6	3.412538000	-0.701511000	0.072881000
1	3.026652000	-1.727452000	-0.036691000
6	4.452064000	-0.475066000	-1.023307000
1	4.854358000	0.543790000	-0.958911000
1	4.025523000	-0.606259000	-2.023356000
1	5.286503000	-1.176461000	-0.914095000
6	-1.067274000	2.902927000	-1.078535000

1	-3.057156000	-1.071346000	1.235207000
6	-2.942037000	-2.905993000	0.134648000
1	-2.422094000	-3.461207000	0.922436000
1	-2.590863000	-3.281621000	-0.834548000
1	-4.011986000	-3.125050000	0.212286000
6	3.668263000	0.086467000	-1.098970000
1	3.124149000	0.979709000	-1.426835000
1	4.718751000	0.361006000	-0.962780000
1	3.630103000	-0.654197000	-1.906404000
6	-3.468712000	-0.643897000	-0.817981000
1	-4.540567000	-0.838740000	-0.711288000
1	-3.314067000	0.437377000	-0.738434000
1	-3.181427000	-0.957834000	-1.828426000

1	-1.255639000	2.786498000	-2.156471000
6	-0.805469000	4.373563000	-0.801086000
1	0.110597000	4.726764000	-1.286240000
1	-0.718641000	4.570835000	0.274303000
1	-1.638619000	4.978401000	-1.173319000
6	4.059050000	-0.577994000	1.442905000
1	3.333091000	-0.684416000	2.256948000
1	4.821862000	-1.353339000	1.567798000
1	4.560269000	0.389658000	1.563334000
6	-2.319155000	2.439204000	-0.337282000
1	-3.180576000	3.063493000	-0.599245000
1	-2.569460000	1.399181000	-0.578013000
1	-2.168758000	2.509991000	0.748816000
6	-0.599811000	-0.373233000	1.748217000
1	-0.083453000	0.564361000	1.537803000
6	-2.021534000	-0.227952000	2.185961000
1	-2.637103000	0.103944000	1.338308000
1	-2.417321000	-1.195670000	2.515309000
6	-2.121217000	0.801139000	3.304009000
1	-1.740308000	1.775809000	2.975814000
1	-3.159077000	0.935750000	3.621464000
1	-1.536946000	0.492526000	4.177522000
6	0.130610000	-1.518034000	1.819598000
1	1.211390000	-1.508649000	1.700467000
1	-0.304529000	-2.430884000	2.219019000

INT2

Atomic Number	X	Y	Z
28	-0.477871000	-0.680361000	-0.279938000
6	-1.926010000	0.617823000	0.280635000
6	-2.472646000	-0.415460000	-0.470778000
1	-2.895134000	-0.220232000	-1.453408000
1	-2.734105000	-1.363749000	0.001082000
6	-1.108449000	0.155383000	1.346590000
1	-1.417901000	-0.714611000	1.927708000
1	-0.422846000	0.842138000	1.838927000
6	-1.876277000	2.028328000	-0.197015000
1	-2.053602000	2.096259000	-1.273323000
1	-2.663615000	2.600956000	0.306992000
1	-0.922280000	2.503834000	0.047742000
6	1.614460000	-0.520293000	-0.353187000
1	1.739228000	-0.729379000	-1.421156000
6	2.100783000	0.813742000	0.108365000
1	1.562710000	1.608275000	-0.426019000
1	1.886578000	0.935677000	1.176818000
6	3.595641000	0.950544000	-0.154075000
1	3.821198000	0.847281000	-1.221047000
1	3.960101000	1.928189000	0.173071000
1	4.158340000	0.180095000	0.383580000
6	1.238875000	-1.543453000	0.465090000
1	1.107004000	-2.552464000	0.075711000
1	1.256437000	-1.431846000	1.547843000

INT3

Atomic Number	X	Y	Z
28	1.044180000	0.040423000	-0.627409000
6	2.465142000	-1.192196000	0.168097000
6	1.793506000	-1.823902000	-0.879066000
1	1.206742000	-2.720375000	-0.695126000
1	2.102874000	-1.655298000	-1.911690000
6	2.979736000	0.078638000	-0.158891000
1	3.415737000	0.249727000	-1.143119000
1	3.329807000	0.733219000	0.636156000
6	2.372520000	-1.653387000	1.583483000
1	1.555412000	-2.363313000	1.734025000
1	3.308328000	-2.162055000	1.843992000
1	2.259358000	-0.812449000	2.274961000
14	-1.593431000	-1.159132000	-0.768023000
6	-1.335349000	-2.028039000	0.866595000
1	-0.549321000	-2.785194000	0.759765000
1	-2.261340000	-2.594524000	1.044621000
1	-1.795455000	-2.135789000	-1.863291000
6	-2.955486000	0.120670000	-0.703337000
1	-2.665733000	0.921798000	-0.009518000
1	-3.048460000	0.587549000	-1.692226000
1	-0.369144000	-0.388136000	-1.319223000
6	0.110421000	1.990965000	-0.444512000
1	-0.770976000	1.880926000	-1.077439000
6	-0.143102000	2.330469000	0.988743000
1	-0.840904000	1.609109000	1.430040000
1	0.795048000	2.267000000	1.556630000
6	-0.738609000	3.729969000	1.090870000

1	-1.676005000	3.798226000	0.526468000
1	-0.954337000	3.989192000	2.131217000
1	-0.049044000	4.478810000	0.686554000
6	1.329640000	2.095938000	-1.037726000
1	1.436089000	2.045023000	-2.119830000
1	2.185548000	2.466295000	-0.480348000
6	-4.284054000	-0.500161000	-0.277217000
1	-4.236513000	-0.900550000	0.741697000
1	-5.092375000	0.237737000	-0.297967000
1	-4.578246000	-1.323399000	-0.939019000
6	-1.048257000	-1.105738000	2.043284000
1	-0.905420000	-1.671301000	2.970325000
1	-0.138195000	-0.515762000	1.875303000
1	-1.869134000	-0.399823000	2.214882000

TS_{3-4}

Atomic Number	X	Y	Z
28	1.130976000	-0.137468000	-0.556971000
6	2.319717000	-1.599283000	0.196791000
6	1.246897000	-2.161044000	-0.503154000
1	0.515316000	-2.761542000	0.033047000
1	1.324399000	-2.342919000	-1.575352000
6	3.079921000	-0.681730000	-0.544191000
1	3.208510000	-0.826842000	-1.616719000
1	3.839414000	-0.084544000	-0.049292000
6	2.440725000	-1.679266000	1.682682000
1	1.524573000	-2.052607000	2.147034000
1	3.252355000	-2.368093000	1.943158000
1	2.692033000	-0.703389000	2.111808000
14	-1.616584000	-0.891795000	-0.472782000
6	-1.661898000	-1.234466000	1.373565000
1	-0.637716000	-1.377910000	1.739643000
1	-2.151398000	-2.213024000	1.481113000
1	-1.523271000	-2.130482000	-1.274181000
6	-3.034595000	0.166949000	-1.083833000
1	-3.067543000	1.102576000	-0.510998000
1	-2.837417000	0.449235000	-2.125566000
1	-0.423808000	-0.001859000	-0.925336000
6	0.717671000	1.952245000	-0.647342000
1	0.208343000	2.096790000	-1.601425000
6	-0.036497000	2.336430000	0.590756000
1	-1.076814000	1.996683000	0.525333000
1	0.411424000	1.841020000	1.464335000
6	-0.009508000	3.848307000	0.778294000
1	-0.447107000	4.359666000	-0.086080000
1	-0.577142000	4.142601000	1.665816000
1	1.018330000	4.208187000	0.895369000
6	2.067470000	1.755484000	-0.642665000
1	2.643224000	1.762028000	-1.563830000
1	2.626500000	1.863130000	0.285524000
6	-4.359144000	-0.585663000	-0.974882000
1	-4.583235000	-0.872190000	0.059314000
1	-5.195527000	0.025003000	-1.330032000
1	-4.350342000	-1.504302000	-1.572537000
6	-2.386631000	-0.198627000	2.226837000

INT4

Atomic Number	X	Y	Z
28	1.128389000	-0.034578000	-0.581417000
6	2.417445000	-1.430654000	0.158816000
6	1.489973000	-2.022126000	-0.705061000
1	0.792079000	-2.762587000	-0.321275000
1	1.681279000	-2.056253000	-1.777953000
6	3.117507000	-0.346028000	-0.391633000
1	3.373378000	-0.348216000	-1.450939000
1	3.738194000	0.274024000	0.248013000
6	2.432748000	-1.691953000	1.628493000
1	1.549935000	-2.245879000	1.955925000
1	3.316956000	-2.291056000	1.874368000
1	2.505658000	-0.757813000	2.196021000
14	-1.459528000	-0.965364000	-0.496605000
6	-1.226743000	-1.204677000	1.359320000
1	-0.282996000	-0.738354000	1.669554000
1	-1.090275000	-2.281497000	1.524731000
1	-1.455958000	-2.243696000	-1.241953000
6	-2.962832000	0.040882000	-0.995898000
1	-3.100453000	0.873569000	-0.295254000
1	-2.767772000	0.493897000	-1.976362000
1	-0.340132000	-0.133986000	-1.202513000
6	0.466828000	2.000386000	-0.556352000
1	-0.079736000	2.112521000	-1.494246000
6	-0.294977000	2.275148000	0.704756000
1	-1.253758000	1.742779000	0.707738000
1	0.279174000	1.916439000	1.569777000
6	-0.555339000	3.771238000	0.835403000
1	-1.112214000	4.150978000	-0.028171000
1	-1.138502000	3.989910000	1.734508000
1	0.387521000	4.325177000	0.896804000
6	1.829742000	1.959328000	-0.584503000
1	2.380122000	2.042613000	-1.517793000
1	2.393654000	2.117680000	0.332077000
6	-4.220346000	-0.823804000	-1.057273000
1	-4.435783000	-1.306720000	-0.096670000
1	-5.098940000	-0.227094000	-1.323616000
1	-4.124229000	-1.617355000	-1.806539000
6	-2.372025000	-0.680386000	2.220007000

1	-2.424899000	-0.518876000	3.273119000	1	-2.197828000	-0.909507000	3.276317000
1	-1.887900000	0.775564000	2.205725000	1	-2.479423000	0.406632000	2.138474000
1	-3.420225000	-0.045682000	1.897989000	1	-3.333336000	-1.127052000	1.944671000

TS_{4-5}

Atomic Number	X	Y	Z
28	0.960616000	-0.192388000	-0.496098000
6	1.950865000	-1.839484000	0.048349000
6	0.697292000	-2.202604000	-0.524973000
1	0.030784000	-2.806438000	0.086787000
1	0.664681000	-2.437492000	-1.589006000
6	2.801084000	-1.085542000	-0.754807000
1	2.749107000	-1.169245000	-1.839636000
1	3.716969000	-0.673442000	-0.344908000
6	2.180467000	-1.983637000	1.517167000
1	1.249322000	-1.847936000	2.078297000
1	2.544325000	-2.995077000	1.732267000
1	2.926964000	-1.271983000	1.880669000
14	-1.403955000	-0.751294000	-0.347361000
6	-1.629543000	-0.865035000	1.515525000
1	-1.092323000	-0.020568000	1.970552000
1	-1.124345000	-1.770920000	1.874766000
1	-1.816288000	-1.986902000	-1.058326000
6	-2.457336000	0.618039000	-1.125946000
1	-2.469575000	1.483078000	-0.447697000
1	-1.976866000	0.962710000	-2.050768000
1	-0.143138000	0.843553000	-0.598497000
6	0.746762000	1.879689000	-0.458412000
1	0.355294000	2.359085000	-1.361857000
6	0.260171000	2.477709000	0.847344000
1	-0.834602000	2.446037000	0.897070000
1	0.636156000	1.866028000	1.678574000
6	0.747950000	3.909819000	0.978187000
1	0.386626000	4.525841000	0.147158000
1	0.391776000	4.360954000	1.908365000
1	1.842492000	3.955509000	0.977040000
6	2.091409000	1.417332000	-0.534601000
1	2.633900000	1.489936000	-1.473564000
1	2.701782000	1.464534000	0.366664000
6	-3.874529000	0.142652000	-1.429099000
1	-4.396735000	-0.203121000	-0.530425000
1	-4.477351000	0.945936000	-1.866973000
1	-3.869805000	-0.688174000	-2.143547000
6	-3.089761000	-0.860257000	1.958519000
1	-3.172190000	-0.954257000	3.046578000
1	-3.598342000	0.067783000	1.674536000
1	-3.649467000	-1.692535000	1.516167000

INT5

Atomic Number	X	Y	Z
28	0.644083000	-0.607061000	-0.436751000
6	0.487104000	-2.337321000	0.417770000
6	-0.954140000	-2.005704000	0.368890000
1	-1.415760000	-2.258960000	1.333417000
1	-1.469486000	-2.536634000	-0.440007000
6	1.170034000	-2.536213000	-0.767433000
1	0.634099000	-2.724925000	-1.696691000
1	2.228195000	-2.778430000	-0.753904000
6	1.157804000	-2.375410000	1.750794000
1	0.862418000	-1.515765000	2.365447000
1	0.846049000	-3.276657000	2.293335000
1	2.246243000	-2.392067000	1.652838000
14	-1.931502000	-0.249192000	0.299647000
6	-1.453761000	0.882253000	1.717711000
1	-0.376274000	1.092358000	1.702798000
1	-1.638660000	0.334963000	2.652431000
1	-3.264591000	-0.838543000	0.580848000
6	-2.067814000	0.583206000	-1.390898000
1	-1.489713000	1.517115000	-1.384062000
1	-1.603965000	-0.054064000	-2.156920000
1	0.442863000	1.048208000	-0.564203000
6	1.574285000	1.291365000	-0.772435000
1	1.444091000	1.871229000	-1.694196000
6	2.008192000	2.141100000	0.412940000
1	1.224112000	2.870112000	0.651594000
1	2.111010000	1.489281000	1.292591000
6	3.315188000	2.853585000	0.124490000
1	3.217552000	3.512848000	-0.745553000
1	3.627198000	3.467248000	0.974316000
1	4.120239000	2.140869000	-0.087446000
6	2.314174000	0.035014000	-0.985289000
1	2.550055000	-0.264836000	-2.005900000
1	3.091712000	-0.218344000	-0.261437000
6	-3.520961000	0.875543000	-1.760044000
1	-4.009931000	1.506259000	-1.008209000
1	-3.590814000	1.397245000	-2.720291000
1	-4.106653000	-0.046328000	-1.840853000
6	-2.247361000	2.185083000	1.690684000
1	-2.011992000	2.816784000	2.553562000
1	-2.029440000	2.771251000	0.789512000
1	-3.328324000	2.001171000	1.707878000

TS_{4-5}

Atomic Number	X	Y	Z
28	-0.091876000	0.679350000	-0.095322000
6	0.962854000	2.294503000	-0.107804000
6	2.119961000	1.385274000	0.102832000
1	2.673724000	1.677427000	1.002579000

INT6

Atomic Number	X	Y	Z
28	-0.075543000	0.615944000	0.288933000
6	0.470894000	2.346110000	-0.399024000
6	1.797586000	1.708702000	-0.212752000
1	2.395954000	2.231660000	0.537895000

1	2.790373000	1.385392000	-0.766953000	1	2.339325000	1.664616000	-1.168862000
6	0.259428000	2.211161000	-1.308210000	6	-0.398288000	1.778056000	-1.319740000
1	0.695732000	1.706134000	-2.171423000	1	-0.026484000	1.111244000	-2.098881000
1	-0.550146000	2.905045000	-1.510401000	1	-1.381681000	2.208829000	-1.477998000
6	0.609055000	3.261736000	0.968282000	6	0.102439000	3.509721000	0.451592000
1	0.643517000	2.781421000	1.953112000	1	0.403708000	3.348858000	1.492360000
1	1.343739000	4.076976000	0.983633000	1	0.637859000	4.399948000	0.097729000
1	-0.382941000	3.693464000	0.809557000	1	-0.970415000	3.713987000	0.408228000
14	1.986596000	-0.580246000	0.397433000	14	2.146049000	-0.240166000	0.205489000
6	0.539861000	-0.967201000	1.577042000	6	1.004077000	-0.858212000	1.607858000
1	-0.416609000	-0.399012000	1.439685000	1	-0.038410000	-0.439666000	1.720141000
1	0.868419000	-0.608416000	2.561520000	1	1.468217000	-0.482875000	2.528301000
1	3.252088000	-0.854654000	1.111234000	1	3.521770000	-0.139508000	0.733457000
6	1.924720000	-1.500184000	-1.237386000	6	2.071183000	-1.251887000	-1.366879000
1	0.881604000	-1.571111000	-1.579228000	1	1.024002000	-1.507971000	-1.581192000
1	2.440685000	-0.878665000	-1.982182000	1	2.396290000	-0.600034000	-2.189250000
1	-1.331624000	-1.212138000	-0.750444000	1	-1.394824000	-1.747605000	-0.238212000
6	-2.246081000	-0.584759000	-0.774376000	6	-2.181979000	-1.001383000	-0.426437000
1	-2.531272000	-0.558837000	-1.833528000	1	-2.117053000	-0.741035000	-1.493056000
6	-3.308684000	-1.304983000	0.053677000	6	-3.537337000	-1.659758000	-0.151232000
1	-3.360903000	-2.353004000	-0.267009000	1	-3.601029000	-2.580235000	-0.745495000
1	-2.989307000	-1.318114000	1.105931000	1	-3.575957000	-1.969653000	0.902400000
6	-4.674402000	-0.656449000	-0.069811000	6	-4.717978000	-0.761616000	-0.469400000
1	-5.008418000	-0.646720000	-1.114176000	1	-4.663639000	-0.391735000	-1.501000000
1	-5.428201000	-1.193007000	0.514498000	1	-5.666567000	-1.296728000	-0.360014000
1	-4.661801000	0.381854000	0.281717000	1	-4.758113000	0.110264000	0.192733000
6	-1.958821000	0.816669000	-0.287130000	6	-1.946433000	0.228268000	0.418871000
1	-2.310569000	1.622556000	-0.930704000	1	-2.540584000	1.094609000	0.118611000
1	-2.248686000	1.008951000	0.756998000	1	-2.103717000	0.038934000	1.491226000
6	2.564954000	-2.884865000	-1.174345000	6	2.938840000	-2.507709000	-1.322488000
1	2.059127000	-3.539254000	-0.455986000	1	2.616767000	-3.204952000	-0.541811000
1	2.530901000	-3.383167000	-2.148494000	1	2.900013000	-3.045973000	-2.274778000
1	3.616692000	-2.822041000	-0.873590000	1	3.988492000	-2.260570000	-1.128547000
6	0.188199000	-2.451079000	1.609120000	6	0.855451000	-2.377157000	1.635069000
1	-0.578361000	-2.663796000	2.360561000	1	0.218906000	-2.698490000	2.464797000
1	-0.190000000	-2.796293000	0.640164000	1	0.415850000	-2.761027000	0.708752000
1	1.066165000	-3.058283000	1.856533000	1	1.831087000	-2.857830000	1.762868000

TS_{6-7}

Atomic Number	X	Y	Z
28	0.124801000	0.522223000	-0.262602000
6	-0.245318000	2.320307000	0.379333000
6	-1.616091000	1.772836000	0.323591000
1	-2.269791000	2.399882000	-0.289437000
1	-2.026292000	1.644154000	1.332148000
6	0.649303000	1.735180000	1.261410000
1	0.291532000	1.134147000	2.098462000
1	1.670266000	2.098377000	1.320925000
6	0.140370000	3.403222000	-0.565761000
1	-0.248953000	3.206333000	-1.570796000
1	-0.302070000	4.350106000	-0.231469000
1	1.224977000	3.529345000	-0.610921000
14	-2.225877000	-0.057922000	-0.373846000

INT7

Atomic Number	X	Y	Z
28	0.270050000	0.293904000	-0.039456000
6	-0.167937000	2.160538000	0.405359000
6	-1.488959000	1.544858000	0.643768000
1	-2.299382000	2.212431000	0.315110000
1	-1.650686000	1.247417000	1.684875000
6	0.903110000	1.743987000	1.183085000
1	0.735234000	1.241170000	2.136203000
1	1.886473000	2.176812000	1.029584000
6	-0.025611000	3.148452000	-0.700550000
1	-0.597958000	2.843310000	-1.583790000
1	-0.427832000	4.116161000	-0.375783000
1	1.021796000	3.290960000	-0.977877000
14	-2.136861000	0.017686000	-0.482588000

6	-0.921135000	-1.043907000	-1.374163000	6	-0.945862000	-1.471803000	-0.502945000
1	0.034484000	-0.510736000	-1.668184000	1	0.122576000	-1.304841000	-0.830786000
1	-1.356989000	-1.064498000	-2.381652000	1	-1.264675000	-2.048780000	-1.382969000
1	-3.310912000	0.350413000	-1.287290000	1	-2.323699000	0.549443000	-1.849294000
6	-2.854391000	-0.978634000	1.121243000	6	-3.729607000	-0.445849000	0.368011000
1	-1.990519000	-1.320736000	1.709148000	1	-3.495954000	-0.747194000	1.397679000
1	-3.383007000	-0.253473000	1.753903000	1	-4.334409000	0.467374000	0.447674000
1	1.536395000	-1.573951000	0.957865000	1	2.027420000	-1.810216000	0.687816000
6	2.364634000	-0.892464000	0.714487000	6	2.720847000	-0.989619000	0.452727000
1	2.548371000	-0.297179000	1.619281000	1	2.913048000	-0.463607000	1.398977000
6	3.603477000	-1.734289000	0.404834000	6	4.029770000	-1.597216000	-0.059878000
1	3.790762000	-2.404924000	1.253266000	1	4.394156000	-2.312115000	0.689019000
1	3.388958000	-2.380890000	-0.458343000	1	3.821261000	-2.180890000	-0.967393000
6	4.840033000	-0.898851000	0.129802000	6	5.104929000	-0.565723000	-0.347374000
1	5.041276000	-0.210743000	0.960546000	1	5.289093000	0.066420000	0.530395000
1	5.726914000	-1.526599000	-0.001692000	1	6.052922000	-1.042884000	-0.614970000
1	4.729674000	-0.296340000	-0.778665000	1	4.827124000	0.093499000	-1.177280000
6	1.979028000	0.013769000	-0.434756000	6	2.089368000	-0.043375000	-0.539463000
1	2.574315000	0.929799000	-0.497854000	1	2.621848000	0.905179000	-0.645513000
1	2.037550000	-0.512247000	-1.398784000	1	1.965100000	-0.493759000	-1.536336000
6	-3.782251000	-2.136977000	0.767870000	6	-4.494968000	-1.540843000	-0.365917000
1	-3.285063000	-2.895612000	0.154379000	1	-3.925087000	-2.476045000	-0.407513000
1	-4.148630000	-2.638043000	1.669318000	1	-5.444593000	-1.761665000	0.131362000
1	-4.658491000	-1.787526000	0.210306000	1	-4.727100000	-1.250332000	-1.396770000
6	-0.573217000	-2.447858000	-0.889167000	6	-0.974180000	-2.310190000	0.771236000
1	0.308022000	-2.835060000	-1.411283000	1	-0.241251000	-3.121394000	0.730969000
1	-0.362510000	-2.481434000	0.184368000	1	-0.755414000	-1.710868000	1.664465000
1	-1.399065000	-3.137901000	-1.083172000	1	-1.960780000	-2.761812000	0.914802000

TS_{7-8}

Atomic Number	X	Y	Z
28	0.398882000	0.350389000	-0.136590000
6	-0.116364000	2.073665000	0.556324000
6	-1.440577000	1.415998000	0.616553000
1	-2.210643000	2.073651000	0.191879000
1	-1.717847000	1.108686000	1.632375000
6	0.915684000	1.560115000	1.343665000
1	0.698117000	0.935748000	2.210998000
1	1.898626000	2.020631000	1.311235000
6	0.071596000	3.226000000	-0.368203000
1	-0.428756000	3.048105000	-1.326555000
1	-0.383543000	4.122161000	0.072319000
1	1.131073000	3.431033000	-0.542293000
14	-1.955477000	-0.204685000	-0.458426000
6	-1.304345000	-1.793451000	0.319538000
1	-0.211132000	-1.910597000	0.201291000
1	-1.720049000	-2.608392000	-0.292237000
1	-1.333426000	-0.030078000	-1.814720000
6	-3.816281000	-0.087584000	-0.468600000
1	-4.141868000	0.084861000	0.566714000
1	-4.089805000	0.816783000	-1.026908000
1	2.098060000	-1.683431000	0.708082000
6	2.831238000	-0.937994000	0.365002000
1	3.172759000	-0.399083000	1.259641000

INT8

Atomic Number	X	Y	Z
28	0.439581000	0.311526000	0.052317000
6	-0.103668000	2.185891000	0.222304000
6	-1.244827000	1.402150000	0.736510000
1	-2.202361000	1.791335000	0.359519000
1	-1.261367000	1.289879000	1.824610000
6	1.127830000	2.024865000	0.846807000
1	1.187749000	1.684493000	1.880979000
1	2.004949000	2.521742000	0.444655000
6	-0.277351000	2.984390000	-1.021458000
1	-0.920844000	2.469266000	-1.742805000
1	-0.767540000	3.934063000	-0.773299000
1	0.684800000	3.208993000	-1.488124000
14	-1.669015000	-0.472822000	0.001858000
6	-2.484885000	-1.406886000	1.380755000
1	-1.824826000	-1.385321000	2.256531000
1	-2.550708000	-2.459199000	1.071815000
1	-0.249538000	-1.152419000	-0.317129000
6	-2.644962000	-0.343205000	-1.571495000
1	-3.514104000	0.301101000	-1.378813000
1	-2.035276000	0.173174000	-2.323400000
1	2.132926000	-1.637239000	1.097723000
6	2.846984000	-0.946343000	0.626352000
1	3.144297000	-0.226993000	1.403114000

6	4.019072000	-1.678615000	-0.257053000	6	4.076456000	-1.750558000	0.193032000
1	4.381702000	-2.416770000	0.469504000	1	4.458164000	-2.295382000	1.066145000
1	3.671198000	-2.249374000	-1.129316000	1	3.765429000	-2.513276000	-0.534542000
6	5.154726000	-0.757450000	-0.661052000	6	5.180917000	-0.894576000	-0.398175000
1	5.482357000	-0.143223000	0.186911000	1	5.461728000	-0.085724000	0.288161000
1	6.022154000	-1.325122000	-1.012210000	1	6.080169000	-1.485944000	-0.597867000
1	4.861843000	-0.077747000	-1.468907000	1	4.877200000	-0.434017000	-1.344653000
6	2.176926000	0.026290000	-0.590779000	6	2.186636000	-0.218166000	-0.520983000
1	2.747587000	0.937431000	-0.788706000	1	2.752179000	0.647470000	-0.876172000
1	1.871331000	-0.448221000	-1.549377000	1	1.960477000	-0.882101000	-1.368077000
6	-4.496244000	-1.317779000	-1.056661000	6	-3.091540000	-1.713099000	-2.078578000
1	-4.289598000	-2.217226000	-0.466703000	1	-3.756634000	-2.210932000	-1.364769000
1	-5.582801000	-1.189488000	-1.084450000	1	-3.635071000	-1.621855000	-3.023602000
1	-4.165190000	-1.513019000	-2.083080000	1	-2.239171000	-2.378816000	-2.256182000
6	-1.691379000	-1.951355000	1.784531000	6	-3.869972000	-0.858150000	1.715675000
1	-1.386024000	-2.926584000	2.175940000	1	-4.331757000	-1.430921000	2.525184000
1	-1.217720000	-1.186184000	2.410953000	1	-3.827394000	0.187461000	2.041178000
1	-2.774730000	-1.866902000	1.930513000	1	-4.545248000	-0.909953000	0.854447000

TS_{8-9}

Atomic Number	X	Y	Z
28	-0.419545000	0.270040000	-0.099779000
6	0.126121000	2.158696000	-0.081680000
6	1.285836000	1.428292000	-0.626212000
1	2.227064000	1.794992000	-0.189719000
1	1.333181000	1.407432000	-1.719103000
6	-1.085789000	2.057496000	-0.752315000
1	-1.121566000	1.816311000	-1.814816000
1	-1.966201000	2.526946000	-0.327161000
6	0.262922000	2.849399000	1.228829000
1	0.905330000	2.289012000	1.916512000
1	0.738073000	3.825375000	1.068604000
1	-0.710733000	3.018004000	1.695129000
14	1.712576000	-0.487781000	-0.038459000
6	2.560323000	-1.297537000	-1.475115000
1	1.907605000	-1.226225000	-2.353654000
1	2.650358000	-2.367851000	-1.244115000
1	0.300044000	-1.192852000	0.206677000
6	2.659765000	-0.485438000	1.557197000
1	3.525117000	0.181065000	1.438795000
1	2.031063000	-0.041601000	2.339166000
1	-3.294579000	-0.097476000	-1.367058000
6	-3.400591000	0.039267000	-0.280701000
1	-3.586379000	1.106392000	-0.115138000
6	-4.630650000	-0.744546000	0.189271000
1	-4.725623000	-0.643035000	1.279699000
1	-5.523306000	-0.271501000	-0.240358000
6	-4.608478000	-2.213235000	-0.193457000
1	-3.792003000	-2.754978000	0.296188000
1	-5.541445000	-2.712332000	0.087364000
1	-4.483010000	-2.333785000	-1.276739000
6	-2.141903000	-0.391185000	0.429252000
1	-2.148175000	-0.123523000	1.497012000
1	-1.964440000	-1.469877000	0.330179000

INT9

Atomic Number	X	Y	Z
28	-0.390780000	0.186955000	-0.258942000
6	0.017103000	2.072513000	0.100993000
6	1.270221000	1.503745000	-0.432946000
1	2.139373000	1.853672000	0.144435000
1	1.417341000	1.660324000	-1.505572000
6	-1.117268000	2.017063000	-0.697662000
1	-1.036915000	1.949597000	-1.782519000
1	-2.063936000	2.364314000	-0.299134000
6	-0.016747000	2.545387000	1.511482000
1	0.594662000	1.911403000	2.162377000
1	0.400939000	3.558666000	1.561107000
1	-1.040070000	2.582302000	1.893258000
14	1.777426000	-0.446340000	-0.088514000
6	2.864411000	-0.963004000	-1.499199000
1	2.332199000	-0.772555000	-2.439354000
1	2.993873000	-2.051942000	-1.434642000
1	0.405956000	-1.268435000	-0.167052000
6	2.503846000	-0.650534000	1.607574000
1	3.318607000	0.078104000	1.719609000
1	1.743338000	-0.382291000	2.351521000
1	-3.625602000	0.694819000	-0.685076000
6	-3.360726000	0.079834000	0.186267000
1	-3.220676000	0.771317000	1.029020000
6	-4.535019000	-0.847810000	0.507587000
1	-4.289176000	-1.444092000	1.397857000
1	-5.399757000	-0.229354000	0.781216000
6	-4.911937000	-1.766236000	-0.640873000
1	-4.116074000	-2.483901000	-0.868224000
1	-5.814359000	-2.342633000	-0.413549000
1	-5.108306000	-1.190753000	-1.554336000
6	-2.084641000	-0.676072000	-0.073511000
1	-1.850516000	-1.369810000	0.748745000
1	-2.090718000	-1.231910000	-1.023655000

6	3.110531000	-1.891177000	1.949124000	6	3.015776000	-2.071407000	1.837458000
1	3.793943000	-2.317641000	1.206881000	1	3.819064000	-2.329284000	1.138985000
1	3.635339000	-1.881472000	2.908806000	1	3.414160000	-2.184919000	2.849976000
1	2.261883000	-2.577544000	2.049236000	1	2.220133000	-2.815630000	1.716316000
6	3.933849000	-0.690589000	-1.752968000	6	4.219097000	-0.258017000	-1.475735000
1	4.421657000	-1.194298000	-2.592551000	1	4.843217000	-0.582794000	-2.313442000
1	3.866586000	0.373301000	-2.007156000	1	4.114508000	0.830300000	-1.552191000
1	4.599804000	-0.781681000	-0.887786000	1	4.771923000	-0.473288000	-0.554716000

$TS_{9\text{-}10}$

Atomic Number	**X**	**Y**	**Z**
28	0.358064000	-0.754319000	-0.836390000
6	-0.254867000	-2.051783000	0.728126000
6	-1.648452000	-1.517157000	0.507474000
1	-2.224744000	-1.541885000	1.444229000
1	-2.191365000	-2.098405000	-0.247337000
6	0.400561000	-2.780625000	-0.231132000
1	-0.128075000	-3.149580000	-1.111509000
1	1.377215000	-3.208281000	-0.024997000
6	0.344588000	-1.804934000	2.071504000
1	0.203286000	-0.771052000	2.404701000
1	-0.173836000	-2.439183000	2.802659000
1	1.408348000	-2.051871000	2.097553000
14	-1.624611000	0.312732000	-0.078499000
6	-3.139813000	0.721714000	-1.081349000
1	-3.238560000	-0.018837000	-1.884783000
1	-2.999380000	1.694522000	-1.568779000
1	-0.461721000	0.494561000	-1.252936000
6	-1.214078000	1.577896000	1.227441000
1	-1.920103000	1.442299000	2.059146000
1	-0.218934000	1.364827000	1.637915000
1	2.930258000	-1.145815000	-0.086372000
6	2.802483000	-0.065554000	0.064580000
1	2.466946000	0.087247000	1.100021000
6	4.173717000	0.609578000	-0.115776000
1	4.884941000	0.092442000	0.539839000
1	4.520404000	0.444194000	-1.144215000
6	4.162718000	2.092177000	0.202759000
1	3.757656000	2.275360000	1.205653000
1	5.174243000	2.508723000	0.173999000
1	3.555495000	2.660891000	-0.509496000
6	1.789275000	0.472278000	-0.896944000
1	1.471104000	1.500032000	-0.707361000
1	2.042487000	0.331584000	-1.960696000
6	-1.279063000	3.003777000	0.687683000
1	-2.291598000	3.267539000	0.363895000
1	-0.979657000	3.730325000	1.449262000
1	-0.613630000	3.143184000	-0.173430000
6	-4.385015000	0.730888000	-0.196101000
1	-5.282193000	0.959423000	-0.779769000
1	-4.548653000	-0.241832000	0.282703000
1	-4.313495000	1.482729000	0.598422000

$TS_{10\text{-}11}$

Atomic

10

Atomic Number	**X**	**Y**	**Z**
28	0.779093000	-0.292653000	-0.242563000
6	-0.405288000	-2.136843000	0.254606000
6	-1.806486000	-1.678570000	-0.019228000
1	-2.494250000	-1.983199000	0.777193000
1	-2.175172000	-2.079467000	-0.971043000
6	0.487777000	-2.330713000	-0.758342000
1	0.166931000	-2.266701000	-1.796981000
1	1.446889000	-2.804718000	-0.564432000
6	-0.064354000	-2.425630000	1.679488000
1	-0.340490000	-1.588211000	2.332847000
1	-0.651370000	-3.288291000	2.019859000
1	0.996431000	-2.651105000	1.815430000
14	-1.740841000	0.198195000	-0.169438000
6	-2.966366000	0.852471000	-1.416665000
1	-2.780021000	0.360082000	-2.379207000
1	-2.790223000	1.923647000	-1.574234000
1	-0.383118000	0.533358000	-0.931760000
6	-1.758202000	1.107041000	1.461396000
1	-2.663479000	0.790872000	1.999748000
1	-0.914150000	0.760690000	2.072723000
1	2.210458000	-0.743390000	0.375139000
6	2.706130000	0.348537000	0.381698000
1	2.995286000	0.359561000	1.439453000
6	3.889551000	0.212959000	-0.564139000
1	4.392709000	-0.745556000	-0.393314000
1	3.513773000	0.194099000	-1.595730000
6	4.868004000	1.356554000	-0.377034000
1	5.251088000	1.380985000	0.649672000
1	5.724170000	1.258702000	-1.050654000
1	4.391467000	2.323070000	-0.576198000
6	1.693602000	1.345239000	0.045165000
1	1.233654000	1.915048000	0.853136000
1	1.822389000	1.907640000	-0.881499000
6	-1.731567000	2.622711000	1.298589000
1	-2.636840000	2.987874000	0.801492000
1	-1.665168000	3.128730000	2.267022000
1	-0.875234000	2.954120000	0.697887000
6	-4.395656000	0.594690000	-0.944681000
1	-5.126611000	0.961869000	-1.672037000
1	-4.588027000	-0.475670000	-0.803447000
1	-4.606801000	1.094827000	0.007723000

INT11

Atomic

Number	X	Y	Z
28	-0.928596000	0.493937000	-0.047824000
6	0.217352000	2.133642000	0.249672000
6	1.326634000	1.396720000	-0.410183000
1	2.269542000	1.656861000	0.098133000
1	1.410865000	1.669861000	-1.468875000
6	-0.867908000	2.549270000	-0.472444000
1	-0.868372000	2.508515000	-1.560619000
1	-1.652506000	3.132027000	0.001439000
6	0.346130000	2.391895000	1.715352000
1	0.646853000	1.483353000	2.252426000
1	1.133855000	3.135247000	1.890440000
1	-0.585508000	2.769458000	2.143883000
14	1.654300000	-0.538561000	-0.428626000
6	3.218677000	-0.638316000	-1.464237000
1	3.012909000	-0.180833000	-2.440821000
1	3.395183000	-1.703726000	-1.664219000
1	0.588847000	-1.269241000	-1.167564000
6	1.890694000	-1.217354000	1.300493000
1	2.680155000	-0.630554000	1.791342000
1	0.980745000	-1.047791000	1.890210000
1	-2.392348000	0.735046000	0.433867000
6	-2.747442000	-0.447487000	0.409340000
1	-3.100171000	-0.454750000	1.447792000
6	-3.862396000	-0.437399000	-0.623639000
1	-4.477639000	0.460331000	-0.497672000
1	-3.414249000	-0.378640000	-1.623756000
6	-4.719397000	-1.682947000	-0.497216000
1	-5.170400000	-1.752587000	0.499200000
1	-5.529864000	-1.677356000	-1.231532000
1	-4.125172000	-2.589572000	-0.657444000
6	-1.605495000	-1.293186000	0.165756000
1	-1.109189000	-1.779807000	1.005992000
1	-1.567006000	-1.842439000	-0.775578000
6	2.250842000	-2.699680000	1.288670000
1	3.189242000	-2.884331000	0.752863000
1	2.374130000	-3.095385000	2.302137000
1	1.473651000	-3.298185000	0.797306000
6	4.444685000	-0.009291000	-0.816937000
1	5.331888000	-0.131129000	-1.447216000
1	4.317772000	1.067049000	-0.652353000
1	4.673020000	-0.466997000	0.152700000

Number	X	Y	Z
28	-0.866138000	0.499928000	0.044019000
6	0.162669000	2.188458000	0.150025000
6	0.991413000	1.273875000	-0.660560000
1	2.037695000	1.416157000	-0.352581000
1	0.897438000	1.425838000	-1.739825000
6	-1.068874000	2.560712000	-0.321019000
1	-1.337991000	2.440562000	-1.369764000
1	-1.721007000	3.180254000	0.287650000
6	0.646876000	2.561618000	1.511903000
1	1.032577000	1.688867000	2.051548000
1	1.474139000	3.276644000	1.427183000
1	-0.145984000	3.024487000	2.104182000
14	1.485052000	-0.731411000	-0.480476000
6	3.064755000	-0.641261000	-1.500639000
1	2.815285000	-0.243819000	-2.493937000
1	3.338421000	-1.692906000	-1.670446000
1	0.676277000	-1.759067000	-1.168310000
6	1.865671000	-1.135409000	1.309350000
1	2.575175000	-0.382116000	1.680331000
1	0.966315000	-1.037154000	1.928629000
1	-2.315004000	0.634897000	0.651243000
6	-2.626620000	-0.529636000	0.487862000
1	-2.943808000	-0.691439000	1.525234000
6	-3.777322000	-0.433149000	-0.502531000
1	-4.409480000	0.427275000	-0.255554000
1	-3.363230000	-0.244974000	-1.502129000
6	-4.600466000	-1.707008000	-0.500720000
1	-5.030804000	-1.896138000	0.489353000
1	-5.424967000	-1.643956000	-1.216669000
1	-3.987662000	-2.575104000	-0.768698000
6	-1.471790000	-1.318628000	0.097173000
1	-0.972192000	-1.927700000	0.850200000
1	-1.487151000	-1.759104000	-0.900150000
6	2.456385000	-2.536760000	1.441633000
1	3.380293000	-2.645771000	0.861464000
1	2.697711000	-2.774363000	2.482840000
1	1.755650000	-3.301922000	1.086075000
6	4.237803000	0.111623000	-0.893285000
1	5.121061000	0.055325000	-1.538336000
1	4.026252000	1.178840000	-0.752754000
1	4.523128000	-0.298437000	0.082208000

TS_{11-12}

Atomic

Number	X	Y	Z
28	-0.793463000	0.461761000	0.023697000
6	0.121920000	2.231481000	0.141150000
6	0.956602000	1.310274000	-0.621625000
1	1.991371000	1.338399000	-0.267008000
1	0.899212000	1.405151000	-1.708428000
6	-1.131970000	2.507033000	-0.346120000
1	-1.380222000	2.347791000	-1.395341000
1	-1.832406000	3.092242000	0.242830000
6	0.561589000	2.654336000	1.503292000
1	1.361762000	3.399008000	1.417533000

INT12

Atomic

Number	X	Y	Z
28	-0.739745000	0.664412000	0.088049000
6	-0.205542000	2.455887000	-0.666114000
6	0.359011000	1.415177000	-1.415946000
1	1.437963000	1.312379000	-1.485763000
1	-0.216227000	0.971204000	-2.230116000
6	-1.599279000	2.348276000	-0.514281000
1	-2.210310000	1.960556000	-1.330042000
1	-2.112183000	2.958557000	0.225527000
6	0.608223000	3.386414000	0.167446000
1	0.661781000	4.357324000	-0.338451000

1	-0.260138000	3.098140000	2.070071000	1	0.146715000	3.553213000	1.145481000
1	0.971472000	1.809293000	2.068643000	1	1.629741000	3.023501000	0.303144000
14	1.371797000	-0.845630000	-0.357689000	14	1.171722000	-1.119808000	0.341607000
6	2.799330000	-0.745073000	-1.588884000	6	1.359626000	-1.685528000	-1.438998000
1	2.384320000	-0.576929000	-2.592007000	1	0.870645000	-1.018086000	-2.154007000
1	3.154710000	-1.787243000	-1.603597000	1	0.828570000	-2.646019000	-1.506144000
1	0.693081000	-2.078938000	-0.820208000	1	1.517240000	-2.317258000	1.156314000
6	1.973663000	-1.016706000	1.410534000	6	2.324250000	0.220490000	1.005516000
1	2.560759000	-0.126188000	1.673365000	1	2.581734000	0.933277000	0.214602000
1	1.114706000	-1.026952000	2.093374000	1	1.779692000	0.797996000	1.766226000
1	-2.274595000	0.644375000	0.603520000	1	-2.142859000	0.591708000	1.021900000
6	-2.579149000	-0.514054000	0.500129000	6	-2.132180000	-0.565932000	0.969142000
1	-2.915043000	-0.626265000	1.538153000	1	-2.640198000	-0.719793000	1.929231000
6	-3.711123000	-0.482253000	-0.516002000	6	-2.996711000	-1.042494000	-0.192998000
1	-4.350747000	0.387999000	-0.330027000	1	-3.833605000	-0.344410000	-0.312656000
1	-3.277888000	-0.347977000	-1.516376000	1	-2.417446000	-0.996346000	-1.128386000
6	-4.530237000	-1.757276000	-0.458905000	6	-3.526872000	-2.448960000	0.019291000
1	-4.975862000	-1.894086000	0.533102000	1	-4.106971000	-2.511104000	0.947062000
1	-5.343146000	-1.736361000	-1.190307000	1	-4.181004000	-2.747488000	-0.804617000
1	-3.911063000	-2.636478000	-0.669701000	1	-2.720436000	-3.187828000	0.079318000
6	-1.422669000	-1.344639000	0.177012000	6	-0.740538000	-1.187599000	1.056260000
1	-0.960450000	-1.919998000	0.978770000	1	-0.428451000	-1.222445000	2.106041000
1	-1.452329000	-1.867143000	-0.778690000	1	-0.824564000	-2.219690000	0.692043000
6	2.810958000	-2.280632000	1.588027000	6	3.593159000	-0.372458000	1.612558000
1	3.706209000	-2.266533000	0.955761000	1	4.159885000	-0.958431000	0.879691000
1	3.147709000	-2.396124000	2.623564000	1	4.259264000	0.412489000	1.986840000
1	2.241213000	-3.180801000	1.328528000	1	3.365060000	-1.037861000	2.452136000
6	3.963822000	0.193284000	-1.315800000	6	2.831122000	-1.873524000	-1.798532000
1	4.802236000	-0.015619000	-1.989058000	1	2.948655000	-2.305908000	-2.797731000
1	3.698427000	1.245118000	-1.467953000	1	3.372389000	-0.919806000	-1.791245000
1	4.342077000	0.090986000	-0.291238000	1	3.338052000	-2.544463000	-1.094332000

$TS_{12\text{-}13}$

Atomic Number	X	Y	Z
28	-1.099822000	0.171904000	0.062352000
6	-1.962266000	1.829466000	-0.657464000
6	-0.689928000	1.655922000	-1.219930000
1	0.089316000	2.384962000	-1.023298000
1	-0.586898000	1.070532000	-2.133753000
6	-2.797406000	0.707432000	-0.801783000
1	-2.747433000	0.096531000	-1.703722000
1	-3.713996000	0.635532000	-0.220915000
6	-2.273443000	2.931897000	0.296342000
1	-2.787919000	3.735172000	-0.243864000
1	-2.938542000	2.595636000	1.096698000
1	-1.364516000	3.356325000	0.731780000
14	1.619226000	-0.166769000	0.342235000
6	1.841262000	-0.731417000	-1.433288000
1	1.098490000	-0.284493000	-2.102579000
1	1.668378000	-1.816610000	-1.458767000
1	2.674254000	-0.883495000	1.112264000
6	1.959571000	1.657176000	0.696786000
1	2.006530000	2.195010000	-0.258608000
1	1.122865000	2.093472000	1.257350000
1	-2.137004000	-0.934856000	0.815187000

INT13

Atomic Number	X	Y	Z
28	-1.360419000	0.051471000	-0.051344000
6	-3.003383000	-1.074779000	0.095966000
6	-1.912837000	-1.813473000	-0.397202000
1	-1.921579000	-2.171196000	-1.424084000
1	-1.247329000	-2.332905000	0.292412000
6	-2.727200000	-0.401461000	1.298636000
1	-2.085946000	-0.861701000	2.051385000
1	-3.395581000	0.382592000	1.646040000
6	-4.180072000	-0.734149000	-0.752429000
1	-4.981645000	-1.454463000	-0.551485000
1	-4.566686000	0.262133000	-0.522172000
1	-3.940191000	-0.795985000	-1.817407000
14	1.855542000	-0.088510000	-0.156095000
6	1.419820000	-0.695146000	1.569632000
1	0.512258000	-1.313214000	1.497641000
1	1.150210000	0.165726000	2.196599000
1	3.016603000	0.839597000	-0.081348000
6	2.249976000	-1.509771000	-1.323176000
1	1.579522000	-2.346239000	-1.074501000
1	1.978720000	-1.203496000	-2.343283000
1	-1.014931000	1.556924000	0.692935000

6	-1.269787000	-1.668837000	1.007512000	6	-0.344726000	1.951328000	-0.156477000
1	-1.670132000	-2.084926000	1.940442000	1	-1.012601000	2.518056000	-0.816254000
6	-1.249822000	-2.715451000	-0.099410000	6	0.572773000	2.921428000	0.585357000
1	-2.283706000	-3.034614000	-0.276835000	1	-0.049527000	3.587888000	1.192638000
1	-0.906594000	-2.257360000	-1.039084000	1	1.213531000	2.374175000	1.288800000
6	-0.390604000	-3.922608000	0.228838000	6	1.415860000	3.740402000	-0.373457000
1	-0.665753000	-4.347299000	1.201547000	1	0.783735000	4.270243000	-1.095548000
1	-0.518997000	-4.705205000	-0.524268000	1	2.001963000	4.489008000	0.167311000
1	0.677808000	-3.679816000	0.259141000	1	2.119429000	3.118632000	-0.937179000
6	0.077654000	-1.014076000	1.336910000	6	0.385842000	0.856973000	-0.941275000
1	0.037757000	-0.492110000	2.300759000	1	-0.315215000	0.086160000	-1.431326000
1	0.746862000	-1.869372000	1.489769000	1	0.730882000	1.285049000	-1.892414000
6	3.267227000	1.850829000	1.458562000	6	3.706065000	-1.963387000	-1.288570000
1	4.118657000	1.431927000	0.909181000	1	4.010314000	-2.288635000	-0.287291000
1	3.477990000	2.912170000	1.628807000	1	3.887320000	-2.800581000	-1.971352000
1	3.241915000	1.358545000	2.436934000	1	4.380768000	-1.151083000	-1.581501000
6	3.254693000	-0.410083000	-1.914049000	6	2.543842000	-1.494575000	2.222996000
1	3.429120000	-0.784879000	-2.927930000	1	2.292032000	-1.784154000	3.248756000
1	3.440023000	0.670423000	-1.932653000	1	2.755800000	-2.415826000	1.668412000
1	4.014469000	-0.861252000	-1.264883000	1	3.476525000	-0.919098000	2.267181000

$Et_2(n$Bu)SiH **$^{i}Pr_2C_6H_4$**

Atomic Number	X	Y	Z	Atomic Number	X	Y	Z
14	-0.504796000	-0.163192000	-0.002744000	6	-1.414742000	0.261854000	-0.036182000
6	-0.978769000	1.650858000	-0.194756000	6	-0.692562000	-0.925566000	0.103392000
1	-1.021249000	1.868979000	-1.272599000	6	-0.695304000	1.443485000	-0.176727000
1	-0.161544000	2.269288000	0.201632000	1	-1.223610000	-1.868820000	0.214420000
1	-0.241894000	-0.434151000	1.444533000	1	-1.233540000	2.382839000	-0.288835000
6	-1.913231000	-1.297226000	-0.547971000	6	0.692561000	-0.925568000	0.103375000
1	-2.406165000	-0.831473000	-1.414286000	6	0.695304000	1.443483000	-0.176746000
1	-1.468402000	-2.227960000	-0.927947000	1	1.223609000	-1.868823000	0.214393000
1	1.876147000	1.426914000	-1.255286000	1	1.233540000	2.382835000	-0.288869000
6	2.190986000	0.424856000	-0.931879000	6	1.414741000	0.261850000	-0.036221000
1	2.990068000	0.123601000	-1.626496000	6	-2.925348000	0.264193000	-0.032262000
6	2.782857000	0.518871000	0.469421000	1	-3.245076000	1.308098000	-0.163399000
1	3.594507000	1.258281000	0.459029000	6	-3.493151000	-0.548906000	-1.189825000
1	2.029843000	0.912049000	1.168757000	1	-3.222250000	-1.607887000	-1.097628000
6	3.315137000	-0.804195000	0.990477000	1	-3.119412000	-0.191374000	-2.155443000
1	4.026882000	-1.246433000	0.281540000	1	-4.587484000	-0.488832000	-1.206140000
1	3.834388000	-0.679622000	1.946384000	6	2.925348000	0.264187000	-0.032314000
1	2.513389000	-1.534077000	1.149827000	1	3.245075000	1.308077000	-0.163573000
6	1.011591000	-0.538617000	-1.060053000	6	3.493158000	-0.549048000	-1.189778000
1	0.655333000	-0.543251000	-2.101661000	1	3.119417000	-0.191639000	-2.155440000
1	1.327818000	-1.572359000	-0.860293000	1	3.222276000	-1.608022000	-1.097450000
6	-2.934956000	-1.618226000	0.537419000	1	4.587490000	-0.488961000	-1.206100000
1	-3.408249000	-0.712646000	0.935007000	6	-3.484751000	-0.233917000	1.295780000
1	-3.737477000	-2.268018000	0.169085000	1	-4.579065000	-0.171684000	1.303638000
1	-2.465078000	-2.130789000	1.384982000	1	-3.212918000	-1.282510000	1.469644000
6	-2.295636000	2.032302000	0.471805000	1	-3.104915000	0.353334000	2.138867000
1	-2.513666000	3.101733000	0.369962000	6	3.484744000	-0.233767000	1.295789000
1	-3.140784000	1.487838000	0.034275000	1	3.104916000	0.353591000	2.138804000
1	-2.284606000	1.805045000	1.545197000	1	3.212893000	-1.282336000	1.469778000
				1	4.579059000	-0.171551000	1.303642000

$[Pt(SiH_4)(PH_3)_2]$ (Energy: -142.050492942 hartree)

Atomic Number	X	Y	Z
78	-2.239467	-0.080460	0.340775
15	-4.400655	0.387712	0.261794
15	-0.069591	-0.511762	0.381629
1	-5.037057	0.447798	-0.995754
1	-5.326309	-0.451372	0.917181
1	-4.849424	1.622996	0.774795
1	0.409665	-1.642496	1.076023
1	0.603829	-0.723866	-0.839666
1	0.805684	0.448635	0.931195
1	-1.225299	4.521363	-1.768369
14	-1.515116	3.204729	-1.179127
1	-0.468752	2.271340	-1.602408
1	-1.526904	3.336547	0.278300
1	-2.823461	2.761297	-1.665779

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