

*Supporting Information for*

## **Mechanistic Studies on Rhodium-Catalyzed Enantioselective Silylation of Aryl C–H Bonds**

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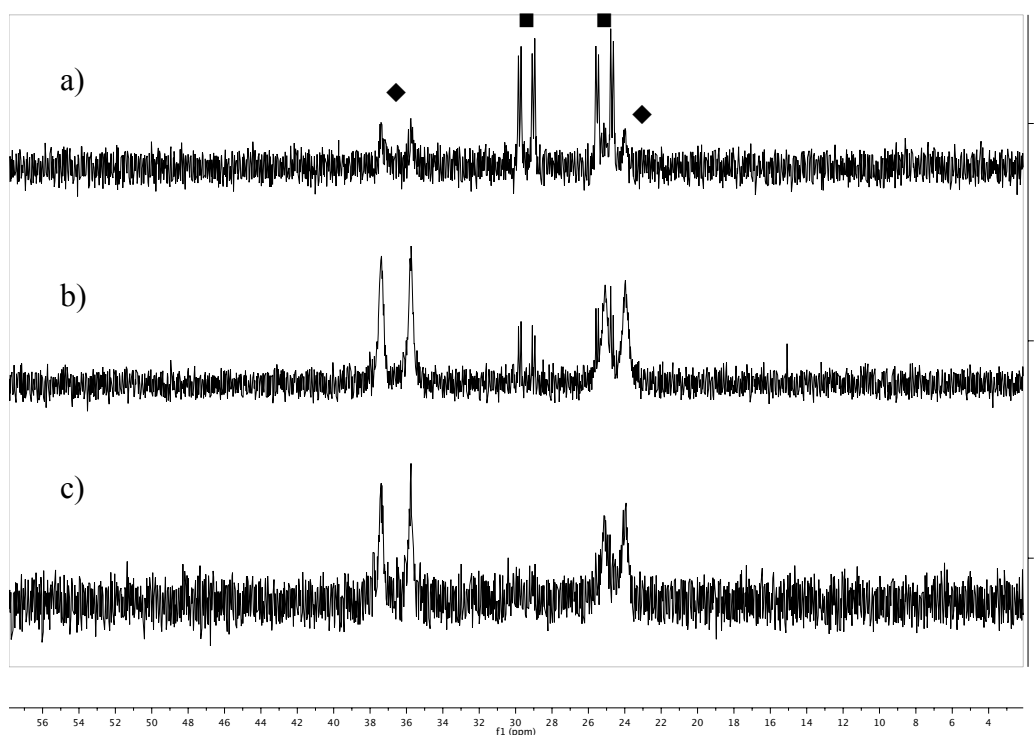
## Materials and Methods

All air-sensitive manipulations were assembled in an N<sub>2</sub>-filled glovebox using oven-dried glassware. [Rh(cod)Cl]<sub>2</sub> was prepared according to the standard procedure.<sup>1</sup> [Rh(C<sub>2</sub>H<sub>4</sub>)Cl]<sub>2</sub>, **L1**, and **L2** were purchased from Strem and were used as received. Silanes **2a**, **2a-d**<sub>10</sub>, and **2a-d**<sub>2</sub> were prepared from the hydrosilylation of benzophenone and benzophenone-*d*<sub>10</sub><sup>2</sup> and the dehydrogenative silylation of benzhydrol-*d*<sub>2</sub><sup>3</sup> according to our previous publication.<sup>4</sup> The silane **2b-d**<sub>1</sub> was prepared according to our previous publication.<sup>5</sup> Norbornene (nbe) was purchased from Aldrich and was used as received. Tetrahydrofuran (THF) was degassed by purging with nitrogen and then dried with a solvent purification system containing activated alumina. All other solvents and reagents were used as received.

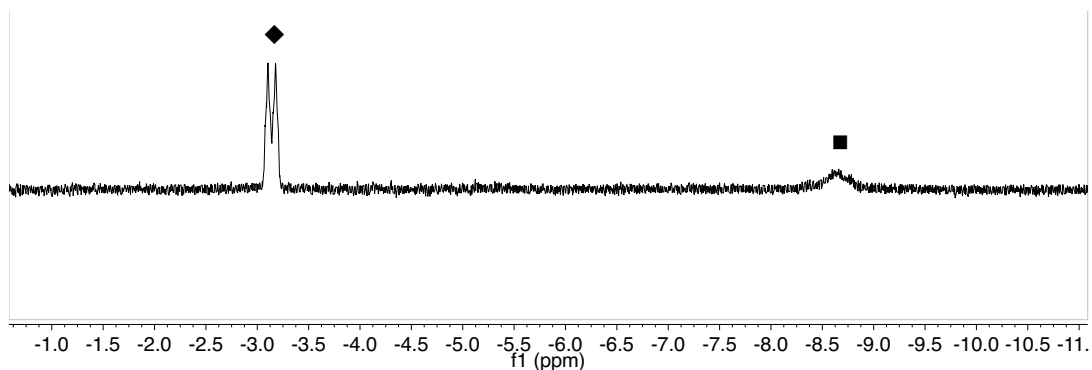
Reaction temperatures above 23 °C refer to the temperature of an aluminum heating block, which was controlled by an electronic temperature modulator. NMR spectra were recorded on Bruker AVQ-400, AV-500, DRX-500 and AV-600 instruments. <sup>1</sup>H NMR chemical shifts (δ) are reported in ppm relative to the residual solvent signal. <sup>31</sup>P NMR chemical shifts were reported relative to an external H<sub>3</sub>PO<sub>4</sub> (85% aqueous) sample. Elemental analysis was conducted at the Micro Analytical Facility in the College of Chemistry, University of California, Berkeley. Chiral SFC analysis was conducted on a Waters chromatography system.

## Observation of the Resting States

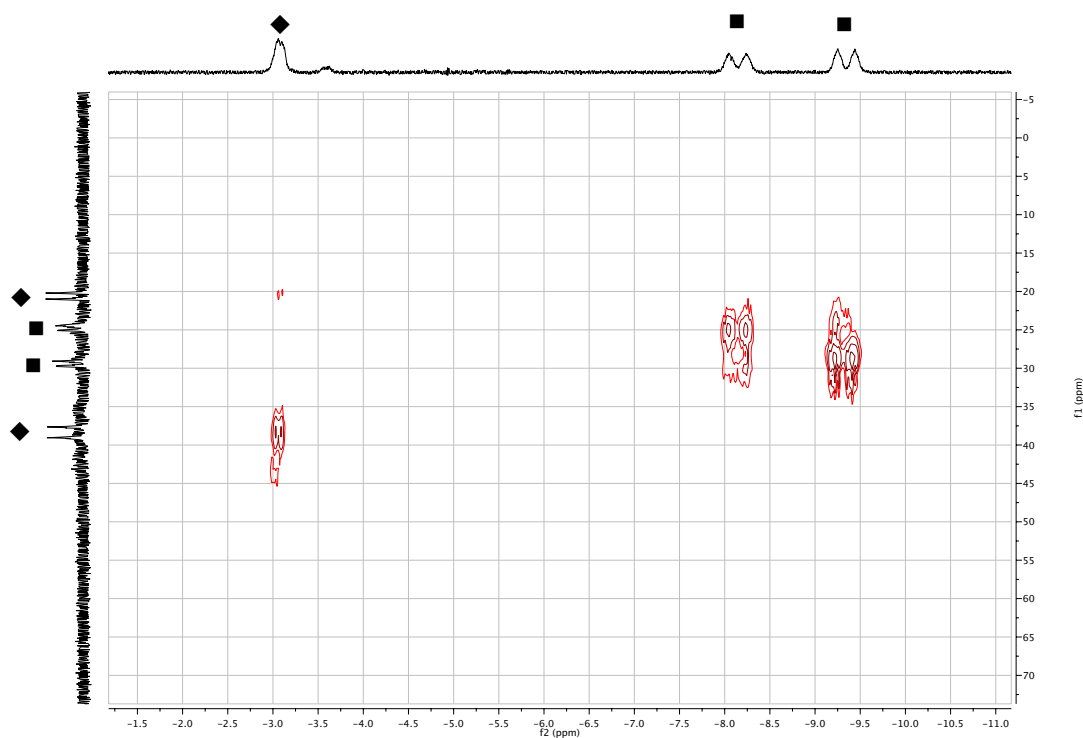
Diethyl(hydrido)silyl ether **2a** (54.1 mg, 0.200 mmol) was treated with norbornene (22.6 mg, 0.240 mmol), and a freshly prepared stock solution of a rhodium precursor ( $[\text{Rh}(\text{C}_2\text{H}_4)\text{Cl}]_2$  or  $[\text{Rh}(\text{cod})\text{Cl}]_2$ , 5  $\mu\text{mol}$ , 2.5 mol %) and **L1** (10  $\mu\text{mol}$ , 5.0 mol %) in THF (0.4 mL) in a 4 mL vial. The solution was transferred to a J-Young NMR tube. The reaction was monitored by  $^{31}\text{P}$  NMR spectroscopy at 50 °C. A higher catalyst loading of 5 mol % (in contrast to 1 mol % used in preparative reactions) was used to facilitate the observation of the resting states.



**Figure S1.**  $^{31}\text{P}$  NMR spectra of catalytic reaction of **2a** conducted with 2.5 mol% of  $[\text{Rh}(\text{C}_2\text{H}_4)\text{Cl}]_2$ , 5 mol% of **L1**, and 1.2 equivalent of norbornene at (a) 5 min (~40% conversion), (b) 10 min (~70% conversion) and (c) 15 min (~90% conversion). **4a** (■), **5** (◆).

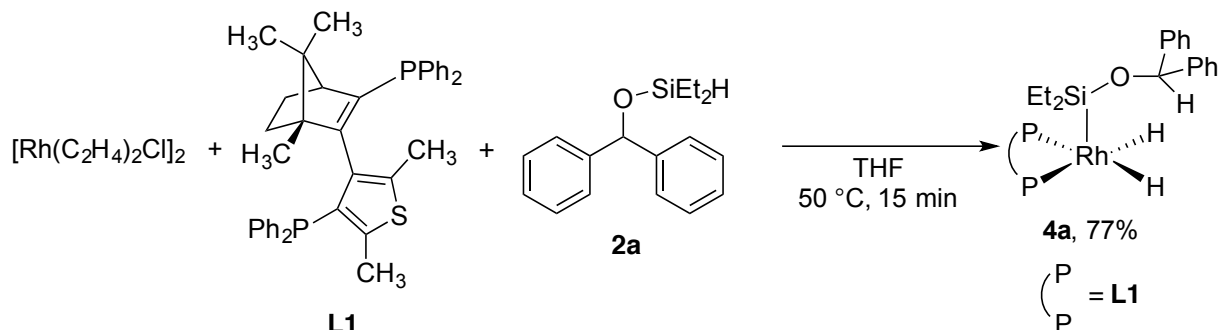


**Figure S2.**  $^1\text{H}$  NMR spectrum of catalytic reaction of **2a** conducted with 2.5 mol% of  $[\text{Rh}(\text{C}_2\text{H}_4)\text{Cl}]_2$ , 5 mol% of **L1**, and 1.2 equivalent of norbornene at 10 min (71% conversion). **4a** (■), **5** (◆).

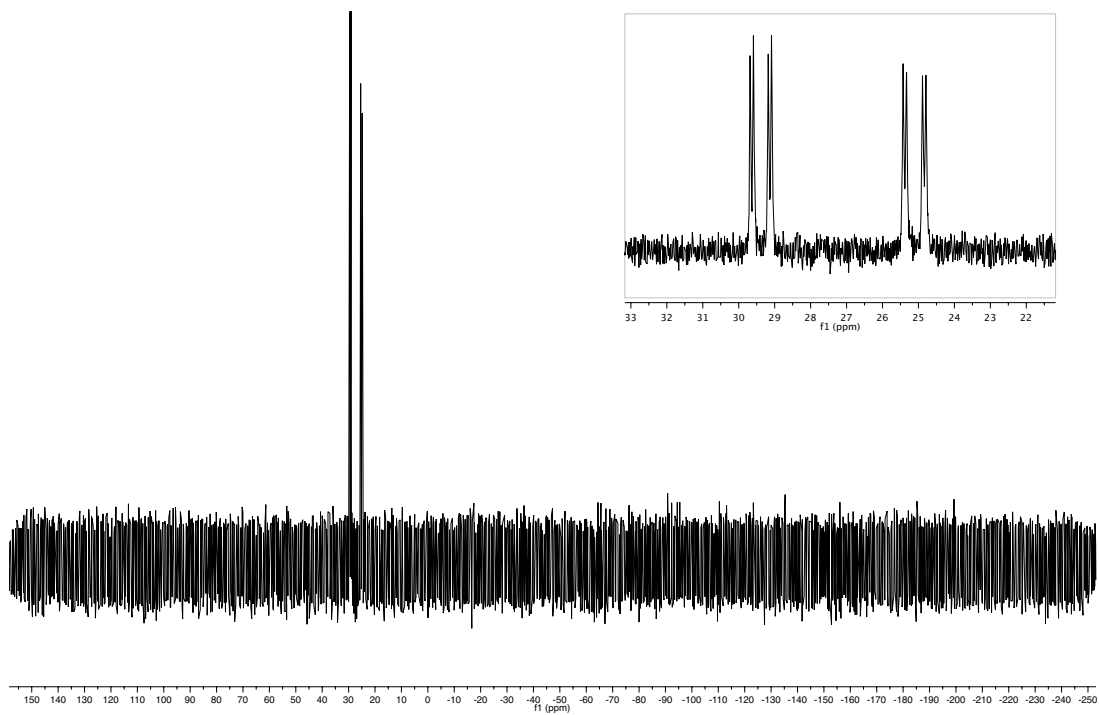
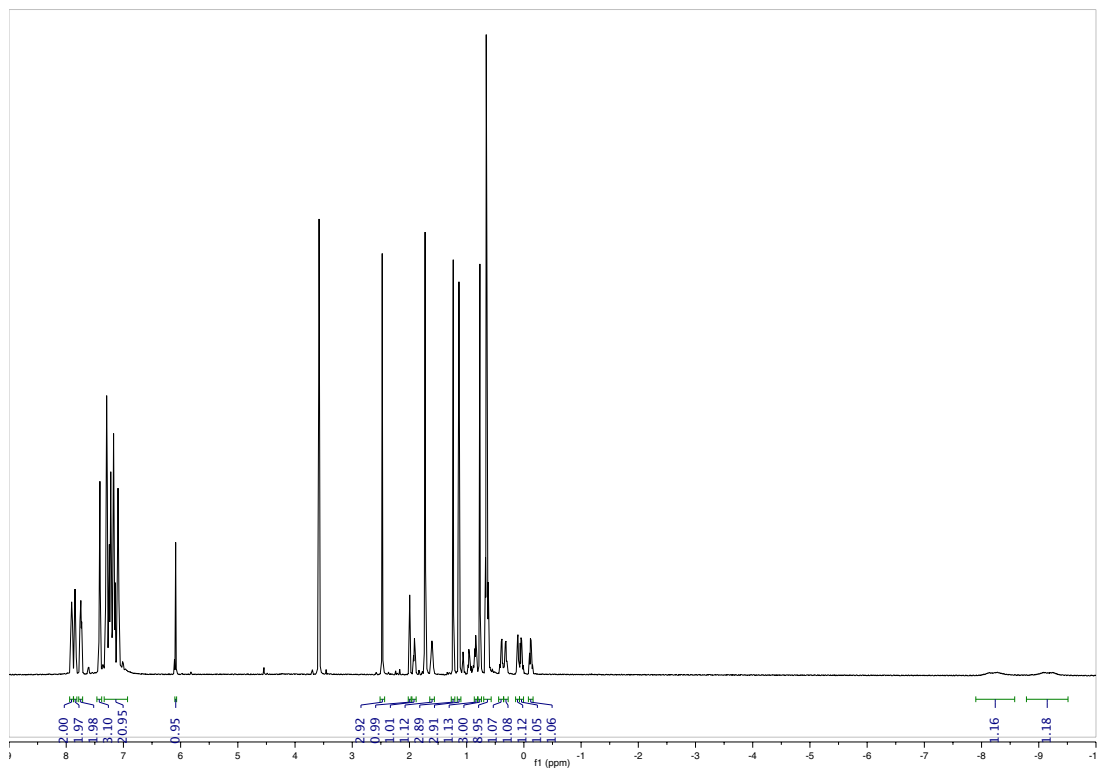


**Figure S3.**  $^{31}\text{P}$ - $^1\text{H}$  HMBC spectrum at  $-80\text{ }^\circ\text{C}$  of silylation reaction of **2a** conducted with 2.5 mol% of  $[\text{Rh}(\text{C}_2\text{H}_4)\text{Cl}]_2$ , 5 mol% of **L1**, and norbornene. **4a** (■), **5** (◆, major isomer labeled).

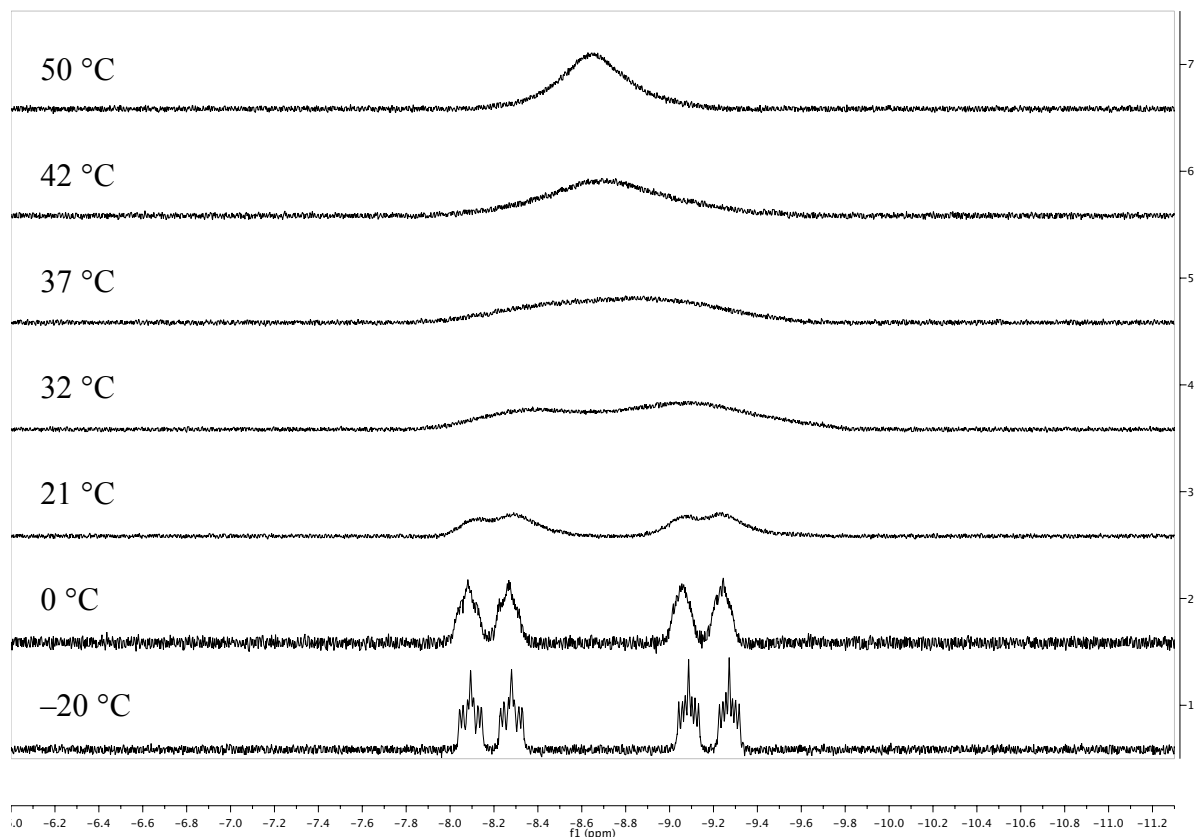
## Synthesis and Characterization of Complex 4a



To a solution of  $[\text{Rh}(\text{C}_2\text{H}_4)_2\text{Cl}]_2$  (11.7 mg, 0.0301 mmol) and **L1** (36.9 mg, 0.0600 mmol) in THF (1.2 mL) was added **2a** (163 mg, 0.603 mmol), and the mixture was stirred at 50 °C for 15 min, during which time the mixture turned from dark red to orange. The volatile materials were evaporated, and the residual mixture was washed with pentane to afford complex **4a** as a yellow solid (45.5 mg, 77% yield).  $^1\text{H NMR}$  (600 MHz,  $\text{THF-}d_8$ )  $\delta$  7.90 (t,  $J=7.2$  Hz, 2H), 7.85 (t,  $J=9.3$  Hz 2H), 7.74 (t,  $J=8.1$  Hz, 2H), 7.41 (s, 3H), 7.34 – 6.93 (m, 21H), 6.09 (s, 1H), 2.48 (s, 3H), 2.00 (s, 1H), 1.91 (t,  $J = 9.9$  Hz, 1H), 1.61 (td,  $J = 8.7, 4.4$  Hz, 1H), 1.23 (s, 3H), 1.13 (s, 3H), 0.84 (t,  $J = 10.6$  Hz, 1H), 0.77 (s, 3H), 0.71 – 0.59 (m, 9H), 0.44 – 0.35 (m, 1H), 0.35 – 0.28 (m, 1H), 0.11 (t,  $J = 10.1$  Hz, 1H), 0.08 – 0.01 (m, 1H), -0.07 – -0.17 (m, 1H), -8.21 (br d,  $J = 76.1$  Hz, 1H), -9.16 (br d,  $J = 78.0$  Hz, 1H).  $^{31}\text{P NMR}$  (243 MHz,  $\text{THF-}d_8$ )  $\delta$  29.39 (dd,  $J_{\text{P-Rh}} = 122.6$ ,  $J_{\text{P-P}} = 22.6$  Hz), 25.11 (dd,  $J_{\text{P-Rh}} = 131.2$ ,  $J_{\text{P-P}} = 22.6$  Hz). Anal. Calcd (%) for  $\text{C}_{57}\text{H}_{63}\text{OP}_2\text{RhSSi}$ : C, 69.22, H, 6.42, S 3.24. Found: C, 69.14, H, 6.56, S 3.56.



**Figure S4.**  $^1\text{H}$  and  $^{31}\text{P}$  NMR spectra of complex **4a**.



**Figure S5.** Variable-temperature  $^1\text{H}$  spectra of complex **4a** (hydride region) between 50 °C and -20 °C, measured by a 500 MHz NMR spectrometer. Hydride signals at -20 °C:  $^1\text{H}$  NMR (500 MHz,  $\text{THF-}d_8$ )  $\delta$  -8.19 (dddd,  $J = 93.2, 24.9, 17.7, 8.0$  Hz, 1H), -9.18 (dddd,  $J = 92.7, 22.7, 15.0, 8.0$  Hz, 1H).

Single crystals of **4a** suitable for X-ray diffraction were obtained from a dilute solution of **4a** and **2a** in pentane at 25 °C. A yellow rod 0.060 x 0.040 x 0.030 mm in size was mounted on a cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 40 mm and exposure time was 10 seconds per frame using a scan width of 0.5°. Data collection was 100.0% complete to 25.000° in  $\theta$ . A total of 71036 reflections were collected covering the indices,  $-26 \leq h \leq 26$ ,  $-25 \leq k \leq 27$ ,  $-11 \leq l \leq 11$ . 9051 reflections were found to be symmetry independent, with an

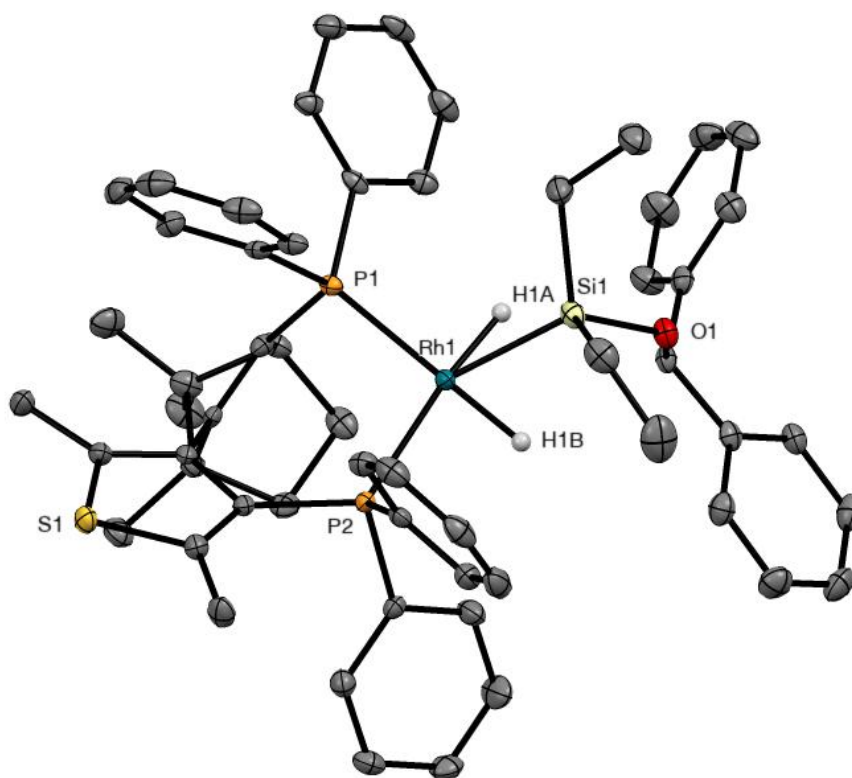
$R_{\text{int}}$  of 0.0342. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be  $P 2_1 2_1 2$  (No. 18). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014. The absolute stereochemistry was unambiguously determined to be *R* at C16 and *S* at C14, respectively.

Table S1. Crystal data and structure refinement for **4a**.

Empirical formula	$C_{57}H_{63}OP_2RhSSi$	
Formula weight	989.07	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P 2_1 2_1 2$	
Unit cell dimensions	$a = 22.1200(17)$ Å	$\alpha = 90^\circ$ .
	$b = 22.8814(16)$ Å	$\beta = 90^\circ$ .
	$c = 9.7523(7)$ Å	$\gamma = 90^\circ$ .
Volume	$4936.0(6)$ Å <sup>3</sup>	
Z	4	
Density (calculated)	$1.331$ Mg/m <sup>3</sup>	
Absorption coefficient	$0.517$ mm <sup>-1</sup>	
F(000)	2072	
Crystal size	$0.060 \times 0.040 \times 0.030$ mm <sup>3</sup>	
Theta range for data collection	1.280 to 25.392°.	
Index ranges	$-26 \leq h \leq 26, -25 \leq k \leq 27, -11 \leq l \leq 11$	
Reflections collected	71036	
Independent reflections	9051 [ $R_{\text{int}} = 0.0342$ ]	



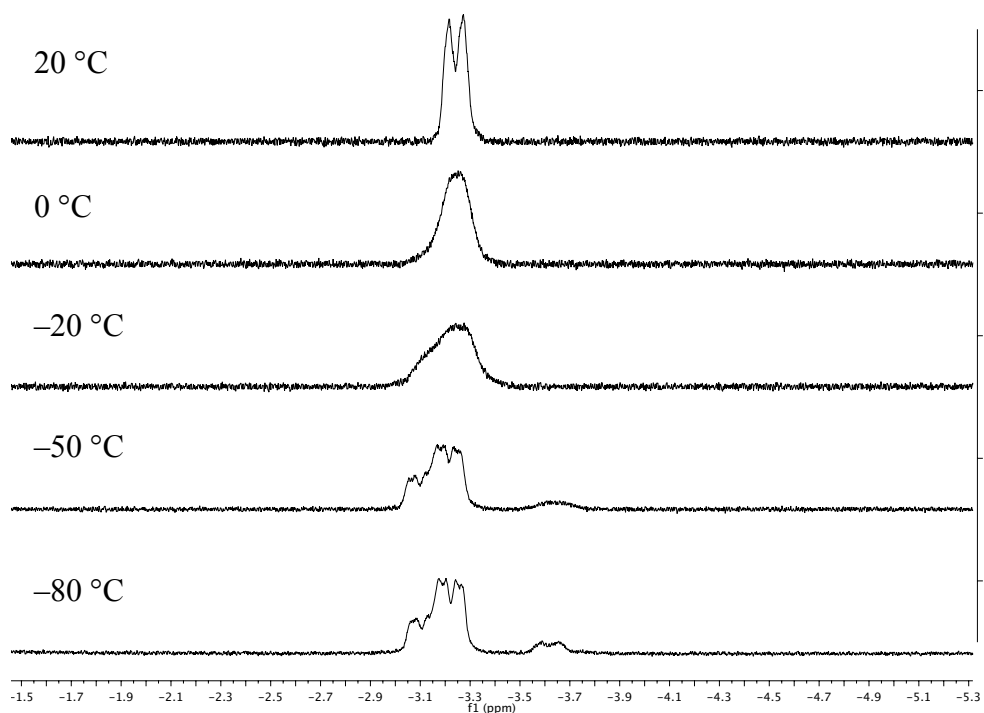
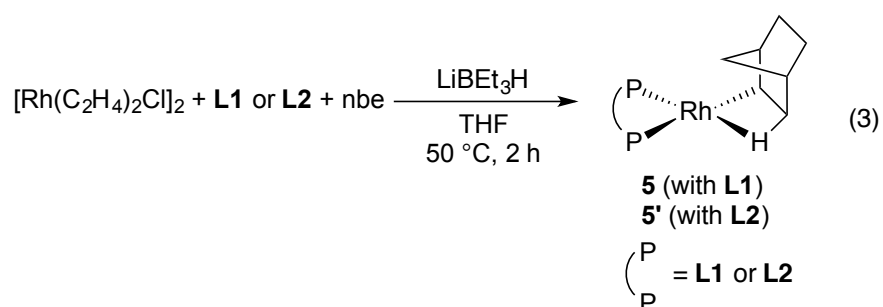
Completeness to theta = 25.000°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.928 and 0.852
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	9051 / 0 / 581
Goodness-of-fit on F <sup>2</sup>	1.048
Final R indices [I>2sigma(I)]	R1 = 0.0207, wR2 = 0.0457
R indices (all data)	R1 = 0.0224, wR2 = 0.0466
Absolute structure parameter	-0.022(5)
Extinction coefficient	n/a
Largest diff. peak and hole	0.474 and -0.274 e.Å <sup>-3</sup>



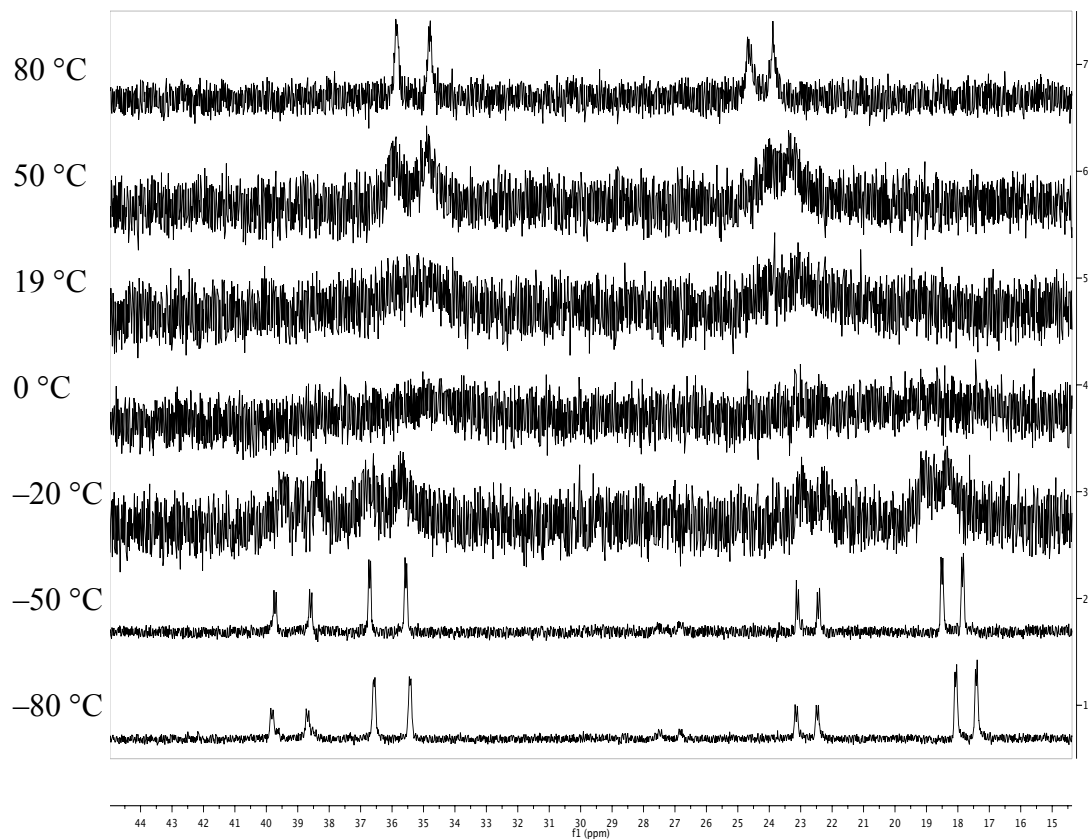
**Figure S6.** ORTEP diagram of **4a** (thermal ellipsoids at the 50% probability level). Hydrogen atoms have been omitted except for the hydrides bound to rhodium. Selected bond lengths (Å): Rh1–P1 = 2.2763(8), Rh1–P2 = 2.3456(8), Rh1–H1A = 1.48(3), Rh1–H1B = 1.49(3), Rh1–Si1 = 2.3126(8). Selected bond angles (°): P1–Rh1–Si1 = 115.52(3), P2–Rh1–Si1 = 129.64(3), H1A–Rh1–Si1 = 53(1), H1B–Rh1–Si1 = 63(1).

## Synthesis and Characterization of Complex **5** and **5'**

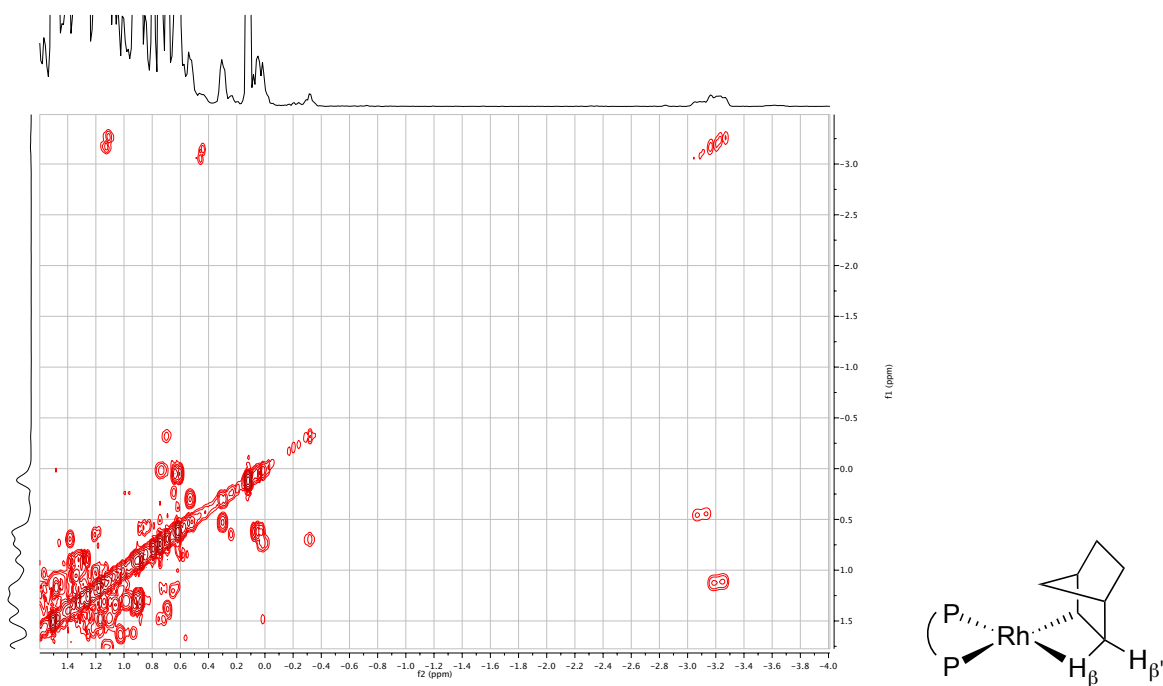
To a solution of  $[\text{Rh}(\text{C}_2\text{H}_4)_2\text{Cl}]_2$  (1.9 mg, 0.0050 mmol) and **L1** (6.1 mg, 0.010 mmol, for complex **5**) or **L2** (6.7 mg, 0.010 mmol, for complex **5'**) in THF (0.4 mL) was added norbornene (37.7 mg, 0.400 mmol), and the mixture was stirred at 50 °C for 2 hours. The volatile materials were evaporated to afford a mixture containing complex **5** or **5'** as a brown solid.



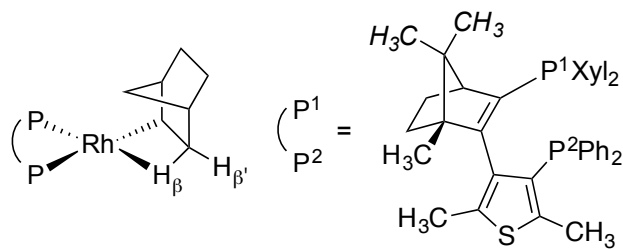
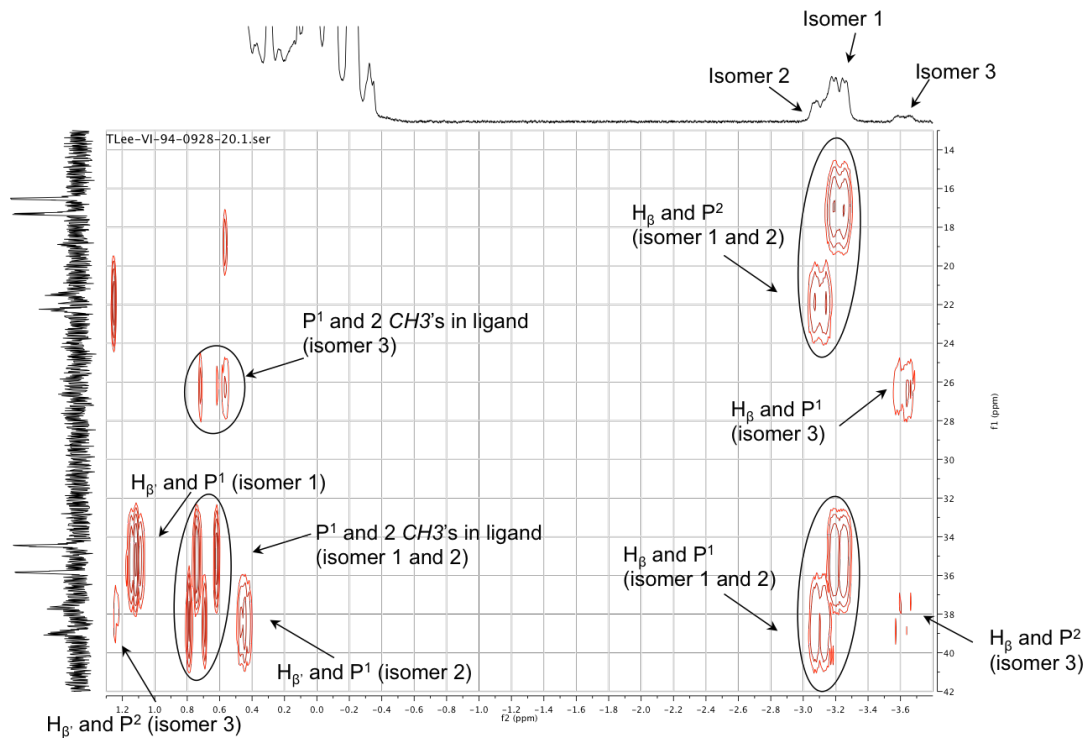
**Figure S7.** Variable-temperature  $^1\text{H}$  spectra of complex **5'** (hydride region) between 19 °C and  $-80$  °C. Three hydride signals corresponding to three isomers were observed at  $-80$  °C:  $\delta$  -3.11 (dd,  $J = 33.7, 13.3$  Hz), -3.22 (dd,  $J = 32.8, 12.9$  Hz), -3.62 (br d,  $J = 35$  Hz).



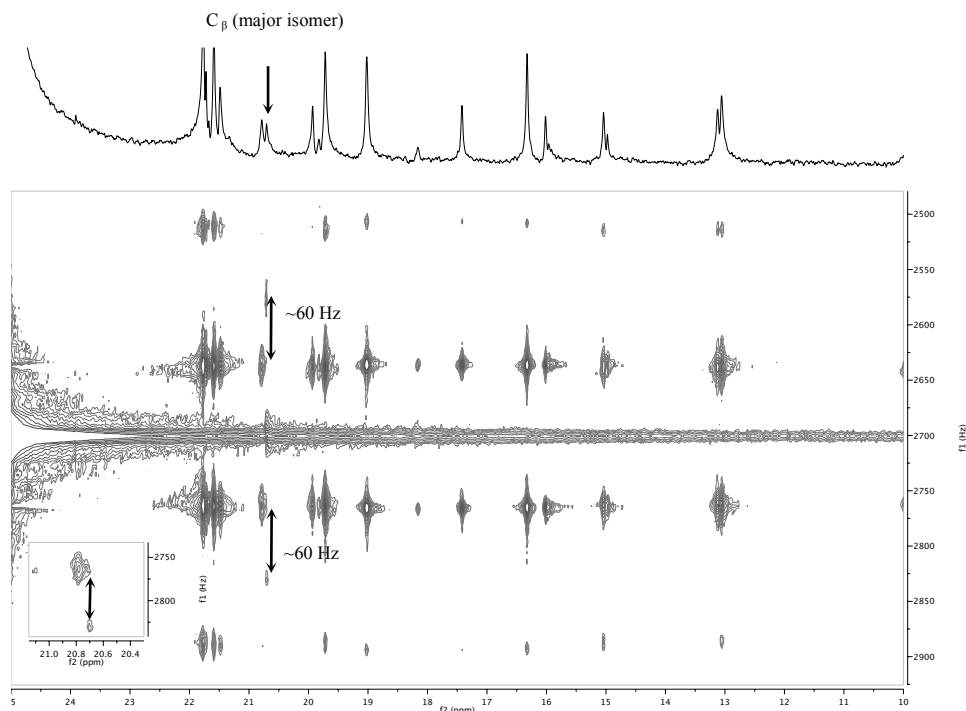
**Figure S8.** Variable-temperature  $^{31}\text{P}$  spectra of complex **5'** between 80 °C and -80 °C.. Three sets of signals corresponding to three isomers were observed at -80 °C.



**Figure S9.**  $^{13}\text{C}$ - $^1\text{H}$  COSY spectrum of **5'** at  $-80\text{ }^\circ\text{C}$  showing the correlation between agostic  $\text{H}_\beta$  and non-agostic  $\text{H}_{\beta'}$  resonances.

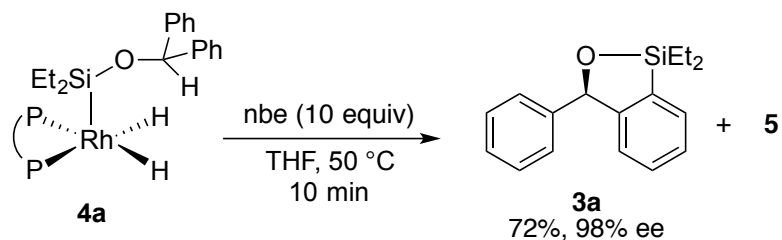


**Figure S10.**  $^{31}\text{P}$ - $^1\text{H}$  HMBC spectrum of **5'** at  $-80\text{ }^\circ\text{C}$  showing the correlation between the agostic  $\text{H}_\beta$  and the ligand resonances.

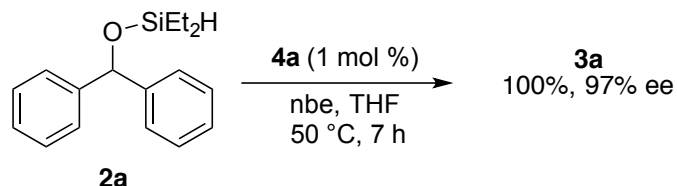


**Figure S11.** 2D  $J$ -resolved  $^{13}\text{C}$  NMR spectrum of **5'** showing  $^1J_{\text{C-H}}$  coupling constant of the agostic C–H bond of the major isomer.

### Examination of the Reactivity of Complex **4**



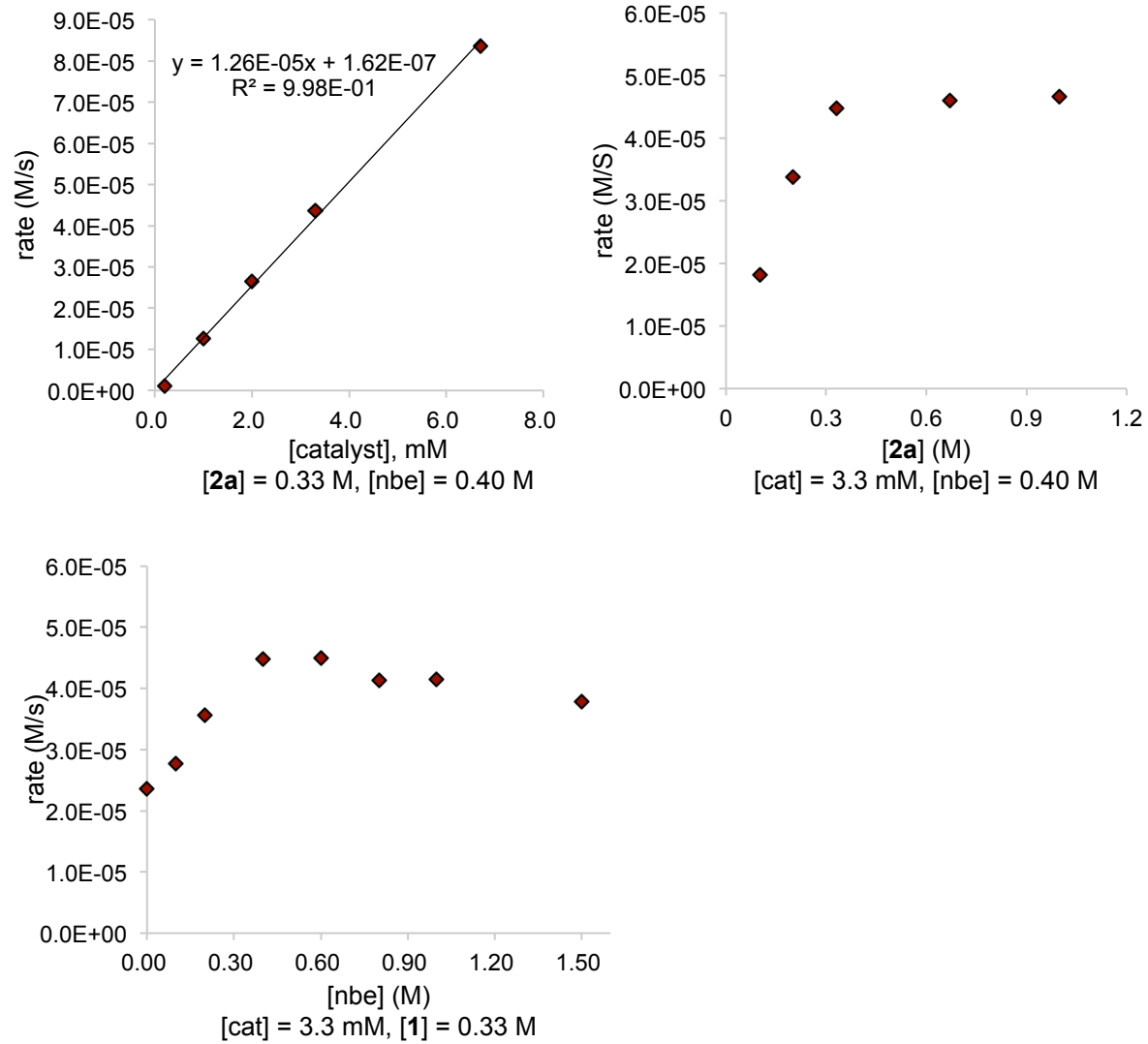
To a J-Young NMR tube was added complex **4a** (9.9 mg, 0.010 mmol), norbornene (9.6 mg, 0.10 mmol) and THF- $d_8$  (0.30 mL). The resulting mixture was heated at 50 °C for 10 min. The  $^1\text{H}$  NMR spectrum of this reaction mixture showed that **4a** was fully consumed and that **3a** and **5** formed in an equal amounts at this time. The yield of **3a** was determined by  $^1\text{H}$  NMR spectroscopy using 1,3,5-trimethoxybenzene as the internal standard added at the end of the reaction, and the enantiomeric excess was determined by chiral SFC analysis.



Diethyl(hydrido)silyl ether **2a** (41.1 mg, 0.153 mmol) was treated with norbornene (16.4 mg, 0.174 mmol), and a solution of **4a** (1.5 mg, 1.5  $\mu\text{mol}$ , 1.0 mol %) in THF (0.4 mL) in a 4 mL vial. The resulting mixture was heated at 50  $^\circ\text{C}$  for 7 hours. The formation of **3a** was monitored by GC analysis with dodecane as the internal standard. The enantiomeric excess was determined by chiral SFC analysis.

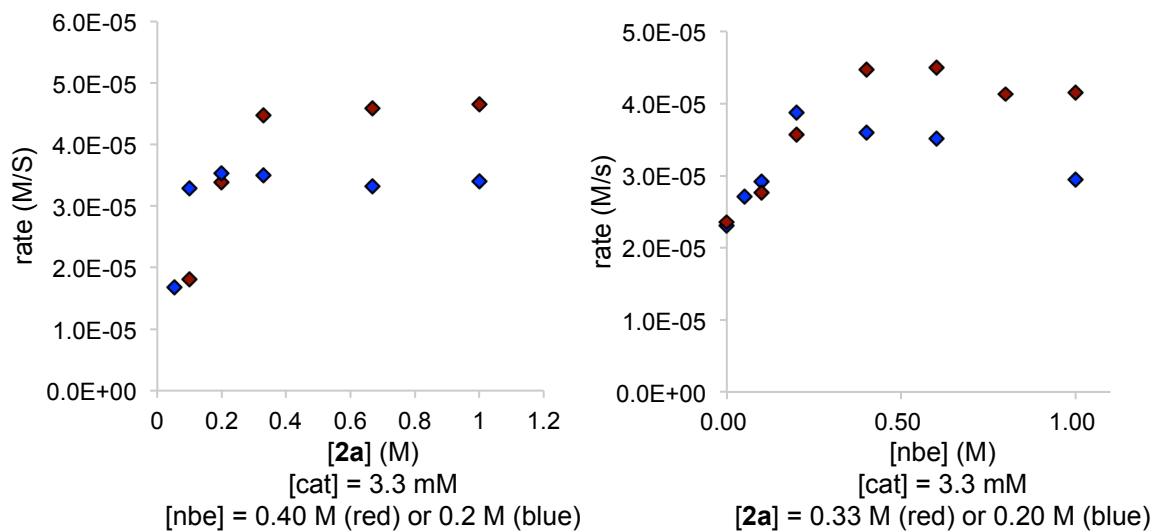
#### Determination of the Experimental Rate Law

Silylation of **2a** was conducted in THF with a total volume of 300  $\mu\text{L}$  by using the combination of  $[\text{Rh}(\text{cod})\text{Cl}]_2$  and **L1** (Rh:L ratio = 1:1.25) as the catalyst. The concentrations of each reagent under the standard conditions for the catalytic silylation are: 0.33 M **2a**, 0.40 M norbornene, and 3.3 mM catalyst. To determine the rate dependence on one reagent, the concentration of that reagent was varied while the concentration of other reagents and the total volume (300  $\mu\text{L}$ ) were held constant. The concentration of **2a** was varied between 0.10 and 1.0 M. The concentration of norbornene was varied between 0 and 1.5 M. The concentration of the catalyst was varied between 0.20 and 6.7 mM. The rate law of the reaction was determined by the method of initial rates at 50  $^\circ\text{C}$  monitored by GC analysis with dodecane as the internal standard.



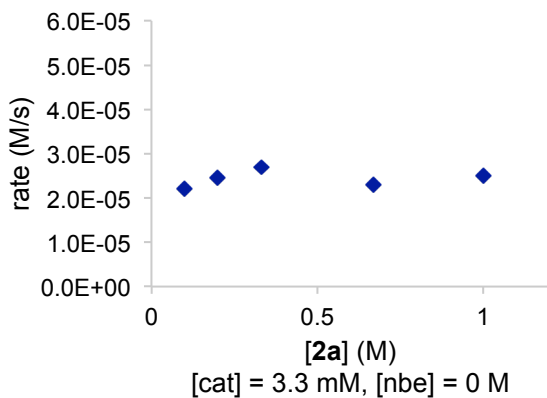
**Figure S12.** Determination of the rate law for the silylation of **2a**.

Additional sets of data points were obtained to illustrate the saturation of the rate at high  $[2a]$  and  $[nbe]$ . The rate dependence on  $[2a]$  at  $[nbe] = 0.20$  M and on  $[nbe]$  at  $[2a] = 0.20$  M were measured.



**Figure S13.** Determination of the rate law for the silylation of **2a** illustrating the saturation of the rate at high  $[2a]$  at two concentrations of  $nbe$ , and the saturation of the rate at high  $[nbe]$  at two concentrations of **2a**.

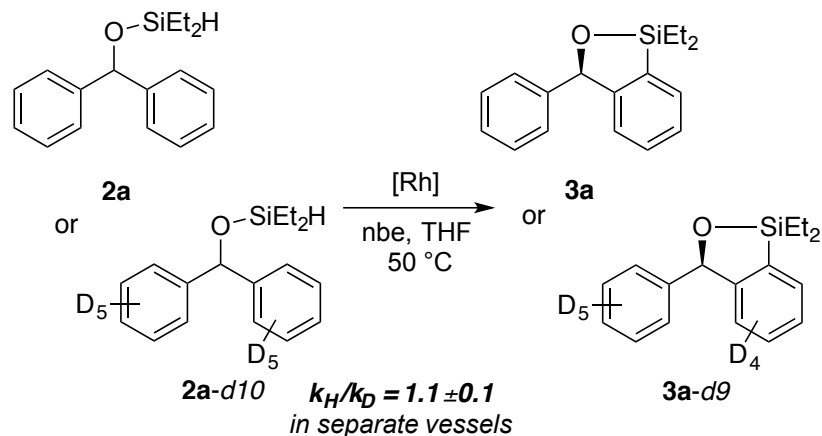
The rate dependence on  $[2a]$  at  $[nbe] = 0$  M was measured.



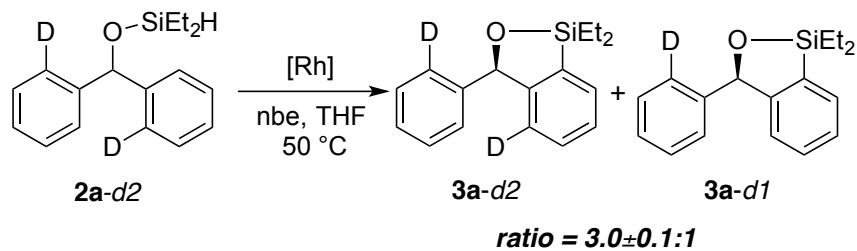
**Figure S14.** Determination of the rate law for the silylation of **2a**  $[2a]$  at  $[nbe] = 0$  M



## Determination of the Kinetic Isotope Effect

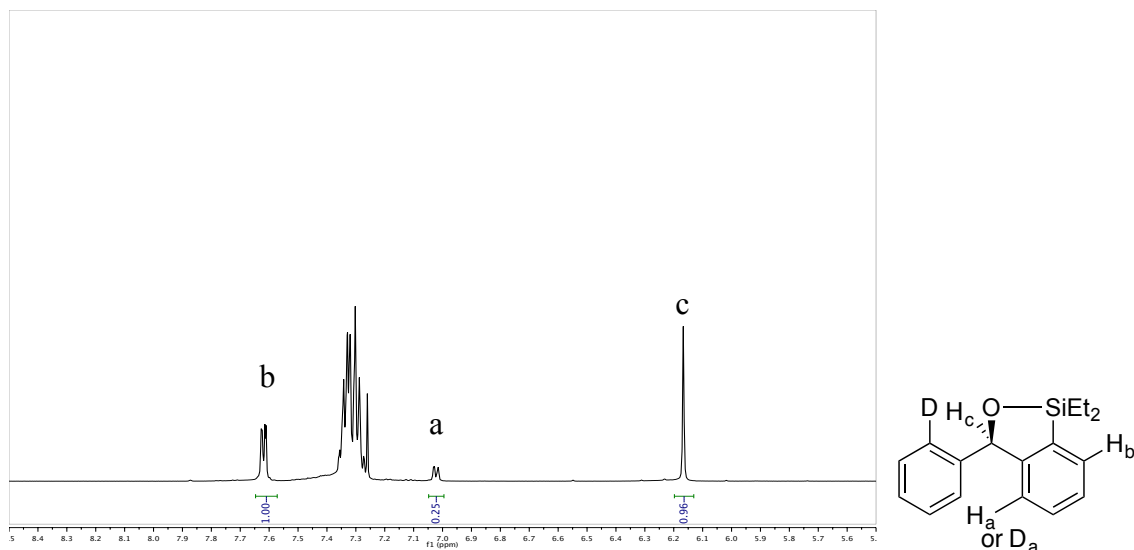


Silylation of **2a-d<sub>10</sub>** was conducted in THF with a total volume of 300  $\mu\text{L}$  under the standard conditions. The concentrations of each reagent under the standard conditions were 0.33 M **2a-d<sub>10</sub>**, 0.40 M norbornene and 3.3 mM catalyst. The initial rate of the reaction at 50  $^\circ\text{C}$  was determined by GC analysis with dodecane as the internal standard. From the initial rates for the silylation of **2a** and **2a-d<sub>10</sub>**, the kinetic isotope effect was determined to be  $k_{\text{H}}/k_{\text{D}} = 1.1 \pm 0.1$  (average of two experiments).



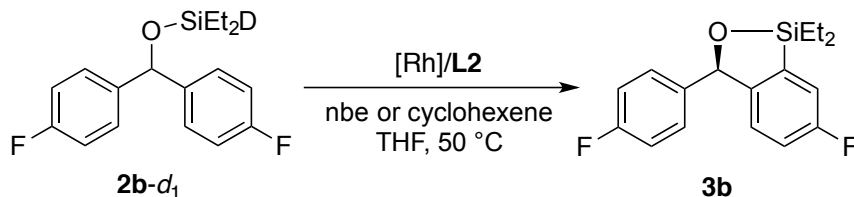
Diethyl(hydrido)silyl ether **2a-d<sub>2</sub>** (27.2 mg, 0.100 mmol) was treated with norbornene (11.3 mg, 0.120 mmol), and a solution of  $[\text{Rh}(\text{cod})\text{Cl}]_2$  (1.0  $\mu\text{mol}$ , 1.0 mol %) and **L2** (2.5  $\mu\text{mol}$ , 2.5 mol %) in THF (0.4 mL) in a 4 mL vial. The resulting mixture was heated at 50  $^\circ\text{C}$  for 24

h. The ratio of **3a-d<sub>2</sub>** and **3a-d<sub>1</sub>** was determined to be 3.0±0.1 : 1 by <sup>1</sup>H NMR analysis (average of two experiments).



**Figure S15.** <sup>1</sup>H spectrum of the mixture of **3a-d<sub>2</sub>** and **3a-d<sub>1</sub>**.

### Deuterium Labeling Study

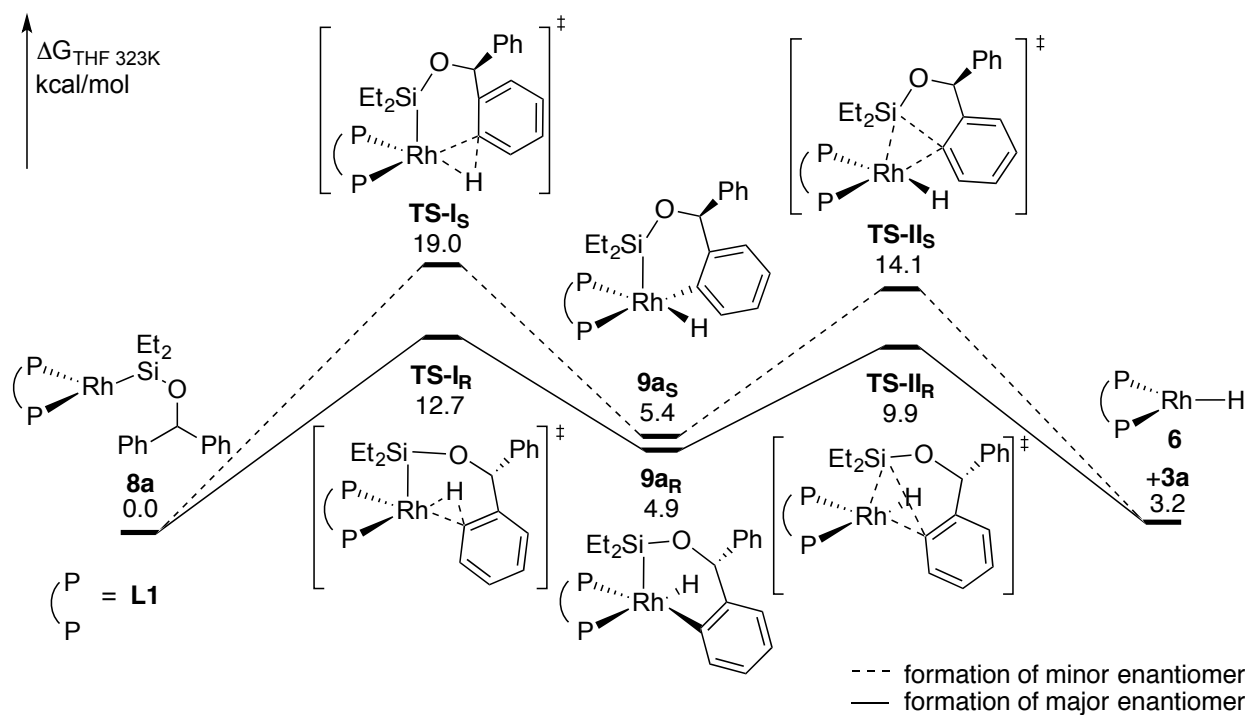


To a J-Young NMR tube was added diethyl(hydrido)silyl ether **2b-d<sub>1</sub>** (30.7 mg, 0.100 mmol), norbornene (11.3 mg, 0.120 mmol) or cyclohexene (12 μL, 0.12 mmol), and a solution of [Rh(cod)Cl]<sub>2</sub> (2.0 μmol, 2.0 mol %) and **L2** (5.0 μmol, 5.0 mol %) in THF (0.4 mL) and THF-*d*<sub>8</sub> (2 μL, standard) in a 4 mL vial. The resulting mixture was heated at 50 °C. The incorporation of deuterium was determined by <sup>2</sup>H NMR analysis.

## Computational Studies

All DFT calculations were performed with the Gaussian 09 software package.<sup>6</sup> Geometries for intermediates and transition states were optimized with the lanl2dz basis set<sup>7,8</sup> for rhodium and the 6-31G(d,p) basis set<sup>9-11</sup> for all other atoms with the B3LYP functional.<sup>12,13</sup> Frequency calculations were conducted on these structures at the same level of theory (at 323 K) to obtain thermodynamic energy corrections and to ensure that all transition states had only one imaginary frequency and all ground states had only positive frequencies. Single-point energy calculations were conducted with the lanl2tz basis set<sup>8,14</sup> for rhodium and the 6-311++G\*\* basis set<sup>15</sup> for all other atoms with the M06 functional.<sup>16</sup> A solvent correction (THF, SMD)<sup>17</sup> was included for the single-point energy calculations.

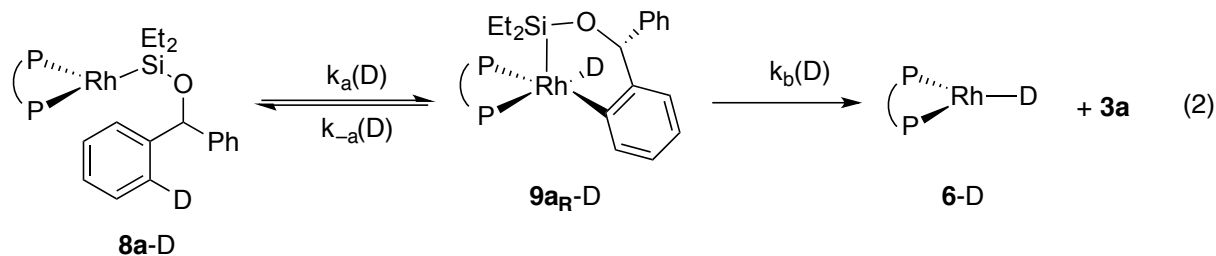
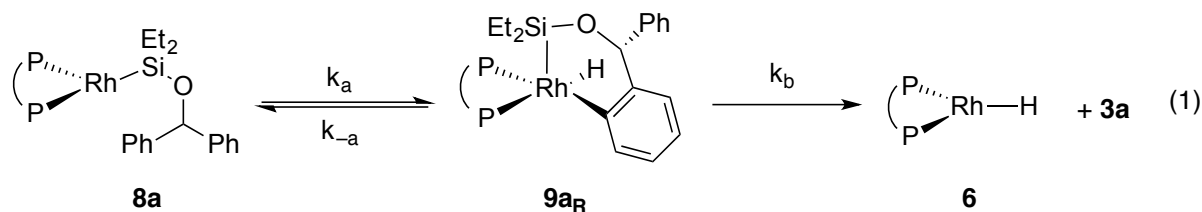
Multiple isomers can be envisioned for each structure. For example, **9a<sub>R</sub>**, a five-coordinate rhodium complex with a non-C<sub>2</sub> symmetric bisphosphine ligand **L1**, can have two diastereomers based on whether phosphorus (P1) of **L1** is trans or cis to the hydride (See Figure 2 to see which phosphorus is P1), and each diastereomer has at least two rotamers based on how the backbone is oriented. At the beginning of the study, we focused on **9a<sub>R</sub>** and **9a<sub>S</sub>**, and we calculated eight structures for each. We found that the structures that resembled the experimental solid-state structure of **4a** were lowest in the energy among the calculated structures. Because of this similarity between the computational and experimental data, we focused on the structures similar to the experimental solid-state structure of **4a** for other intermediates and transition states.



**Figure S16.** Computed pathways for the C–H oxidative addition and C–Si reductive elimination.

#### *Calculation of Theoretical intramolecular KIE*

The intramolecular KIE was calculated by DFT using the following assumptions: 1) only the C–H/D oxidative addition and C–Si reductive elimination steps described in the Figure S13 affect the ratio between C–D and C–H silylation products, 2) the pathway that forms the minor enantiomer is negligible, and 3) the concentration of intermediate **IIa** can be treated with the steady-state approximation. Based on these assumptions, the comparison of the rates of reactions in equation 1 and 2 provides the intramolecular KIE.



From equation 1,

$$\frac{d[9a_R]}{dt} = k_a[8a] - k_{-a}[9a_R] - k_b[9a_R] = 0$$

$$[9a_R] = \frac{k_a[8a]}{k_{-a} + k_b}$$

From equation 2,

$$\frac{d[9a_{R-D}]}{dt} = k_a(D)[8a-D] - k_{-a}(D)[9a_{R-D}] - k_b(D)[9a_{R-D}] = 0$$

$$[9a_{R-D}] = \frac{k_a(D)[8a-D]}{k_{-a}(D) + k_b(D)}$$

Thus,

$$\text{intramolecular KIE} = \frac{\text{rate of reaction in Eq. 1}}{\text{rate of reaction in Eq. 2}} = \frac{k_b[9a_R]}{k_b(D)[9a_{R-D}]} = \frac{\frac{k_b k_a}{k_{-a} + k_b}}{\frac{k_b(D) k_a(D)}{k_{-a}(D) + k_b(D)}}$$

Microscopic rate constants  $k_a$ ,  $k_{-a}$ , and  $k_b$  were calculated by using the Eyring equation:

$$k_a = 1.59 \times 10^4 \text{ s}^{-1}$$

$$k_{-a} = 3.14 \times 10^7 \text{ s}^{-1}$$

$$k_b = 2.57 \times 10^9 \text{ s}^{-1}$$

$k_a(\text{D})$ ,  $k_{-a}(\text{D})$ , and  $k_b(\text{D})$  were calculated by dividing each microscopic rate constant  $k_a$ ,  $k_{-a}$ , and  $k_b$  by its corresponding KIE. The KIE's for each step were calculated from the zero-point energy difference in the reactants ( $\Delta\text{ZPE}_{\text{reactant}}$ ) and the zero-point energy difference in the transition state ( $\Delta\text{ZPE}_{\text{TS}}$ ).  $\Delta\text{ZPE}$  is the difference of the zero-point energy between the protiated structure and the deuterated structure. The expression for the microscopic KIE's is:

$$\text{KIE} = e^{\frac{\Delta\text{ZPE}_{\text{reactant}} - \Delta\text{ZPE}_{\text{TS}}}{RT}}$$

Zero-point energies for deuterated structures were determined from frequency calculations. The corresponding hydrogen atoms were substituted with deuterium in optimized structures of **8a**, **TS-I<sub>R</sub>**, **9a<sub>R</sub>**, and **TS-II<sub>R</sub>** in these frequency calculations. The microscopic KIE's are:

$$\text{KIE}_a = 4.21$$

$$\text{KIE}_{-a} = 1.39$$

$$\text{KIE}_b = 0.962$$

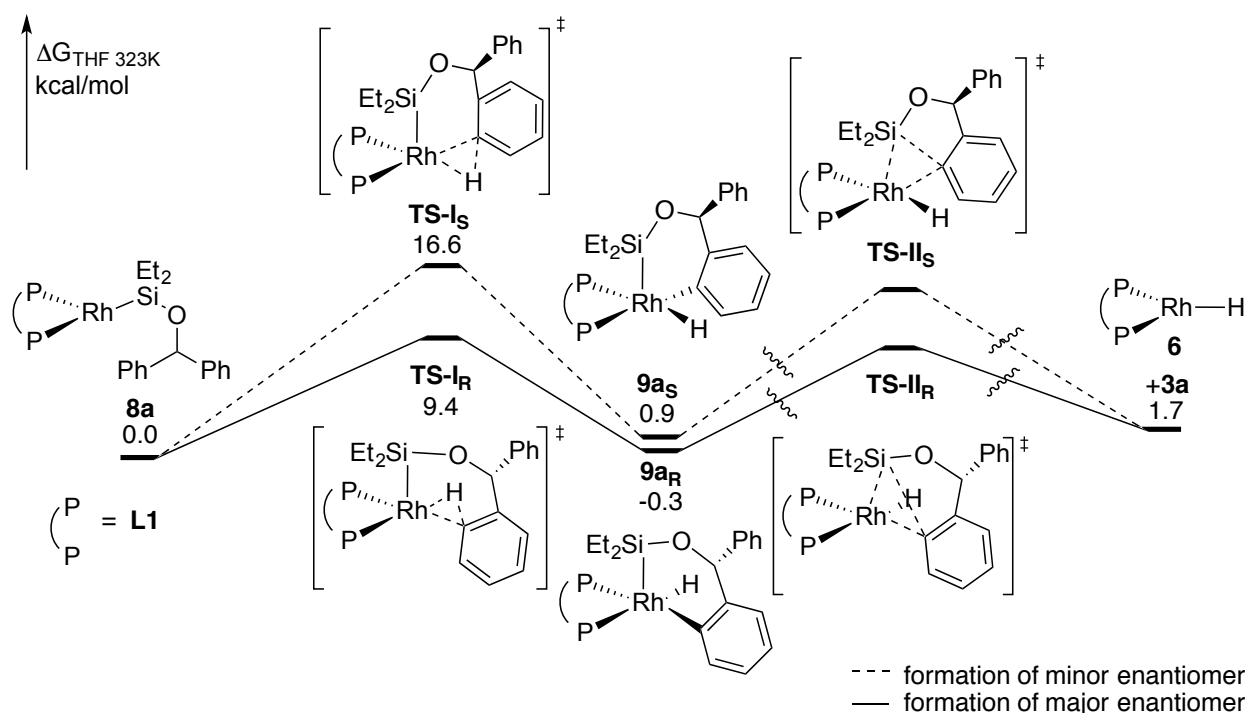
From these values, the theoretical intramolecular KIE was calculated to be 4.20.

#### *Calculation with the M06 functional.*

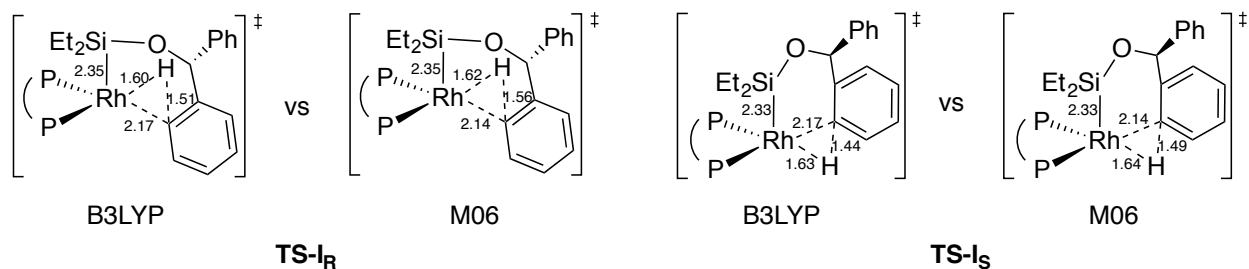
We optimized the geometry of the structures by using the M06 functional to ensure the consistency of results from different functionals. The computational details are identical as described above (S19) except the use of the M06 functional for geometry optimization. We were unable to calculate **TS-II<sub>R</sub>** and **TS-II<sub>S</sub>** in this set of calculation.

Comparison of the energies from these calculations with M06 to those with the B3LYP functionals suggested that the discrepancy between the two functionals is not significant

enough to affect the conclusion in our study. Both calculations suggest that **TS-I<sub>S</sub>** is 6-7 kcal/mol higher than **TS-I<sub>R</sub>** (Figure S16–17). Differences of the lengths of the bonds that break and form during **TS-I<sub>S</sub>** and **TS-I<sub>R</sub>** between the two functionals are within 0.05 Å (Figure S18).



**Figure S17.** Computed pathways for the C–H oxidative addition and C–Si reductive elimination (M06 functional).

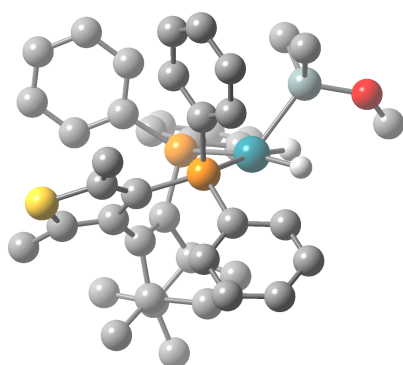
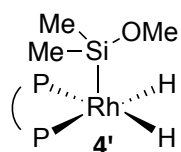


**Figure S18.** Comparison of **TS-I<sub>R</sub>** and **TS-I<sub>S</sub>** computed with the B3LYP and M06 functionals (All distances are in Å.)

## Cartesian Coordinates of Computed Structures

All distances in the figures below are in Å.

Structures computed with the B3LYP functional:



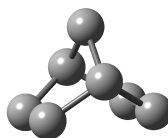
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ZPE=-3222.780754

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C	-0.88742600	-2.14485000	-0.46298800	C
C	-1.43324200	-0.86413100	-2.96082900	C
C	-0.46794900	-2.07717300	-2.87933500	C
C	-3.59178900	-3.38016000	-0.98738100	C
C	-3.12623500	-3.21482000	-3.40240400	C
C	-0.57221800	-4.41239200	-1.78947900	C
C	0.18515500	-2.43463500	0.52771900	C
C	0.11229900	-3.54132700	1.34803000	C
C	2.30662100	-2.32753300	1.57731400	C
C	1.44825300	-1.70253700	0.69112000	C
C	-1.01509100	-4.50537200	1.57838700	C
C	3.72224200	-2.03667500	1.99986100	C
C	2.94761100	-0.62166500	-1.55137500	C
C	3.29751100	0.31527000	-2.53902400	C
C	4.14421600	-0.03907700	-3.58989500	C
C	4.63958100	-1.34089100	-3.68693100	C
C	4.28553500	-2.28461100	-2.72274500	C
C	3.45012900	-1.92804300	-1.66173100	C
C	2.96871700	0.75536200	1.03083700	C
C	2.48978500	1.04754400	2.31851800	C
C	3.29073800	1.72693600	3.23575100	C
C	4.57541000	2.14457000	2.87612100	C
C	5.05053300	1.87408400	1.59352500	C
C	4.25466700	1.18271300	0.67659000	O
O	0.38668200	4.77913400	-1.81241800	Si
Si	0.33631800	3.77560000	-0.45454600	P
P	-1.73027600	0.46767300	0.42170600	P
P	1.83092400	-0.09332700	-0.16030300	S
S	1.56500300	-3.73790800	2.27724200	Rh
Rh	0.05783500	1.48596600	-0.83051500	H
H	-4.29649500	-0.00491000	1.93791800	H
H	-6.58907000	0.83740500	1.63571700	H
H	-7.11050300	2.42632000	-0.20554400	H
H	-5.29834100	3.16313200	-1.74423400	H
H	-2.98773100	2.32299800	-1.43101600	H
H	-2.46849300	-1.97682900	2.04413800	H
H	-2.40722100	-2.42639400	4.47591800	H
H	-1.55931400	-0.69459200	6.04394800	H
H	-0.77763300	1.49504300	5.15822900	H
C	-3.47584900	1.08784900	0.26145100	C
C	-4.50591700	0.68061500	1.12394700	C
C	-5.80568900	1.16005000	0.95540300	C
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C	-5.08280700	2.46422300	-0.94086700	C
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C	-2.09700800	-1.21677100	2.72223200	C
C	-2.06124200	-1.46937500	4.09471800	C
C	-1.58614600	-0.49650900	4.97627100	C
C	-1.14599500	0.73139500	4.47899200	C
C	-1.17553200	0.98147700	3.10576700	C
C	-1.74609700	-1.09584400	-0.53471900	C
C	-2.49428500	-1.20776300	-1.86698900	C
C	-2.63603600	-2.75264200	-2.01661600	C

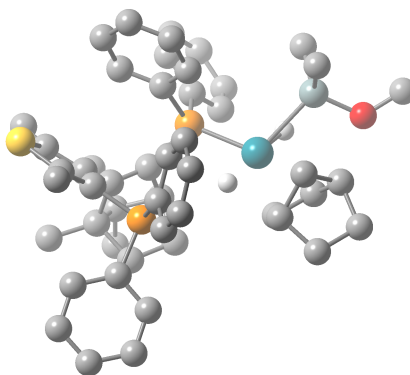
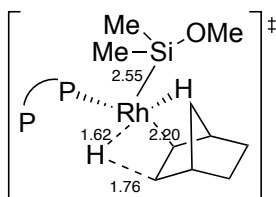


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H	-1.90034600	-0.77650100	-3.94679000
H	-0.93662100	0.09092400	-2.75126500
H	0.55730800	-1.79460200	-2.63179500
H	-0.42221100	-2.62641600	-3.82563100
H	-4.62723800	-3.12040400	-1.23446800
H	-3.40631900	-3.03665400	0.03084900
H	-3.52382600	-4.47416200	-1.00234500
H	-3.17691400	-4.30888000	-3.44246900
H	-2.50074200	-2.88504700	-4.23216200
H	-4.13948200	-2.83850300	-3.58374100
H	0.49771300	-4.44663900	-1.56073900
H	-0.70808500	-4.83789700	-2.78945800
H	-1.08387300	-5.06787500	-1.07998100
H	-1.86026800	-4.27693600	0.93062900
H	-1.36640700	-4.45328200	2.61595800
H	-0.71321000	-5.54180000	1.38986500
H	4.31077200	-1.63659200	1.17335100
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H	3.76411800	-1.30733200	2.81461600
H	2.88917700	1.31936100	-2.48817000
H	4.40499600	0.70221000	-4.33998500
H	5.28952200	-1.61899800	-4.51180100
H	4.65728100	-3.30314300	-2.79308500
H	3.17985400	-2.67511900	-0.92363000
H	1.49255600	0.73295400	2.60978700
H	2.90840900	1.93483700	4.23142300
H	5.19663900	2.67870200	3.58919900
H	6.04579300	2.19711400	1.30123700
H	4.64563200	0.97110700	-0.31284100
H	-0.96053400	2.46843500	-1.53134100
H	1.07876600	2.03220600	-1.91332800
C	2.00060000	4.18847200	0.34274900
H	2.12735500	3.69899200	1.31154700
H	2.83034200	3.88786600	-0.30201200
H	2.05966400	5.27380100	0.49054200
C	-1.02313100	4.46313400	0.68948000
H	-2.02827900	4.28657100	0.29532900
H	-0.97669900	4.01015400	1.68596400
H	-0.88560000	5.54493300	0.81082400
C	-0.55962700	4.80204700	-2.85359900
H	-0.65294000	3.81737300	-3.33527500
H	-1.55779800	5.10879800	-2.50399200
H	-0.23079900	5.52658200	-3.60740500



G=-272.461427  
ZPE=-272.429973

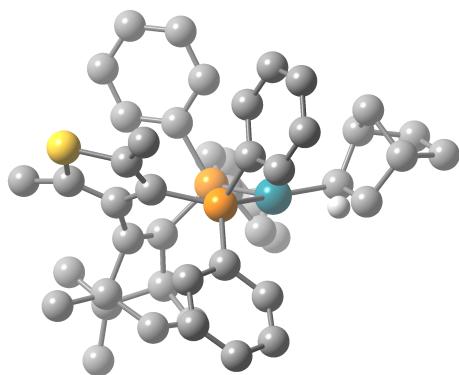
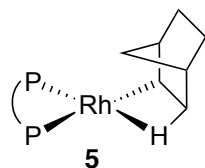
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C	-0.08743300	1.12855900	0.32241700
C	-0.08839900	-1.12799500	0.32360600
C	1.19107700	-0.78133700	-0.51560100
H	1.14781900	1.20551900	-1.52207900
H	2.08894000	1.17573200	-0.02801000
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H	2.08741600	-1.17775000	-0.02688600
C	-0.04201200	0.00094800	1.38059700
H	-0.91339900	0.00178600	2.04137200
H	0.87592700	0.00096800	1.98008300
C	-1.27837900	0.67023500	-0.50861500
H	-1.92009500	1.32761200	-1.08593800
C	-1.27899100	-0.67005900	-0.50787600
H	-1.92091000	-1.32756800	-1.08481200
H	-0.11904600	2.15744400	0.68751700
H	-0.12090900	-2.15634400	0.69012500



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ZPE=-3495.196150

Si	-4.56557100	0.94635100	0.22117500	P	-1.31950200	-1.21056300	0.24360500
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O	-5.51367600	1.80742300	-0.88107300	H	-2.07677500	-3.61739700	2.00598100
C	-2.53811300	-2.62993500	0.13665700	H	-3.69236700	-5.43504000	1.70386400
C	-2.67521500	-3.63752700	1.10343600	H	-5.11763700	-5.53206000	-0.33318800
C	-3.60045900	-4.67153800	0.93610700	H	-4.91863900	-3.73887300	-2.05212600
C	-4.40195900	-4.72515000	-0.20360500	H	-3.33141300	-1.88072300	-1.72285500
C	-4.28784100	-3.72213000	-1.16760000	H	0.14760200	-3.14886300	2.08410600
C	-3.37719500	-2.68065000	-0.99035400	H	0.65630300	-3.05436900	4.49548300
C	-0.80510600	-1.21460300	2.01889700	H	-0.00382500	-1.06862700	5.83539700
C	-0.14403600	-2.27656900	2.65521700	H	-1.16749000	0.83370000	4.72944000
C	0.14199500	-2.22391400	4.02003300	H	-1.65601800	0.73588100	2.28954200
C	-0.22665400	-1.10681200	4.77281900	H	-1.30036800	-2.47128500	-2.44104800
C	-0.87844000	-0.04052500	4.15258500	H	0.06294200	-1.21142600	-4.12210200
C	-1.16097700	-0.09409400	2.78532700	H	0.06756500	-0.15689600	-2.70692100
C	0.06741400	-1.92122100	-0.75734800	H	2.42850900	-0.54227500	-2.47779000
C	-0.25130200	-2.27778900	-2.22057000	H	2.38844800	-1.62112400	-3.85914300
C	0.71719200	-3.46744700	-2.47793500	H	-0.51642500	-5.21639800	-2.11947100
C	1.95390900	-2.64147100	-1.95460300	H	0.11737700	-4.52240900	-0.63517400
C	1.40441500	-2.10864300	-0.59614700	H	1.17916000	-5.46040300	-1.70592300
C	0.37882900	-1.13531500	-3.07667500	H	1.53703100	-4.71716500	-4.06426700
C	1.89879500	-1.39316700	-2.90647700	H	1.10470200	-3.10741600	-4.63969400
C	0.36065400	-4.73155000	-1.67692100	H	-0.15710100	-4.28768200	-4.29040400
C	0.81224800	-3.90254000	-3.95357600	H	4.09267600	-2.65417200	-1.56850500
C	3.31325800	-3.32706600	-1.93927400	H	3.59445500	-3.62813000	-2.95431200
C	2.33846700	-1.82363100	0.53435000	H	3.32354700	-4.22345200	-1.31209500
C	2.82680200	-2.82310200	1.34895500	H	1.76890600	-4.54037900	0.62475800
C	3.84584300	-0.57875700	1.87587600	H	2.10581300	-4.59301500	2.35926900
C	2.94337100	-0.52360000	0.83231400	H	3.39895800	-4.90089100	1.20181100
C	2.50771700	-4.28929500	1.38480500	H	5.05956500	1.19938100	1.78104000
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C	4.02619400	1.28643800	-1.17836300	H	4.09720400	1.06764600	3.24899800
C	3.91809200	2.26143400	-2.18745400	H	2.98725100	2.81150300	-2.30350400
C	4.98397500	2.52849000	-3.04663800	H	4.88063100	3.29128000	-3.81344900
C	6.17280900	1.80438000	-2.93267000	H	7.00016100	2.00232600	-3.60815000
C	6.28523300	0.81614000	-1.95406300	H	7.20278300	0.24081500	-1.86463100
C	5.22326600	0.56057300	-1.08308800	H	5.32336000	-0.21424700	-0.33001600
C	2.57240100	2.35226900	1.10340600	H	1.10562000	1.37689200	2.35887400
C	1.70868200	2.26714200	2.21012800	H	0.95958400	3.21421000	3.98740900
C	1.62478500	3.30891700	3.13325100	H	2.31547100	5.28231800	3.67655700
C	2.38513500	4.46846700	2.96051800	H	3.83176800	5.46568300	1.71210700
C	3.23281400	4.57056800	1.85771300	H	4.00498600	3.61952100	0.09506700
C	3.32829200	3.52297500	0.93784800	C	-6.80362000	2.30255700	-0.57936300
				H	-6.78669900	3.03129300	0.24421700
				H	-7.19527500	2.80790600	-1.46839900
				H	-7.50400000	1.49882500	-0.31017500
				C	-4.33887100	2.00188700	1.78570900

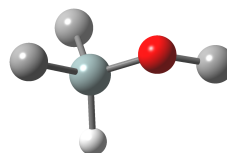
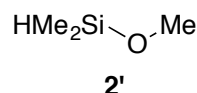
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H	-3.82990500	1.42937200	2.56646700	C	0.52232000	5.81638400	0.45919200
C	-5.55069400	-0.56460200	0.80557500	C	0.88403600	6.14571000	-0.84660500
H	-6.44298400	-0.25817200	1.36467500	C	0.98571900	5.13656400	-1.80703500
H	-5.87242000	-1.18963100	-0.03275200	C	0.73414500	3.81019800	-1.45772100
H	-4.94840700	-1.19464300	1.46863300	C	-0.16002100	1.69043800	2.07291900
C	-2.53884300	2.73024900	-1.62221700	C	-1.32942800	2.12554000	2.71394800
C	-2.79975600	4.03865300	-0.87112400	C	-1.40846100	2.15639600	4.10745100
H	-3.16694300	2.46182000	-2.46651700	C	-0.31679400	1.75664600	4.88135300
C	-1.12688100	2.57129500	-1.63274600	C	0.85462000	1.32776500	4.25488500
C	-2.33633400	5.17401600	-1.83869300	C	0.93087400	1.29277700	2.86090600
C	-1.63935700	4.05466300	0.14933200	C	-1.63738100	1.39278700	-0.44661200
H	-3.81228300	4.16594600	-0.48558800	C	-2.12964200	2.05376900	-1.73636200
C	-0.54955700	3.78373600	-0.90542400	C	-3.67530900	1.90670600	-1.60260300
H	-0.58560500	1.27974000	-0.56501800	C	-3.56660000	0.36648100	-1.28971800
H	-0.58699300	2.14965300	-2.47641700	C	-2.48556900	0.37033700	-0.16984600
C	-0.78549200	4.98134300	-1.88172600	C	-1.79252600	1.02525200	-2.86542700
H	-2.80394100	5.08954900	-2.82438200	C	-2.77489400	-0.13581600	-2.55497400
H	-2.60047400	6.15731300	-1.43305100	C	-4.28038000	2.77169900	-0.48405700
H	-1.69961300	3.25794300	0.89491400	C	-4.45692600	2.24979500	-2.88576600
H	-1.51717900	5.02237500	0.64845500	C	-4.85474600	-0.40969200	-1.05539100
H	0.47451100	3.68482200	-0.54370800	C	-2.38404400	-0.70578500	0.85446400
H	-0.41001700	4.77332200	-2.88904200	C	-3.32050300	-0.82794200	1.85817400
H	-0.26246300	5.87170500	-1.51703600	C	-1.70117700	-2.75964200	1.81936900
				C	-1.40985600	-1.80689800	0.86239500
				C	-4.41537900	0.10854500	2.27796200
				C	-1.07805300	-4.08661100	2.16464100
				C	-0.37571700	-2.86417100	-1.65011500
				C	0.33352000	-2.70271000	-2.85112200
				C	0.03643000	-3.48530300	-3.96802200
				C	-0.98831100	-4.43157800	-3.90568500
				C	-1.71298000	-4.58978500	-2.72254600
				C	-1.40882100	-3.81319500	-1.60295600
				C	1.32175800	-2.86648800	0.70571800
				C	1.77336900	-2.43821100	1.96738900
				C	2.76662100	-3.14385300	2.64558600
				C	3.34314200	-4.27972800	2.06939500
				C	2.91223400	-4.70455000	0.81289300
				C	1.90814800	-4.00570700	0.13648800
				P	0.04608500	1.66805400	0.23166700
				P	0.10882700	-1.79445400	-0.20937400
				S	-3.08221600	-2.28598100	2.77323600
				Rh	1.43978700	0.13507200	-0.59549600
				H	-0.02632500	4.25636200	1.82611600
				H	0.44521400	6.59272200	1.21567100
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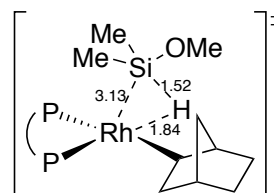
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H	-2.32214900	2.49503200	4.58872300
H	-0.37964700	1.77975600	5.96570300
H	1.70923600	1.01815600	4.85024900
H	1.83579000	0.95160400	2.36588800
H	-1.76224700	3.06449000	-1.91888100
H	-1.96815800	1.45604200	-3.85655600
H	-0.74459400	0.71694400	-2.81276900
H	-2.26949000	-1.08111100	-2.35341400
H	-3.46598300	-0.31880400	-3.38487600
H	-4.24258500	3.82977100	-0.76690500
H	-3.75210300	2.66790600	0.46368900
H	-5.33493100	2.52046400	-0.32038500
H	-5.52944900	2.08291700	-2.73425900
H	-4.15631900	1.67528800	-3.76235600
H	-4.32736900	3.31101400	-3.12782700
H	-4.64604000	-1.45325800	-0.79974900
H	-5.46605600	-0.40965100	-1.96441900
H	-5.46139800	0.01366700	-0.25061300
H	-4.47178700	0.96378700	1.60566500
H	-4.23009100	0.49259900	3.28815500
H	-5.39531000	-0.38202400	2.28880400
H	-0.65613400	-4.57431000	1.28563600
H	-1.83202800	-4.75552000	2.59119000
H	-0.27006000	-3.98308900	2.89605300
H	1.11178300	-1.94608000	-2.90663600
H	0.59679700	-3.34737800	-4.88858500
H	-1.22733000	-5.03569400	-4.77642000
H	-2.51859900	-5.31716000	-2.67078200
H	-1.98825300	-3.93291900	-0.69308400
H	1.33838900	-1.55336400	2.42226000
H	3.09500600	-2.80321200	3.62389500
H	4.12122400	-4.82539400	2.59549900
H	3.35268900	-5.58615700	0.35493500
H	1.57958700	-4.35580600	-0.83643900
C	5.41125600	2.15825800	-0.65864800
C	4.13159900	1.64561800	0.06246000
C	4.95631100	-0.22739800	-0.91383600
C	5.96265100	0.86930500	-1.35189300
H	5.18592400	2.95870500	-1.37054400
H	6.13463800	2.55627000	0.06309000
H	6.01937300	0.96291600	-2.44183000
H	6.96978900	0.62667600	-0.99625800
C	4.59459800	0.24109800	0.51142300
H	3.79536200	-0.35331800	0.96534300
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C	3.09126200	1.31207600	-1.01988300

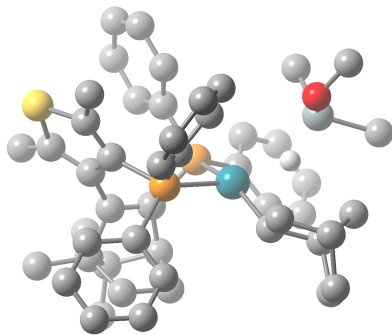
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H	3.73680100	0.07785800	-2.76218900
H	3.77439700	2.31575500	0.84901200
H	5.33474600	-1.24912300	-1.01156200



G=-484.933094  
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O	-0.98520600	-0.64516400	-0.32197100
C	-2.28239400	-0.16159900	-0.01914100
H	-2.44666500	0.84747400	-0.42203900
H	-3.01563000	-0.83354000	-0.47521300
H	-2.46832500	-0.13506600	1.06400700
C	1.81049200	-1.12067200	-0.18978200
H	1.64059900	-2.15143400	0.13546900
H	1.91169200	-1.12468600	-1.27990300
H	2.76253500	-0.78456100	0.23549700
C	0.68928900	1.77594200	-0.20225200
H	0.81938500	1.83832600	-1.28798300
H	-0.14479700	2.43003100	0.07326000
H	1.59212600	2.18326700	0.26732000
Si	0.40403800	-0.00366700	0.34943500
H	0.26987700	-0.01919200	1.84031100



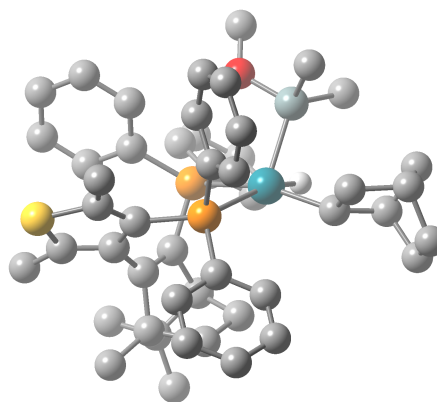
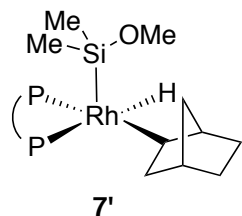


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H	2.16690500	1.89831100	-0.12063600
O	3.79914900	1.49269800	1.84057400
C	-0.69713400	3.31322000	-0.62619900
C	-1.14371800	4.49989700	-0.02514500
C	-0.90597300	5.74058200	-0.62446800
C	-0.22172900	5.81974500	-1.83706000
C	0.23321600	4.64729600	-2.44582600
C	0.00569600	3.41046500	-1.84216200
C	-1.82909200	1.92987600	1.68455600
C	-3.09917300	2.53020900	1.70800400
C	-3.76976800	2.73319300	2.91476800
C	-3.18557100	2.32812400	4.11830400
C	-1.93170500	1.71703300	4.10734100
C	-1.26016400	1.52006000	2.89783800
C	-2.11511900	0.80660000	-0.95576300
C	-2.41410800	1.13034100	-2.41778600
C	-3.85533100	0.54815000	-2.57427800
C	-3.42975800	-0.84441300	-1.95956100
C	-2.70425800	-0.37820700	-0.66783300
C	-1.55764000	0.11729800	-3.24516900
C	-2.25494800	-1.23449900	-2.93322100
C	-4.91987200	1.33042500	-1.78743600
C	-4.35749600	0.48222600	-4.03010400
C	-4.48376800	-1.93751300	-1.84590600
C	-2.58830800	-1.12303700	0.61844800
C	-3.67878400	-1.26189300	1.45107600
C	-1.58936700	-2.28016600	2.42914500
C	-1.36269600	-1.71026500	1.19062000
C	-5.07724500	-0.73092700	1.32461300
C	-0.73433000	-3.03651700	3.41544400

C	-0.04263300	-3.15359700	-0.87622000
C	0.80115600	-3.37799500	-1.97642600
C	0.60100800	-4.46635200	-2.82719000
C	-0.44778100	-5.35751500	-2.59740200
C	-1.29066200	-5.15365700	-1.50426900
C	-1.08990300	-4.06500200	-0.65281100
C	1.50459300	-2.47233400	1.43261300
C	2.21685600	-1.62130300	2.29372100
C	3.16538100	-2.13411000	3.17916300
C	3.44389200	-3.50305100	3.19658900
C	2.77001900	-4.35199800	2.31810400
C	1.80632700	-3.84196800	1.44454400
P	-0.86782700	1.61754900	0.12190000
P	0.26881300	-1.70168600	0.27087000
S	-3.25528300	-2.09737700	2.90831700
H	-1.67381700	4.46465100	0.91976600
H	-1.25916700	6.64578900	-0.13785500
H	-0.04038000	6.78447400	-2.30238300
H	0.77093400	4.69445900	-3.38887200
H	0.38418200	2.50677500	-2.31233800
H	-3.56345400	2.84773100	0.77934400
H	-4.74794600	3.20685100	2.91644300
H	-3.70914100	2.48376000	5.05741900
H	-1.47696100	1.38858500	5.03768900
H	-0.29256000	1.02673700	2.88309500
H	-2.28692400	2.17529500	-2.70701400
H	-1.58619500	0.35708400	-4.31297300
H	-0.51150200	0.13357300	-2.92702300
H	-1.59016800	-1.96244400	-2.47259600
H	-2.65820800	-1.70172500	-3.83787700
H	-5.09357100	2.30412000	-2.26012400
H	-4.63209100	1.51223200	-0.75229100
H	-5.87910800	0.79935400	-1.79028900
H	-5.35002300	0.01914700	-4.06927900
H	-3.70841300	-0.07539500	-4.70535400
H	-4.45956200	1.49599100	-4.43435500
H	-4.07211100	-2.82700000	-1.35836000
H	-4.82681100	-2.23875000	-2.84152200
H	-5.36221600	-1.62305200	-1.27637100
H	-5.20114800	-0.17491600	0.39820700
H	-5.30838000	-0.04933500	2.15101200
H	-5.82141900	-1.53576400	1.34220500
H	-0.36033500	-3.97479200	2.99880500
H	-1.32250500	-3.28119700	4.30489600
H	0.13388100	-2.45918100	3.73816900
H	1.62005600	-2.70013500	-2.17375100
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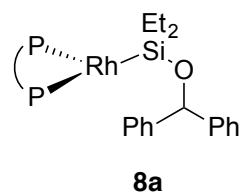
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H	3.70011600	-1.45883800	3.84144300
H	4.19137300	-3.90195200	3.87685200
H	2.99161000	-5.41584700	2.31013800
H	1.28795200	-4.51952400	0.77516100
C	4.88617000	1.82082200	2.69207800
H	4.56198400	2.40812300	3.56261900
H	5.32669300	0.88712300	3.05360600
H	5.66596600	2.38456800	2.16277200
C	1.79060800	3.59099800	2.14543300
H	1.13603500	2.94382800	2.73245300
H	2.40587100	4.17513900	2.84099100
H	1.16390900	4.29236000	1.58698500
C	4.01618200	3.84149100	0.06483700
H	4.61291100	4.45029300	0.75409500
H	4.69860500	3.33692500	-0.62387500
H	3.39194100	4.52638500	-0.52036000
C	2.69610800	-0.43910100	-1.45890700
C	3.57035000	0.63364300	-2.18873700
H	2.08330500	-0.92022600	-2.23178000
C	3.78003400	-1.43200400	-0.93547700
C	4.00008300	0.02944800	-3.55251100
C	4.91438700	0.58685300	-1.42828900
H	3.10487000	1.61876300	-2.29134300
C	5.08617800	-0.93684500	-1.59502100
H	3.88227600	-1.37628300	0.15323100
H	3.56164100	-2.47984500	-1.17783900
C	4.98834900	-1.10737700	-3.13133500
H	3.14528100	-0.34014100	-4.12909300
H	4.50873900	0.78206300	-4.16911200
H	4.84010400	0.87560100	-0.37738500
H	5.70569500	1.17399000	-1.91225200
H	5.99320000	-1.36886400	-1.15909100
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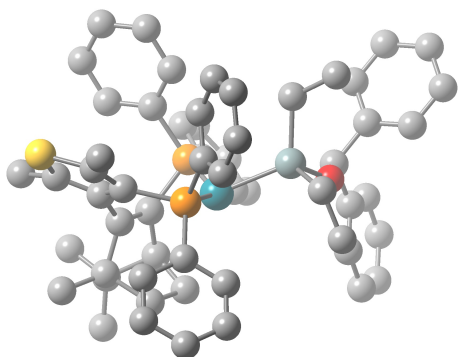


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O	0.01233800	3.04653800	2.18515900
C	-2.27470100	2.80837200	-0.45600000
C	-3.33125400	3.40572300	0.24737100
C	-3.87209100	4.62473200	-0.16963000
C	-3.37139600	5.27019600	-1.29923100
C	-2.31322000	4.69294600	-2.00389300
C	-1.76422700	3.48264200	-1.57993400
C	-2.49457200	0.74703500	1.56377200
C	-3.84295300	0.37066900	1.44548500
C	-4.60144900	0.06120500	2.57454800
C	-4.02099700	0.11159600	3.84425100
C	-2.68407300	0.48588300	3.97443900
C	-1.92716600	0.80709100	2.84415800
C	-2.01168200	-0.00450600	-1.19468000
C	-2.13122200	0.31549000	-2.68720200
C	-3.07486600	-0.82367100	-3.18256100
C	-2.18926800	-1.93918100	-2.50344900
C	-2.03300800	-1.35628800	-1.07044700
C	-0.75915500	-0.10191900	-3.30617300
C	-0.79596000	-1.64856700	-3.17512800
C	-4.51442300	-0.69578000	-2.65810100
C	-3.18407500	-0.93562000	-4.71613000
C	-2.62066000	-3.39214000	-2.64889000
C	-1.83361400	-2.18486800	0.15326100
C	-2.86841600	-2.92004900	0.69205400
C	-0.70798900	-3.25480700	1.94670500
C	-0.57955200	-2.36351800	0.89692700
C	-4.31984400	-2.98175800	0.31680000

C	0.26948600	-3.83077200	2.93853200	H	3.30118700	-5.54453100	-3.07934900
C	1.72695200	-2.84953200	-0.72748700	H	1.56530800	-6.19074200	-1.41647000
C	2.69721900	-2.49857900	-1.68005600	H	0.56212700	-4.49221800	0.05451500
C	3.26449800	-3.46229900	-2.51659100	H	0.74648100	-0.37533700	3.03777800
C	2.86442600	-4.79521600	-2.42528600	H	2.18583700	-0.33113500	5.04202800
C	1.89090500	-5.15695400	-1.49255900	H	4.37935700	-1.50973600	5.03418900
C	1.32720900	-4.19495200	-0.65337500	H	5.10880300	-2.72978600	2.99247900
C	2.08983700	-1.60327300	1.87670300	H	3.65897700	-2.80215600	1.00152900
C	1.69812000	-0.89696300	3.02581000	C	-0.23311300	4.14520900	3.04221200
C	2.51120400	-0.87359200	4.15874200	H	-0.43287100	5.06697700	2.47978900
C	3.74286500	-1.53379100	4.15446600	H	-1.11766600	3.91697300	3.64771100
C	4.15083600	-2.21753800	3.00939300	H	0.60609900	4.33715500	3.72748700
C	3.33068800	-2.25530500	1.87875400	C	1.59468800	4.66837200	0.42393900
P	-1.47674500	1.21310400	0.07957700	H	0.65994000	4.99817200	-0.04296900
P	0.99853200	-1.53415800	0.38053400	H	1.86765800	5.40277400	1.19175100
S	-2.34455700	-3.83235500	2.07166500	H	2.37164300	4.68526500	-0.34530800
H	-3.73567100	2.92680300	1.13082800	C	2.83820400	2.62290400	2.34369300
H	-4.68735600	5.06803500	0.39576000	H	2.80677100	3.37322900	3.14510900
H	-3.79431200	6.21690300	-1.62340600	H	2.78768600	1.63346700	2.80426300
H	-1.90407700	5.18918700	-2.87964400	H	3.80786300	2.71475500	1.84776000
H	-0.91844400	3.06741800	-2.11787700	C	2.83820000	1.13216200	-1.24015400
H	-4.30751700	0.33044800	0.46588800	C	3.39074300	2.34448100	-2.05224200
H	-5.64622300	-0.21669300	2.46273800	H	2.52950700	0.37260900	-1.97931400
H	-4.60987700	-0.13348200	4.72376600	C	4.11538300	0.64697700	-0.47482900
H	-2.22678100	0.53741000	4.95883500	C	4.21688900	1.78240100	-3.24001800
H	-0.90625100	1.15453200	2.94993900	C	4.53019700	2.89096500	-1.16547200
H	-2.44820400	1.33139900	-2.92645600	H	2.63382500	3.06938100	-2.36086900
H	-0.68080200	0.22014700	-4.34940200	C	5.24809600	1.53089500	-1.04665300
H	0.07362400	0.35600700	-2.76326700	H	4.02745100	0.80059600	0.60473400
H	0.02034700	-2.04984900	-2.57476600	H	4.32849600	-0.41951200	-0.61532700
H	-0.73794500	-2.14049700	-4.15155600	C	5.47058300	1.16543000	-2.53505800
H	-5.01851600	0.14274900	-3.15159100	H	3.65349900	1.04810000	-3.82631100
H	-4.55979300	-0.51690500	-1.58417200	H	4.51015500	2.58766400	-3.92531400
H	-5.09677000	-1.59688800	-2.88307500	H	4.19571600	3.28246200	-0.20300300
H	-3.82593400	-1.78067000	-4.98968200	H	5.13321300	3.65896600	-1.66531300
H	-2.23086300	-1.06948600	-5.22791600	H	6.16367000	1.51834300	-0.44621800
H	-3.65186500	-0.03167300	-5.12288700	H	5.54948400	0.08200900	-2.68129100
H	-1.93927100	-4.05947800	-2.11149700	H	6.39802800	1.60834700	-2.91495300
H	-2.60568300	-3.68771400	-3.70349600				
H	-3.62975800	-3.57426500	-2.26972800				
H	-4.52495700	-2.35069200	-0.54558000				
H	-4.94888700	-2.63013100	1.14217800				
H	-4.63400800	-4.00362400	0.07484400				
H	1.22464100	-4.07730900	2.47223000				
H	-0.13636600	-4.74795000	3.37547700				
H	0.48015700	-3.13569200	3.75651500				
H	3.00616500	-1.46672500	-1.77801900				
H	4.01405700	-3.16440600	-3.24427900				





G = -3761.935139 Hartree

ZPE<sub>H</sub> = -3761.817271 Hartree

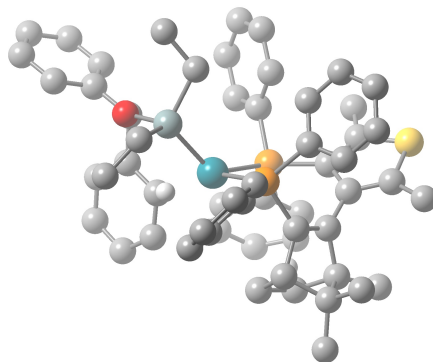
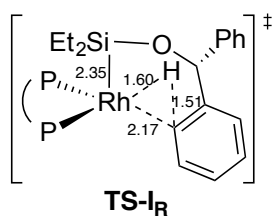
ZPE<sub>D</sub> = -3761.820593 Hartree

C	4.07738700	-1.17848400	-2.30424400
C	4.29677600	-1.17106900	-0.92267400
C	4.53512900	-2.24126000	-3.08955000
C	4.97620200	-2.25014700	-0.34104600
C	5.21183000	-3.31097600	-2.50310700
H	4.36404900	-2.22774100	-4.16296000
C	5.42895900	-3.31212700	-1.12241400
H	5.15330800	-2.25504000	0.73106300
H	5.56805600	-4.13615400	-3.11343600
H	5.95315000	-4.14118700	-0.65461900
Si	1.92412400	2.16526600	-0.37942200
C	3.85598900	0.00595600	-0.05002200
C	2.42524200	3.04031400	1.25169900
C	3.52130700	4.11921600	1.20136100
H	2.69450600	2.26369400	1.97979800
H	1.49597500	3.48525100	1.63551700
H	3.70183000	4.55033100	2.19388300
H	4.47214100	3.71584200	0.84245000
H	3.23938000	4.94333100	0.53731600
C	2.28961500	3.36598700	-1.82116700
C	2.16301300	2.77250100	-3.23247500
H	1.62456600	4.23308600	-1.71398100
H	3.30826700	3.75113100	-1.67612800
H	1.16657700	2.35139200	-3.40876600
H	2.35067700	3.52255200	-4.01058900
H	2.88027500	1.95866900	-3.37904800
Rh	0.32758800	0.52113300	-0.31600800
H	3.54206700	-0.35034800	-2.75438000
O	2.91592400	0.78833600	-0.77373800
H	3.38439700	-0.39868100	0.85599700
C	5.07325900	0.82077000	0.38270900

C	5.46836700	0.84303900	1.72404100
C	5.83167300	1.53036600	-0.55907000
C	6.59976200	1.56032300	2.12265900
H	4.88498100	0.29628900	2.46125700
C	6.95653500	2.25188100	-0.16310000
H	5.53698100	1.50974200	-1.60408400
C	7.34574000	2.26761300	1.18015700
H	6.89302300	1.56955800	3.16886200
H	7.53516600	2.79856600	-0.90266600
H	8.22414000	2.82815800	1.48725300
C	-1.78594900	3.39341700	-0.44923800
C	-2.52431600	4.33514500	0.28316800
C	-2.69772500	5.63559800	-0.19780300
C	-2.14669400	6.01460300	-1.42179500
C	-1.41153600	5.08603300	-2.16170400
C	-1.22554300	3.79259000	-1.67299000
C	-2.05706400	1.72861200	1.88091300
C	-3.40158800	1.71537300	2.28085400
C	-3.74596000	1.84766100	3.62764900
C	-2.75162900	2.00005100	4.59570800
C	-1.41032500	2.01992800	4.20971200
C	-1.06639000	1.88131400	2.86349600
C	-2.86471200	0.74583100	-0.78234100
C	-3.20675800	1.06553600	-2.24015900
C	-4.63543400	0.45940200	-2.37423400
C	-4.17462200	-0.92338400	-1.77564300
C	-3.42881900	-0.45522300	-0.49319600
C	-2.33850300	0.07119800	-3.07888100
C	-3.00089700	-1.29526800	-2.75775700
C	-5.70266600	1.21179100	-1.56111900
C	-5.15962100	0.39078000	-3.82169700
C	-5.21446600	-2.02841100	-1.65065400
C	-3.26346200	-1.32740700	0.70116400
C	-4.32466400	-1.61979900	1.53079000
C	-2.25328900	-2.92289500	2.13337700
C	-2.04633500	-2.05838900	1.07624000
C	-5.70771000	-1.03870300	1.56994800
C	-1.35552500	-3.91970500	2.81571900
C	-0.23489100	-3.15879300	-0.92758200
C	0.79361300	-3.07626000	-1.88135300
C	0.98452500	-4.09652600	-2.81314000
C	0.13292200	-5.20353400	-2.82456500
C	-0.90345200	-5.28792300	-1.89333800
C	-1.08360700	-4.27623700	-0.94742400
C	0.84071700	-2.15772100	1.58012500
C	0.88544000	-1.34246600	2.72647200
C	1.84006100	-1.56098700	3.71974400
C	2.78243000	-2.58485600	3.57911700



C	2.75872700	-3.38480000	2.43672900
C	1.79710100	-3.17362900	1.44410800
P	-1.52341500	1.63104200	0.10704600
P	-0.40921800	-1.74894200	0.26530800
S	-3.88574800	-2.79845700	2.72994300
H	-2.96346800	4.06322100	1.23618200
H	-3.26606000	6.35203100	0.38920800
H	-2.28301300	7.02625300	-1.79364100
H	-0.97206500	5.36994900	-3.11394800
H	-0.63115600	3.08137600	-2.23743400
H	-4.18208400	1.60236500	1.53662000
H	-4.79257500	1.83412800	3.92015500
H	-3.02103000	2.10243400	5.64314500
H	-0.62974000	2.14131900	4.95577300
H	-0.02354600	1.88512800	2.56139200
H	-3.10396200	2.11218700	-2.53021800
H	-2.38653500	0.30912600	-4.14627600
H	-1.28946300	0.11651300	-2.76962500
H	-2.31345700	-2.00750500	-2.29881400
H	-3.39911100	-1.77875000	-3.65629600
H	-5.91575800	2.17978500	-2.02836400
H	-5.39471400	1.40709400	-0.53355800
H	-6.64501100	0.65189100	-1.53860100
H	-6.14769600	-0.08255900	-3.84753800
H	-4.51386900	-0.15914700	-4.50681100
H	-5.27742300	1.40406900	-4.22255800
H	-4.79444800	-2.91554200	-1.16620900
H	-5.56459400	-2.33039900	-2.64351900
H	-6.09041500	-1.71948300	-1.07357000
H	-5.84144100	-0.31004900	0.77109700
H	-5.88824000	-0.52609300	2.52230400
H	-6.48089100	-1.80789600	1.46224400
H	-0.69713300	-4.41667300	2.10167200
H	-1.95332800	-4.68943400	3.31295600
H	-0.72057000	-3.44719100	3.57194500
H	1.45487700	-2.21411600	-1.89125100
H	1.79755700	-4.02002400	-3.52898700
H	0.27333600	-5.99322600	-3.55736200
H	-1.57332800	-6.14355600	-1.89937100
H	-1.89397200	-4.34980700	-0.22904400
H	0.16291900	-0.54179600	2.84401700
H	1.84800300	-0.93020300	4.60464300
H	3.52564300	-2.75545800	4.35293700
H	3.48655100	-4.18198200	2.31324300
H	1.79354600	-3.80911600	0.56545600



G = -3761.914822 Hartree

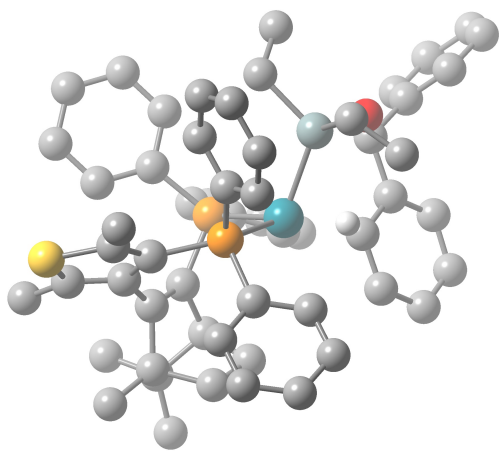
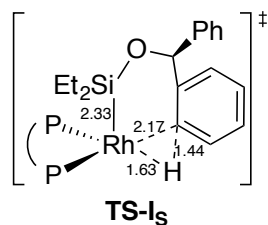
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ZPE<sub>D</sub> = -3761.804465 Hartree

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C	3.45930100	0.05834600	-1.50947900
C	1.75058600	-0.07817300	-3.21486500
C	4.37579300	-0.46655200	-2.42962700
C	2.67392800	-0.58706000	-4.12943400
H	0.73095800	0.08752500	-3.54827400
C	3.99246800	-0.79797300	-3.73110200
H	5.40770800	-0.61124800	-2.12763900
H	2.36057700	-0.81472400	-5.14527800
H	4.72543900	-1.19440000	-4.42851300
Si	1.91713100	2.25964400	0.54413800
C	3.89553300	0.46908300	-0.09561000
C	1.83419200	2.19618700	2.45714900
C	3.04501800	2.84463900	3.15471800
H	1.75670900	1.14675700	2.76470000
H	0.90821500	2.68693900	2.78306300
H	2.97590700	2.74849300	4.24550100
H	3.98131400	2.37903300	2.83424200
H	3.11813700	3.91360300	2.92813300
C	1.87063900	4.08957300	0.02505100
C	2.29411100	4.37210600	-1.42434000
H	0.86889300	4.49332200	0.21329600
H	2.54550700	4.62261700	0.70971600
H	1.63239900	3.87005300	-2.13856400
H	2.26802000	5.44454400	-1.65201300

H	3.30956200	4.01160000	-1.61396900	C	-0.57278900	-5.26307100	-2.11443400
Rh	0.53267400	0.64180400	-0.44653900	C	-0.77359500	-4.25327800	-1.17160600
H	1.37079000	1.49170700	-1.51281200	C	1.13925700	-2.20734100	1.51545100
O	3.50198500	1.81946300	0.13482400	C	0.99512400	-1.59402800	2.77186600
H	3.37724700	-0.19407400	0.61346700	C	1.92830300	-1.80742700	3.78642300
C	5.38742600	0.34502500	0.17164100	C	3.03203400	-2.63455800	3.56575800
C	5.91890400	-0.85540100	0.65778100	C	3.18556400	-3.24862400	2.32305800
C	6.25425900	1.41750500	-0.07187600	C	2.25089500	-3.03631100	1.30562300
C	7.28974400	-0.98856400	0.88707000	P	-1.51925600	1.57967500	0.24133000
H	5.25162200	-1.68835500	0.86442400	P	-0.09198000	-1.81650600	0.17591300
C	7.62417300	1.28763300	0.15993800	S	-3.51821600	-3.12986000	2.57476200
H	5.84056200	2.35397800	-0.42944800	H	-2.65133800	4.11922500	1.50408900
C	8.14775100	0.08397000	0.63753500	H	-2.85175100	6.42273900	0.67761300
H	7.68570200	-1.92628400	1.26805300	H	-2.10749300	7.00545700	-1.62362500
H	8.28465300	2.12951100	-0.03028300	H	-1.10595700	5.24199500	-3.07062100
H	9.21437400	-0.01495800	0.81963700	H	-0.83534800	2.94474900	-2.21414000
C	-1.77315800	3.34004900	-0.31203400	H	-4.31159900	2.13266100	1.18439900
C	-2.31879000	4.34622400	0.49817800	H	-5.36800400	2.12467400	3.41144600
C	-2.43304400	5.65838500	0.02872800	H	-4.02674700	1.56430400	5.43134400
C	-2.01415400	5.98634300	-1.25947100	H	-1.61099500	1.02087300	5.19128200
C	-1.45636300	4.99637800	-2.07216400	H	-0.55633200	1.04043300	2.95324100
C	-1.32184900	3.69352000	-1.59609600	H	-3.12835200	2.05319500	-2.45671000
C	-2.35245500	1.57194300	1.90464700	H	-2.31442500	0.39228000	-4.17803100
C	-3.71628300	1.87801100	2.05503500	H	-1.16852800	0.23262400	-2.84554800
C	-4.31405700	1.87801100	3.31504000	H	-1.99044700	-1.98966600	-2.44087700
C	-3.56034500	1.56568600	4.45028600	H	-3.13019600	-1.79470000	-3.75921700
C	-2.20692900	1.26104300	4.31534600	H	-5.89467300	1.87867900	-1.88219800
C	-1.61026800	1.26685900	3.05114500	H	-5.30801300	1.04303800	-0.44443700
C	-2.72487400	0.63171900	-0.78375400	H	-6.51944600	0.27926400	-1.48729500
C	-3.13296200	0.98976700	-2.21529100	H	-6.01115700	-0.32127800	-3.81061700
C	-4.51035600	0.27151700	-2.34647400	H	-4.39402900	-0.24320400	-4.50798500
C	-3.92122000	-1.09336600	-1.82296800	H	-5.26682700	1.24288200	-4.13727500
C	-3.18424000	-0.62091100	-0.53546100	H	-4.34147700	-3.16823000	-1.33314700
C	-2.21690700	0.11200300	-3.12450500	H	-5.24442300	-2.54710800	-2.71679400
C	-2.74931400	-1.31990900	-2.84906800	H	-5.72018500	-2.09726200	-1.07675400
C	-5.61479300	0.89843700	-1.47991200	H	-5.61783200	-0.67919800	0.72828900
C	-5.06191600	0.22549600	-3.78485200	H	-5.55142400	-0.81036400	2.48325700
C	-4.86027600	-2.28758100	-1.72439000	H	-6.15020400	-2.16893000	1.52130500
C	-2.96483100	-1.52011700	0.63246000	H	-0.24237200	-4.54664500	1.78782400
C	-4.00635000	-1.89231300	1.45574600	H	-1.53905800	-5.08059200	2.86217200
C	-1.89280600	-3.17209900	1.95293000	H	-0.40554100	-3.82887100	3.38900900
C	-1.72125300	-2.22830000	0.95774000	H	1.98827600	-2.37513200	-1.81930900
C	-5.40748300	-1.36371500	1.54825100	H	2.34974500	-4.16427400	-3.46003300
C	-0.96716300	-4.20883000	2.52963200	H	0.70862900	-6.02938700	-3.67157000
C	0.14775800	-3.20124200	-1.03844400	H	-1.29813300	-6.06754500	-2.20052900
C	1.27104500	-3.18382000	-1.88453700	H	-1.65275400	-4.28241300	-0.53720100
C	1.47377500	-4.20071600	-2.81910900	H	0.13011500	-0.97049400	2.96928100
C	0.55298100	-5.24253000	-2.93890200	H	1.79083600	-1.32722300	4.75128500

H	3.76001600	-2.80020000	4.35431200
H	4.03170800	-3.90556700	2.14061500
H	2.38628700	-3.53729500	0.35400600



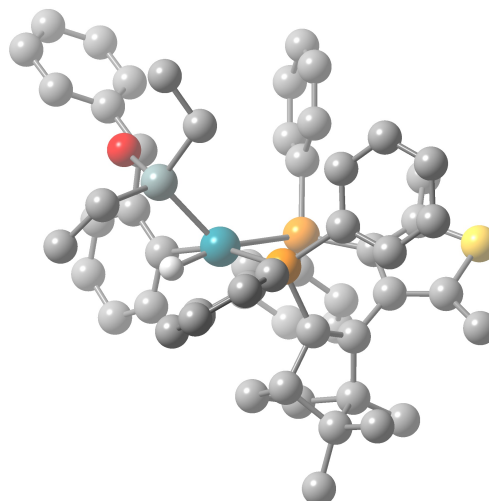
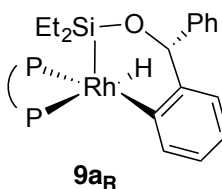
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ZPE = -3761.793247 Hartree

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C	3.47812600	-0.30415100	-1.57915600
C	1.75851800	-0.21861400	-3.28096000
C	4.40264800	0.12481400	-2.53917300
C	2.68571400	0.22142200	-4.22565900
H	0.73402500	-0.39922700	-3.59590300
C	4.01754000	0.39690500	-3.85365800
H	5.44051300	0.25763000	-2.25207100
H	2.36923800	0.40623300	-5.24913900
H	4.75669800	0.72338700	-4.57982800
Si	1.78722400	-2.10041500	0.72386600
C	3.89012300	-0.53177100	-0.12146300
C	5.38549500	-0.46418600	0.14376600
C	5.98667900	0.75878200	0.46557200
C	6.18420500	-1.61137600	0.06737900
C	7.36108000	0.83797700	0.69943700
H	5.37418700	1.65536600	0.53031500
C	7.55711000	-1.53470500	0.30418500
H	5.71520400	-2.56180000	-0.16308800
C	8.15090100	-0.31021900	0.61961200

H	7.81185900	1.79410400	0.95153300
H	8.16488800	-2.43378800	0.24583800
H	9.21961600	-0.25271000	0.80704700
C	1.70734000	-3.96898900	0.36975900
C	1.99262200	-4.41631800	-1.06931500
H	0.74995800	-4.37135600	0.71301900
H	2.46994300	-4.39339400	1.04120100
H	2.03976100	-5.50908900	-1.15137800
H	1.21127900	-4.07132000	-1.75548400
H	2.94441700	-4.01292000	-1.42901700
C	2.93359500	-1.60950100	3.35568900
H	2.78096900	-1.53664900	4.43996000
H	3.67432800	-2.39427800	3.17589900
H	3.39081100	-0.67194100	3.02181700
Rh	0.48684700	-0.61567300	-0.51507200
H	1.28655800	-1.57350700	-1.56587300
O	3.39949900	-1.79040300	0.31948800
H	3.41789000	0.27413800	0.46381000
H	0.87019100	-1.13316500	2.86535100
C	1.61045700	-1.90082900	2.62571900
H	1.19239000	-2.84691800	2.99229300
C	1.42176100	2.96493200	0.42682600
C	1.45477400	4.09851200	1.25559200
C	2.39198100	5.10949300	1.03941000
C	3.31001400	5.00704300	-0.00838800
C	3.28280600	3.88801100	-0.84152400
C	2.34712200	2.87340100	-0.62330800
C	-0.20257200	1.81607500	2.44752600
C	-1.38569300	2.38503300	2.93407900
C	-1.58490300	2.55110600	4.30741600
C	-0.59987100	2.16210900	5.21454400
C	0.59333700	1.61171200	4.73999900
C	0.78806200	1.43825700	3.37054500
C	-1.25036400	2.21703800	-0.30531300
C	-1.03872300	3.08786600	-1.55091900
C	-2.40513500	3.82292900	-1.66508700
C	-3.21148500	2.47173500	-1.56337000
C	-2.55208000	1.82286500	-0.30591100
C	-1.09281600	2.09513600	-2.75250000
C	-2.58132200	1.65901300	-2.75486600
C	-2.64023400	4.83904600	-0.53417900
C	-2.60947200	4.58798800	-2.98673600
C	-4.72997200	2.54253600	-1.65121000
C	-3.30555900	0.87596700	0.56710400
C	-4.35910700	1.33014400	1.33653700
C	-4.21973100	-1.18264500	1.30485400
C	-3.18629700	-0.59083900	0.59803000
C	-4.79360600	2.72688900	1.67764500

C	-4.65380000	-2.61094600	1.51446700	H	-3.81206100	-3.18176100	-5.28580800
C	-2.45586100	-2.04014400	-1.80700800	H	-5.37537600	-2.31715500	-3.55488800
C	-1.58335300	-2.52182700	-2.79700500	H	-4.51960700	-1.59316700	-1.35760900
C	-2.06849500	-2.93921400	-4.03764500	H	-1.39299500	-2.12731500	2.67747700
C	-3.43447400	-2.86703900	-4.31703700	H	-1.31290800	-4.20343100	4.00125600
C	-4.31116600	-2.38193700	-3.34547200	H	-1.63781500	-6.41078200	2.89481900
C	-3.82740500	-1.97533700	-2.10009000	H	-2.03982500	-6.50462500	0.44074200
C	-1.78051600	-3.12219900	0.79769900	H	-2.13517700	-4.43075600	-0.88411900
C	-1.53786000	-3.08188500	2.18043400				
C	-1.49380000	-4.25684000	2.93127100				
C	-1.67601100	-5.49567900	2.31108800				
C	-1.90145500	-5.54710500	0.93515100				
C	-1.95301600	-4.37069600	0.18330900				
P	0.18821700	1.58492400	0.65158500				
P	-1.75133700	-1.52915700	-0.15728900				
S	-5.24918300	0.01714800	2.03497500				
H	0.75102000	4.19267900	2.07586800				
H	2.40451800	5.97839000	1.69191700				
H	4.04112200	5.79388500	-0.17215300				
H	3.99164600	3.79301500	-1.65915800				
H	2.33639300	2.00482700	-1.27100500				
H	-2.14885300	2.70694000	2.23963000				
H	-2.51054300	2.99398200	4.66534700				
H	-0.75594900	2.29221000	6.28162900				
H	1.37412100	1.31599600	5.43489600				
H	1.72443800	1.01992000	3.01583700				
H	-0.15355900	3.72381100	-1.53040700				
H	-0.80588800	2.58854500	-3.68623900				
H	-0.40169800	1.26292100	-2.60931500				
H	-2.71696000	0.58578000	-2.61263800				
H	-3.07944900	1.91792200	-3.69507200				
H	-2.00365200	5.71741100	-0.68852200				
H	-2.40487600	4.43952000	0.45285000				
H	-3.67762900	5.19357500	-0.52960400				
H	-3.60170300	5.05253000	-3.00619800				
H	-2.51918200	3.97079800	-3.88096900				
H	-1.87388600	5.39634600	-3.06868200				
H	-5.18424200	1.55732400	-1.50761300				
H	-5.02793000	2.89998900	-2.64271000				
H	-5.16647400	3.22076100	-0.91425900				
H	-4.17842200	3.46705800	1.16916900				
H	-4.70836300	2.90757100	2.75620200				
H	-5.83876100	2.90805100	1.40312100				
H	-4.43991000	-3.22894100	0.64267900				
H	-5.73320600	-2.64567600	1.69145700				
H	-4.15954100	-3.07502300	2.37282500				
H	-0.51886100	-2.55883500	-2.58587300				
H	-1.37612600	-3.31263900	-4.78700100				
				H	-3.81206100	-3.18176100	-5.28580800
				H	-5.37537600	-2.31715500	-3.55488800
				H	-4.51960700	-1.59316700	-1.35760900
				H	-1.39299500	-2.12731500	2.67747700
				H	-1.31290800	-4.20343100	4.00125600
				H	-1.63781500	-6.41078200	2.89481900
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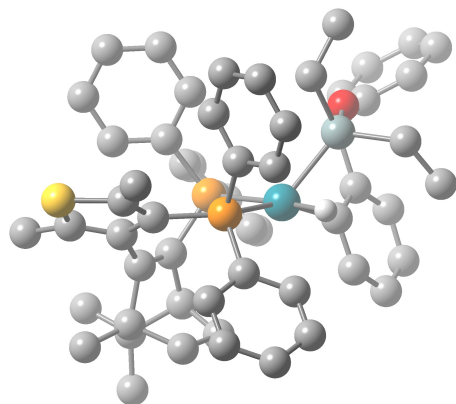
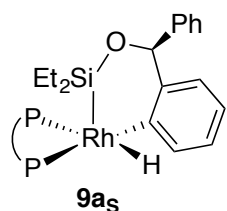


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 ZPE<sub>D</sub> = -3761.817199 Hartree

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C	3.42238600	0.10162300	-1.44650900
C	1.70573900	-0.11303800	-3.11634200
C	4.35991600	-0.35431600	-2.38477700
C	2.64320300	-0.55624600	-4.05435200
H	0.67216100	-0.03179100	-3.43799100
C	3.97906200	-0.69082200	-3.68493800
H	5.40346700	-0.43742400	-2.09896900
H	2.32399800	-0.79643100	-5.06608100
H	4.72233300	-1.03493800	-4.39935000
Si	1.90398700	2.45964700	0.22444100
C	3.86249500	0.55387200	-0.04824200

C	1.58875300	2.78017400	2.08437000	C	-5.68611100	0.46009700	-1.59077300
C	2.65434800	3.66713000	2.75598100	C	-4.95928900	-0.00424900	-3.89662400
H	1.55685000	1.80624000	2.58797700	C	-4.51678100	-2.59321600	-1.98972100
H	0.59576100	3.23202700	2.20125800	C	-2.84385700	-1.72620100	0.52741600
H	2.47124500	3.76770400	3.83308000	C	-3.87955300	-2.25827700	1.26907300
H	3.65538300	3.24603800	2.62369500	C	-1.64516700	-3.19813800	1.94728100
H	2.66325200	4.67724000	2.33350700	C	-1.53611600	-2.24458900	0.95093700
C	1.97185500	4.16555500	-0.61802400	C	-5.34887100	-1.95232000	1.25437800
C	2.35433900	4.16911300	-2.10555500	C	-0.63476100	-4.09500900	2.61133300
H	1.00318900	4.66329200	-0.47534200	C	0.46132900	-3.11540700	-0.94157000
H	2.70367800	4.76068500	-0.05453400	C	1.66560200	-3.12165100	-1.66907900
H	1.64100800	3.59299500	-2.70640100	C	1.95450400	-4.15994600	-2.55608600
H	2.38422800	5.18682700	-2.51353200	C	1.04413500	-5.19951600	-2.74929100
H	3.33928100	3.71816800	-2.26055000	C	-0.15889300	-5.19811800	-2.04318500
Rh	0.46325000	0.76623800	-0.55592300	C	-0.44712700	-4.16806400	-1.14592300
H	0.56795800	2.08383800	-1.36663600	C	1.28850300	-1.96038400	1.61966800
O	3.50035400	1.92325600	0.12008800	C	1.11423500	-1.18138000	2.77507800
H	3.32143900	-0.05479400	0.69075100	C	1.99514400	-1.29034600	3.85058900
C	5.34864200	0.40824100	0.23929600	C	3.07765500	-2.17114200	3.78659100
C	5.86134800	-0.81563300	0.68699800	C	3.26398600	-2.94323800	2.64030300
C	6.23100300	1.47817000	0.04923500	C	2.37833700	-2.83987000	1.56385300
C	7.22617700	-0.97218700	0.93315100	P	-1.70984200	1.50940900	0.30088900
H	5.18357200	-1.64976600	0.84750900	P	0.08901800	-1.71617000	0.22241700
C	7.59610400	1.32496600	0.29799200	S	-3.30019200	-3.40453300	2.43521300
H	5.83251000	2.43018300	-0.28280300	H	-3.35445900	3.64898700	1.68017800
C	8.09985600	0.09964400	0.73875700	H	-3.91648800	5.96240100	1.07694500
H	7.60630800	-1.92861100	1.28277600	H	-3.09797500	6.94129000	-1.05924000
H	8.26791000	2.16622700	0.14866400	H	-1.67718000	5.56500000	-2.57308100
H	9.16231300	-0.01787800	0.93392800	H	-1.07205700	3.25951400	-1.94732900
C	-2.19049400	3.26425700	-0.10130400	H	-4.48145900	1.07555300	1.35274300
C	-2.98437300	4.05315200	0.74534000	H	-5.41279100	0.92633200	3.63056100
C	-3.30546200	5.36883400	0.40254100	H	-3.91002900	1.07198700	5.60861700
C	-2.84665100	5.91834600	-0.79397600	H	-1.46513400	1.39046000	5.27153000
C	-2.05185700	5.14625100	-1.64342600	H	-0.54111600	1.55577300	2.99258500
C	-1.71792000	3.83756600	-1.29457500	H	-3.32762900	1.97251700	-2.36556500
C	-2.43654400	1.30686400	1.99935200	H	-2.26690300	0.53546800	-4.15578500
C	-3.81515700	1.13573000	2.20541400	H	-1.14372200	0.46219700	-2.79955400
C	-4.34217500	1.05314700	3.49414600	H	-1.67330200	-1.87545800	-2.52042100
C	-3.49960200	1.13833800	4.60512900	H	-2.76643700	-1.76728500	-3.88749700
C	-2.12987500	1.31483900	4.41568200	H	-6.09866200	1.39514400	-1.98582500
C	-1.60443100	1.40001200	3.12348400	H	-5.43620500	0.63331300	-0.54423400
C	-2.81056900	0.50022400	-0.77137600	H	-6.48658900	-0.28729700	-1.63624600
C	-3.20818500	0.90148100	-2.19514000	H	-5.84580400	-0.64151300	-3.98962400
C	-4.47583300	0.02633500	-2.43346600	H	-4.21844300	-0.36953800	-4.60801300
C	-3.73791000	-1.28566400	-1.96190700	H	-5.25229900	1.00323700	-4.21333400
C	-3.12068600	-0.81160700	-0.61575800	H	-3.91814700	-3.41975300	-1.59427700
C	-2.15761000	0.21014000	-3.11654900	H	-4.78706400	-2.84716100	-3.02014900
C	-2.49855600	-1.29407200	-2.93721600	H	-5.44156900	-2.54801100	-1.40883600

H	-5.58807300	-1.21989800	0.48593100	H	-2.54146400	0.59993200	5.07734000
H	-5.66716100	-1.53761500	2.21783500	H	-4.87017200	0.99933900	4.26166300
H	-5.95067000	-2.84937900	1.06951500	Si	-1.91290700	-2.40196800	0.01609900
H	0.07931300	-4.48907800	1.88587800	C	-3.78097200	-0.34569500	-0.12043200
H	-1.13789600	-4.94590000	3.07969400	C	-5.25969000	-0.24990000	-0.46302200
H	-0.06553900	-3.57338900	3.38626600	C	-5.80031900	0.95347600	-0.93086600
H	2.38175500	-2.31834200	-1.55058200	C	-6.10493900	-1.35612700	-0.31072200
H	2.89124000	-4.13947300	-3.10478400	C	-7.16061000	1.05464300	-1.23155200
H	1.26874300	-6.00180900	-3.44648900	H	-5.15231500	1.81680200	-1.06138900
H	-0.87733700	-6.00080300	-2.18482700	C	-7.46303000	-1.25818800	-0.61329100
H	-1.38368900	-4.18834300	-0.60046500	H	-5.68368800	-2.29492700	0.03316100
H	0.27092100	-0.50353800	2.84218400	C	-7.99669700	-0.05155500	-1.07323800
H	1.83658200	-0.68461200	4.73840500	H	-7.56426600	1.99536900	-1.59670400
H	3.76786400	-2.25269900	4.62093500	H	-8.10623800	-2.12605700	-0.49354000
H	4.09792700	-3.63703800	2.58042600	H	-9.05414800	0.02315800	-1.31194300
H	2.53398000	-3.46279300	0.69023700	C	-2.44436400	-3.79505100	1.21022700

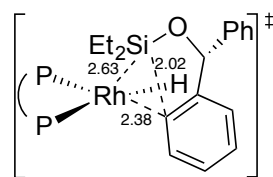


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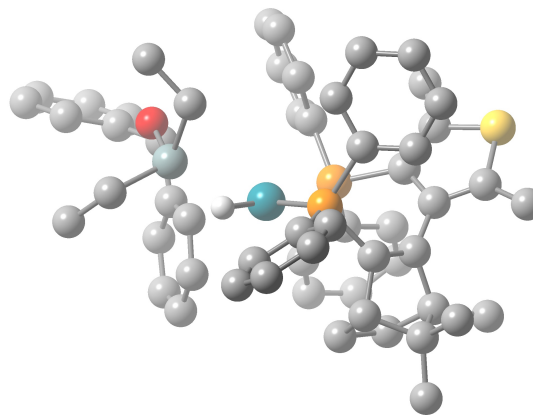
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C	-3.44100900	-0.09363900	1.35271700	C	0.83060000	2.04574700	-3.08238400
C	-1.83459300	-0.06713100	3.15220300	C	0.98507800	1.87966600	-4.45969800
C	-4.41297400	0.37403600	2.25046800	C	0.29559000	0.86481700	-5.12661000
C	-2.80135700	0.41660900	4.03723700	C	-0.55475700	0.01950500	-4.41141500
H	-0.83578300	-0.26451400	3.53516900	C	-0.70415700	0.17935600	-3.03242200
C	-4.10111100	0.63916000	3.58362200	C	1.08036700	2.27899400	0.18600200
H	-5.42632600	0.53721200	1.89879400	C	0.89071700	3.19796700	1.39843500
				C	2.14215900	4.11842100	1.30077400

C	3.11598700	2.88747000	1.17428100	H	1.54192300	5.69769300	2.66804000
C	2.41368200	2.07064800	0.04597300	H	5.18044400	2.24650600	0.93261000
C	1.22618300	2.30730400	2.63731000	H	4.96479800	3.65483600	1.97455200
C	2.75328400	2.08483900	2.47853700	H	4.85044400	3.82946300	0.22272700
C	2.10810200	5.07049300	0.09297700	H	3.62447600	3.74183100	-1.75073700
C	2.37770500	4.99985500	2.54298400	H	4.00171900	3.09101600	-3.34745400
C	4.60745900	3.17015200	1.05967400	H	5.29981100	3.37858000	-2.18713900
C	3.18079800	1.15062800	-0.83653100	H	4.67717400	-2.81886900	-0.65154300
C	4.07743300	1.64342100	-1.76094700	H	5.98728600	-2.14667000	-1.62690100
C	4.29708500	-0.84649200	-1.44933300	H	4.53083600	-2.78235600	-2.40392600
C	3.25729600	-0.31096200	-0.70835700	H	1.12545400	-2.26858600	2.87971100
C	4.26292600	3.03807800	-2.28344500	H	2.27758500	-2.77866600	5.00887200
C	4.89885600	-2.22489200	-1.53723500	H	4.73519600	-2.43657600	5.21330600
C	2.91597400	-1.67094800	1.84245600	H	6.02136900	-1.58564500	3.26047100
C	2.19966200	-2.13635900	2.95828000	H	4.87452400	-1.08830300	1.14005400
C	2.85187400	-2.41683600	4.16065000	H	1.77248500	-2.05281500	-2.59074200
C	4.22906600	-2.22457800	4.27578600	H	1.78285800	-4.19218000	-3.81313300
C	4.95018600	-1.74850700	3.17983300	H	2.06917200	-6.33833800	-2.58488400
C	4.30096500	-1.47430800	1.97514800	H	2.32897000	-6.31055300	-0.11009400
C	2.07899400	-2.95294400	-0.64915600	H	2.35147700	-4.17197600	1.11363700
C	1.90371700	-2.98054400	-2.04192200				
C	1.91095900	-4.19078800	-2.73429700				
C	2.06729800	-5.39572800	-2.04533000				
C	2.21274700	-5.37946200	-0.65767200				
C	2.22050300	-4.16710300	0.03676700				
P	-0.33805300	1.37189700	-0.54677300				
P	2.01750800	-1.32840000	0.24455400				
S	5.07676900	0.38098400	-2.40937100				
H	-1.55814400	3.19429100	-2.61627400				
H	-3.33404800	4.89180100	-2.50801800				
H	-4.49752600	5.35798700	-0.35763000				
H	-3.86206800	4.07870900	1.68403000				
H	-2.10451300	2.36658900	1.57737600				
H	1.35992800	2.84299300	-2.57371900				
H	1.64030400	2.54709700	-5.01289900				
H	0.41649900	0.73779300	-6.19870500				
H	-1.10341400	-0.76592500	-4.92307600				
H	-1.36870300	-0.47812600	-2.48093700				
H	-0.06870000	3.71093100	1.45546200				
H	0.98011700	2.82322900	3.57041900				
H	0.65454600	1.37676800	2.62571000				
H	3.02818100	1.03341500	2.38438000				
H	3.31323300	2.47940200	3.33273800				
H	1.37803200	5.86862700	0.26738500				
H	1.82648200	4.57218900	-0.83524900				
H	3.08113300	5.55371800	-0.05349200				
H	3.28377000	5.60271700	2.41530900	C	2.38657700	0.96245200	-1.28706600
H	2.48255500	4.44403500	3.47521200	C	3.53952600	0.14752800	-1.20950100



TS-II<sub>R</sub>



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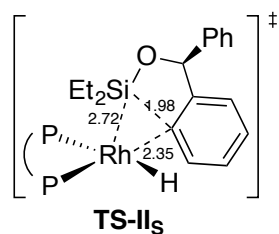
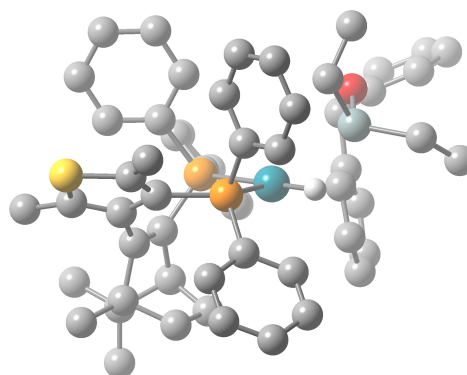
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ZPE<sub>D</sub> = -3761.80903 Hartree

C	1.82849300	1.20289000	-2.55916500	C	-3.40612600	1.13830000	4.69621500
C	4.07383200	-0.44499800	-2.35408500	C	-2.09521900	1.52681400	4.41657900
C	2.34880900	0.59057200	-3.70547700	C	-1.64889600	1.58978300	3.09539200
H	1.00357800	1.90143600	-2.66137300	C	-2.94217900	0.46619800	-0.77716900
C	3.46809900	-0.23567800	-3.59787700	C	-3.29085800	0.89635000	-2.20345200
H	4.98143500	-1.03683700	-2.28810900	C	-4.57604000	0.05595500	-2.47709600
H	1.90101800	0.78195600	-4.67685400	C	-3.87712200	-1.28226400	-2.01776100
H	3.89874600	-0.68719500	-4.48807000	C	-3.27228700	-0.84362900	-0.65427300
Si	2.48153400	2.20728900	0.29964200	C	-2.23132800	0.18961900	-3.10975800
C	4.18844200	0.10000600	0.17855600	C	-2.62822600	-1.30468800	-2.97757400
C	1.86085300	2.76661600	2.03337900	C	-5.78728500	0.49785100	-1.63847900
C	2.96423900	3.34909600	2.93669300	C	-5.03959300	0.06404900	-3.94644700
H	1.41795100	1.89745800	2.52934500	C	-4.68193500	-2.57325400	-2.08421400
H	1.05321700	3.49569000	1.89345200	C	-2.98708500	-1.75665900	0.48416800
H	2.56082800	3.64653800	3.91325600	C	-4.00983900	-2.33929900	1.20399000
H	3.75794400	2.61658800	3.10563900	C	-1.73430000	-3.05532100	2.01759600
H	3.42748000	4.23946400	2.49740100	C	-1.65816500	-2.15134000	0.97354900
C	3.01422900	3.84271900	-0.54908800	C	-5.49530700	-2.13295400	1.12699100
C	4.10673900	3.78336500	-1.62776800	C	-0.70679900	-3.82143700	2.81157800
H	2.10786700	4.30451400	-0.96573000	C	0.18364000	-2.80162100	-1.12341800
H	3.33903400	4.51684700	0.25469400	C	1.00276300	-2.47490300	-2.21329000
H	3.78901700	3.19723400	-2.49523800	C	1.25056600	-3.40659600	-3.22291900
H	4.37007400	4.78606700	-1.98615100	C	0.67500000	-4.67629900	-3.16364600
H	5.02355600	3.32245900	-1.24579200	C	-0.14984800	-5.01032400	-2.08729300
Rh	0.26548100	0.88792800	-0.22000000	C	-0.39373200	-4.08152000	-1.07457400
H	0.50225500	2.46368300	-0.33127200	C	1.24243500	-1.95089600	1.43305500
O	3.82616400	1.28762500	0.85825400	C	1.34570700	-1.15464500	2.58580000
H	3.76318300	-0.75518200	0.72433000	C	2.34743000	-1.39036300	3.52713000
C	5.69799600	-0.08946600	0.15798400	C	3.27298200	-2.41753800	3.32546400
C	6.23706800	-1.38000700	0.07253700	C	3.18848000	-3.20440400	2.17616000
C	6.57125900	1.00141000	0.22480700	C	2.18253400	-2.97236400	1.23373400
C	7.61839400	-1.57662800	0.02418000	P	-1.86302200	1.47243300	0.30681400
H	5.56823100	-2.23757000	0.05416400	P	-0.07803600	-1.52409400	0.20207700
C	7.95274100	0.80707600	0.18350300	S	-3.39180300	-3.38026800	2.44319200
H	6.15673700	1.99746100	0.33243900	H	-4.15444900	3.19063200	1.20839500
C	8.48186200	-0.48087200	0.07670800	H	-4.92397700	5.43592800	0.56761400
H	8.01926500	-2.58458400	-0.04266100	H	-3.65347200	6.77013700	-1.10461100
H	8.61849800	1.66426000	0.23961000	H	-1.59252800	5.81770500	-2.12544500
H	9.55758700	-0.63021600	0.04596000	H	-0.81073800	3.56118600	-1.46302700
C	-2.42867800	3.20348300	-0.09560800	H	-4.50393900	0.63963400	1.51785700
C	-3.59029200	3.75158100	0.47164600	H	-5.29330000	0.52034300	3.85553400
C	-4.02698000	5.02709900	0.11062000	H	-3.75337800	1.08459600	5.72412700
C	-3.31434200	5.77605900	-0.82702400	H	-1.41673100	1.78130300	5.22602600
C	-2.15922200	5.24186000	-1.39901100	H	-0.63077600	1.89768900	2.88351700
C	-1.71914800	3.96869800	-1.03214600	H	-3.37672900	1.97293300	-2.36192500
C	-2.50758300	1.27085700	2.03263500	H	-2.30211100	0.54246600	-4.14367100
C	-3.82471300	0.88734200	2.32525300	H	-1.21668800	0.39116300	-2.75637700
C	-4.26988700	0.82034400	3.64677600	H	-1.83102200	-1.92626300	-2.56980700



H	-2.90491800	-1.74041100	-3.94341000
H	-6.16524900	1.45852400	-2.00593900
H	-5.55040500	0.62542400	-0.58186300
H	-6.60882500	-0.22295000	-1.72431300
H	-5.92240400	-0.57338300	-4.07000700
H	-4.28658700	-0.27811000	-4.65672500
H	-5.33163400	1.07909000	-4.23902700
H	-4.11967700	-3.40940700	-1.65629500
H	-4.90278300	-2.82481000	-3.12697400
H	-5.63572400	-2.50829300	-1.55476000
H	-5.74559300	-1.36264600	0.39888400
H	-5.89271000	-1.81501600	2.09788400
H	-6.02354100	-3.05088500	0.84483600
H	0.00891000	-4.33150500	2.16423100
H	-1.19973800	-4.58068700	3.42557600
H	-0.13431300	-3.17192100	3.47839300
H	1.43949500	-1.48711400	-2.27819800
H	1.88897800	-3.13107100	-4.05730700
H	0.86203000	-5.39947600	-3.95259900
H	-0.60719000	-5.99462200	-2.03544100
H	-1.04583000	-4.34956500	-0.25016100
H	0.63532700	-0.34920000	2.74336400
H	2.41206300	-0.76434900	4.41232500
H	4.05872200	-2.59583000	4.05363100
H	3.90650000	-4.00262500	2.00889700
H	2.12862300	-3.59529900	0.34729200

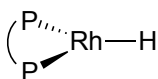


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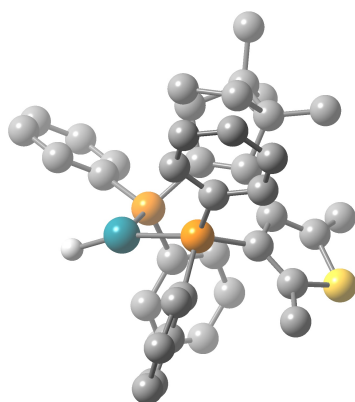
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C	2.44419500	-0.70653200	-1.41090100
C	3.57875700	0.07776200	-1.08229700
C	1.95454600	-0.63423000	-2.73364900
C	4.17415500	0.90798400	-2.02968500
C	2.51238500	0.25162800	-3.66404700
H	1.16265100	-1.30165900	-3.05387200
C	3.62454700	1.01465100	-3.31191700
H	5.07182000	1.46250600	-1.77595900
H	2.10674200	0.30690800	-4.67056500
H	4.09256600	1.66554300	-4.04607700
Si	2.51312400	-2.23633900	-0.14804300
C	4.12215500	-0.13728700	0.33259600
C	5.62257200	0.06572200	0.47530300
C	6.13303700	1.34638500	0.72471200
C	6.51371000	-1.00676800	0.36123900
C	7.50948300	1.55598600	0.83076000
H	5.44798200	2.18310600	0.84322700
C	7.88911900	-0.79982800	0.47369700
H	6.11665900	-2.00412600	0.20830200
C	8.39264700	0.48249600	0.70309700
H	7.89019500	2.55512500	1.02522300
H	8.56931000	-1.64294800	0.38714900
H	9.46364700	0.64199200	0.79235900
C	3.16966500	-3.64405000	-1.26265000
C	4.29042300	-3.33275300	-2.26545500
H	2.29567100	-4.04767500	-1.79518300
H	3.49337500	-4.44898300	-0.58888500
H	4.59808200	-4.23134200	-2.81381600
H	3.97713400	-2.58825700	-3.00332900
H	5.18042600	-2.93635700	-1.76555500
C	2.58735400	-3.87645400	2.22459200
H	2.03062000	-4.39695100	3.01369600
H	3.19584700	-4.62917700	1.71088700
H	3.27425200	-3.17095500	2.70017600
Rh	0.26656500	-0.74560100	-0.52697800

H	0.25027000	-2.20781100	-1.19324100	S	-5.26351000	0.17987600	2.16471000
O	3.73532500	-1.43888400	0.74605300	H	1.20943000	3.19237700	2.72303000
H	3.63105200	0.59757400	0.99181500	H	2.95564300	4.92188600	2.68910200
H	0.99721500	-2.46050800	1.82751200	H	4.14724000	5.46498800	0.57232900
C	1.61973800	-3.15755500	1.26330900	H	3.58845300	4.20920300	-1.50552700
H	0.92546800	-3.87662900	0.81639500	H	1.87459200	2.44421900	-1.46286600
C	1.38708900	2.70125100	0.62460600	H	-1.72074700	2.99765000	2.39593000
C	1.72149600	3.40598800	1.79212600	H	-2.19478500	2.83028700	4.81715900
C	2.71225600	4.39018300	1.77334800	H	-1.13706000	1.03663700	6.17480000
C	3.38235500	4.69357700	0.58746000	H	0.40739600	-0.58478300	5.08790300
C	3.06575500	3.99324800	-0.57818800	H	0.86076200	-0.42644000	2.65787300
C	2.08716400	2.99851200	-0.55580700	H	-0.13869500	3.68700600	-1.54314200
C	-0.40711400	1.28902000	2.35303600	H	-0.96229800	2.62949100	-3.68531900
C	-1.26278500	2.20681600	2.97953500	H	-0.63142700	1.24971200	-2.63167600
C	-1.52708400	2.11347200	4.34678700	H	-2.98353500	0.77395600	-2.55583400
C	-0.93151600	1.10713000	5.11040100	H	-3.28207500	2.14600000	-3.60741300
C	-0.06741000	0.19609800	4.50057800	H	-1.77895700	5.79008800	-0.57729400
C	0.18968800	0.28447900	3.13048500	H	-2.27809900	4.52855400	0.54569700
C	-1.29956400	2.24515400	-0.29654100	H	-3.49127000	5.41740100	-0.39488300
C	-1.06661800	3.11552400	-1.53473200	H	-3.51209200	5.30996700	-2.85938200
C	-2.37478000	3.96017200	-1.58226200	H	-2.55911900	4.15524700	-3.78964800
C	-3.28235400	2.67868100	-1.46463400	H	-1.76493000	5.50724300	-2.98295200
C	-2.62457100	1.96664600	-0.24583200	H	-5.31558600	1.91965900	-1.33707800
C	-1.24847800	2.14473100	-2.74651700	H	-5.10864200	3.27830900	-2.44503400
C	-2.76831700	1.83497900	-2.69159400	H	-5.13965800	3.55857700	-0.70356800
C	-2.49077800	4.97042200	-0.42809500	H	-4.08052600	3.61345400	1.36035500
C	-2.56312900	4.76249600	-2.88412600	H	-4.54199600	3.02688300	2.95895100
C	-4.79272600	2.87068600	-1.47873200	H	-5.75514200	3.13962900	1.68158000
C	-3.37372100	1.02900000	0.62949600	H	-4.54479500	-3.05757500	0.65053400
C	-4.36621500	1.49037600	1.46835300	H	-5.85381000	-2.46595700	1.67627500
C	-4.30640700	-1.02425700	1.34547400	H	-4.30195600	-2.92896600	2.38821500
C	-3.29108200	-0.43742800	0.60821400	H	-0.94432300	-2.55305700	-2.76210300
C	-4.70693900	2.89177600	1.88312400	H	-2.01994900	-3.29686000	-4.86621700
C	-4.76991700	-2.44725800	1.52464300	H	-4.47942800	-3.04898900	-5.16496600
C	-2.77647000	-1.92021700	-1.83303100	H	-5.84322500	-2.06645000	-3.32988500
C	-2.01841000	-2.46244700	-2.88412600	H	-4.77160500	-1.35067700	-1.23265900
C	-2.62743400	-2.87543400	-4.06999800	H	-1.57065800	-1.92057300	2.61297100
C	-4.00621600	-2.73713200	-4.23815200	H	-1.39567400	-3.96231400	3.98095300
C	-4.77016000	-2.18680000	-3.20887100	H	-1.60511400	-6.20601100	2.92024400
C	-4.16267500	-1.78495300	-2.01747000	H	-1.99476000	-6.37014000	0.46784900
C	-1.90834200	-2.97322700	0.75581100	H	-2.19388000	-4.33121600	-0.89953700
C	-1.67247400	-2.89154900	2.13750200				
C	-1.57196900	-4.04679100	2.91204700				
C	-1.68765900	-5.30602400	2.31774500				
C	-1.90511700	-5.39689000	0.94271300				
C	-2.01610700	-4.23991200	0.16684400				
P	0.06868000	1.38443000	0.56893300				
P	-1.93553200	-1.40692900	-0.24454200				



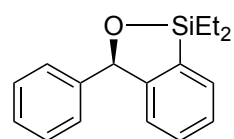
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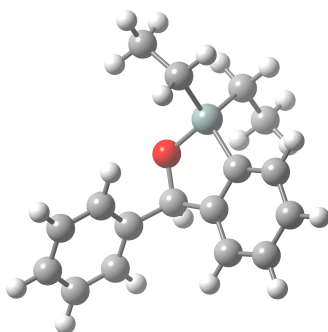
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C	5.67731300	-0.89671800	-1.49792200
C	5.66570000	-0.97592400	-2.89274200
C	4.44869400	-1.03349800	-3.57266400
C	3.24654900	-1.01090100	-2.86202800
C	1.95406300	-1.90273800	0.91802800
C	2.50101900	-1.41881600	2.11479900
C	2.76088600	-2.28380500	3.18053800
C	2.47994400	-3.64535100	3.06347500
C	1.93510400	-4.13803500	1.87532300
C	1.66876400	-3.27434900	0.81276000
C	1.60186500	0.89846400	0.02997900
C	2.29265300	2.02909000	-0.73649000
C	2.45712900	3.11125100	0.37340800
C	0.93781200	3.01411900	0.78317200
C	0.76799700	1.47469100	0.93355100
C	1.17183800	2.64299100	-1.63870900
C	0.24415100	3.32128200	-0.59572400
C	3.46539700	2.72784700	1.46998000
C	2.89450000	4.49334900	-0.14963100
C	0.44025000	3.91088400	1.90846300
C	-0.27955000	0.85809500	1.79548300
C	-0.19176300	0.88194700	3.17007600
C	-2.39541300	-0.04684300	2.36936300
C	-1.54954700	0.28270400	1.33066800
C	0.94519600	1.29767400	4.05704400
C	-3.79254700	-0.60628000	2.39445200
C	-2.82480600	1.36118400	-1.06963900
C	-2.81180700	1.60529800	-2.45245500
C	-3.52795900	2.67330300	-2.99456300
C	-4.25596600	3.52219800	-2.15817500
C	-4.26562800	3.29730400	-0.77991700
C	-3.55673000	2.22319100	-0.23865400
C	-3.10070000	-1.46787900	-0.50147400
C	-2.69019500	-2.73482000	-0.04032800
C	-3.53267600	-3.84123900	-0.16116000
C	-4.78785800	-3.70780300	-0.75877100
C	-5.19633700	-2.46057700	-1.23421300
C	-4.36097100	-1.34852200	-1.10828000
P	1.62588900	-0.83579000	-0.56366900
P	-1.85474100	-0.09273700	-0.45201400
S	-1.63815700	0.26107900	3.91004800
Rh	-0.20408600	-1.33676700	-1.63427600
H	4.50146300	-0.82140200	0.29658200
H	6.62176600	-0.86142500	-0.96167400
H	6.60150800	-0.99995800	-3.44439300
H	4.43226200	-1.10447800	-4.65674900
H	2.29375700	-1.08017200	-3.37861700
H	2.71706500	-0.36193800	2.21979700
H	3.18382300	-1.89155600	4.10169800
H	2.68093200	-4.31764800	3.89290900
H	1.71155400	-5.19677500	1.77656900
H	1.23081500	-3.65001300	-0.10732500
H	3.19961700	1.74644200	-1.27255000
H	1.58942200	3.36484400	-2.34746100
H	0.66315600	1.86647800	-2.21556700
H	-0.77660500	2.93970500	-0.61717500
H	0.17849500	4.40350900	-0.75044900
H	4.48510100	2.76238400	1.07030700
H	3.30483500	1.72490700	1.86571300
H	3.42387300	3.43675400	2.30507200
H	2.93394600	5.21655000	0.67284200
H	2.24513300	4.90818900	-0.92077400
H	3.90442500	4.42860400	-0.57042400
H	-0.61476000	3.71957500	2.12867400
H	0.53064900	4.96374900	1.62028400
H	1.00177900	3.77424400	2.83673900
H	1.77812100	1.67460700	3.46392000
H	1.31208600	0.44692800	4.64312500
H	0.64946600	2.08035800	4.76484600
H	-4.38858000	-0.23352700	1.56029900
H	-4.29849000	-0.32342900	3.32249900
H	-3.79545600	-1.69966100	2.33145800
H	-2.22419800	0.95899700	-3.10023700
H	-3.50774800	2.84881600	-4.06647700
H	-4.80649500	4.35974800	-2.57719400
H	-4.82426200	3.95968800	-0.12429600
H	-3.55742300	2.06421600	0.83539500
H	-1.70993000	-2.84562500	0.41415500

H	-3.20325900	-4.80892400	0.20668800
H	-5.44060300	-4.57044900	-0.85751100
H	-6.16991200	-2.34907000	-1.70370900
H	-4.69579200	-0.38542500	-1.47900300
H	0.70343600	-2.48928400	-2.27220400



**3a**



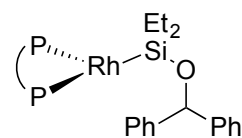
G = -1024.000594 Hartree

ZPE = -1023.945505 Hartree

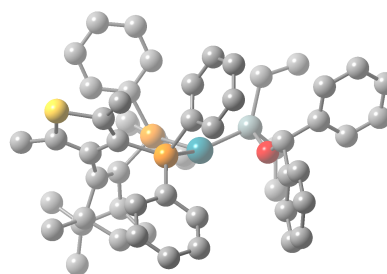
C	-0.00204300	3.52844400	0.67948300
C	0.62678400	2.49646300	-0.01638200
C	-0.01585600	1.26211400	-0.14254000
C	-1.28503700	1.05133900	0.42725000
C	-1.90119300	2.09879900	1.12545200
C	-1.26414600	3.33304100	1.25045400
H	0.49470900	4.48920300	0.78214900
H	1.61313700	2.64906300	-0.44603100
H	-2.88103300	1.95738000	1.57611100
H	-1.74459500	4.14242700	1.79281000
O	-0.31704000	-1.04996000	-0.75335200
C	1.98035500	-0.28934900	-0.49898400
C	2.22965500	-0.99872800	0.68205100
C	3.06382300	0.11445600	-1.28536600
C	3.53578300	-1.29036100	1.06960800
H	1.39430100	-1.33388600	1.28831300
C	4.37481300	-0.16932200	-0.89540400
H	2.88149600	0.64650000	-2.21624500
C	4.61377500	-0.87284200	0.28418200
H	3.71494800	-1.84583100	1.98592000
H	5.20501500	0.14986800	-1.51903700
H	5.63124900	-1.10162400	0.58763600

Si	-1.77027300	-0.71631700	0.04228400
C	-1.97080600	-1.83821300	1.54999000
H	-2.90633200	-1.56949800	2.06101400
H	-1.16669300	-1.59587500	2.25662600
C	-1.95706200	-3.34635700	1.23688500
H	-2.05092300	-3.94627900	2.14877000
H	-2.78247500	-3.62967600	0.57511600
H	-1.02525000	-3.63814200	0.74220000
C	-3.24293500	-0.90676900	-1.12671200
H	-4.15435900	-0.63788800	-0.57322700
H	-3.35249200	-1.97254900	-1.36868500
C	-3.14555800	-0.08337000	-2.42217300
H	-4.02150600	-0.23330400	-3.06267700
H	-3.07064900	0.98815500	-2.20950400
H	-2.26042300	-0.36624200	-3.00095900
C	0.56225700	0.06847800	-0.91473800
H	0.58636000	0.32935400	-1.98379500

Structures computed with the M06 functional:



**8a**



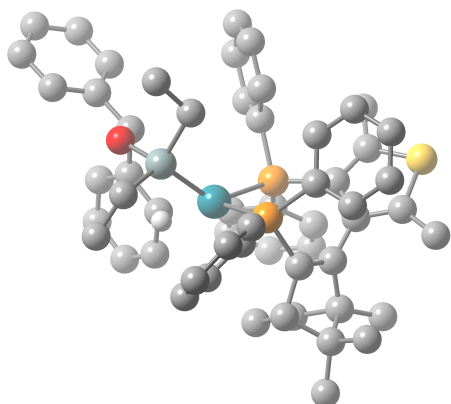
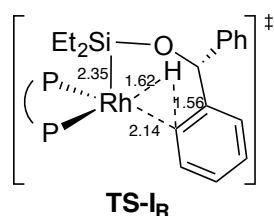
G = -3761.935759 Hartree

ZPE = - 3761.827449 Hartree

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C	3.84775200	-2.19924300	-3.32125300
C	4.63461000	-2.31924300	-0.66203100
C	4.51292800	-3.32537000	-2.84897200
H	3.53634800	-2.14693100	-4.36282500
C	4.90339800	-3.38368600	-1.51215000
H	4.95234200	-2.35556900	0.38053700
H	4.72871000	-4.15584400	-3.51809300

H	5.42488300	-4.26062600	-1.13451400	C	-3.31976600	-0.53325200	-0.52994500
Si	1.95982300	2.25558600	-0.23701300	C	-2.10902200	0.01103500	-3.03785700
C	3.68292200	-0.03936800	-0.17854900	C	-2.70290300	-1.37509300	-2.71916500
C	2.59989100	2.84522100	1.45122300	C	-5.58020000	0.98264100	-1.74500900
C	3.78719900	3.80421100	1.43400700	C	-4.88081100	0.14607000	-3.93309000
H	2.83172500	1.94250200	2.03858500	C	-4.90648000	-2.22178600	-1.74394800
H	1.74618100	3.31670200	1.96203800	C	-3.16132400	-1.33483800	0.69945100
H	4.13660100	4.04029800	2.44710900	C	-4.23392000	-1.66060100	1.49405100
H	4.63945500	3.38428200	0.88543100	C	-2.07562400	-2.61085200	2.35423800
H	3.52325300	4.75310800	0.95080900	C	-1.90934500	-1.86844100	1.20891300
C	2.38616400	3.54923000	-1.55771500	C	-5.65848400	-1.23292500	1.39224800
C	2.22874000	3.02895500	-2.98308200	C	-1.11968800	-3.43704400	3.15448000
H	1.76520400	4.44232900	-1.38855400	C	-0.20940500	-3.16346500	-0.66433000
H	3.42623000	3.86660500	-1.38772100	C	0.79925700	-3.23129900	-1.63053100
H	1.24169300	2.57264100	-3.14889800	C	0.93098100	-4.35099200	-2.44290900
H	2.36534800	3.81554400	-3.73558800	C	0.03076300	-5.40626800	-2.32236100
H	2.96693700	2.24322100	-3.18425600	C	-0.99032900	-5.33952000	-1.37950200
Rh	0.37778000	0.61417300	-0.34449400	C	-1.10823400	-4.22842100	-0.54920500
H	3.01722600	-0.26596600	-2.81694400	C	0.96662600	-1.84295800	1.62483900
O	2.80224000	0.85777400	-0.81162200	C	1.01297800	-0.90464200	2.66704700
H	3.21959900	-0.45549800	0.73706400	C	1.99989700	-0.97739000	3.64269400
C	4.97469700	0.64391100	0.21519000	C	2.96956200	-1.97854400	3.58611500
C	5.47605200	0.53491400	1.51002400	C	2.94154200	-2.90057700	2.54563900
C	5.68534000	1.38163100	-0.73408500	C	1.94939000	-2.83304300	1.56874300
C	6.67308000	1.15721200	1.85655200	P	-1.53608700	1.62840700	0.09228000
H	4.91566900	-0.03643800	2.25213000	P	-0.31918600	-1.61011400	0.32234100
C	6.87617400	2.00760100	-0.38857800	S	-3.74113300	-2.61404600	2.85307100
H	5.28837900	1.45631400	-1.74674800	H	-3.64417400	3.64820500	0.77253700
C	7.37341400	1.89528300	0.90912700	H	-4.17244300	5.86846600	-0.17485100
H	7.05607400	1.06941700	2.87101400	H	-2.75535100	6.83248800	-1.96840600
H	7.42313200	2.58184900	-1.13318400	H	-0.80530000	5.54573700	-2.83005900
H	8.30642500	2.38477800	1.17928200	H	-0.29275500	3.30388500	-1.87626500
C	-1.91916400	3.33860100	-0.48949400	H	-4.14263200	1.16409900	1.52841700
C	-3.02009300	4.06039700	-0.01972400	H	-4.75626300	1.32519800	3.92108200
C	-3.31718000	5.31108200	-0.55109900	H	-3.05130400	1.96954500	5.60421100
C	-2.52251500	5.85178800	-1.55918500	H	-0.72634900	2.46721600	4.87853900
C	-1.43188000	5.13492500	-2.04021200	H	-0.10846900	2.26840500	2.48343000
C	-1.13655800	3.88470600	-1.50600200	H	-3.02078100	2.01291300	-2.58382600
C	-2.08420500	1.70873000	1.84660400	H	-2.11072400	0.22360700	-4.11380900
C	-3.39160300	1.44790800	2.26325800	H	-1.07694400	0.13101500	-2.67352500
C	-3.73559100	1.53853000	3.60889800	H	-2.00730400	-2.03876400	-2.19233700
C	-2.78072000	1.90289400	4.55286500	H	-3.01377300	-1.91235100	-3.62519700
C	-1.47816600	2.17872600	4.14696900	H	-5.81559600	1.92509300	-2.25703000
C	-1.13303400	2.07659500	2.80404900	H	-5.34067600	1.23047900	-0.70666900
C	-2.80396800	0.68556600	-0.80957700	H	-6.49593600	0.37484800	-1.75484100
C	-3.07400200	0.95979000	-2.27914900	H	-5.86018300	-0.34710100	-3.99394700
C	-4.44367600	0.27258400	-2.47535500	H	-4.19041200	-0.41583000	-4.56716200
C	-3.94804300	-1.05774400	-1.83014200	H	-4.99465000	1.14549800	-4.37378500

H	-4.42917000	-3.07842600	-1.24845800	C	4.02912600	-1.18960200	-3.46619800
H	-5.20128200	-2.54647600	-2.75016100	H	5.38309800	-0.75345900	-1.85638200
H	-5.82169500	-1.98323700	-1.18949700	H	2.45656100	-1.45606200	-4.91770200
H	-5.79229000	-0.53234600	0.56266200	H	4.79725500	-1.65734600	-4.07860000
H	-5.98692000	-0.72761000	2.31045200	Si	1.78619600	2.40918800	0.14890900
H	-6.33589900	-2.08136500	1.23085800	C	3.75657000	0.55516000	-0.05862500
H	-0.47958000	-4.04160000	2.50231800	C	1.56185000	2.70360300	2.01288800
H	-1.66261200	-4.11960600	3.81676300	C	2.56507000	3.71467600	2.56387200
H	-0.45677100	-2.82196900	3.77542600	H	1.68146600	1.73427600	2.52152100
H	1.49121800	-2.39603300	-1.74303500	H	0.52879000	3.03355700	2.20386300
H	1.73681400	-4.38586700	-3.17394600	H	2.49156200	3.81852500	3.65382000
H	0.11980600	-6.27747500	-2.96765200	H	3.59303600	3.41455700	2.32555400
H	-1.70105300	-6.15814100	-1.28679900	H	2.40677900	4.71068200	2.13189000
H	-1.91503500	-4.17993300	0.18231300	C	1.78010400	4.09085900	-0.71025200
H	0.25303400	-0.12540800	2.72035800	C	1.97811900	4.02830500	-2.21940100
H	2.01150500	-0.24870900	4.45103900	H	0.85854900	4.63382500	-0.45312100
H	3.74085600	-2.03883300	4.35102400	H	2.60718600	4.65369800	-0.25036200
H	3.69383400	-3.68534700	2.49040000	H	1.14413200	3.51017100	-2.71266900
H	1.94175400	-3.56478100	0.76247700	H	2.05321500	5.02600200	-2.67068800



G = - 3761.920819 Hartree

ZPE = - 3761.815974 Hartree

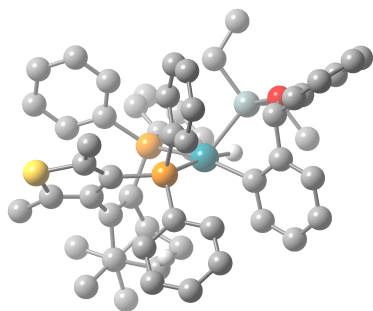
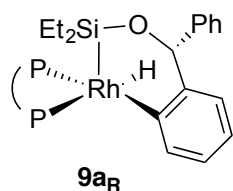
C	2.05879000	0.00917600	-1.85367800	C	-3.74888600	1.71593300	1.96110900
C	3.39595400	-0.06498200	-1.40723700	C	-4.39617000	1.66552700	3.18886800
C	1.75754300	-0.47450400	-3.13423100	C	-3.67226700	1.39248000	4.34827900
C	4.35710300	-0.67911100	-2.21243800	C	-2.29823500	1.20059600	4.27511300
C	2.72641700	-1.07262300	-3.93505900	C	-1.65116900	1.26343200	3.04253800
H	0.73436800	-0.41068300	-3.50516100	C	-2.71219300	0.57535900	-0.77598500



C	4.30580100	0.05403900	-2.53170200	C	1.07894000	1.03598000	4.65285800
C	2.66267400	0.38507300	-4.25371400	C	1.17637000	0.99791900	3.26868400
H	0.66216800	-0.21858500	-3.76714100	C	-0.99024400	2.25011600	-0.15421600
C	3.97971200	0.47646700	-3.81764900	C	-0.77787000	3.12173000	-1.38287100
H	5.33603200	0.12611200	-2.18586000	C	-2.06114400	3.97960100	-1.38099900
H	2.39457200	0.69135600	-5.26330700	C	-2.98002800	2.72536800	-1.26285300
H	4.75486000	0.85723600	-4.47916000	C	-2.31739800	1.98425400	-0.08137300
Si	1.53944100	-2.34335800	0.41296000	C	-1.00585300	2.16768600	-2.58169000
C	3.64938300	-0.83006800	-0.23737000	C	-2.52058200	1.90465400	-2.50650000
C	5.10280300	-0.74257600	0.13996200	C	-2.10792100	4.96310600	-0.21449700
C	5.60048800	0.44853900	0.66920400	C	-2.27022600	4.80557200	-2.64883000
C	5.96911200	-1.81565800	-0.06178600	C	-4.47753600	2.92377600	-1.24292500
C	6.94956700	0.57062700	0.98573600	C	-3.09392900	1.09021400	0.80766000
H	4.91745900	1.28599600	0.82995500	C	-4.02460600	1.61235000	1.67598200
C	7.31733500	-1.69536400	0.25754000	C	-4.11420700	-0.89068600	1.57397400
H	5.56996600	-2.74419000	-0.46380000	C	-3.10833200	-0.36682600	0.78882100
C	7.81121600	-0.50246700	0.77924600	C	-4.28344900	3.02507100	2.07812900
H	7.32727400	1.50324200	1.39972000	C	-4.65342900	-2.27370300	1.77140700
H	7.98794200	-2.53756500	0.09964600	C	-2.79869900	-1.58000900	-1.77707000
H	8.86601800	-0.41173900	1.02976500	C	-2.08216200	-1.91265600	-2.93181500
C	1.26730900	-4.15185600	-0.04984300	C	-2.72829300	-2.03122000	-4.15845900
C	1.27473100	-4.46910600	-1.53724400	C	-4.09885700	-1.80857000	-4.24836900
H	0.35379600	-4.52815800	0.42924100	C	-4.82249200	-1.48195300	-3.10550600
H	2.10770900	-4.66062400	0.45278400	C	-4.17847900	-1.37157300	-1.87741100
H	1.26716700	-5.54918500	-1.72992500	C	-2.00427000	-3.01670500	0.59541800
H	0.39383000	-4.04091100	-2.03429000	C	-1.65541800	-3.14050900	1.94385200
H	2.16070500	-4.04912700	-2.03138300	C	-1.67510200	-4.38142000	2.56946000
C	2.82767000	-2.03886600	2.95454100	C	-2.03274100	-5.51978600	1.85086600
H	2.75105000	-1.92478600	4.04451600	C	-2.36330100	-5.40801200	0.50393400
H	3.47086600	-2.90307600	2.74954800	C	-2.34618100	-4.16478600	-0.12264500
H	3.37017700	-1.16591300	2.56692500	P	0.41885000	1.41631200	0.64964000
Rh	0.36710300	-0.65980700	-0.68609000	P	-1.87984400	-1.35737700	-0.18617700
H	1.04915000	-1.63245700	-1.82375800	S	-4.95659400	0.36627200	2.42827500
O	3.15644800	-2.13195800	-0.00014900	H	1.58415600	3.61226900	2.35513800
H	3.10813900	-0.10177000	0.40402400	H	3.46142300	5.16776200	1.98845900
H	0.78577500	-1.38253000	2.61215700	H	4.75303200	5.09717100	-0.13146100
C	1.45218500	-2.20082700	2.31192200	H	4.12371800	3.45774700	-1.90218100
H	0.98227100	-3.12854500	2.67043900	H	2.25039200	1.91056500	-1.54147400
C	1.78551100	2.64313800	0.43590400	H	-1.72149500	2.56203900	2.46284600
C	2.13835000	3.57443600	1.41877000	H	-1.91807700	2.60628600	4.92791300
C	3.19849100	4.45164300	1.21270200	H	-0.12833900	1.62427800	6.33920300
C	3.91994600	4.41493700	0.02274200	H	1.88056800	0.62001600	5.25982500
C	3.56828000	3.50340400	-0.96765100	H	2.06368400	0.56670700	2.80344400
C	2.50997000	2.62446100	-0.76194000	H	0.16512200	3.67919700	-1.41017300
C	0.16067900	1.52612600	2.46185300	H	-0.70503700	2.63108100	-3.52969300
C	-0.94269300	2.11796400	3.07482700	H	-0.40757500	1.25201500	-2.47471800
C	-1.04767900	2.14614700	4.46363400	H	-2.77726300	0.84636600	-2.39592800
C	-0.04302300	1.60138600	5.25523900	H	-3.04518700	2.25697700	-3.40414100



H	-1.41566900	5.79303900	-0.40689100	C	1.64496500	-0.39206100	-3.06995300
H	-1.81255600	4.51605400	0.73978800	C	4.29608900	-0.49681900	-2.30244000
H	-3.10909800	5.40320300	-0.10425700	C	2.60450100	-0.86891700	-3.96153500
H	-3.19467400	5.39313700	-2.56920300	H	0.60473200	-0.38558800	-3.39610800
H	-2.33180800	4.22257900	-3.57108200	C	3.93665900	-0.93513400	-3.57343800
H	-1.44459500	5.51986500	-2.76632600	H	5.34222100	-0.52804200	-2.00102800
H	-4.99427100	1.95899000	-1.14563900	H	2.30354000	-1.19807300	-4.95537800
H	-4.80767000	3.37895800	-2.18565200	H	4.69630100	-1.30914800	-4.25702700
H	-4.81800300	3.56997000	-0.42623600	Si	1.85041500	2.53405400	-0.03519200
H	-3.62007100	3.71400100	1.54888700	C	3.73192800	0.57113400	-0.06068900
H	-4.11379400	3.16436200	3.15469400	C	1.44547100	2.99624600	1.75862400
H	-5.31900800	3.32744300	1.87609100	C	2.36383500	4.08910300	2.30268300
H	-4.56062400	-2.87865000	0.86535200	H	1.55138900	2.08012100	2.35966800
H	-5.71645000	-2.22525500	2.03271800	H	0.39192800	3.30610300	1.82907500
H	-4.13930400	-2.81664700	2.57340600	H	2.19351400	4.27193900	3.37109400
H	-1.00258500	-2.05402800	-2.85637700	H	3.41982800	3.81961500	2.17811600
H	-2.15560800	-2.28746500	-5.04714000	H	2.20379300	5.04129900	1.78295000
H	-4.60227200	-1.88612400	-5.20951300	C	2.01947500	4.13000100	-1.03292600
H	-5.89394000	-1.30527100	-3.17030400	C	2.30416500	3.88455700	-2.51089500
H	-4.75000700	-1.08762300	-0.99449900	H	1.11372200	4.74261600	-0.89892000
H	-1.38286000	-2.25141400	2.51419900	H	2.84741600	4.69621300	-0.58064900
H	-1.40721300	-4.45884700	3.62136000	H	1.47054800	3.36346800	-3.00304000
H	-2.04818900	-6.49162700	2.33854500	H	2.47917200	4.81651900	-3.06244500
H	-2.63829900	-6.29307100	-0.06553200	H	3.18939700	3.24828900	-2.63897600
H	-2.61530300	-4.08731400	-1.17493000	Rh	0.40679700	0.67986500	-0.56032400

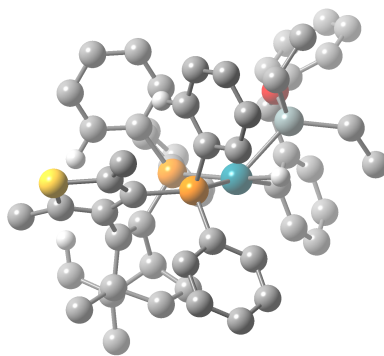
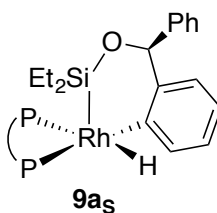


G = -3761.936275 Hartree

ZPE = -3761.828734 Hartree

C	1.97591400	0.03067300	-1.77528200	C	-2.38266400	1.22881700	1.99495000
C	3.33607700	-0.01057700	-1.41046200	C	-3.75010800	1.03056100	2.20969500
				C	-4.25038100	0.88437700	3.49816500

C	-3.39048700	0.93545700	4.59283100	H	-2.54931400	-1.74735500	-3.85668200
C	-2.03251200	1.15347800	4.39305100	H	-6.02623000	1.28369500	-2.08862800
C	-1.53542000	1.30284400	3.10136000	H	-5.38137800	0.57028900	-0.61131300
C	-2.77470900	0.51003300	-0.76997600	H	-6.36590000	-0.40871600	-1.72497300
C	-3.13999300	0.89397800	-2.19303900	H	-5.68009900	-0.70869600	-4.03363600
C	-4.35347000	-0.02531400	-2.46298200	H	-4.03517000	-0.45088900	-4.61929200
C	-3.59046900	-1.29647500	-1.97241700	H	-5.07254900	0.93358000	-4.26148900
C	-3.04528800	-0.80693900	-0.62214900	H	-3.64843300	-3.43539500	-1.67530800
C	-2.04172800	0.24978100	-3.07192200	H	-4.59500600	-2.86363000	-3.05331700
C	-2.32981600	-1.25614100	-2.89971400	H	-5.21259000	-2.64876400	-1.40636400
C	-5.59176200	0.36889300	-1.66491600	H	-5.52824500	-1.30731400	0.33296600
C	-4.79091500	-0.07361900	-3.92630800	H	-5.69517800	-1.48610200	2.08265100
C	-4.30548800	-2.62628000	-2.02153700	H	-5.82668500	-2.90484600	1.03658500
C	-2.77891500	-1.65916900	0.55858900	H	0.06369200	-4.22942800	2.37428000
C	-3.81972100	-2.16665600	1.30007000	H	-1.08038700	-4.27554500	3.71956900
C	-1.58351100	-2.85697200	2.20113500	H	0.07956800	-2.94615400	3.58700700
C	-1.47894500	-2.04836400	1.09167700	H	2.30519600	-2.46471300	-1.48953900
C	-5.29045700	-1.95763200	1.17720600	H	2.57464400	-4.31687300	-3.07502100
C	-0.57616800	-3.60919600	3.01190400	H	0.76189200	-6.00148000	-3.36377600
C	0.32699400	-3.06165600	-0.85087900	H	-1.31768600	-5.80848100	-2.01508200
C	1.50173000	-3.18926100	-1.60434900	H	-1.59210800	-3.95752800	-0.41736500
C	1.65647100	-4.24476500	-2.49609200	H	0.74295100	-0.09245600	2.58024500
C	0.64246700	-5.18375300	-2.65651800	H	2.45231700	-0.25236100	4.36554800
C	-0.52285200	-5.07357600	-1.90535500	H	4.09295300	-2.12509300	4.34359200
C	-0.67716000	-4.02496600	-1.00429600	H	3.99367000	-3.82144800	2.53520000
C	1.39398000	-1.86105000	1.55462400	H	2.28486000	-3.66169200	0.76713900
C	1.45940900	-0.91105600	2.57824100				
C	2.41661500	-1.00444900	3.58026400				
C	3.33411600	-2.05269500	3.56836000				
C	3.27969200	-3.00057300	2.55273100				
C	2.31968000	-2.90513000	1.54777000				
P	-1.67276500	1.47566900	0.31311400				
P	0.10714100	-1.60982900	0.26324900				
S	-3.24463000	-3.10225700	2.63541600				
H	-3.12811200	3.61540200	1.84538600				
H	-3.59153600	5.98025700	1.34329500				
H	-2.85846200	6.97396300	-0.81046000				
H	-1.63249300	5.56962900	-2.45889200				
H	-1.13132400	3.21027900	-1.94401600				
H	-4.42856400	1.00378000	1.35847000				
H	-5.31787600	0.73504500	3.65013000				
H	-3.78326200	0.81535400	5.59987200				
H	-1.35620600	1.21075000	5.24282700				
H	-0.47660100	1.50222700	2.94676400				
H	-3.30667800	1.96408700	-2.36777700				
H	-2.12666500	0.57085900	-4.11732300				
H	-1.04493000	0.54451900	-2.71500400				
H	-1.49566900	-1.81192600	-2.45395100				



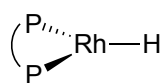
G = - 3761.934285 Hartree  
ZPE = - 3761.827970 Hartree

C	2.14123000	0.10368500	-1.70211900	C	2.19629500	3.06478300	-0.28292900
C	3.41514800	0.31453100	-1.14650400	C	-0.11273500	0.71736100	2.31576500
C	1.91790200	0.54756600	-3.01530400	C	-1.04695000	1.32046600	3.15958800
C	4.39978500	0.98360200	-1.88244400	C	-1.29371600	0.79190200	4.42306300
C	2.89111300	1.23442000	-3.73412000	C	-0.58497500	-0.32259200	4.86386900
H	0.95433800	0.35280400	-3.49083300	C	0.38172300	-0.90124700	4.04498200
C	4.14118500	1.45653700	-3.16264200	C	0.61308500	-0.38972400	2.77183200
H	5.38188100	1.14141600	-1.43910100	C	-1.19679100	2.24928100	0.02960400
H	2.67872500	1.57940500	-4.74486300	C	-1.03662600	3.23972900	-1.11251200
H	4.91824500	1.97754800	-3.71815100	C	-2.31384800	4.09429800	-0.96632200
Si	2.05258300	-2.23037300	-0.53537600	C	-3.23377200	2.83866000	-0.92627500
C	3.68184000	-0.16660100	0.27257100	C	-2.51807500	1.98748600	0.13940400
C	5.14125500	-0.15525000	0.64766700	C	-1.32765900	2.40305700	-2.38725200
C	5.69425800	0.96788300	1.26067200	C	-2.84008500	2.13764100	-2.26320900
C	5.96337600	-1.23809700	0.33926600	C	-2.31054500	4.95891000	0.29138400
C	7.05262700	1.01143300	1.55993200	C	-2.56913700	5.03562500	-2.14129100
H	5.04851100	1.81701700	1.49533800	C	-4.72600000	3.03964300	-0.80907000
C	7.31920000	-1.19908200	0.64334600	C	-3.23134300	0.97421400	0.93726700
H	5.52197500	-2.11402600	-0.13552100	C	-4.13768500	1.34622200	1.89942900
C	7.86787100	-0.07369200	1.25357900	C	-4.12360100	-1.12911900	1.49385900
H	7.47467600	1.89238900	2.03950800	C	-3.17536600	-0.46537900	0.74123200
H	7.95254500	-2.05057700	0.40282000	C	-4.39806300	2.68649200	2.49718300
H	8.92875700	-0.04480900	1.49294600	C	-4.59103800	-2.55097200	1.54343300
C	2.97477600	-3.15265300	-1.90920400	C	-2.86837500	-1.48271700	-1.92328900
C	3.38796900	-2.47849700	-3.20738100	C	-2.16453200	-1.61269800	-3.12588500
H	2.31875100	-4.01276900	-2.12912000	C	-2.84433300	-1.68195200	-4.33811900
H	3.85825000	-3.58511600	-1.41173000	C	-4.23328600	-1.61378400	-4.36488000
H	3.86123300	-3.18908200	-3.89730400	C	-4.94302700	-1.48545000	-3.17464500
H	2.52314100	-2.04348600	-3.72341900	C	-4.26606500	-1.42003300	-1.96201900
H	4.09988000	-1.66267300	-3.03101200	C	-1.86808000	-2.97262000	0.38606000
C	2.62193900	-4.52215900	1.08389400	C	-1.55241500	-3.09525200	1.74277000
H	2.27192000	-5.25235400	1.82618200	C	-1.46495700	-4.34941200	2.33383000
H	3.04421700	-5.09312900	0.24768800	C	-1.68039900	-5.49689000	1.57430400
H	3.44079600	-3.94994300	1.53779700	C	-1.97212800	-5.38119800	0.21834600
Rh	0.38385500	-0.58192200	-0.83129200	C	-2.06065600	-4.12498900	-0.37655500
H	0.50636300	-2.00391000	-1.69191100	P	0.22665200	1.28253500	0.61089900
O	3.14325500	-1.44740200	0.49475500	P	-1.92307600	-1.29149100	-0.34977200
H	3.17062800	0.53985700	0.95762200	S	-4.98132900	-0.02568700	2.52720400
H	1.02159800	-3.13438300	1.50416100	H	1.44553200	2.59153900	2.99971200
C	1.48803600	-3.60534600	0.62922100	H	3.27224200	4.23013300	3.24541100
H	0.69534100	-4.18949500	0.14031300	H	4.43631000	5.11638000	1.23782500
C	1.53477700	2.55764400	0.84277000	H	3.74389900	4.34792600	-1.02744400
C	1.93524000	2.98708600	2.11189800	H	1.92416000	2.71691700	-1.27871100
C	2.97056700	3.90683900	2.25157600	H	-1.58871300	2.20137700	2.82037800
C	3.62135200	4.40458000	1.12644100	H	-2.04040200	1.25455800	5.06603100
C	3.22982800	3.98335700	-0.14072700	H	-0.78095600	-0.73527800	5.85110200
				H	0.94722300	-1.76645500	4.38606400
				H	1.35211800	-0.85755800	2.11732400

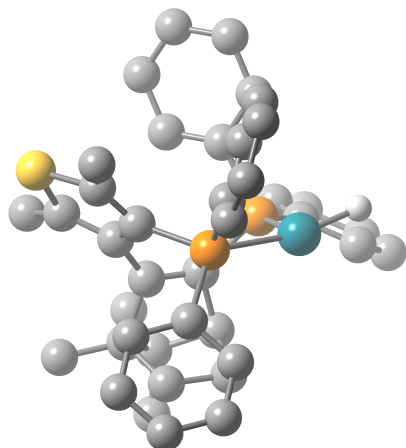
H	-0.09646600	3.80208000	-1.12920500
H	-1.07412200	2.95939900	-3.29799700
H	-0.73489600	1.47759600	-2.39271400
H	-3.09978300	1.07274000	-2.24059800
H	-3.40501900	2.57452000	-3.09723700
H	-1.59257600	5.78041900	0.17145600
H	-2.02315400	4.40824200	1.19226700
H	-3.29544300	5.41718200	0.45837800
H	-3.49528000	5.60293300	-1.97912000
H	-2.65288700	4.53746600	-3.11087200
H	-1.75230100	5.76557300	-2.21544500
H	-5.24752600	2.07327700	-0.77750000
H	-5.09999900	3.58612200	-1.68437000
H	-5.01580900	3.60450600	0.08399900
H	-3.81838300	3.46178300	1.98832500
H	-4.11129300	2.70367700	3.55804900
H	-5.45808500	2.96513700	2.44527900
H	-4.44975900	-3.05994100	0.58632600
H	-5.65949200	-2.58312200	1.78495700
H	-4.05900400	-3.14118100	2.29920100
H	-1.07463800	-1.64172700	-3.09971000
H	-2.28383800	-1.77852000	-5.26521700
H	-4.76345800	-1.65528300	-5.31378000
H	-6.02900700	-1.42662600	-3.19007500
H	-4.82722900	-1.28367600	-1.03872600
H	-1.38411300	-2.20262000	2.34816900
H	-1.21903900	-4.42806900	3.39126100
H	-1.61321300	-6.47920400	2.03613700
H	-2.13534900	-6.27342800	-0.38199900
H	-2.29674500	-4.04240400	-1.43720600

G = -2737.931711 Hartree  
ZPE = - 2737.849704 Hartree

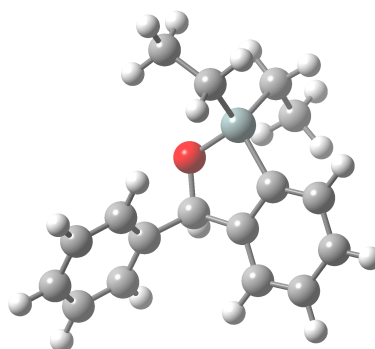
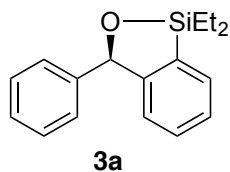
C	3.27576100	-1.16212200	-1.21082600
C	4.33548300	-1.19267900	-0.29843200
C	5.64834100	-1.24442900	-0.74999300
C	5.91410100	-1.26433300	-2.11763000
C	4.86471200	-1.23809900	-3.02943400
C	3.54871900	-1.18786900	-2.57727200
C	1.44664800	-2.08130300	0.80466300
C	1.76101200	-1.72713800	2.11801600
C	1.64175200	-2.65703900	3.14683900
C	1.22335600	-3.95441500	2.87154400
C	0.92169900	-4.32111400	1.56243300
C	1.02543200	-3.38921700	0.53657700
C	1.65724400	0.75633500	0.05011800
C	2.43656600	1.83867800	-0.67751100
C	2.67015200	2.86098300	0.45599900
C	1.15962600	2.88247500	0.84433500
C	0.86388700	1.37647400	0.95422800
C	1.37978200	2.54854700	-1.56540900
C	0.51124600	3.27451600	-0.52057800
C	3.62680300	2.35274600	1.53126900
C	3.22428100	4.20352300	-0.01482400
C	0.72029500	3.78884700	1.96994000
C	-0.22823300	0.80178700	1.76485100
C	-0.18199000	0.79911600	3.13792700
C	-2.31018800	-0.19040200	2.24681500
C	-1.45094400	0.20552100	1.24755900
C	0.92068300	1.20356800	4.05622200
C	-3.70133100	-0.74156400	2.22308600
C	-2.60763000	1.58890500	-0.97536200
C	-2.60897800	1.97648700	-2.31876900
C	-3.19636300	3.17443100	-2.70893900
C	-3.77531500	4.00638600	-1.75456700
C	-3.77453400	3.63208200	-0.41371300
C	-3.19687200	2.42741600	-0.02516400
C	-3.08961800	-1.23668400	-0.69501800
C	-2.75058500	-2.56663900	-0.40526200
C	-3.69550200	-3.57745400	-0.53609900
C	-4.98172000	-3.27861700	-0.98013700
C	-5.31619200	-1.96587000	-1.29665900
C	-4.37603700	-0.94889000	-1.15718900
P	1.55017500	-0.92734000	-0.62115100
P	-1.74940000	0.01572700	-0.55899700
S	-1.61226400	0.09756600	3.81328500
Rh	-0.16195200	-1.07097900	-1.95570400



6



H	4.13111500	-1.17888500	0.77198800
H	6.46727900	-1.27098200	-0.03433200
H	6.94241200	-1.30343700	-2.47052900
H	5.06912500	-1.25759400	-4.09765000
H	2.71160000	-1.17072300	-3.27493600
H	2.08687300	-0.71300000	2.34028400
H	1.87895000	-2.36609600	4.16852800
H	1.12898400	-4.67975100	3.67662300
H	0.59762300	-5.33555100	1.34038300
H	0.76810500	-3.65761500	-0.48885000
H	3.33493300	1.50475000	-1.21099300
H	1.85625800	3.24800100	-2.26262400
H	0.81518000	1.81494500	-2.15776700
H	-0.54534200	2.98828700	-0.54984500
H	0.53812000	4.36502000	-0.64739400
H	4.63841900	2.26537000	1.11222100
H	3.35451700	1.36832100	1.92237400
H	3.68510300	3.05645400	2.37326400
H	3.31655600	4.89488100	0.83342600
H	2.62181400	4.69819600	-0.78087700
H	4.23149100	4.06336500	-0.42900700
H	-0.35109800	3.66175900	2.17622500
H	0.87874100	4.83897200	1.69322800
H	1.26491900	3.60876400	2.90418400
H	1.80856300	1.49765100	3.48918900
H	1.20789300	0.37361500	4.71552000
H	0.63698800	2.04570500	4.70037200
H	-4.34859100	-0.16383500	1.55410200
H	-4.14278300	-0.70637700	3.22462900
H	-3.73289000	-1.78157500	1.87754100
H	-2.12116900	1.33513000	-3.05493100
H	-3.18875500	3.46710600	-3.75642900
H	-4.22154100	4.95163000	-2.05547600
H	-4.22143300	4.28403900	0.33376500
H	-3.17707100	2.14553100	1.02760600
H	-1.74287500	-2.79628100	-0.05551900
H	-3.42590900	-4.60318800	-0.29437900
H	-5.72044900	-4.06985000	-1.08622100
H	-6.31761100	-1.72907000	-1.64979300
H	-4.65074300	0.07884600	-1.39183800
H	0.79585900	-2.10297400	-2.75152500



G = -1024.001264 Hartree

ZPE = - 1023.948326 Hartree

C	0.12345400	3.51896500	-0.64987300
C	-0.51089100	2.52070800	0.07818300
C	0.08422700	1.26564300	0.17595000
C	1.30276000	0.99817900	-0.46070400
C	1.92708500	2.01273200	-1.18892100
C	1.34212400	3.26944600	-1.28158700
H	-0.33469400	4.50233400	-0.73028900
H	-1.46788400	2.71387900	0.56245700
H	2.87747000	1.82523000	-1.68824000
H	1.83050900	4.05950500	-1.84748300
O	0.33557100	-1.01765700	0.84434100
C	-1.91563300	-0.21512100	0.54014500
C	-2.14345800	-0.94464400	-0.62651700
C	-3.00437200	0.23891100	1.27913300
C	-3.43965100	-1.21361400	-1.04456400
H	-1.29276900	-1.31316500	-1.19910700
C	-4.30532200	-0.02310400	0.85895400
H	-2.82934000	0.79390700	2.20113600
C	-4.52493200	-0.75124600	-0.30378800
H	-3.60719200	-1.78809800	-1.95284400
H	-5.14738600	0.33277700	1.44816500
H	-5.53968800	-0.96499000	-0.63111100
Si	1.72100800	-0.77685900	-0.07305600
C	1.72828000	-1.96261900	-1.52663700
H	2.68884200	-1.87954900	-2.05578400
H	0.96001600	-1.63533300	-2.24186100
C	1.47503300	-3.40662900	-1.09432500
H	1.47463600	-4.09766900	-1.94492400
H	2.24142400	-3.75772800	-0.39172700
H	0.50680400	-3.49997200	-0.58803900
C	3.24274900	-0.99560100	1.00049200
H	4.13494000	-0.76753300	0.39813900
H	3.33180000	-2.05692500	1.27391300

C	3.19380100	-0.12129700	2.25101800
H	4.07172900	-0.26223500	2.89149500
H	3.14354300	0.94320800	1.98955700
H	2.30521500	-0.34981500	2.85223700
C	-0.50662400	0.11159600	0.97359500
H	-0.53843800	0.40562300	2.03903400

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