Supporting Information

Density Functional Theory Study of the Mechanism of the Rhodium(I)-Catalyzed Conjugated Diene Assisted Allylic C－H Bond Activation and Addition to Alkenes Using Ene-2-dienes as Substrates

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1. Computational Detail

All calculations were performed with the Gaussian 03 program.[1] Density functional theory calculations using the B3LYP functional[2a-b] were used to locate all the stationary points in the gas phase. For the integration grid in the DFT calculations, the parameter Integral=FineGrid was applied. The default convergance criterion (RMS density matrix = 1.00×10^{-8}) for geometry optimization was used. The 6-31G(d) basis set[2c] was applied for all elements except Rh, which used the basis set of LANL2DZ and its pseudo potential.[2d] The keyword "5D" in Gaussian 03 pragram was used to specify that five d-type orbitals were used as basis sets in all elements of the calculations. This method has been successfully applied to study structures and reaction mechanisms for Rh-catalyzed reactions. [3] Frequency calculations at the same level had been performed to confirm each stationary point to be either a minimum or a transition structure.

Solvation energies in 1,2-dichloroethane were evaluated by a self-consistent reaction field (SCRF) using the CPCM model, where simple united atom topological model (UA0) was used to define the atomic radii. Solvation calculations were carried out using the optimized gas-phase structures. The reported energies are the zero-point energy-corrected enthalpies ($\Delta H_{\text{gas 298K}}$), Gibbs free energies ($\Delta G_{\text{gas 298K}}$), both in the gas phase, and the Gibbs free energies in 1,2-dichloroethane solution ($\Delta G_{\text{DCE 298K}}$). Unless specifically mentioned, all discussed relative energies in the paper are referred to the $\Delta G_{\text{DCE 298K}}$ values.

2. Comparison of DFT Methods of M06 and B3LYP

We compared the computed energies of the competitive alkene insertion step and the reductive elimination step of the reaction of substrate **1a** obtained from the M06 and the B3LYP calculations. The M06 method has been proved to perform better than B3LYP in calculating the energy barriers of several catalytic reactions.[3] The M06 calculations were performed using Gaussian 09.[4] Geometry optimization of all the minima and transition states involved was carried out at the B3LYP level of theory at 298K. LANL2DZ basis set and pseudo potential were used for the rhodium atom, and the 6-31G(d) basis set was used for other atoms. The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum or a transition state and to evaluate its zero-point vibrational energy (ZPVE). Solvent effects were computed based on the gas-phase optimized structures using the same basis sets. Solvation energies in dichloroethane were evaluated by a self-consistent reaction field (SCRF) using the CPCM model, where universal force field model (UFF) was used to define the atom radii. Discussed energies are Gibbs free energies in dichloroethane ($\Delta G_{\mathrm{DCE\ 298\ K}}$) unless specified. The Gibbs free energy ($\Delta G_{\mathrm{gas\ 298K}}$) and the enthalpies ($\Delta H_{\mathrm{gas\ 298\ K}}$) in gas phase are also given for reference. The results are shown in Figure S1.

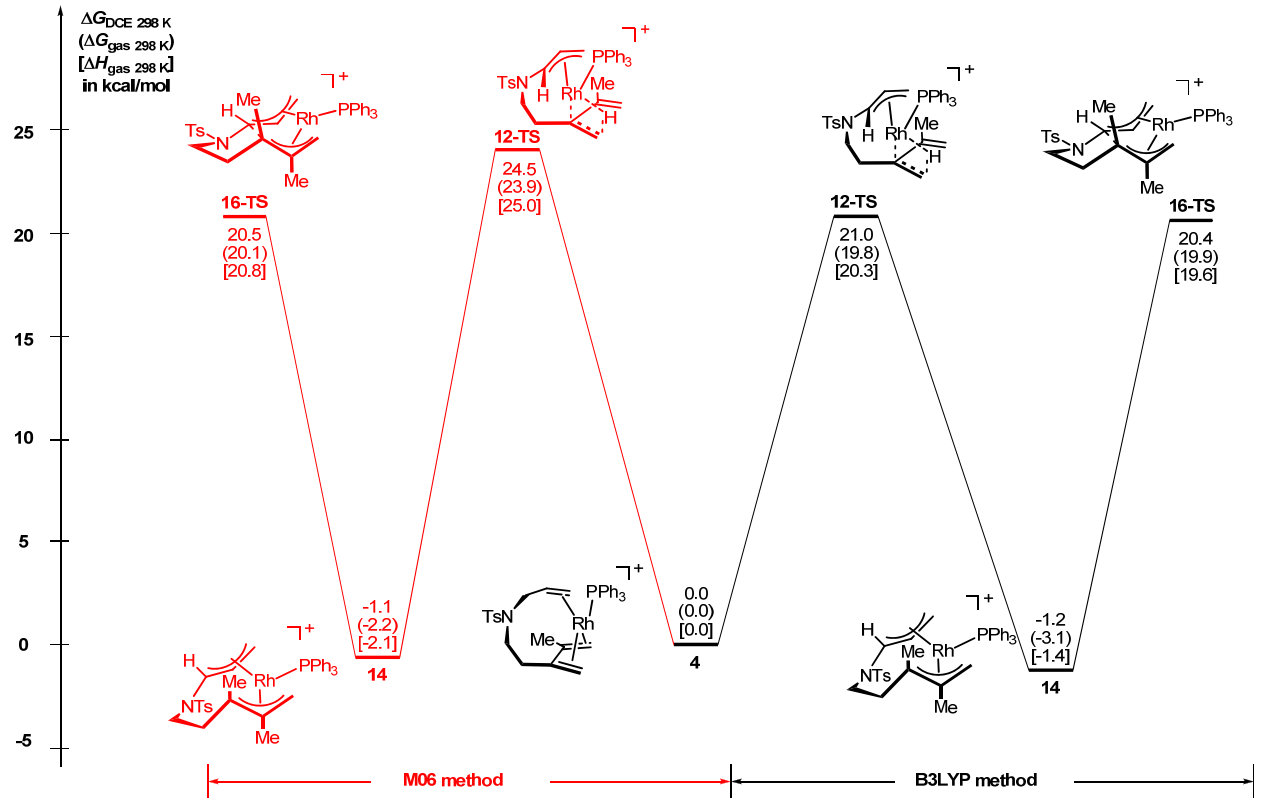

Figure S1. The alkene insertion and reductive elimination steps of reaction of **1a** using both B3LYP and M06 methods (Reaction 1).

The activation free energies computed by the M06 method for the alkene insertion step and the reductive elimination are 24.5 kcal/mol and 21.6 kcal/mol, respectively. According to our D-labeled study of this reaction, which shows the alkene insertion step is reversible (unpublished results), we believe the energy provide by M06 method is too high for the alkene insertion step compared with that obtained by B3LYP method. So we believe that B3LYP method is suitable for studying the present reaction.

3. Comparison of Basis Sets in the B3LYP Method

We have calculated the potential energy surface for reaction 1 using a bigger basis set (LANL2DZ basis set and pseudo potential are used for the rhodium atom, and the 6-311G(d,p) basis set is used for other atoms) by performing the single-point energy calculations in the gas phase and DCE solution on the optimized geometries shown in Figure 3. The salvation energies were computed by using the CPCM model of the self-consistent reaction field (SCRF), where simple united atom topological model (UA0) was used to define the atom radii. Discussed energies are Gibbs free energies in dichloroethane ($\Delta G_{\mathrm{DCE\ 298}}$) unless specified. The Gibbs free energy ($\Delta G_{\mathrm{gas\ 298\ K}}$) and the enthalpies ($\Delta H_{\mathrm{gas\ 298\ K}}$) in gas phase are also given for reference. These new data (Shown in Figure S2) do not show much difference for the key steps from the reported ones in Figure 2, which were computed using a smaller basis set (LANL2DZ basis set and pseudo potential for the rhodium atom, and the 6-31G(d) basis set for other atoms). Therefore, we think the basis set (LANL2DZ + ECP for Rh and 6-31G(d) for other atoms) used for calculations in the main text is appropriate for studying the present reaction.

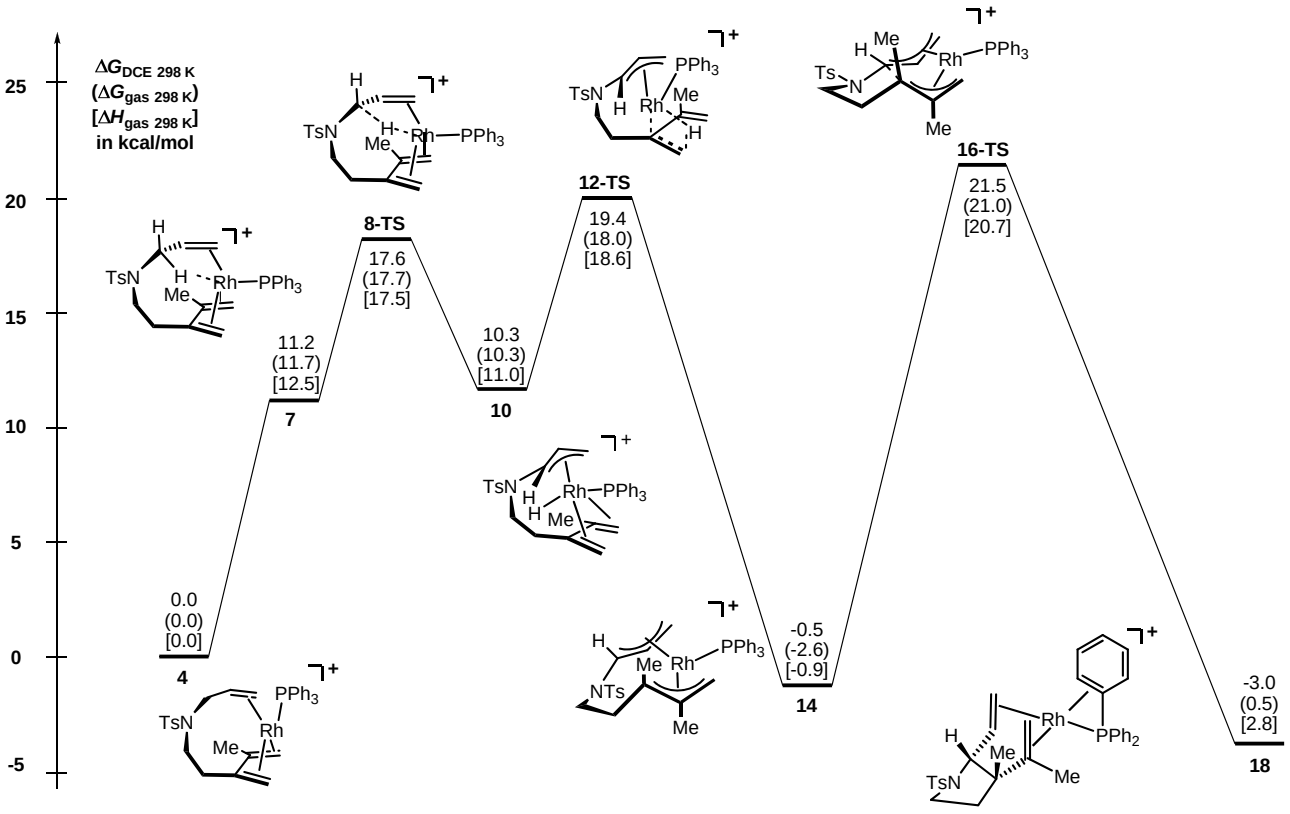

Figure S2. The potential energy surface of allylic C—H activation/addition reaction of **1a** using bigger basis set (Reaction 1).

4. Discussion of the Initiation Step in Reaction 1

We also considered the initiation step of reaction 1 (Figure S3). It shows that, the dissociation of the triphenylphosphine from the rhodium center is very easy, which only needs 4.6 kcal/mol to form $[Rh(PPh_3)_2]^+$ from $[Rh(PPh_3)_3]^+$. When $[Rh(PPh_3)_2]^+$ is formed, it easily coordinates to the substrate to form the substrate—Rh complex **6**, which will then dissociate another triphenyl phosphine ligand to generate a more stable substrate—Rh complex **4**. This process is exergonic by 22.3 kcal/mol.

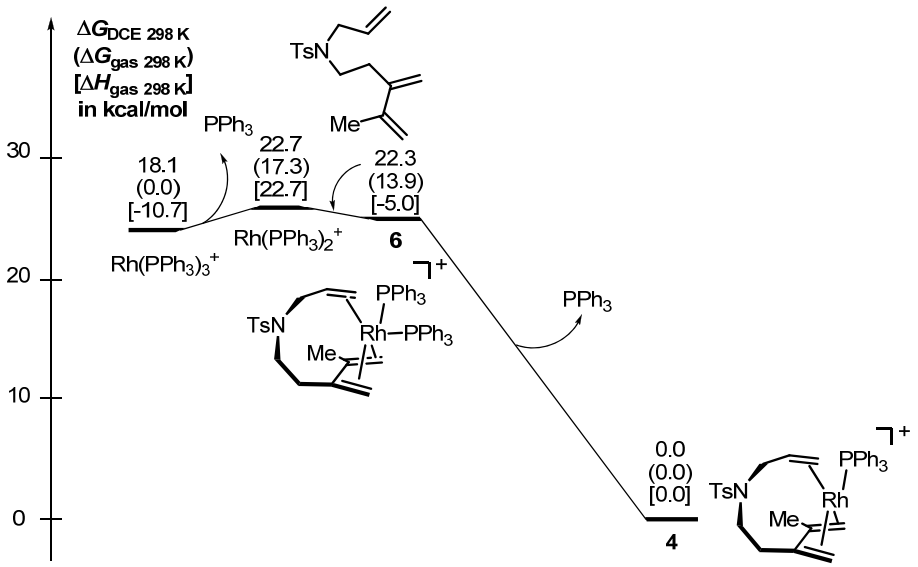

Figure S3. The potential energy surface of the initiation step of reaction 1.

5. Potential Energy Surface of the Bis-ene Substrate 1b

We also calculated the potential energy surface of the reaction for bis-ene **1b**. Similar conclusions can be reached as those obtained in Figure 4 in the text, demonstrating that treating the alkene in Figure 4 as a speculator group is appropriate to appreciate the important role of diene in the target reaction.

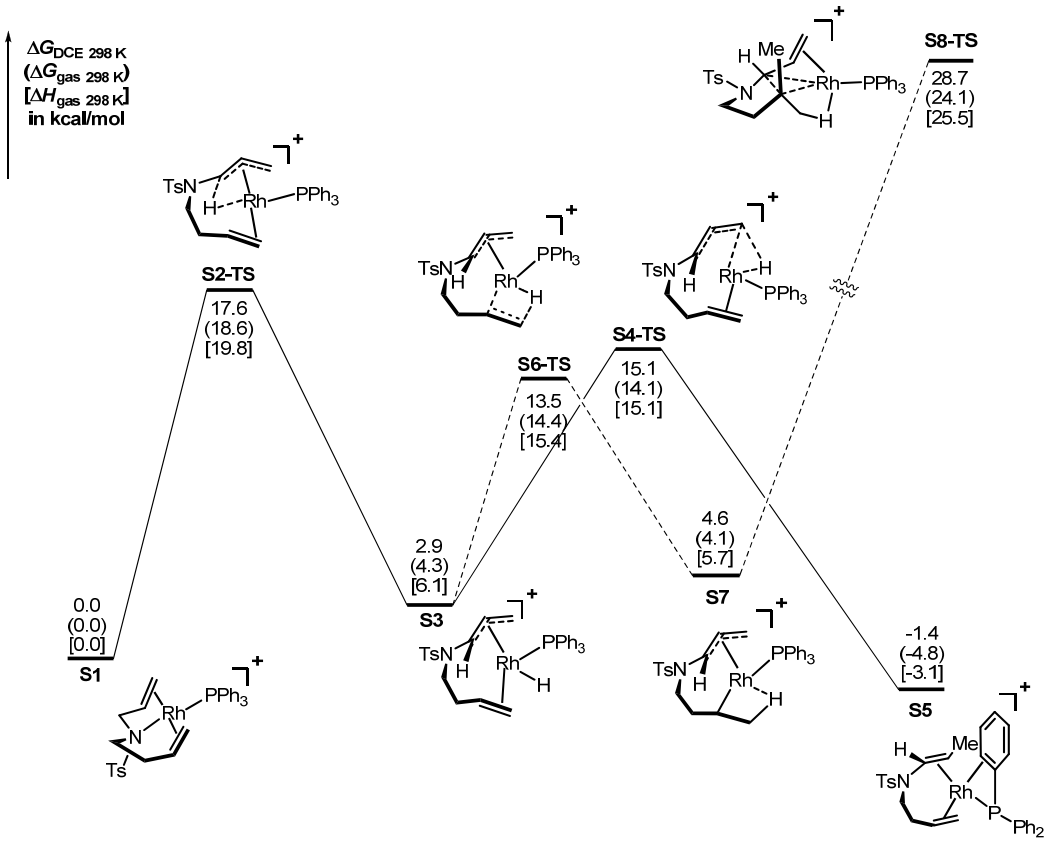

Figure S4. Potential energy surface of the bis-ene **1b**.

6. Potential Energy Surface of Reaction 1 at 338K

We found that the energy surface of reaction 1 at 298 K and 338 K are very similar with energy differences about 0.1-0.2 kcal/mol. Therefore, it is reasonable and convenient to compute and discuss all the computed energy surfaces at 298K.

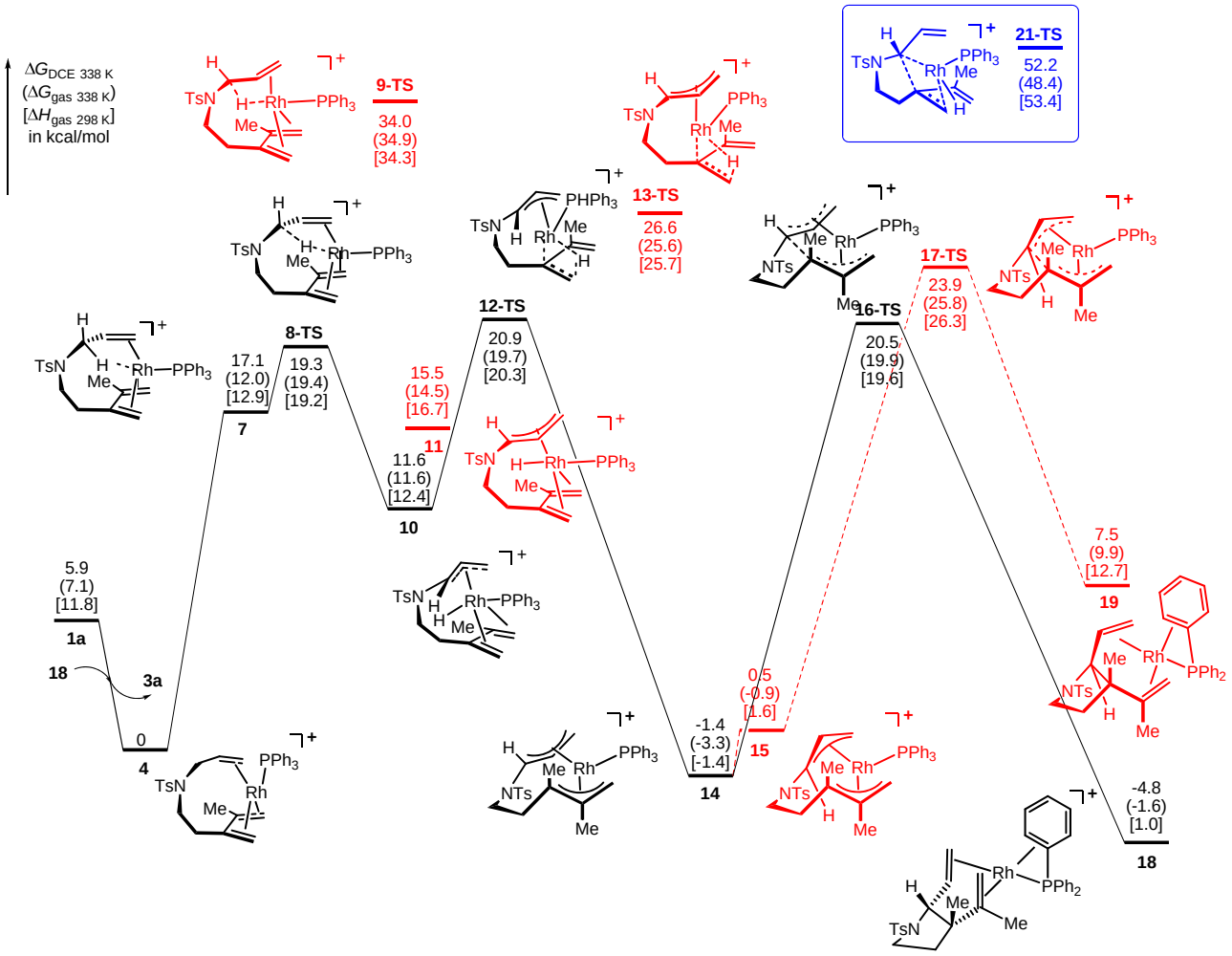

Figure S5. Potential energy surface of reaction 1 at 338 K.

7. Computed Energies of All Stationary Points

Table S1. Sum of electronic and zero-point energies (*E*, in Hartree), sum of electronic and thermal enthalpies (*H*, in Hartree), sum of electronic and thermal free energies (*G*, in Hartree), thermal correction to Gibbs free energy (TCGFE, in Hartree), total free energy in solution (E_{sol}, in Hartree), and thermo corrected Gibbs free energy in 1,2-dichloroethane solution (G_{sol}, which equals to E_{sol} + TCGFE, in Hartree). Relative energies ($\Delta H_{298\ K}$, $\Delta G_{298\ K}$, and $\Delta G_{sol\ 298\ K}$) are reported in kcal/mol. (These data are obtained by B3LYP method. LANL2DZ basis set and pseudo potential were used for the rhodium atom, and the 6-31G(d) basis set was used for other atoms.)

Structure	*E*	*H*	*G*	TCGEF	E_{sol}	G_{sol}	ΔH	ΔG	ΔG_{sol}
				Reaction 1					
1a	-1264.531325	-1264.507552	-1264.586427	0.314470	-1264.893992	-1264.579522			
2a	-1264.571087	-1264.550308	-1264.621685	0.326488	-1264.954166	-1264.627678			
3a	-1264.547542	-1264.524784	-1264.600776	0.318287	-1264.915375	-1264.597088			
PPh_3	-1036.007294	-1035.990388	-1036.054504	0.227119	-1036.281395	-1036.054276			
4	-2409.933139	-2409.892175	-2410.008146	0.575552	-2410.608464	-2410.032912	0.0	0.0	0.0
trans-4	-2409.927891	-2409.927891	-2410.003237	0.575392	-2410.604177	-2410.028785	3.3	3.1	2.6
4'	-2409.925181	-2409.883383	-2410.002471	0.571884	-2410.591295	-2410.019411	5.5	3.6	8.5
5	-3445.948508	-3445.890568	-3446.044130	0.832880	-3446.888127	-3446.055247	-5.0	11.6	20.0
6	-3445.962141	-3445.902679	-3446.063777	0.824404	-3446.894374	-3446.069970	-12.6	-0.7	10.8
7	-2409.912490	-2409.871660	-2409.988855	0.572487	-2410.578053	-2410.005566	12.9	12.1	17.2
8-TS	-2409.902106	-2409.861626	-2409.977331	0.570089	-2410.572280	-2410.002191	19.2	19.3	19.3
9-TS	-2409.877843	-2409.837436	-2409.952638	0.570307	-2410.549205	-2409.978898	34.3	34.8	33.9
10	-2409.913561	-2409.872452	-2409.989459	0.571005	-2410.585239	-2410.014234	12.4	11.7	11.7
11	-2409.906918	-2409.865559	-2409.984640	0.568531	-2410.576295	-2410.007764	16.7	14.8	15.8
12-TS	-2409.900764	-2409.859832	-2409.976665	0.568827	-2410.568248	-2409.999421	20.3	19.8	21.0
13-TS	-2409.891947	-2409.851195	-2409.967373	0.569510	-2410.560065	-2409.990555	25.7	25.6	26.6
14	-2409.935619	-2409.894396	-2410.013080	0.572776	-2410.607541	-2410.034765	-1.4	-3.1	-1.2
15	-2409.930979	-2409.889581	-2410.009037	0.571859	-2410.603540	-2410.031681	1.6	-0.6	0.8
16-TS	-2409.901238	-2409.861003	-2409.976474	0.574113	-2410.574440	-2410.000327	19.6	19.9	20.4
17-TS	-2409.896374	-2409.855695	-2409.973205	0.572064	-2410.570202	-2409.998138	22.9	22.8	21.8
18	-2409.931682	-2409.890602	-2410.010272	0.571709	-2410.611843	-2410.040134	1.0	-1.3	-4.5
19	-2409.912943	-2409.871837	-2409.991830	0.571674	-2410.592032	-2410.020358	12.8	10.2	7.9
20	-1145.283189	-1145.264179	-1145.334434	0.224940	-1145.635395	-1145.410455	86.3	54.8	8.8
21-TS	-2409.848736	-2409.807038	-2409.930015	0.562174	-2410.510901	-2409.948727	53.4	49.0	52.8
22	-2409.889927	-2409.848328	-2409.970098	0.565316	-2410.556194	-2409.990878	27.5	23.9	26.4
32-TS	-2409.899186	-2409.858474	-2409.973935	0.570467	-2410.567335	-2409.996868	21.1	21.5	22.6
33	-2409.929125	-2409.887461	-2410.007145	0.571236	-2410.598879	-2410.027643	3.0	0.6	3.3
				Reaction 2					
23	-2409.912680	-2409.871227	-2409.989926	0.572187	-2410.586123	-2410.013936	0.0	0.0	0.0
24-TS	-2409.882129	-2409.840799	-2409.959849	0.566376	-2410.552148	-2409.985772	19.1	18.9	17.7
25	-2409.908940	-2409.867200	-2409.987067	0.566943	-2410.578909	-2410.011966	2.5	1.8	1.2
26-TS	-2409.897196	-2409.855599	-2409.975708	0.565323	-2410.559107	-2409.993784	9.8	8.9	12.6
27	-2409.914684	-2409.872798	-2409.992273	0.571760	-2410.584573	-2410.012813	-1.0	-1.5	0.7
28-TS	-2409.897829	-2409.856508	-2409.975256	0.567222	-2410.558606	-2409.991384	9.2	9.2	14.2
29	-2409.909268	-2409.867498	-2409.989011	0.567755	-2410.577118	-2410.009363	2.3	0.6	2.9
30-TS	-2409.863018	-2409.822220	-2409.939336	0.571944	-2410.534019	-2409.962075	30.8	31.7	32.5
31	-2409.895310	-2409.853728	-2409.975855	0.568658	-2410.572174	-2410.003516	9.4	7.6	6.4
				Reaction 3					
34-TS	-2409.896803	-2409.856826	-2409.971713	0.575235	-2410.572617	-2409.997382	22.2	22.9	22.3
35	-2409.954251	-2409.914543	-2410.028887	0.578631	-2410.629002	-2410.050371	-14.0	-13.0	-11.0
36-TS	-2409.861702	-2409.821995	-2409.937158	0.576353	-2410.534712	-2409.958359	44.0	44.5	46.8
37	-2409.919002	-2409.879584	-2409.993934	0.579620	-2410.593353	-2410.013733	7.9	8.9	12.0

Structure	E	H	G	TCGEF	E_{sol}	G_{sol}	ΔH	ΔG	ΔG_{sol}
Reaction 2 using bis-ene 1b									
S1	-2293.270407	-2293.232679	-2293.343085	0.515234	-2293.886598	-2293.371364	0.0	0.0	0.0
S2-TS	-2293.238928	-2293.201174	-2293.313375	0.507746	-2293.851025	-2293.343279	19.8	18.5	17.5
S3	-2293.261218	-2293.22292	-2293.336213	0.508108	-2293.874888	-2293.366780	6.1	4.1	2.6
S4-TS	-2293.246572	-2293.208686	-2293.320623	0.508184	-2293.855559	-2293.347375	15.1	14.0	14.9
S5	-2293.276009	-2293.237612	-2293.350738	0.512524	-2293.886092	-2293.373568	-3.1	-5.0	-1.6
S6-TS	-2293.245848	-2293.208066	-2293.320100	0.508136	-2293.858026	-2293.349890	15.4	14.3	13.3
S7	-2293.261576	-2293.223669	-2293.336519	0.511262	-2293.875299	-2293.364037	5.7	3.9	4.4
S8-TS	-2293.229778	-2293.192067	-2293.304675	0.510945	-2293.836593	-2293.325648	25.5	23.9	28.5

8. Atoms in Molecules Caculations of Complex 7

We have done the Atoms in Molecules (AIM) calculations [6] of complex **7** and found that there is a bond critical point between Rh and the activated allylic hydrogen. The electron density value of this critical point is 0.0444. The eigenvalues are -0.0379, -0.0153 and 0.2259. The corresponding Laplacian value is 0.1727. The key critical point is labeled by a blue cycle. All these suggest that there exists an agostic interaction between the C—H group and the Rh center.

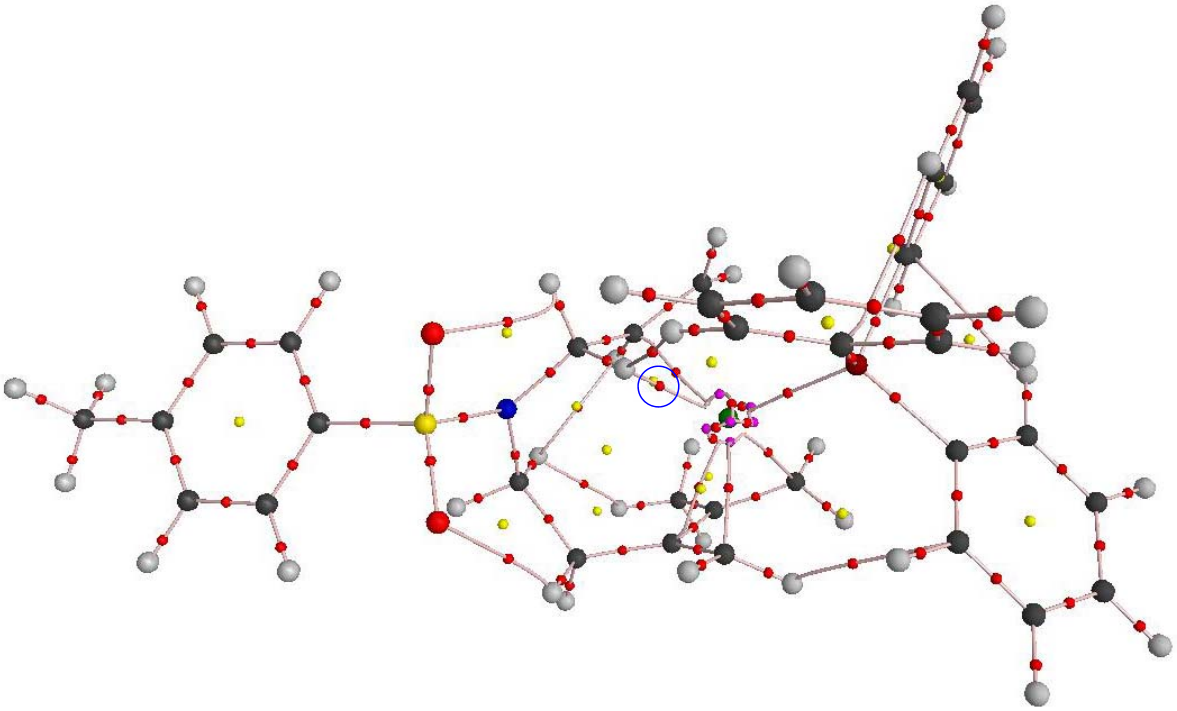

Figure S6. The AIM analysis of complex **7**.

9. References

(1) Full citation of Gaussian 03: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision C.02; Gaussian Inc.: Wallingford CT, 2004.

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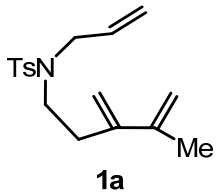
10.Computed Coordinates of All Stationary Points Using B3LYP Method

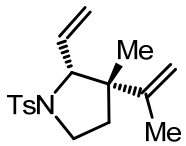


1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.378879	1.159953	0.291120
2	6	0	-0.289074	2.131002	-0.813407
3	6	0	-1.618688	2.787356	-1.074374
4	6	0	-2.228245	2.803698	-2.261058
5	6	0	-1.171407	-0.065281	0.061864
6	6	0	-2.408606	-0.150774	0.973766
7	16	0	0.928623	1.043129	1.346489
8	8	0	1.421267	2.408401	1.549800
9	8	0	0.476803	0.204249	2.459573
10	6	0	2.216457	0.130445	0.487171
11	6	0	2.316476	-1.252949	0.656781
12	6	0	3.290697	-1.957980	-0.048924
13	6	0	4.173733	-1.303996	-0.919349
14	6	0	4.058862	0.086729	-1.063889
15	6	0	3.091902	0.807858	-0.366861
16	6	0	-3.227512	-1.399703	0.703582
17	6	0	-3.322202	-2.372343	1.622255
18	6	0	-3.919031	-1.517502	-0.614679
19	6	0	-3.833683	-2.639282	-1.345105
20	6	0	-4.719031	-0.324557	-1.093248
21	1	0	0.086103	1.653665	-1.732204
22	1	0	0.430238	2.895975	-0.506372
23	1	0	-2.064801	3.289340	-0.216731
24	1	0	-1.800309	2.307858	-3.130346
25	1	0	-0.550089	-0.955759	0.208829
26	1	0	-1.473012	-0.066649	-0.990703
27	1	0	-3.013276	0.752039	0.819709
28	1	0	-2.070710	-0.139343	2.013050
29	1	0	1.654478	-1.759247	1.350960
30	1	0	3.370325	-3.034116	0.084741

31	1	0	4.742379	0.613622	-1.725396
32	1	0	3.030495	1.886798	-0.462700
33	1	0	-3.928447	-3.257707	1.452683
34	1	0	-2.808481	-2.301245	2.577885
35	1	0	-4.361436	-2.743228	-2.290241
36	1	0	-3.230940	-3.483413	-1.022981
37	1	0	-5.250588	-0.556919	-2.021170
38	1	0	-5.458222	-0.018320	-0.341594
39	1	0	-4.078743	0.546473	-1.282454
40	6	0	5.247333	-2.071072	-1.654460
41	1	0	5.495450	-1.597542	-2.610076
42	1	0	6.171934	-2.116664	-1.063737
43	1	0	4.938211	-3.102204	-1.854564
44	1	0	-3.168817	3.325768	-2.413625

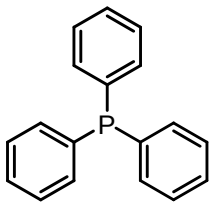


3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.649518	1.867934	-0.041403
2	8	0	-1.015961	2.774656	-1.132271
3	8	0	-0.366784	2.337947	1.315979
4	7	0	0.706684	1.048333	-0.560843
5	6	0	-5.055900	-2.351425	0.380681
6	6	0	-3.962756	-1.314749	0.270832
7	6	0	-3.165733	-0.993503	1.380017
8	6	0	-2.173989	-0.018474	1.298523
9	6	0	-1.966450	0.649336	0.087511
10	6	0	-2.756182	0.357131	-1.028036
11	6	0	-3.742758	-0.623915	-0.928824
12	6	0	1.574286	0.280436	0.376375
13	6	0	1.992505	-0.966043	-0.490218
14	6	0	2.011733	-0.354343	-1.912742
15	6	0	0.792099	0.572895	-1.952911
16	6	0	0.875973	-2.036491	-0.411166
17	6	0	3.317902	-1.592097	-0.050520

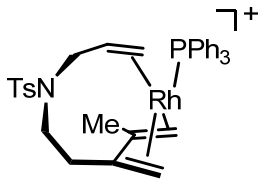
18	6	0	3.403349	-2.114638	1.368303
19	6	0	4.359176	-1.733247	-0.879479
20	6	0	2.725435	1.141585	0.836577
21	6	0	2.890494	1.558708	2.091301
22	1	0	-4.766555	-3.170091	1.048321
23	1	0	-5.302958	-2.779472	-0.596127
24	1	0	-5.976025	-1.911134	0.787302
25	1	0	-3.330297	-1.508598	2.323568
26	1	0	-1.580526	0.245965	2.167339
27	1	0	-2.614517	0.912423	-1.949117
28	1	0	-4.359002	-0.849155	-1.795935
29	1	0	0.994135	-0.036495	1.249239
30	1	0	1.975505	-1.115317	-2.698649
31	1	0	2.922361	0.235544	-2.058838
32	1	0	0.915961	1.415693	-2.637154
33	1	0	-0.115803	0.028495	-2.248901
34	1	0	1.112011	-2.877742	-1.072730
35	1	0	-0.095926	-1.630256	-0.707290
36	1	0	0.764562	-2.426706	0.604915
37	1	0	4.410464	-2.484252	1.583202
38	1	0	2.704164	-2.942191	1.541542
39	1	0	3.170695	-1.332212	2.099265
40	1	0	5.278810	-2.206124	-0.543987
41	1	0	4.347130	-1.400246	-1.911855
42	1	0	3.432996	1.441312	0.064839
43	1	0	2.180607	1.303854	2.874953
44	1	0	3.724553	2.193607	2.377429



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.000435	-0.003713	-1.205932
2	6	0	-1.357576	-0.974650	-0.398688
3	6	0	-1.758330	-2.158889	-1.040183
4	6	0	-2.022092	-0.592087	0.776908

5	6	0	-2.778747	-2.949649	-0.511980
6	1	0	-1.268951	-2.459776	-1.963797
7	6	0	-3.051266	-1.377975	1.300116
8	1	0	-1.738748	0.325346	1.284062
9	6	0	-3.429905	-2.559179	0.660032
10	1	0	-3.072331	-3.864193	-1.020856
11	1	0	-3.557287	-1.065495	2.210213
12	1	0	-4.232027	-3.168580	1.068129
13	6	0	-0.164476	1.660327	-0.405658
14	6	0	0.550118	2.073452	0.729297
15	6	0	-1.045675	2.571818	-1.012115
16	6	0	0.379039	3.358856	1.248428
17	1	0	1.245546	1.390459	1.207882
18	6	0	-1.225438	3.851276	-0.486933
19	1	0	-1.591126	2.276498	-1.905650
20	6	0	-0.510980	4.248858	0.645309
21	1	0	0.942263	3.663418	2.127048
22	1	0	-1.914647	4.540945	-0.967428
23	1	0	-0.642316	5.248749	1.050608
24	6	0	1.524295	-0.688904	-0.402683
25	6	0	2.749222	-0.429348	-1.040723
26	6	0	1.529263	-1.465886	0.765669
27	6	0	3.946991	-0.914354	-0.515962
28	1	0	2.762051	0.153877	-1.958756
29	6	0	2.727253	-1.961941	1.284929
30	1	0	0.593720	-1.687294	1.270048
31	6	0	3.938348	-1.685187	0.648560
32	1	0	4.884905	-0.699905	-1.021800
33	1	0	2.712771	-2.564768	2.189558
34	1	0	4.869394	-2.072814	1.053778



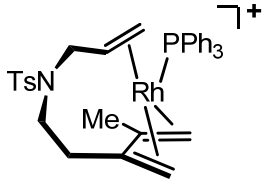
4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.957822	0.167809	-1.885628
2	6	0	0.514608	0.595042	-1.718792
3	6	0	-0.433797	0.387255	-2.697592
4	6	0	2.809324	-2.106193	-1.142161
5	6	0	1.827755	-3.122350	-0.537550
6	6	0	0.362734	-2.990255	-0.917523
7	6	0	-0.655847	-2.990600	0.138830
8	6	0	-0.032285	-2.829732	-2.247141
9	6	0	-0.263843	-3.024315	1.595196
10	6	0	-2.004511	-2.869917	-0.217180
11	7	0	2.486407	-0.709128	-0.836162
12	6	0	4.741482	0.415504	0.375128
13	6	0	5.741190	-0.508341	0.695467
14	6	0	7.073894	-0.166669	0.474626
15	6	0	7.427527	1.083553	-0.054508
16	6	0	6.402648	1.993951	-0.357254
17	6	0	5.064193	1.673649	-0.144954
18	16	0	3.027279	-0.029910	0.602627
19	8	0	2.967362	-1.104201	1.601376
20	8	0	2.250614	1.207854	0.758958
21	1	0	2.083649	-0.357369	-2.836962
22	1	0	2.563778	1.081808	-1.952983
23	1	0	0.340356	1.324400	-0.934538
24	1	0	-1.327502	1.002860	-2.743734
25	1	0	-0.179626	-0.154486	-3.606245
26	1	0	2.857451	-2.197941	-2.231509
27	1	0	3.812968	-2.347563	-0.774695
28	1	0	2.147005	-4.125321	-0.858034
29	1	0	1.948125	-3.086448	0.542895
30	1	0	-0.985037	-3.178336	-2.634987
31	1	0	0.732215	-2.697011	-3.007500
32	1	0	0.079689	-4.036631	1.849289
33	1	0	0.541492	-2.328592	1.840689
34	1	0	-1.122785	-2.796191	2.228637
35	1	0	-2.739157	-2.760172	0.574271
36	1	0	-2.400976	-3.256115	-1.153005
37	1	0	5.480028	-1.463697	1.137924
38	1	0	7.853658	-0.879856	0.728370
39	1	0	6.657716	2.972878	-0.754680
40	1	0	4.282709	2.397746	-0.349330
41	45	0	-0.968261	-1.107165	-1.104182
42	15	0	-2.375957	0.412523	0.115055
43	6	0	-2.157597	2.219745	-0.204699
44	6	0	-1.403156	3.058762	0.629550

45	6	0	-2.746801	2.763760	-1.361632
46	6	0	-1.241689	4.409456	0.310879
47	1	0	-0.952764	2.674470	1.537265
48	6	0	-2.581440	4.112242	-1.675252
49	1	0	-3.363832	2.142137	-2.005065
50	6	0	-1.825604	4.938622	-0.840176
51	1	0	-0.662492	5.047034	0.972468
52	1	0	-3.051224	4.518031	-2.566618
53	1	0	-1.700574	5.990023	-1.082013
54	6	0	-2.096075	0.163730	1.915652
55	6	0	-3.120660	-0.221413	2.794525
56	6	0	-0.785879	0.304686	2.411273
57	6	0	-2.841806	-0.440437	4.146276
58	1	0	-4.135610	-0.351494	2.435075
59	6	0	-0.518833	0.100507	3.765045
60	1	0	0.035194	0.564845	1.749172
61	6	0	-1.545562	-0.272987	4.635723
62	1	0	-3.644047	-0.737584	4.815734
63	1	0	0.496669	0.220763	4.130741
64	1	0	-1.335035	-0.438675	5.688316
65	6	0	-4.170826	0.180108	-0.203744
66	6	0	-5.122412	1.003773	0.426269
67	6	0	-4.609145	-0.781230	-1.125876
68	6	0	-6.480598	0.842316	0.158211
69	1	0	-4.801777	1.775950	1.119519
70	6	0	-5.970440	-0.935731	-1.398980
71	1	0	-3.883203	-1.400999	-1.644094
72	6	0	-6.906977	-0.129228	-0.752466
73	1	0	-7.206244	1.480176	0.654367
74	1	0	-6.295621	-1.681777	-2.118352
75	1	0	-7.965791	-0.248989	-0.962643
76	6	0	8.875481	1.457851	-0.255550
77	1	0	9.002533	2.122432	-1.116016
78	1	0	9.265144	1.986195	0.624338
79	1	0	9.501658	0.573744	-0.409201

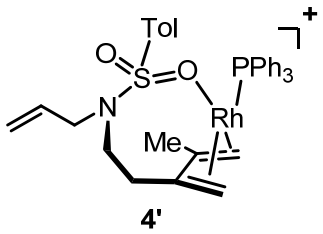


trans-4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.882833	-1.179594	-1.056398
2	1	0	-1.550995	1.225058	-1.037246
3	6	0	-1.866666	0.338843	-1.588315
4	6	0	-2.732672	-1.980592	-1.090666
5	6	0	-1.874817	-3.132713	-0.530454
6	6	0	-0.372563	-3.051406	-0.759957
7	6	0	0.550603	-2.896948	0.362623
8	6	0	0.467108	0.493619	-2.586273
9	6	0	0.058038	-2.807268	1.782151
10	6	0	1.923078	-2.784607	0.068038
11	7	0	-2.315709	-0.656377	-0.601686
12	6	0	-4.716117	0.414451	0.411388
13	6	0	-4.949577	1.690968	-0.113344
14	6	0	-6.249275	2.053912	-0.454197
15	6	0	-7.324568	1.167817	-0.275752
16	6	0	-7.061108	-0.101135	0.259525
17	6	0	-5.767082	-0.486097	0.607464
18	16	0	-3.047044	-0.080628	0.812766
19	8	0	-2.286978	1.119602	1.184445
20	8	0	-3.121508	-1.246725	1.700685
21	1	0	-2.689231	0.626398	-2.266351
22	1	0	-0.961276	-0.961054	-3.140578
23	1	0	1.144794	0.228724	-3.396169
24	1	0	0.633133	1.452395	-2.110908
25	1	0	-3.779393	-2.179016	-0.833449
26	1	0	-2.693856	-1.959944	-2.183763
27	1	0	-2.086063	-3.211609	0.535087
28	1	0	-2.228114	-4.063383	-0.994375
29	1	0	1.149187	-3.488141	-2.278362
30	1	0	-0.510780	-3.079355	-2.900432
31	1	0	-0.819381	-2.168980	1.904446
32	1	0	-0.220773	-3.818212	2.113161
33	1	0	0.849253	-2.452600	2.443925
34	1	0	2.593447	-2.532412	0.883908
35	1	0	2.392828	-3.322948	-0.749405
36	1	0	-4.132121	2.395601	-0.223756
37	1	0	-6.435834	3.046763	-0.855281
38	1	0	-7.881898	-0.795535	0.417411
39	1	0	-5.576619	-1.456473	1.053086

40	6	0	0.168874	-3.082533	-2.052505
41	6	0	-0.721786	-0.175768	-2.431313
42	6	0	-8.732356	1.589312	-0.618512
43	1	0	-9.156891	2.210580	0.180673
44	1	0	-8.760168	2.182624	-1.538490
45	1	0	-9.390776	0.725295	-0.747675
46	15	0	2.337194	0.433141	0.068864
47	6	0	2.177813	2.246446	-0.272999
48	6	0	1.457443	3.118723	0.556445
49	6	0	2.774425	2.758924	-1.440738
50	6	0	1.341457	4.471608	0.226567
51	1	0	0.999814	2.760629	1.470873
52	6	0	2.656285	4.109815	-1.764531
53	1	0	3.348591	2.106705	-2.092865
54	6	0	1.937539	4.970760	-0.931321
55	1	0	0.788696	5.134525	0.885920
56	1	0	3.131919	4.489626	-2.664246
57	1	0	1.848686	6.023862	-1.181625
58	6	0	2.132035	0.256939	1.889425
59	6	0	3.186961	-0.115543	2.737343
60	6	0	0.852371	0.462988	2.437682
61	6	0	2.968950	-0.255505	4.110617
62	1	0	4.178843	-0.295126	2.337179
63	6	0	0.647101	0.339292	3.812006
64	1	0	0.005155	0.709195	1.803562
65	6	0	1.704200	-0.019820	4.651831
66	1	0	3.793968	-0.543841	4.755782
67	1	0	-0.345174	0.511807	4.218282
68	1	0	1.541421	-0.121855	5.720856
69	6	0	4.109743	0.130894	-0.316393
70	6	0	5.111387	0.947411	0.241401
71	6	0	4.480139	-0.881977	-1.212694
72	6	0	6.451958	0.729980	-0.072116
73	1	0	4.843388	1.756715	0.914144
74	6	0	5.823823	-1.092706	-1.531472
75	1	0	3.712801	-1.498643	-1.671656
76	6	0	6.810532	-0.291500	-0.956924
77	1	0	7.216769	1.362797	0.368555
78	1	0	6.096386	-1.878554	-2.230079
79	1	0	7.855752	-0.454826	-1.202859



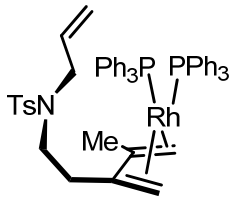
4'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.033356	-1.915224	-0.965304
2	6	0	3.557494	-2.463907	-2.284510
3	6	0	4.044599	-3.574237	-2.842480
4	6	0	2.671288	-3.140815	0.779863
5	6	0	1.232144	-3.389311	1.268776
6	6	0	0.103038	-3.306923	0.256881
7	6	0	-1.266783	-3.027617	0.708406
8	6	0	0.327833	-3.338412	-1.120104
9	6	0	-1.620122	-2.940438	2.170127
10	6	0	-2.248198	-2.792560	-0.299338
11	7	0	2.997948	-1.860983	0.097327
12	6	0	3.446862	0.842347	0.330823
13	6	0	4.421950	0.885914	1.335730
14	6	0	5.370076	1.901766	1.306313
15	6	0	5.358850	2.880197	0.296327
16	6	0	4.363804	2.812482	-0.688548
17	6	0	3.401779	1.802642	-0.681358
18	16	0	2.212014	-0.437735	0.424958
19	8	0	1.681082	-0.528156	1.790606
20	8	0	1.226001	-0.129116	-0.670188
21	1	0	4.859919	-2.520957	-0.575040
22	1	0	4.427761	-0.903815	-1.099721
23	1	0	2.792830	-1.880544	-2.796528
24	1	0	3.704367	-3.924865	-3.812704
25	1	0	4.819463	-4.165690	-2.358223
26	1	0	2.942661	-3.914923	0.055453
27	1	0	3.332406	-3.259401	1.647116
28	1	0	1.238514	-4.417517	1.662103
29	1	0	1.025663	-2.740285	2.117454
30	1	0	-0.421168	-3.670255	-1.829919
31	1	0	1.342511	-3.337509	-1.498722
32	1	0	-1.653122	-3.954467	2.592713

33	1	0	-0.903383	-2.357431	2.752378
34	1	0	-2.606921	-2.492265	2.301678
35	1	0	-3.224292	-2.458671	0.041754
36	1	0	-2.281586	-3.362240	-1.224841
37	1	0	4.432471	0.144020	2.127845
38	1	0	6.130475	1.941605	2.081577
39	1	0	4.336887	3.563211	-1.473430
40	1	0	2.623422	1.767750	-1.434488
41	45	0	-0.645294	-1.376832	-0.497942
42	15	0	-2.024320	0.546722	-0.120301
43	6	0	-1.177390	2.165584	-0.364689
44	6	0	-1.167621	3.186733	0.595097
45	6	0	-0.557637	2.388170	-1.606423
46	6	0	-0.549370	4.409042	0.315972
47	1	0	-1.643486	3.038567	1.558626
48	6	0	0.048818	3.611591	-1.884799
49	1	0	-0.558324	1.607895	-2.363578
50	6	0	0.056430	4.625085	-0.921385
51	1	0	-0.551418	5.193692	1.067256
52	1	0	0.508791	3.776997	-2.855375
53	1	0	0.527040	5.579820	-1.138535
54	6	0	-2.654597	0.558796	1.605184
55	6	0	-4.020924	0.469285	1.909557
56	6	0	-1.717086	0.589341	2.655076
57	6	0	-4.443314	0.422828	3.241238
58	1	0	-4.758805	0.441324	1.114688
59	6	0	-2.146922	0.558283	3.981115
60	1	0	-0.652932	0.629231	2.437822
61	6	0	-3.510551	0.472656	4.277429
62	1	0	-5.504240	0.354304	3.464311
63	1	0	-1.415566	0.594581	4.783675
64	1	0	-3.842592	0.443418	5.311232
65	6	0	-3.486439	0.696425	-1.226348
66	6	0	-4.307284	1.837472	-1.171741
67	6	0	-3.764267	-0.298613	-2.174485
68	6	0	-5.394863	1.963622	-2.033930
69	1	0	-4.091402	2.630250	-0.461232
70	6	0	-4.850993	-0.165862	-3.042222
71	1	0	-3.123753	-1.172845	-2.239191
72	6	0	-5.669141	0.961491	-2.969673
73	1	0	-6.024174	2.847362	-1.981182
74	1	0	-5.054446	-0.941952	-3.774567
75	1	0	-6.514486	1.065048	-3.643836
76	6	0	6.382300	3.988265	0.294203

77	1	0	6.424145	4.496067	-0.673465
78	1	0	6.139733	4.741668	1.054630
79	1	0	7.382836	3.607658	0.525554



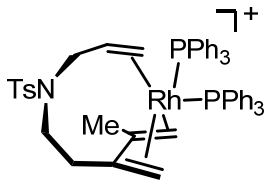
5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.190526	1.714195	-1.106907
2	6	0	4.302001	2.774649	-0.501869
3	6	0	3.926095	3.878742	-1.150814
4	6	0	3.484133	-0.003342	-1.872406
5	6	0	2.137886	0.272161	-1.154620
6	6	0	0.935423	-0.121869	-1.983292
7	6	0	0.463620	-1.511479	-2.021470
8	6	0	0.179155	0.859750	-2.627623
9	6	0	1.207014	-2.623859	-1.325542
10	6	0	-0.745027	-1.777413	-2.681354
11	7	0	4.677468	0.329155	-1.081296
12	6	0	6.688494	-0.801909	0.367208
13	6	0	7.281066	-1.617172	-0.603439
14	6	0	8.652937	-1.836252	-0.553418
15	6	0	9.446802	-1.259894	0.453879
16	6	0	8.824327	-0.451729	1.413666
17	6	0	7.448426	-0.220109	1.381993
18	16	0	4.919065	-0.555002	0.341731
19	8	0	4.241618	-1.840046	0.114365
20	8	0	4.563094	0.251684	1.522815
21	1	0	5.407257	1.953654	-2.154876
22	1	0	6.156887	1.702134	-0.587761
23	1	0	4.005955	2.610569	0.532467
24	1	0	4.221105	4.067786	-2.181652
25	1	0	3.551266	0.592083	-2.789437
26	1	0	3.550009	-1.056176	-2.155429

27	1	0	2.145454	-0.273472	-0.209919
28	1	0	2.076492	1.336441	-0.917533
29	1	0	-0.440883	0.666199	-3.496728
30	1	0	0.446275	1.900277	-2.485582
31	1	0	1.966247	-3.022214	-2.012349
32	1	0	1.735070	-2.310685	-0.423987
33	1	0	0.531414	-3.444807	-1.077987
34	1	0	-1.156688	-2.776964	-2.596374
35	1	0	-1.091615	-1.214364	-3.541795
36	1	0	6.676122	-2.073307	-1.380164
37	1	0	9.119457	-2.467501	-1.305388
38	1	0	9.421400	0.001472	2.200440
39	1	0	6.965456	0.396183	2.132382
40	45	0	-1.118054	-0.232944	-1.091209
41	6	0	10.930930	-1.529238	0.506602
42	1	0	11.130788	-2.538487	0.889126
43	1	0	11.384280	-1.466386	-0.488715
44	1	0	11.445367	-0.820057	1.161613
45	15	0	-1.669802	1.859523	0.057901
46	15	0	-2.646044	-1.703029	0.046319
47	6	0	-1.544942	3.338744	-1.066095
48	6	0	-0.306112	3.983470	-1.233048
49	6	0	-2.642140	3.798653	-1.809693
50	6	0	-0.172638	5.054961	-2.117243
51	1	0	0.559404	3.662795	-0.661685
52	6	0	-2.505056	4.870275	-2.694779
53	1	0	-3.618695	3.344429	-1.688818
54	6	0	-1.271225	5.501496	-2.853758
55	1	0	0.791970	5.543470	-2.224329
56	1	0	-3.371025	5.216231	-3.252141
57	1	0	-1.168001	6.337895	-3.538893
58	6	0	-3.355675	2.034002	0.798051
59	6	0	-3.575657	2.495010	2.104080
60	6	0	-4.468250	1.700780	0.006632
61	6	0	-4.875751	2.647031	2.590736
62	1	0	-2.739272	2.728195	2.751966
63	6	0	-5.766183	1.864285	0.490433
64	1	0	-4.327388	1.299101	-0.991246
65	6	0	-5.973375	2.344421	1.784721
66	1	0	-5.026590	3.004877	3.605276
67	1	0	-6.611512	1.608333	-0.142095
68	1	0	-6.982812	2.472385	2.165069
69	6	0	-0.467161	2.282978	1.386647
70	6	0	-0.461471	3.549853	2.000062

71	6	0	0.513633	1.351438	1.754465
72	6	0	0.490332	3.857423	2.971547
73	1	0	-1.188808	4.301595	1.708704
74	6	0	1.480375	1.665053	2.713851
75	1	0	0.531554	0.381827	1.266644
76	6	0	1.462940	2.917904	3.328059
77	1	0	0.480560	4.836984	3.441233
78	1	0	2.255965	0.943789	2.953036
79	1	0	2.211619	3.168166	4.074324
80	6	0	-4.203539	-1.921040	-0.911658
81	6	0	-5.181196	-2.863361	-0.543088
82	6	0	-4.398547	-1.170776	-2.081508
83	6	0	-6.337845	-3.018373	-1.307051
84	1	0	-5.032950	-3.490267	0.330855
85	6	0	-5.554210	-1.330915	-2.849531
86	1	0	-3.630412	-0.468253	-2.397461
87	6	0	-6.529030	-2.249585	-2.458392
88	1	0	-7.085620	-3.747312	-1.008130
89	1	0	-5.688095	-0.743638	-3.753671
90	1	0	-7.428567	-2.376685	-3.053829
91	6	0	-3.115786	-1.282052	1.782748
92	6	0	-2.082516	-0.949070	2.675182
93	6	0	-4.435096	-1.296330	2.257753
94	6	0	-2.354482	-0.679290	4.016385
95	1	0	-1.058251	-0.888044	2.322437
96	6	0	-4.706250	-1.015158	3.598381
97	1	0	-5.259026	-1.511123	1.588029
98	6	0	-3.669381	-0.717621	4.483217
99	1	0	-1.539340	-0.431213	4.690173
100	1	0	-5.734496	-1.029395	3.948518
101	1	0	-3.885021	-0.507085	5.526831
102	6	0	-2.028077	-3.450613	0.188232
103	6	0	-1.248615	-3.864653	1.279735
104	6	0	-2.282388	-4.373395	-0.842154
105	6	0	-0.734878	-5.161399	1.336898
106	1	0	-1.048992	-3.187559	2.102118
107	6	0	-1.766657	-5.669508	-0.782385
108	1	0	-2.903370	-4.093054	-1.686850
109	6	0	-0.988126	-6.067244	0.305778
110	1	0	-0.139690	-5.462392	2.194267
111	1	0	-1.982658	-6.369088	-1.585039
112	1	0	-0.589130	-7.076239	0.353405
113	1	0	3.333648	4.651039	-0.666850



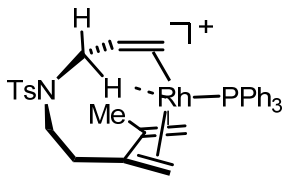
6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.574126	1.277695	0.626214
2	6	0	1.359532	0.434864	0.950017
3	6	0	0.225281	0.975108	1.507030
4	6	0	3.347231	1.489862	-1.784853
5	6	0	2.379936	0.839062	-2.779968
6	6	0	0.897642	0.896146	-2.474510
7	6	0	0.029079	-0.147770	-2.893010
8	6	0	0.265827	2.017567	-1.824725
9	6	0	0.497250	-1.362638	-3.646994
10	6	0	-1.364207	0.016545	-2.575082
11	7	0	3.396388	0.810396	-0.489311
12	6	0	6.087794	0.511295	0.207356
13	6	0	6.991662	0.852091	-0.803201
14	6	0	8.144169	1.560978	-0.470242
15	6	0	8.415120	1.929249	0.855883
16	6	0	7.495084	1.563740	1.850862
17	6	0	6.336364	0.856293	1.539758
18	16	0	4.578942	-0.350446	-0.213434
19	8	0	4.794465	-1.024345	-1.499882
20	8	0	4.125893	-1.084476	0.974392
21	1	0	2.287202	2.314326	0.422787
22	1	0	3.186567	1.304633	1.537558
23	1	0	1.577067	-0.615926	1.099991
24	1	0	-0.431939	0.374412	2.122366
25	1	0	0.134797	2.049139	1.635569
26	1	0	3.104946	2.543990	-1.608648
27	1	0	4.344437	1.476630	-2.233130
28	1	0	2.510041	1.347096	-3.749944
29	1	0	2.711935	-0.189677	-2.925892
30	1	0	-0.599394	2.475860	-2.297947

31	1	0	0.923359	2.761786	-1.385038
32	1	0	0.597460	-1.084123	-4.706094
33	1	0	1.458303	-1.754764	-3.314466
34	1	0	-0.238045	-2.167251	-3.591330
35	1	0	-1.991814	-0.854545	-2.743265
36	1	0	-1.868881	0.942670	-2.829795
37	1	0	6.808030	0.540400	-1.825811
38	1	0	8.851483	1.822799	-1.252880
39	1	0	7.694690	1.827781	2.886201
40	1	0	5.648485	0.548720	2.320228
41	45	0	-0.477269	0.360673	-0.641187
42	15	0	-0.771717	-2.081163	0.141947
43	15	0	-2.521232	1.684896	0.079596
44	6	0	-2.316570	3.532029	0.204639
45	6	0	-1.065192	4.152366	0.312465
46	6	0	-3.467496	4.342945	0.250744
47	6	0	-0.958808	5.538825	0.457280
48	1	0	-0.162559	3.557635	0.276929
49	6	0	-3.362404	5.725072	0.394757
50	1	0	-4.451891	3.892808	0.176253
51	6	0	-2.106252	6.328832	0.496864
52	1	0	0.023048	5.997257	0.536126
53	1	0	-4.263673	6.330553	0.427129
54	1	0	-2.025265	7.406407	0.606463
55	6	0	-3.948572	1.631225	-1.112376
56	6	0	-5.131940	0.910366	-0.895038
57	6	0	-3.818935	2.348060	-2.318422
58	6	0	-6.145212	0.894522	-1.858299
59	1	0	-5.291793	0.381007	0.035708
60	6	0	-4.828565	2.326501	-3.280039
61	1	0	-2.942041	2.964609	-2.495137
62	6	0	-5.995603	1.593204	-3.055745
63	1	0	-7.060213	0.343419	-1.658990
64	1	0	-4.706920	2.894040	-4.198308
65	1	0	-6.785974	1.580824	-3.800484
66	6	0	-3.257268	1.286854	1.737008
67	6	0	-3.220956	2.213815	2.792692
68	6	0	-3.832735	0.026445	1.978335
69	6	0	-3.766973	1.898395	4.039041
70	1	0	-2.777012	3.191683	2.648184
71	6	0	-4.400215	-0.276703	3.217736
72	1	0	-3.838854	-0.732986	1.204444
73	6	0	-4.369528	0.658859	4.253482
74	1	0	-3.727385	2.632090	4.839206

75	1	0	-4.856407	-1.250665	3.371827
76	1	0	-4.807772	0.421995	5.218691
77	6	0	-2.432331	-2.895152	0.071080
78	6	0	-2.675953	-4.089911	0.772368
79	6	0	-3.456652	-2.361973	-0.725019
80	6	0	-3.910267	-4.731655	0.672077
81	1	0	-1.899541	-4.521244	1.396151
82	6	0	-4.692282	-3.007314	-0.826663
83	1	0	-3.302124	-1.429307	-1.255069
84	6	0	-4.920914	-4.194013	-0.129809
85	1	0	-4.081913	-5.653461	1.220676
86	1	0	-5.472266	-2.575947	-1.447753
87	1	0	-5.880546	-4.697131	-0.207306
88	6	0	-0.246201	-2.463327	1.885261
89	6	0	0.887549	-3.227425	2.202604
90	6	0	-1.031780	-1.962554	2.939103
91	6	0	1.228909	-3.471962	3.535984
92	1	0	1.508480	-3.646556	1.420520
93	6	0	-0.692548	-2.213989	4.267592
94	1	0	-1.926748	-1.387998	2.727290
95	6	0	0.444010	-2.967172	4.571481
96	1	0	2.111250	-4.065469	3.757439
97	1	0	-1.319539	-1.820846	5.063064
98	1	0	0.711292	-3.161914	5.606166
99	6	0	0.285056	-3.218284	-0.870229
100	6	0	1.670911	-2.986252	-0.935713
101	6	0	-0.248582	-4.298695	-1.590054
102	6	0	2.503168	-3.822224	-1.680623
103	1	0	2.120579	-2.160841	-0.395756
104	6	0	0.584964	-5.125986	-2.348332
105	1	0	-1.312274	-4.506849	-1.562038
106	6	0	1.960034	-4.894666	-2.392874
107	1	0	3.569138	-3.616798	-1.707387
108	1	0	0.153156	-5.956777	-2.899545
109	1	0	2.604490	-5.543915	-2.978681
110	6	0	9.684879	2.664167	1.210571
111	1	0	10.481883	1.957250	1.475769
112	1	0	10.048547	3.265520	0.371613
113	1	0	9.539030	3.326414	2.069920

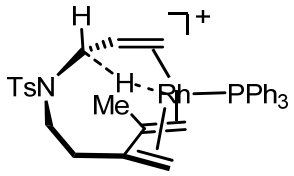


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.604250	-1.045140	0.253628
2	1	0	0.724878	0.486778	0.333780
3	6	0	1.518863	0.111107	1.082322
4	6	0	2.878980	-1.685392	-0.133258
5	6	0	2.018122	-2.160681	-1.347427
6	6	0	0.518031	-2.303976	-1.172439
7	6	0	-0.084477	-3.176497	-0.211800
8	6	0	-0.350892	-0.599139	2.585186
9	6	0	0.654609	-4.221992	0.582158
10	6	0	-1.494033	-2.945915	0.046026
11	7	0	2.716723	-0.322150	0.388827
12	6	0	5.209601	0.695692	-0.163273
13	6	0	5.693895	1.027134	1.107531
14	6	0	7.049439	0.869437	1.370958
15	6	0	7.933752	0.393578	0.386188
16	6	0	7.418858	0.077248	-0.877939
17	6	0	6.061898	0.227752	-1.164963
18	16	0	3.480939	0.927089	-0.526883
19	8	0	2.997541	2.172634	0.078533
20	8	0	3.267213	0.660123	-1.954890
21	1	0	1.735729	1.038347	1.622243
22	1	0	1.333619	-1.848675	2.162415
23	1	0	-0.808916	-1.314943	3.259545
24	1	0	-0.725567	0.416930	2.645073
25	1	0	3.926333	-1.768958	-0.438816
26	1	0	2.769109	-2.368195	0.711157
27	1	0	2.213894	-1.487391	-2.183558
28	1	0	2.427241	-3.139746	-1.632124
29	1	0	-1.329464	-1.787366	-2.248320
30	1	0	0.046778	-0.606745	-2.436591
31	1	0	0.358278	-5.210668	0.207579
32	1	0	1.739968	-4.157285	0.499944
33	1	0	0.376734	-4.193484	1.641510

34	1	0	-1.895968	-3.410677	0.945682
35	1	0	-2.216719	-2.890872	-0.764945
36	1	0	5.023760	1.411159	1.869629
37	1	0	7.433386	1.125306	2.354981
38	1	0	8.088129	-0.285141	-1.653302
39	1	0	5.669838	0.001940	-2.150697
40	6	0	-0.391661	-1.411441	-1.849221
41	6	0	0.840354	-0.904326	1.960401
42	6	0	9.406391	0.255239	0.683717
43	1	0	9.894880	1.238034	0.689926
44	1	0	9.574483	-0.194443	1.668289
45	1	0	9.912580	-0.360510	-0.065191
46	15	0	-2.578242	0.373044	0.038007
47	6	0	-3.458534	0.692910	1.628317
48	6	0	-3.697534	-0.383105	2.502923
49	6	0	-3.879975	1.976419	2.006425
50	6	0	-4.366142	-0.184360	3.710142
51	1	0	-3.358280	-1.381561	2.240103
52	6	0	-4.535486	2.174488	3.224647
53	1	0	-3.699538	2.825731	1.357086
54	6	0	-4.785280	1.097883	4.075109
55	1	0	-4.553242	-1.027984	4.368604
56	1	0	-4.851904	3.175245	3.504232
57	1	0	-5.298400	1.255303	5.019267
58	6	0	-2.342391	2.029708	-0.731992
59	6	0	-3.432968	2.713304	-1.302227
60	6	0	-1.082378	2.645215	-0.737820
61	6	0	-3.258876	3.979631	-1.859298
62	1	0	-4.416775	2.254606	-1.316129
63	6	0	-0.909806	3.913131	-1.296663
64	1	0	-0.219320	2.143589	-0.314215
65	6	0	-1.997521	4.581564	-1.858566
66	1	0	-4.109048	4.494516	-2.297386
67	1	0	0.076233	4.367992	-1.295840
68	1	0	-1.864384	5.565868	-2.297990
69	6	0	-3.833452	-0.426385	-1.058257
70	6	0	-4.954732	-1.100407	-0.552856
71	6	0	-3.625441	-0.406019	-2.450089
72	6	0	-5.844453	-1.742151	-1.418920
73	1	0	-5.153698	-1.112474	0.513090
74	6	0	-4.518290	-1.044267	-3.310763
75	1	0	-2.780480	0.134225	-2.867218
76	6	0	-5.628848	-1.718725	-2.796689
77	1	0	-6.712825	-2.251601	-1.011005

78	1	0	-4.349543	-1.007420	-4.383250
79	1	0	-6.324766	-2.214207	-3.467270



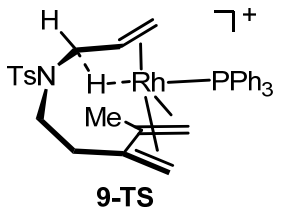
8-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.565109	-1.010694	-0.380370
2	1	0	-0.294298	0.328611	0.071049
3	6	0	-1.485252	0.123627	-0.968705
4	6	0	-2.871890	-1.818382	-0.220335
5	6	0	-2.018815	-2.611076	0.819193
6	6	0	-0.505057	-2.606657	0.706009
7	6	0	0.222451	-3.263226	-0.362637
8	6	0	0.410397	-0.152018	-2.519892
9	6	0	-0.457332	-4.107971	-1.413735
10	6	0	1.616449	-3.032880	-0.454611
11	7	0	-2.620476	-0.378614	-0.351017
12	6	0	-5.106454	0.629000	0.314043
13	6	0	-5.507733	1.377159	-0.799019
14	6	0	-6.846924	1.356566	-1.170856
15	6	0	-7.794294	0.610016	-0.447708
16	6	0	-7.360588	-0.122008	0.666462
17	6	0	-6.022597	-0.117360	1.059011
18	16	0	-3.402116	0.670109	0.818894
19	8	0	-2.828763	1.989914	0.558673
20	8	0	-3.274853	0.016021	2.122690
21	1	0	-1.473022	1.210613	-1.012641
22	1	0	-1.254239	-1.526102	-2.417114
23	1	0	0.906636	-0.697597	-3.315166
24	1	0	0.694727	0.887255	-2.399157
25	1	0	-3.921867	-1.932352	0.061950
26	1	0	-2.784851	-2.254189	-1.217224
27	1	0	-2.290067	-2.246036	1.811135
28	1	0	-2.375992	-3.647283	0.757637

29	1	0	1.245173	-2.182475	1.967793
30	1	0	-0.266540	-1.234897	2.346024
31	1	0	-0.405999	-5.160534	-1.105443
32	1	0	-1.511451	-3.870223	-1.566372
33	1	0	0.060611	-4.031902	-2.374793
34	1	0	2.122426	-3.399958	-1.343616
35	1	0	2.251754	-2.955209	0.419998
36	1	0	-4.789497	1.974468	-1.350949
37	1	0	-7.167988	1.936077	-2.032257
38	1	0	-8.080014	-0.697574	1.242139
39	1	0	-5.695411	-0.664892	1.936300
40	6	0	0.273295	-1.844077	1.626544
41	6	0	-0.817749	-0.610619	-2.035895
42	6	0	-9.248170	0.626136	-0.849189
43	1	0	-9.730661	1.553875	-0.515665
44	1	0	-9.362868	0.575739	-1.937108
45	1	0	-9.797991	-0.209206	-0.406404
46	15	0	2.550156	0.347675	0.047954
47	6	0	2.199551	2.167229	0.026783
48	6	0	1.916136	2.899246	1.189034
49	6	0	2.138376	2.826754	-1.214925
50	6	0	1.570073	4.249870	1.110699
51	1	0	1.981843	2.432882	2.164781
52	6	0	1.790773	4.176072	-1.289208
53	1	0	2.400445	2.300464	-2.127901
54	6	0	1.499643	4.891177	-0.126174
55	1	0	1.361884	4.800489	2.023562
56	1	0	1.759478	4.669137	-2.256776
57	1	0	1.231032	5.941914	-0.182807
58	6	0	3.341577	-0.009677	1.679337
59	6	0	4.681705	-0.415997	1.781090
60	6	0	2.574409	0.073437	2.856556
61	6	0	5.241693	-0.709867	3.027074
62	1	0	5.297649	-0.502235	0.893464
63	6	0	3.141322	-0.204540	4.099950
64	1	0	1.526330	0.351103	2.805535
65	6	0	4.478545	-0.598197	4.188844
66	1	0	6.280195	-1.023231	3.084234
67	1	0	2.534890	-0.121548	4.997402
68	1	0	4.918406	-0.822363	5.156195
69	6	0	3.921831	0.204409	-1.175168
70	6	0	4.982428	1.130444	-1.160114
71	6	0	3.937969	-0.826835	-2.123346
72	6	0	6.032855	1.015335	-2.069062

73	1	0	4.986150	1.942655	-0.439442
74	6	0	4.991133	-0.939584	-3.034638
75	1	0	3.120125	-1.537643	-2.150628
76	6	0	6.039413	-0.020118	-3.008390
77	1	0	6.845049	1.736177	-2.045899
78	1	0	4.989175	-1.743752	-3.765082
79	1	0	6.857628	-0.105403	-3.717637



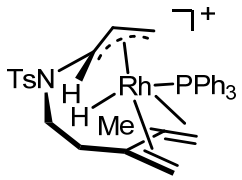
9-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.593106	-0.730822	-0.659975
2	1	0	-0.319107	0.084466	0.514479
3	6	0	-1.614872	0.511830	-0.503456
4	6	0	-2.990310	-1.443456	-1.245036
5	6	0	-2.120230	-2.714435	-1.024514
6	6	0	-0.597752	-2.629610	-1.003351
7	6	0	0.086854	-2.690321	0.277616
8	6	0	0.337572	1.130953	-1.937591
9	6	0	-0.628723	-2.849794	1.598428
10	6	0	1.495697	-2.543979	0.266246
11	7	0	-2.744463	-0.281082	-0.379875
12	6	0	-5.316880	0.362889	0.430908
13	6	0	-5.541543	1.692901	0.057174
14	6	0	-6.799470	2.052676	-0.413307
15	6	0	-7.839309	1.111346	-0.510737
16	6	0	-7.583628	-0.210831	-0.120201
17	6	0	-6.330982	-0.595438	0.355563
18	16	0	-3.718278	-0.107376	1.053060
19	8	0	-3.108917	1.011843	1.770830
20	8	0	-3.820633	-1.446694	1.636379
21	1	0	-1.633269	1.413207	0.099194
22	1	0	-1.282756	-0.106703	-2.567938
23	1	0	0.797845	1.094111	-2.919070

24	1	0	0.628961	1.956807	-1.301624
25	1	0	-4.031909	-1.736390	-1.096933
26	1	0	-2.926698	-1.109199	-2.283660
27	1	0	-2.457929	-3.179354	-0.097562
28	1	0	-2.405616	-3.397282	-1.833430
29	1	0	1.163617	-2.968966	-2.256362
30	1	0	-0.296162	-2.299424	-3.117830
31	1	0	-1.587440	-2.334059	1.658588
32	1	0	-0.814858	-3.919020	1.772011
33	1	0	0.006765	-2.496637	2.414499
34	1	0	1.991558	-2.449919	1.225499
35	1	0	2.115277	-2.955067	-0.522202
36	1	0	-4.753702	2.433033	0.151187
37	1	0	-6.983420	3.083893	-0.702438
38	1	0	-8.377999	-0.949654	-0.178842
39	1	0	-6.146316	-1.612634	0.683668
40	6	0	0.200217	-2.481745	-2.167674
41	6	0	-0.884730	0.477765	-1.749084
42	6	0	-9.206660	1.527309	-0.992925
43	1	0	-9.775086	1.999715	-0.181330
44	1	0	-9.139232	2.255918	-1.807414
45	1	0	-9.787467	0.669990	-1.345200
46	15	0	2.657895	0.305734	0.015339
47	6	0	2.738683	2.156898	-0.005424
48	6	0	2.352005	2.924094	1.104398
49	6	0	3.140414	2.820198	-1.179157
50	6	0	2.374743	4.319193	1.043374
51	1	0	2.052716	2.443275	2.028901
52	6	0	3.163717	4.213930	-1.234760
53	1	0	3.449503	2.249612	-2.049696
54	6	0	2.780158	4.967913	-0.123634
55	1	0	2.083357	4.896630	1.916073
56	1	0	3.486391	4.708738	-2.146392
57	1	0	2.801731	6.052946	-0.166261
58	6	0	3.048641	-0.125349	1.772604
59	6	0	4.314963	-0.568264	2.182050
60	6	0	2.027005	-0.019274	2.734666
61	6	0	4.557129	-0.877721	3.523446
62	1	0	5.116987	-0.685254	1.462623
63	6	0	2.276394	-0.316462	4.074562
64	1	0	1.027757	0.282254	2.433128
65	6	0	3.544492	-0.746737	4.473096
66	1	0	5.542988	-1.223280	3.821068
67	1	0	1.477140	-0.219201	4.803888

68	1	0	3.737608	-0.985609	5.514797
69	6	0	4.128816	-0.166637	-0.987012
70	6	0	5.380785	0.442071	-0.775596
71	6	0	4.004193	-1.126223	-2.000686
72	6	0	6.483179	0.070932	-1.544051
73	1	0	5.492572	1.214382	-0.020541
74	6	0	5.109490	-1.493566	-2.771944
75	1	0	3.031224	-1.563769	-2.199632
76	6	0	6.350665	-0.900811	-2.540343
77	1	0	7.444282	0.546033	-1.369920
78	1	0	4.997443	-2.236599	-3.556414
79	1	0	7.210823	-1.185116	-3.139534



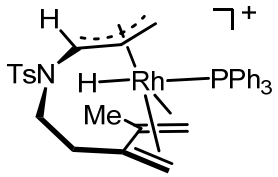
10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.460469	-0.606037	0.228706
2	1	0	-0.117023	0.747150	-0.438588
3	6	0	-0.285988	-1.535278	-1.814125
4	6	0	3.004209	-1.755362	-0.055064
5	6	0	2.027339	-2.323752	-1.127033
6	6	0	0.522943	-2.269168	-0.923283
7	6	0	-0.130978	-3.073544	0.128664
8	6	0	-0.164905	0.213776	2.268249
9	6	0	0.676512	-3.995484	1.018453
10	6	0	-1.488721	-2.989135	0.327075
11	7	0	2.876527	-0.316074	0.183220
12	6	0	5.422958	0.648587	-0.313735
13	6	0	5.786807	1.362432	0.834139
14	6	0	7.099968	1.281014	1.282811
15	6	0	8.057509	0.507565	0.602705
16	6	0	7.661380	-0.188883	-0.547869
17	6	0	6.350409	-0.123802	-1.017578
18	16	0	3.754970	0.760919	-0.915743

19	8	0	3.207583	2.087704	-0.640941
20	8	0	3.680575	0.144004	-2.238943
21	1	0	1.707668	1.282846	0.712504
22	1	0	1.303366	-1.396747	2.233793
23	1	0	-0.753726	-0.248819	3.053591
24	1	0	-0.257865	1.294515	2.206307
25	1	0	4.025146	-1.946224	-0.394447
26	1	0	2.904705	-2.259394	0.907056
27	1	0	2.270648	-1.836697	-2.072762
28	1	0	2.308750	-3.379704	-1.241606
29	1	0	-1.293765	-1.849486	-2.060756
30	1	0	0.203478	-0.934578	-2.574736
31	1	0	1.110087	-4.803296	0.415081
32	1	0	1.505095	-3.508843	1.538517
33	1	0	0.038005	-4.459609	1.773942
34	1	0	-1.932501	-3.519020	1.165139
35	1	0	-2.185964	-2.611887	-0.408137
36	1	0	5.061868	1.980522	1.353462
37	1	0	7.392705	1.833586	2.171510
38	1	0	8.390160	-0.783888	-1.091069
39	1	0	6.054755	-0.642724	-1.922936
40	6	0	1.819778	0.214004	0.856920
41	6	0	1.038530	-0.415752	1.853863
42	6	0	9.485163	0.458620	1.086770
43	1	0	10.026867	1.363565	0.782700
44	1	0	9.535382	0.403792	2.179282
45	1	0	10.021417	-0.400626	0.674034
46	15	0	-2.672842	0.340596	0.025181
47	6	0	-2.743057	2.084965	-0.570284
48	6	0	-3.877207	2.565780	-1.248364
49	6	0	-1.693405	2.974631	-0.295975
50	6	0	-3.949357	3.901212	-1.647557
51	1	0	-4.703893	1.899079	-1.470457
52	6	0	-1.769125	4.310056	-0.693037
53	1	0	-0.807126	2.625429	0.223701
54	6	0	-2.896166	4.775386	-1.372450
55	1	0	-4.829186	4.255418	-2.176936
56	1	0	-0.943946	4.982592	-0.477712
57	1	0	-2.952339	5.812980	-1.688465
58	6	0	-3.768613	-0.558366	-1.157290
59	6	0	-4.840011	-1.355653	-0.727163
60	6	0	-3.489142	-0.478520	-2.534643
61	6	0	-5.615391	-2.056750	-1.655157
62	1	0	-5.083361	-1.421499	0.328091

63	6	0	-4.270297	-1.174252	-3.456719
64	1	0	-2.673878	0.146804	-2.888705
65	6	0	-5.333686	-1.968577	-3.018316
66	1	0	-6.446018	-2.664423	-1.307662
67	1	0	-4.050045	-1.093515	-4.517341
68	1	0	-5.940850	-2.510764	-3.737289
69	6	0	-3.614241	0.358756	1.615175
70	6	0	-4.421307	1.446769	1.982403
71	6	0	-3.538575	-0.748272	2.477756
72	6	0	-5.137274	1.422922	3.181426
73	1	0	-4.494007	2.316486	1.339043
74	6	0	-4.264749	-0.774548	3.668394
75	1	0	-2.907164	-1.591931	2.217218
76	6	0	-5.064240	0.314124	4.024809
77	1	0	-5.753201	2.275352	3.453157
78	1	0	-4.200356	-1.641097	4.320609
79	1	0	-5.623048	0.298513	4.956007



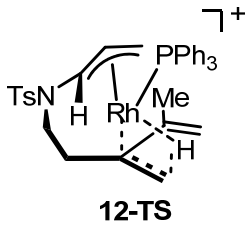
11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.423892	-0.613832	-0.329588
2	1	0	-0.008856	0.630624	0.462072
3	6	0	-0.328653	-1.585606	1.667574
4	6	0	3.116583	-1.817540	0.104551
5	6	0	2.076670	-2.170161	1.199201
6	6	0	0.598256	-2.271658	0.861411
7	6	0	0.084048	-3.266092	-0.122402
8	6	0	-0.374563	0.116439	-2.454147
9	6	0	1.034312	-4.223231	-0.812778
10	6	0	-1.238051	-3.315329	-0.444488
11	7	0	2.844335	-0.570253	-0.631569
12	6	0	5.160962	0.675402	0.094907
13	6	0	5.856322	0.481131	1.290005

14	6	0	7.245418	0.362186	1.246856
15	6	0	7.944070	0.440257	0.034521
16	6	0	7.213257	0.643230	-1.150239
17	6	0	5.829143	0.767475	-1.131990
18	16	0	3.395081	0.895427	0.143710
19	8	0	2.952843	0.877309	1.541687
20	8	0	3.006646	1.985083	-0.752321
21	1	0	1.576788	-1.576325	-1.899780
22	1	0	1.079338	1.459619	-1.580633
23	1	0	-0.494399	-0.820250	-2.996290
24	1	0	3.203071	-2.609784	-0.642822
25	1	0	4.098992	-1.729925	0.574008
26	1	0	2.388826	-3.141969	1.607900
27	1	0	2.185854	-1.445028	2.008045
28	6	0	0.855782	0.437059	-1.851442
29	1	0	1.668494	-3.736234	-1.562265
30	1	0	1.702648	-4.705523	-0.090822
31	1	0	0.476121	-5.010528	-1.324947
32	1	0	-1.585500	-3.995521	-1.216734
33	1	0	-2.011868	-2.773774	0.082876
34	1	0	5.319343	0.437694	2.231464
35	1	0	7.794045	0.213022	2.172591
36	1	0	7.740630	0.712218	-2.097988
37	1	0	5.276537	0.941317	-2.049464
38	6	0	1.674000	-0.620545	-1.389382
39	15	0	-2.638418	0.311113	0.058852
40	6	0	9.448294	0.333958	-0.005940
41	1	0	9.778028	-0.349122	-0.796510
42	1	0	9.900587	1.311577	-0.215253
43	1	0	9.853183	-0.022474	0.945315
44	6	0	-2.742782	2.054259	-0.541441
45	6	0	-1.651453	2.922167	-0.357703
46	6	0	-3.896315	2.543623	-1.175413
47	6	0	-1.719202	4.249394	-0.782983
48	1	0	-0.743485	2.566433	0.120654
49	6	0	-3.955668	3.869403	-1.609216
50	1	0	-4.749953	1.894828	-1.337466
51	6	0	-2.871213	4.725261	-1.412673
52	1	0	-0.868411	4.906534	-0.627691
53	1	0	-4.853741	4.230814	-2.101856
54	1	0	-2.920964	5.755932	-1.751562
55	6	0	-3.139028	0.383590	1.831359
56	6	0	-3.613558	-0.776067	2.471325
57	6	0	-2.984493	1.556900	2.584193

58	6	0	-3.928562	-0.757754	3.830098
59	1	0	-3.768110	-1.691271	1.905669
60	6	0	-3.296485	1.569330	3.945396
61	1	0	-2.632281	2.467965	2.112246
62	6	0	-3.767575	0.414952	4.571657
63	1	0	-4.304778	-1.658505	4.306699
64	1	0	-3.177562	2.488067	4.512454
65	1	0	-4.013971	0.429146	5.629275
66	6	0	-4.031801	-0.562540	-0.773137
67	6	0	-5.346785	-0.491648	-0.278868
68	6	0	-3.793946	-1.267740	-1.963480
69	6	0	-6.391891	-1.116602	-0.960545
70	1	0	-5.556371	0.049059	0.638200
71	6	0	-4.841612	-1.888345	-2.645216
72	1	0	-2.785611	-1.332201	-2.359038
73	6	0	-6.142198	-1.815876	-2.143425
74	1	0	-7.401972	-1.055148	-0.565941
75	1	0	-4.641249	-2.429342	-3.565691
76	1	0	-6.957662	-2.302197	-2.670823
77	1	0	-1.035139	0.921948	-2.755681
78	1	0	0.042328	-0.919475	2.440076
79	1	0	-1.316762	-1.986322	1.858191



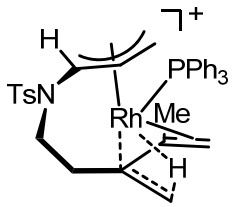
12-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.584619	-0.954095	-0.356386
2	1	0	0.223353	-0.193754	1.014239
3	6	0	0.063453	-1.787083	1.659180
4	6	0	-2.864591	-1.993757	-0.389277
5	6	0	-1.996489	-2.831521	0.599322
6	6	0	-0.486889	-2.630977	0.626078
7	6	0	0.416926	-3.346839	-0.265238
8	6	0	0.461745	-0.202479	-2.498066

9	6	0	-0.130046	-4.269508	-1.330816
10	6	0	1.784134	-3.110535	-0.177834
11	7	0	-2.610013	-0.550145	-0.421763
12	6	0	-5.031965	0.534025	0.322586
13	6	0	-5.365572	1.397639	-0.727769
14	6	0	-6.697103	1.500938	-1.111382
15	6	0	-7.703552	0.763633	-0.461618
16	6	0	-7.336616	-0.085809	0.590837
17	6	0	-6.006580	-0.206890	0.993809
18	16	0	-3.334290	0.413692	0.838309
19	8	0	-2.683960	1.721472	0.732841
20	8	0	-3.266350	-0.374802	2.072289
21	1	0	-1.311007	1.017062	-0.849912
22	1	0	-1.150164	-1.632607	-2.480748
23	1	0	0.991764	-0.738647	-3.279121
24	1	0	0.699723	0.853387	-2.409852
25	1	0	-3.914920	-2.140220	-0.124033
26	1	0	-2.759607	-2.362474	-1.411948
27	1	0	-2.378961	-2.642185	1.603272
28	1	0	-2.213971	-3.881869	0.371764
29	1	0	1.023415	-1.999332	2.119459
30	1	0	-0.656415	-1.341012	2.341109
31	1	0	-0.401312	-5.233695	-0.880874
32	1	0	-1.026048	-3.882844	-1.824519
33	1	0	0.623502	-4.469932	-2.097128
34	1	0	2.443842	-3.519403	-0.937182
35	1	0	2.267727	-2.804434	0.741249
36	1	0	-4.599833	1.985753	-1.222850
37	1	0	-6.965289	2.170594	-1.924203
38	1	0	-8.101674	-0.655888	1.110355
39	1	0	-5.730218	-0.847740	1.824084
40	6	0	-1.466433	-0.040932	-1.021705
41	6	0	-0.795985	-0.684561	-2.090850
42	6	0	-9.145736	0.909721	-0.879080
43	1	0	-9.543765	1.883189	-0.565827
44	1	0	-9.252475	0.853728	-1.968031
45	1	0	-9.775007	0.134491	-0.433211
46	15	0	2.504059	0.444190	-0.021384
47	6	0	2.134738	2.209538	-0.403332
48	6	0	3.004956	3.011800	-1.157590
49	6	0	0.923525	2.763786	0.052632
50	6	0	2.676578	4.340637	-1.436709
51	1	0	3.938861	2.606746	-1.531068
52	6	0	0.606258	4.094953	-0.218134

53	1	0	0.223128	2.159597	0.622603
54	6	0	1.482055	4.886211	-0.965747
55	1	0	3.359839	4.947720	-2.023656
56	1	0	-0.328850	4.506907	0.150069
57	1	0	1.231540	5.920360	-1.183628
58	6	0	4.043964	0.035186	-0.940938
59	6	0	5.281598	0.560369	-0.525327
60	6	0	4.003166	-0.796092	-2.069089
61	6	0	6.445818	0.264435	-1.233651
62	1	0	5.337387	1.193721	0.354893
63	6	0	5.170697	-1.090693	-2.776371
64	1	0	3.057513	-1.222537	-2.385275
65	6	0	6.392514	-0.560522	-2.360394
66	1	0	7.395363	0.674668	-0.902247
67	1	0	5.125232	-1.737815	-3.647736
68	1	0	7.301651	-0.792425	-2.907576
69	6	0	3.052207	0.407869	1.741115
70	6	0	2.730626	1.427219	2.648452
71	6	0	3.752591	-0.720543	2.205130
72	6	0	3.096369	1.316420	3.992250
73	1	0	2.205833	2.315330	2.312885
74	6	0	4.116238	-0.826313	3.547825
75	1	0	4.045310	-1.504705	1.512176
76	6	0	3.784899	0.190965	4.446205
77	1	0	2.847023	2.118067	4.681534
78	1	0	4.665580	-1.699150	3.889246
79	1	0	4.069407	0.109583	5.491155



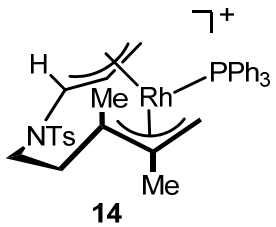
13-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.509886	-0.824015	-0.369893
2	1	0	-0.076465	-0.041556	0.977305

3	6	0	0.039747	-1.585065	1.696740
4	6	0	3.093373	-2.057102	-0.279195
5	6	0	2.135048	-2.683521	0.783127
6	6	0	0.627323	-2.464335	0.714466
7	6	0	-0.234883	-3.203990	-0.196925
8	6	0	-0.490803	-0.024547	-2.431998
9	6	0	0.348956	-4.147041	-1.224311
10	6	0	-1.609813	-2.989168	-0.145465
11	7	0	2.760630	-0.691731	-0.717515
12	6	0	5.015208	0.575257	0.161629
13	6	0	5.810718	0.161609	1.232108
14	6	0	7.197644	0.190751	1.087574
15	6	0	7.795531	0.629590	-0.101681
16	6	0	6.964666	1.044131	-1.158416
17	6	0	5.580360	1.026828	-1.037223
18	16	0	3.246923	0.600356	0.350725
19	8	0	2.911228	0.200043	1.722053
20	8	0	2.694233	1.821222	-0.233976
21	1	0	1.492642	-1.534519	-2.069940
22	1	0	0.846345	1.422165	-1.443750
23	1	0	-0.455935	-0.893903	-3.087228
24	1	0	3.123744	-2.667211	-1.186525
25	1	0	4.107474	-2.055346	0.127118
26	1	0	2.321608	-3.764487	0.750863
27	1	0	2.467251	-2.337629	1.762409
28	6	0	0.696429	0.404827	-1.773421
29	1	0	1.244690	-3.759506	-1.718088
30	1	0	0.631104	-5.093218	-0.743847
31	1	0	-0.388834	-4.383451	-1.995607
32	1	0	-2.243570	-3.422776	-0.913324
33	1	0	-2.118808	-2.698913	0.764790
34	1	0	5.351247	-0.161601	2.159890
35	1	0	7.824087	-0.127001	1.916340
36	1	0	7.412529	1.391652	-2.085589
37	1	0	4.949048	1.364723	-1.852582
38	6	0	1.588245	-0.639564	-1.459231
39	15	0	-2.536283	0.378470	0.030753
40	6	0	9.296162	0.683189	-0.244854
41	1	0	9.618911	0.280044	-1.210887
42	1	0	9.653218	1.719548	-0.191924
43	1	0	9.797087	0.119035	0.546791
44	6	0	-2.341111	2.173363	-0.343675
45	6	0	-1.161688	2.829327	0.054962
46	6	0	-3.326946	2.905655	-1.024154

47	6	0	-0.984983	4.189146	-0.201979
48	1	0	-0.373930	2.279023	0.561066
49	6	0	-3.139784	4.264016	-1.289262
50	1	0	-4.240298	2.422615	-1.353036
51	6	0	-1.973396	4.909154	-0.876865
52	1	0	-0.069954	4.679701	0.116969
53	1	0	-3.910187	4.815916	-1.820099
54	1	0	-1.831871	5.965725	-1.085013
55	6	0	-3.071239	0.286258	1.793586
56	6	0	-3.729053	-0.869860	2.252661
57	6	0	-2.764618	1.300960	2.712387
58	6	0	-4.069000	-1.004677	3.599529
59	1	0	-4.011032	-1.653140	1.554713
60	6	0	-3.107345	1.161489	4.058892
61	1	0	-2.270861	2.208600	2.381766
62	6	0	-3.756073	0.009759	4.506902
63	1	0	-4.586617	-1.898509	3.936087
64	1	0	-2.872051	1.960862	4.755704
65	1	0	-4.023807	-0.093750	5.554322
66	6	0	-4.025240	-0.169218	-0.902628
67	6	0	-5.315890	0.189581	-0.471993
68	6	0	-3.888224	-0.929964	-2.073295
69	6	0	-6.437827	-0.201449	-1.203048
70	1	0	-5.446634	0.768101	0.437335
71	6	0	-5.013082	-1.318098	-2.803714
72	1	0	-2.899840	-1.225121	-2.408713
73	6	0	-6.288804	-0.954557	-2.370282
74	1	0	-7.428453	0.080572	-0.858238
75	1	0	-4.891713	-1.907173	-3.708372
76	1	0	-7.164230	-1.259398	-2.936333
77	1	0	-1.228095	0.722799	-2.707064
78	1	0	0.736405	-1.114083	2.383911
79	1	0	-0.931595	-1.795262	2.133368

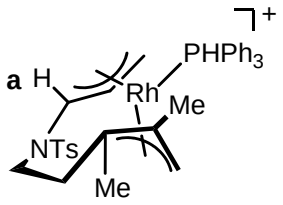


14

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.541771	-0.275566	-1.623227
2	6	0	0.629060	0.797196	-1.588547
3	6	0	-0.536904	0.624784	-2.372739
4	6	0	3.164044	-1.910472	-0.984910
5	6	0	2.235980	-2.912454	-0.239983
6	6	0	0.776143	-2.907729	-0.633208
7	6	0	-0.222284	-2.794502	0.366181
8	6	0	0.494144	-3.508156	-2.002230
9	6	0	0.128579	-2.707078	1.841477
10	6	0	-1.590743	-2.663786	-0.018050
11	7	0	2.706439	-0.515075	-0.926047
12	6	0	4.937624	0.568622	0.236805
13	6	0	5.818472	-0.136538	1.061022
14	6	0	7.189522	0.038900	0.881157
15	6	0	7.689609	0.908091	-0.099455
16	6	0	6.775237	1.605759	-0.907878
17	6	0	5.403126	1.449664	-0.745911
18	16	0	3.185457	0.401807	0.488670
19	8	0	2.951020	-0.446482	1.660831
20	8	0	2.533640	1.702515	0.356349
21	1	0	1.467527	-0.930446	-2.488268
22	1	0	0.749586	1.635767	-0.917103
23	1	0	-1.252281	1.436758	-2.416507
24	1	0	-0.512801	-0.016196	-3.254346
25	1	0	3.251187	-2.169602	-2.045248
26	1	0	4.169184	-1.967593	-0.562313
27	1	0	2.647843	-3.907275	-0.465519
28	1	0	2.360128	-2.748598	0.828445
29	1	0	0.564499	-4.603719	-1.934899
30	1	0	1.239970	-3.195500	-2.741350
31	1	0	0.518594	-3.676656	2.178647
32	1	0	0.881265	-1.948057	2.067233
33	1	0	-0.760318	-2.483271	2.432617
34	1	0	-2.331798	-2.605692	0.772954
35	1	0	-1.954080	-3.126624	-0.931038
36	1	0	5.435011	-0.795134	1.832854
37	1	0	7.881618	-0.504589	1.518407
38	1	0	7.146148	2.286059	-1.669618
39	1	0	4.706396	2.007625	-1.362960
40	45	0	-0.676244	-0.836926	-0.768821
41	1	0	-0.488805	-3.264048	-2.407311

42	15	0	-2.531379	0.323390	0.055204
43	6	0	9.174378	1.116848	-0.263440
44	1	0	9.438175	1.321639	-1.305730
45	1	0	9.510425	1.975524	0.332375
46	1	0	9.742697	0.243979	0.071392
47	6	0	-2.489312	2.165306	-0.151709
48	6	0	-1.818987	2.999502	0.756934
49	6	0	-3.088312	2.747400	-1.284345
50	6	0	-1.753285	4.377306	0.539946
51	1	0	-1.363197	2.589370	1.650418
52	6	0	-3.020044	4.124937	-1.497102
53	1	0	-3.628527	2.130118	-1.995821
54	6	0	-2.350814	4.944307	-0.586268
55	1	0	-1.238515	5.006448	1.260372
56	1	0	-3.497255	4.555817	-2.372694
57	1	0	-2.301045	6.016788	-0.750092
58	6	0	-2.617949	0.056264	1.879011
59	6	0	-3.781781	-0.376775	2.532619
60	6	0	-1.451760	0.264099	2.638919
61	6	0	-3.783930	-0.572735	3.916151
62	1	0	-4.689039	-0.568172	1.971038
63	6	0	-1.463651	0.084599	4.022063
64	1	0	-0.524560	0.547490	2.148364
65	6	0	-2.631261	-0.333984	4.664817
66	1	0	-4.692595	-0.910731	4.406099
67	1	0	-0.556583	0.259351	4.593589
68	1	0	-2.639033	-0.480705	5.740945
69	6	0	-4.177849	-0.116727	-0.633806
70	6	0	-5.343677	0.559726	-0.226596
71	6	0	-4.279711	-1.111823	-1.616079
72	6	0	-6.581158	0.221906	-0.772220
73	1	0	-5.284058	1.357708	0.507680
74	6	0	-5.520201	-1.444613	-2.165594
75	1	0	-3.381264	-1.614494	-1.959543
76	6	0	-6.672023	-0.783124	-1.740013
77	1	0	-7.474004	0.748173	-0.447225
78	1	0	-5.583522	-2.216142	-2.927614
79	1	0	-7.637311	-1.041107	-2.165936



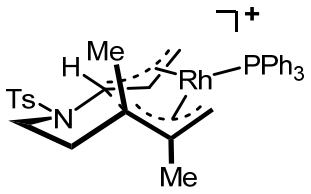
15

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.657572	-0.036861	-1.242263
2	6	0	0.806935	1.060950	-1.049529
3	6	0	-0.364717	1.097176	-1.848694
4	6	0	3.109879	-1.844045	-0.615018
5	6	0	2.261275	-2.736508	0.344321
6	6	0	0.779374	-2.451000	0.534522
7	6	0	-0.181853	-2.873290	-0.404755
8	6	0	0.446651	-2.063654	1.962060
9	6	0	0.203832	-3.601355	-1.679212
10	6	0	-1.562747	-2.550488	-0.196043
11	7	0	2.806588	-0.412324	-0.568709
12	6	0	5.257942	0.496899	0.246153
13	6	0	6.159942	-0.295919	0.959340
14	6	0	7.508264	-0.262493	0.604847
15	6	0	7.965493	0.551873	-0.440428
16	6	0	7.031325	1.342398	-1.133701
17	6	0	5.682627	1.327090	-0.798137
18	16	0	3.543155	0.507832	0.719535
19	8	0	3.388488	-0.271430	1.950648
20	8	0	3.003618	1.860430	0.602458
21	1	0	1.541935	-0.597185	-2.170195
22	1	0	0.964865	1.768444	-0.247691
23	1	0	-0.352438	0.664073	-2.848333
24	1	0	2.969877	-2.153933	-1.655076
25	1	0	4.168174	-1.990062	-0.385599
26	1	0	2.386324	-3.763954	-0.021047
27	1	0	2.734901	-2.687707	1.326502
28	1	0	1.075749	-1.227965	2.284246
29	1	0	0.698880	-2.910917	2.618914
30	1	0	1.159158	-3.280875	-2.100928
31	1	0	0.281962	-4.677113	-1.470774

32	1	0	-0.562751	-3.476035	-2.448534
33	1	0	-2.268781	-2.883993	-0.953202
34	1	0	-1.975680	-2.530980	0.805352
35	1	0	5.813611	-0.909659	1.783876
36	1	0	8.216797	-0.873771	1.156748
37	1	0	7.370178	1.984644	-1.942184
38	1	0	4.973657	1.956789	-1.325726
39	45	0	-0.598664	-0.662612	-0.596657
40	1	0	-0.597133	-1.803503	2.134249
41	15	0	-2.677478	0.291403	-0.030926
42	6	0	9.429337	0.606250	-0.800263
43	1	0	9.574205	0.596970	-1.885857
44	1	0	9.886786	1.529097	-0.421200
45	1	0	9.980923	-0.235933	-0.373003
46	6	0	-2.389829	2.013693	0.568938
47	6	0	-1.327416	2.235895	1.465196
48	6	0	-3.167996	3.106475	0.158639
49	6	0	-1.067659	3.515024	1.957339
50	1	0	-0.695726	1.407222	1.775199
51	6	0	-2.897478	4.387896	0.645998
52	1	0	-3.981384	2.969580	-0.545126
53	6	0	-1.853411	4.595026	1.547641
54	1	0	-0.246476	3.667163	2.651762
55	1	0	-3.507294	5.224126	0.316223
56	1	0	-1.647496	5.592564	1.924436
57	6	0	-3.606865	-0.518827	1.347468
58	6	0	-4.490726	-1.574777	1.060048
59	6	0	-3.413436	-0.144387	2.686549
60	6	0	-5.165118	-2.234586	2.087367
61	1	0	-4.668328	-1.874142	0.031625
62	6	0	-4.088813	-0.810275	3.711771
63	1	0	-2.754876	0.679778	2.937485
64	6	0	-4.964055	-1.856124	3.416682
65	1	0	-5.851405	-3.041451	1.846618
66	1	0	-3.935080	-0.501079	4.741644
67	1	0	-5.491264	-2.369089	4.215714
68	6	0	-3.922801	0.386334	-1.378988
69	6	0	-5.243527	0.803401	-1.127727
70	6	0	-3.562985	0.019353	-2.683932
71	6	0	-6.169749	0.872694	-2.167581
72	1	0	-5.552199	1.063099	-0.119551
73	6	0	-4.493879	0.086471	-3.722853
74	1	0	-2.554084	-0.331104	-2.879201
75	6	0	-5.795854	0.517419	-3.466791

76	1	0	-7.185389	1.198262	-1.962217
77	1	0	-4.202564	-0.203010	-4.728484
78	1	0	-6.521028	0.568982	-4.273746
79	1	0	-1.035185	1.941741	-1.729676



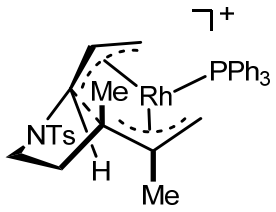
16-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.973662	-0.816039	-0.908455
2	6	0	1.655280	-0.696141	-1.307971
3	6	0	1.053777	-2.434126	-0.684406
4	6	0	3.517512	-2.008569	-0.778877
5	6	0	2.426552	-2.874904	-0.132509
6	6	0	-0.174373	0.753202	-2.215418
7	6	0	-0.041216	-2.376218	0.353943
8	6	0	0.708613	-3.207558	-1.967639
9	6	0	0.291933	-2.045837	1.788926
10	6	0	-1.355164	-2.778920	0.038605
11	7	0	2.988898	-0.635780	-0.777766
12	6	0	5.197694	0.545698	0.246581
13	6	0	6.139591	-0.011699	1.112326
14	6	0	7.494157	0.219207	0.869689
15	6	0	7.915500	0.997913	-0.216051
16	6	0	6.939291	1.553218	-1.063327
17	6	0	5.584633	1.338061	-0.840720
18	16	0	3.463820	0.323881	0.589246
19	8	0	3.326903	-0.467606	1.820560
20	8	0	2.766214	1.606280	0.464199
21	1	0	1.741995	-0.993040	-2.356411
22	1	0	0.878371	1.154362	-0.361400
23	1	0	-0.695484	1.703216	-2.206283
24	1	0	-0.062609	0.290310	-3.195692
25	1	0	3.700982	-2.292856	-1.822155

26	1	0	4.470670	-2.061345	-0.250830
27	1	0	2.579312	-3.938231	-0.351265
28	1	0	2.483122	-2.740795	0.946979
29	1	0	0.438134	-4.242801	-1.730366
30	1	0	1.573370	-3.240171	-2.638285
31	1	0	0.696198	-2.939518	2.285321
32	1	0	1.038033	-1.255072	1.892469
33	1	0	-0.610703	-1.755967	2.329760
34	1	0	-2.077721	-2.843705	0.846840
35	1	0	-1.565560	-3.415290	-0.817255
36	1	0	5.815367	-0.601132	1.963206
37	1	0	8.233646	-0.207780	1.541315
38	1	0	7.248960	2.168660	-1.903911
39	1	0	4.838567	1.781574	-1.491790
40	6	0	0.721371	0.456584	-1.171531
41	1	0	-0.123350	-2.770782	-2.535078
42	6	0	9.380822	1.240724	-0.480905
43	1	0	9.589532	2.310426	-0.595962
44	1	0	10.005845	0.858099	0.330609
45	1	0	9.697981	0.749311	-1.409205
46	15	0	-2.699978	0.310216	0.031346
47	6	0	-2.489402	0.368792	1.852197
48	6	0	-3.380747	-0.277514	2.722915
49	6	0	-1.365446	1.025861	2.388099
50	6	0	-3.159680	-0.251280	4.102254
51	1	0	-4.249463	-0.796709	2.332577
52	6	0	-1.157257	1.059642	3.765903
53	1	0	-0.645854	1.508622	1.732885
54	6	0	-2.054332	0.420097	4.626210
55	1	0	-3.857880	-0.753690	4.765451
56	1	0	-0.289885	1.577087	4.165020
57	1	0	-1.888553	0.442280	5.699289
58	6	0	-4.343455	-0.442221	-0.306863
59	6	0	-5.507714	0.211172	0.137829
60	6	0	-4.463395	-1.630403	-1.040431
61	6	0	-6.762608	-0.333271	-0.128374
62	1	0	-5.433839	1.145425	0.686840
63	6	0	-5.723532	-2.167244	-1.314015
64	1	0	-3.572360	-2.130214	-1.405778
65	6	0	-6.872268	-1.523291	-0.854016
66	1	0	-7.655213	0.175324	0.223957
67	1	0	-5.804997	-3.086048	-1.887490
68	1	0	-7.852024	-1.941790	-1.065143
69	6	0	-2.943208	2.048763	-0.526474

70	6	0	-2.855046	3.154859	0.330763
71	6	0	-3.267868	2.256004	-1.880025
72	6	0	-3.078051	4.444430	-0.160934
73	1	0	-2.626591	3.021283	1.382024
74	6	0	-3.491785	3.542494	-2.364014
75	1	0	-3.353218	1.408703	-2.555728
76	6	0	-3.393055	4.641540	-1.504613
77	1	0	-3.008670	5.292614	0.513897
78	1	0	-3.746023	3.688004	-3.409928
79	1	0	-3.566712	5.644762	-1.882622



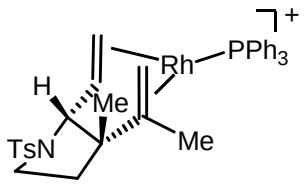
17-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.658969	-0.087241	-0.492248
2	6	0	-1.218082	1.816266	-0.323291
3	45	0	0.708025	0.203713	-0.368924
4	6	0	-3.461370	1.263289	-1.309827
5	6	0	-2.216192	2.166602	-1.438642
6	6	0	-1.029977	-0.938599	0.539191
7	6	0	0.206388	2.267920	-0.557674
8	6	0	-1.731314	2.190309	1.067681
9	6	0	0.825548	3.301610	0.357088
10	6	0	0.884982	1.879624	-1.733885
11	7	0	-3.076784	0.180473	-0.371118
12	6	0	-5.654989	-0.653633	-0.063330
13	6	0	-5.946049	-0.365405	1.274574
14	6	0	-7.220755	0.085658	1.600140
15	6	0	-8.212644	0.240601	0.615973
16	6	0	-7.891044	-0.066926	-0.713692
17	6	0	-6.618737	-0.516608	-1.064265
18	16	0	-4.041587	-1.271479	-0.489414
19	8	0	-3.537446	-2.138744	0.578333

20	8	0	-4.047481	-1.726181	-1.885149
21	1	0	-1.388322	-0.395677	-1.513885
22	1	0	-1.299733	-0.750171	1.574148
23	1	0	-0.019576	-2.304313	-0.783907
24	1	0	-3.741445	0.860553	-2.290397
25	1	0	-4.322197	1.791415	-0.893867
26	1	0	-1.750567	2.039276	-2.419050
27	1	0	-2.482813	3.226379	-1.349928
28	1	0	-2.728884	1.790324	1.246305
29	1	0	-1.783851	3.282781	1.146953
30	1	0	0.322291	4.269455	0.220798
31	1	0	0.749123	3.039138	1.414362
32	1	0	1.880746	3.438138	0.113114
33	1	0	1.858673	2.314579	-1.933075
34	1	0	0.364616	1.503426	-2.612647
35	1	0	-5.193251	-0.507686	2.042749
36	1	0	-7.456940	0.311561	2.636672
37	1	0	-8.648055	0.039253	-1.485785
38	1	0	-6.377065	-0.771347	-2.090580
39	6	0	-0.076469	-1.888049	0.219225
40	1	0	-1.067351	1.832152	1.858578
41	15	0	2.909806	-0.189355	0.077413
42	6	0	-9.600650	0.696376	0.992902
43	1	0	-10.146308	1.083667	0.127587
44	1	0	-10.183349	-0.138185	1.403835
45	1	0	-9.571176	1.478059	1.759247
46	6	0	3.116194	-1.141144	1.639825
47	6	0	2.295794	-0.821138	2.736136
48	6	0	4.061515	-2.169083	1.773580
49	6	0	2.431316	-1.502056	3.945666
50	1	0	1.545115	-0.040842	2.637132
51	6	0	4.186919	-2.855378	2.983549
52	1	0	4.696211	-2.443727	0.938101
53	6	0	3.377637	-2.522636	4.070498
54	1	0	1.794989	-1.241744	4.786727
55	1	0	4.918749	-3.652923	3.072902
56	1	0	3.478541	-3.059260	5.009289
57	6	0	3.932876	1.326468	0.289420
58	6	0	4.380623	2.025021	-0.846911
59	6	0	4.224033	1.840337	1.562317
60	6	0	5.101874	3.210838	-0.709001
61	1	0	4.187881	1.631946	-1.841082
62	6	0	4.945051	3.029006	1.695198
63	1	0	3.903278	1.310484	2.453029

64	6	0	5.382684	3.717642	0.563024
65	1	0	5.451098	3.734072	-1.594561
66	1	0	5.170887	3.410406	2.686846
67	1	0	5.947004	4.639460	0.669437
68	6	0	3.768246	-1.135875	-1.240576
69	6	0	5.172621	-1.166401	-1.319556
70	6	0	3.016852	-1.860533	-2.178493
71	6	0	5.804535	-1.919526	-2.309090
72	1	0	5.772427	-0.597243	-0.615806
73	6	0	3.652720	-2.610681	-3.168963
74	1	0	1.932201	-1.828560	-2.139402
75	6	0	5.046562	-2.643049	-3.233469
76	1	0	6.889301	-1.936858	-2.360505
77	1	0	3.059329	-3.164509	-3.890598
78	1	0	5.542063	-3.225243	-4.004904
79	1	0	0.404083	-2.456888	1.007120



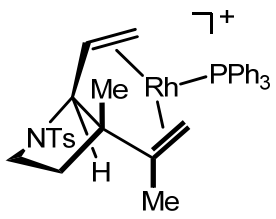
18

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.036428	-0.055217	-0.516716
2	6	0	1.937956	-1.086032	-0.566682
3	6	0	1.206730	-2.068408	0.392064
4	6	0	3.210816	-1.263944	1.508690
5	6	0	1.729081	-1.581066	1.766545
6	6	0	0.620563	0.667239	-1.883399
7	6	0	-0.317245	-2.030683	0.231427
8	6	0	1.693351	-3.516589	0.121721
9	6	0	-1.108594	-2.539502	1.420279
10	6	0	-0.883375	-2.092067	-1.065430
11	7	0	3.245092	-0.832741	0.086306
12	6	0	5.829882	-0.033226	-0.239680
13	6	0	5.755136	1.283474	-0.703609
14	6	0	6.702789	2.205277	-0.270182

15	6	0	7.726454	1.834915	0.618249
16	6	0	7.782035	0.504429	1.055442
17	6	0	6.842996	-0.435685	0.631707
18	16	0	4.641735	-1.233662	-0.816194
19	8	0	4.284286	-0.950715	-2.210640
20	8	0	5.121213	-2.566730	-0.421755
21	1	0	2.093569	-1.522006	-1.555617
22	1	0	1.395762	0.962131	0.079053
23	1	0	0.345334	1.710076	-2.024084
24	1	0	0.634916	0.052053	-2.780002
25	1	0	3.836831	-2.150301	1.654297
26	1	0	3.589275	-0.467172	2.156143
27	1	0	1.609063	-2.326492	2.558033
28	1	0	1.194183	-0.675310	2.077291
29	1	0	1.313560	-4.208378	0.881239
30	1	0	2.785948	-3.575948	0.130020
31	1	0	-0.752491	-3.542190	1.694057
32	1	0	-0.990452	-1.908224	2.305637
33	1	0	-2.175744	-2.618073	1.198639
34	1	0	-1.874542	-2.515922	-1.206076
35	1	0	-0.244233	-2.158852	-1.943861
36	1	0	4.981844	1.570707	-1.408463
37	1	0	6.657716	3.227995	-0.635777
38	1	0	8.578024	0.194332	1.727265
39	1	0	6.903200	-1.470183	0.951821
40	6	0	1.214189	0.241122	-0.717696
41	1	0	1.353096	-3.866956	-0.858131
42	6	0	8.733877	2.851188	1.098454
43	1	0	8.946548	3.599593	0.328284
44	1	0	8.357752	3.388027	1.979443
45	1	0	9.677736	2.376737	1.383749
46	15	0	-3.255632	0.193250	0.139905
47	6	0	-3.687131	0.508730	1.885531
48	6	0	-2.650806	0.601824	2.831451
49	6	0	-5.019434	0.655651	2.304680
50	6	0	-2.941890	0.863139	4.170131
51	1	0	-1.619309	0.463672	2.517221
52	6	0	-5.304159	0.909342	3.646417
53	1	0	-5.831587	0.568389	1.590413
54	6	0	-4.268988	1.016658	4.578179
55	1	0	-2.135941	0.936598	4.894414
56	1	0	-6.336577	1.021879	3.963761
57	1	0	-4.496601	1.212389	5.621857
58	6	0	-4.742412	-0.447938	-0.696554

59	6	0	-5.735125	0.407535	-1.206795
60	6	0	-4.908212	-1.838979	-0.804173
61	6	0	-6.870348	-0.126333	-1.817666
62	1	0	-5.623610	1.485065	-1.130305
63	6	0	-6.047890	-2.365862	-1.411593
64	1	0	-4.153255	-2.513322	-0.409925
65	6	0	-7.027399	-1.510606	-1.920895
66	1	0	-7.632137	0.540016	-2.211441
67	1	0	-6.168343	-3.442162	-1.489934
68	1	0	-7.912099	-1.921856	-2.397780
69	6	0	-2.763539	1.774296	-0.660681
70	6	0	-2.815089	1.894936	-2.071194
71	6	0	-2.133678	2.794935	0.089163
72	6	0	-2.289361	3.023089	-2.699542
73	1	0	-3.292354	1.120722	-2.663602
74	6	0	-1.602173	3.914604	-0.553757
75	1	0	-2.100609	2.728863	1.172327
76	6	0	-1.684527	4.032751	-1.943749
77	1	0	-2.354572	3.115070	-3.779609
78	1	0	-1.138541	4.701113	0.034207
79	1	0	-1.281901	4.912018	-2.437935



19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.789680	-0.325708	-0.495338
2	6	0	-1.299229	-1.422759	-1.478414
3	45	0	1.103090	0.451267	-0.566377
4	6	0	-3.525416	-1.990000	-0.707265
5	6	0	-2.138793	-2.617475	-0.960420
6	6	0	-1.296490	1.030326	-0.925612
7	6	0	0.245632	-1.533183	-1.357534
8	6	0	-1.728569	-1.155232	-2.942030

9	6	0	0.785660	-2.728069	-0.599291
10	6	0	1.090260	-0.859037	-2.265310
11	7	0	-3.260979	-0.532498	-0.462408
12	6	0	-5.722633	0.144799	0.468337
13	6	0	-6.129669	1.047309	-0.519248
14	6	0	-7.477084	1.110899	-0.859032
15	6	0	-8.427343	0.292471	-0.225334
16	6	0	-7.989840	-0.592348	0.770025
17	6	0	-6.643485	-0.673451	1.124144
18	16	0	-4.007879	0.092350	0.953872
19	8	0	-3.477399	1.452202	1.099875
20	8	0	-3.865636	-0.864901	2.062653
21	1	0	-1.353261	-0.548831	0.490691
22	1	0	-1.501659	1.330050	-1.949802
23	1	0	-0.632194	1.740561	0.975413
24	1	0	-4.013519	-2.450508	0.154718
25	1	0	-4.190924	-2.086471	-1.569766
26	1	0	-1.738862	-3.001274	-0.018060
27	1	0	-2.189445	-3.448960	-1.670401
28	1	0	-2.816025	-1.091971	-3.026085
29	1	0	-1.386645	-1.978144	-3.578827
30	1	0	0.452199	-2.757881	0.442391
31	1	0	0.434854	-3.655156	-1.073712
32	1	0	1.878109	-2.746354	-0.599064
33	1	0	2.096767	-1.232575	-2.430871
34	1	0	0.693220	-0.286782	-3.097032
35	1	0	-5.404641	1.693527	-1.002832
36	1	0	-7.801369	1.813406	-1.622409
37	1	0	-8.712611	-1.222326	1.281707
38	1	0	-6.308071	-1.347377	1.904994
39	6	0	-0.669191	1.909303	-0.100085
40	1	0	-1.324759	-0.230524	-3.358557
41	15	0	3.214779	0.021966	0.113850
42	6	0	-9.882653	0.355323	-0.620627
43	1	0	-10.535344	0.047975	0.202114
44	1	0	-10.171177	1.365600	-0.927857
45	1	0	-10.086083	-0.313296	-1.467527
46	6	0	2.948990	1.752879	0.640682
47	6	0	2.836602	2.746831	-0.365021
48	6	0	2.673782	2.099372	1.983530
49	6	0	2.482070	4.055126	-0.021208
50	1	0	3.073738	2.506570	-1.397102
51	6	0	2.319252	3.404362	2.309086
52	1	0	2.757118	1.349260	2.763314

53	6	0	2.224374	4.382410	1.309761
54	1	0	2.416599	4.814301	-0.794897
55	1	0	2.123589	3.665896	3.344656
56	1	0	1.953894	5.400208	1.575048
57	6	0	4.688343	-0.097404	-0.953086
58	6	0	4.872026	-1.265815	-1.715011
59	6	0	5.641041	0.931898	-1.030518
60	6	0	5.984962	-1.396060	-2.544135
61	1	0	4.157581	-2.082515	-1.653339
62	6	0	6.751454	0.795400	-1.865637
63	1	0	5.525891	1.833775	-0.438083
64	6	0	6.923455	-0.363904	-2.623823
65	1	0	6.118842	-2.302238	-3.127319
66	1	0	7.484199	1.595232	-1.917562
67	1	0	7.788606	-0.465888	-3.272136
68	6	0	3.518633	-1.028814	1.571591
69	6	0	4.811639	-1.464698	1.906443
70	6	0	2.430070	-1.397969	2.382533
71	6	0	5.008847	-2.251101	3.041570
72	1	0	5.659522	-1.192982	1.286059
73	6	0	2.635576	-2.180429	3.517962
74	1	0	1.426802	-1.072152	2.120186
75	6	0	3.924755	-2.608240	3.846747
76	1	0	6.010368	-2.584598	3.296405
77	1	0	1.791284	-2.460074	4.141117
78	1	0	4.083394	-3.222270	4.728390
79	1	0	-0.387600	2.897691	-0.450651

$[Rh(PPh_3)]^+$

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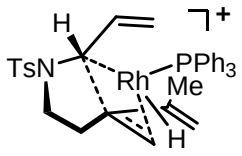
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.121877	0.095273	2.274339
2	15	0	0.013106	-0.006557	0.095312
3	6	0	-1.689063	-0.132646	-0.515940
4	6	0	-2.246330	0.809254	-1.398899
5	6	0	-2.490431	-1.180034	-0.012293
6	6	0	-3.583809	0.697915	-1.775318
7	1	0	-1.638939	1.617042	-1.793700

8	6	0	-3.827861	-1.278160	-0.390870
9	1	0	-2.063998	-1.924651	0.655922
10	6	0	-4.373984	-0.339581	-1.270956
11	1	0	-4.009692	1.420106	-2.465185
12	1	0	-4.440722	-2.086533	-0.004090
13	1	0	-5.415552	-0.419000	-1.567622
14	6	0	0.802863	1.516805	-0.488121
15	6	0	1.928496	1.501294	-1.329974
16	6	0	0.302137	2.746481	-0.009978
17	6	0	2.535929	2.701928	-1.694426
18	1	0	2.323664	0.560496	-1.699089
19	6	0	0.920502	3.940425	-0.375951
20	1	0	-0.576972	2.769109	0.630411
21	6	0	2.036264	3.917539	-1.217740
22	1	0	3.399733	2.689146	-2.352085
23	1	0	0.531883	4.885183	-0.008450
24	1	0	2.516058	4.848615	-1.504245
25	6	0	0.975858	-1.456877	-0.409392
26	6	0	0.514699	-2.360937	-1.382105
27	6	0	2.208320	-1.689715	0.235229
28	6	0	1.282512	-3.478654	-1.706474
29	1	0	-0.432818	-2.191632	-1.883194
30	6	0	2.965106	-2.812910	-0.092260
31	1	0	2.580608	-0.987983	0.978463
32	6	0	2.501904	-3.706621	-1.062173
33	1	0	0.928957	-4.171877	-2.463650
34	1	0	3.913648	-2.989343	0.405513
35	1	0	3.093326	-4.580654	-1.318069



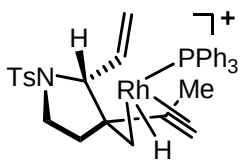
21-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.703670	0.431033	0.249962
2	6	0	-0.869470	2.033950	-0.984241

3	6	0	-1.799043	1.013301	0.741314
4	6	0	-3.413596	1.974977	-0.749952
5	6	0	-2.213492	2.199622	-1.696193
6	1	0	0.248933	-1.012079	0.002439
7	6	0	-0.206156	3.254213	-0.430092
8	6	0	-0.876178	1.680379	2.929831
9	6	0	-1.015183	4.517936	-0.233309
10	6	0	1.101824	3.256704	-0.090186
11	7	0	-3.063069	0.863469	0.132305
12	6	0	-5.196158	-0.820609	-0.170003
13	6	0	-5.663962	-0.927570	1.145140
14	6	0	-7.032966	-1.026626	1.361675
15	6	0	-7.943626	-1.027892	0.289343
16	6	0	-7.441675	-0.926827	-1.014731
17	6	0	-6.071467	-0.825543	-1.256962
18	16	0	-3.444503	-0.735317	-0.468051
19	8	0	-2.726910	-1.644319	0.429386
20	8	0	-3.210753	-0.773349	-1.917530
21	1	0	-1.380632	0.024551	0.966321
22	1	0	-2.268514	2.843601	1.871769
23	1	0	-0.312001	0.753063	3.013897
24	1	0	-4.334185	1.750812	-1.293395
25	1	0	-3.609486	2.853618	-0.127558
26	1	0	-2.287203	1.472785	-2.505934
27	1	0	-2.276890	3.196743	-2.143891
28	1	0	0.899242	1.426182	-2.131182
29	1	0	-0.457991	0.228789	-2.128485
30	1	0	-1.250748	4.979008	-1.201081
31	1	0	-1.969256	4.343804	0.273207
32	1	0	-0.454723	5.252512	0.350408
33	1	0	1.559562	4.125495	0.373005
34	1	0	1.790870	2.444941	-0.321832
35	1	0	-4.968292	-0.941939	1.977616
36	1	0	-7.405561	-1.110972	2.379178
37	1	0	-8.129838	-0.933744	-1.855372
38	1	0	-5.684155	-0.765347	-2.268208
39	6	0	0.043768	1.026736	-1.581549
40	6	0	-1.679771	1.930031	1.883563
41	6	0	-9.424869	-1.152073	0.547703
42	1	0	-9.666910	-2.136512	0.966950
43	1	0	-9.765542	-0.402129	1.270860
44	1	0	-10.005686	-1.027842	-0.370400
45	15	0	2.776448	-0.473668	0.000947
46	6	0	2.997561	-1.893539	-1.134463

47	6	0	4.290785	-2.216703	-1.586673
48	6	0	1.914764	-2.696280	-1.524542
49	6	0	4.490656	-3.325705	-2.407484
50	1	0	5.139931	-1.603577	-1.300959
51	6	0	2.121161	-3.804169	-2.348016
52	1	0	0.909782	-2.458623	-1.191605
53	6	0	3.406717	-4.120147	-2.789838
54	1	0	5.492588	-3.566382	-2.750526
55	1	0	1.274308	-4.415185	-2.645878
56	1	0	3.564290	-4.980749	-3.433445
57	6	0	4.040785	0.748480	-0.529940
58	6	0	5.036806	1.231831	0.331672
59	6	0	3.977780	1.234339	-1.849406
60	6	0	5.951154	2.186584	-0.119933
61	1	0	5.111322	0.859341	1.347739
62	6	0	4.894337	2.185194	-2.294379
63	1	0	3.228244	0.852625	-2.537730
64	6	0	5.880845	2.665908	-1.428453
65	1	0	6.723044	2.548717	0.552941
66	1	0	4.841785	2.546787	-3.317175
67	1	0	6.595307	3.406324	-1.776061
68	6	0	3.236801	-1.043312	1.684387
69	6	0	3.679076	-2.350420	1.936040
70	6	0	3.067471	-0.154346	2.763529
71	6	0	3.955543	-2.756042	3.243108
72	1	0	3.806902	-3.050728	1.117519
73	6	0	3.350841	-0.563972	4.066092
74	1	0	2.729288	0.864542	2.585757
75	6	0	3.793404	-1.867185	4.307227
76	1	0	4.298701	-3.769733	3.427870
77	1	0	3.225534	0.132167	4.890408
78	1	0	4.009927	-2.188198	5.321863
79	1	0	-0.785761	2.380653	3.754631



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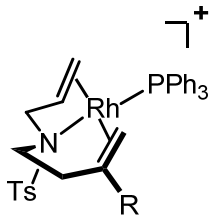
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.775774	1.505058	0.340489
2	6	0	0.940823	2.106265	0.719317
3	6	0	1.979227	1.746741	-0.395788
4	6	0	2.934465	1.275930	1.819679
5	6	0	1.881579	2.396592	1.915841
6	1	0	-1.306398	1.431330	-1.116805
7	6	0	-0.099448	3.216329	0.436279
8	6	0	2.932583	2.937925	-2.383322
9	6	0	-0.053329	4.090646	-0.793016
10	6	0	-1.058866	3.454945	1.393206
11	7	0	2.964933	0.937991	0.377133
12	6	0	5.018630	-0.809590	-0.035654
13	6	0	5.786933	0.008565	-0.871392
14	6	0	7.168816	-0.140481	-0.871663
15	6	0	7.799390	-1.096504	-0.055156
16	6	0	7.002264	-1.899773	0.769512
17	6	0	5.612830	-1.766784	0.785520
18	16	0	3.240395	-0.672368	-0.068052
19	8	0	2.760248	-0.784163	-1.455080
20	8	0	2.697656	-1.571298	0.962748
21	1	0	1.528854	1.121124	-1.167675
22	1	0	3.175254	3.626475	-0.414693
23	1	0	2.527533	2.188566	-3.060257
24	1	0	2.637814	0.399383	2.404460
25	1	0	3.920990	1.602130	2.163574
26	1	0	1.361200	2.386850	2.878098
27	1	0	2.342522	3.384355	1.802227
28	1	0	-0.120017	0.690670	2.064299
29	1	0	0.368619	-0.053042	0.512338
30	1	0	0.787889	4.789878	-0.718813
31	1	0	0.095440	3.521319	-1.712643
32	1	0	-0.972159	4.677595	-0.880903
33	1	0	-1.769606	4.268244	1.266970
34	1	0	-0.996358	3.030845	2.394377
35	1	0	5.309298	0.750921	-1.503219
36	1	0	7.772922	0.492958	-1.516323
37	1	0	7.471979	-2.642525	1.408627
38	1	0	4.996390	-2.392754	1.421233
39	6	0	0.050409	0.870250	0.993738
40	6	0	2.725482	2.877431	-1.066508
41	6	0	9.300290	-1.253787	-0.082862

42	1	0	9.633013	-1.667734	-1.043057
43	1	0	9.804292	-0.288686	0.042978
44	1	0	9.649090	-1.924676	0.707406
45	15	0	-2.796060	-0.520383	-0.133332
46	6	0	-1.800675	-1.972611	-0.594880
47	6	0	-2.202381	-3.264900	-0.210952
48	6	0	-0.637716	-1.808431	-1.364334
49	6	0	-1.447693	-4.371065	-0.599913
50	1	0	-3.095355	-3.406884	0.389951
51	6	0	0.118901	-2.918378	-1.739658
52	1	0	-0.310073	-0.818434	-1.664595
53	6	0	-0.287267	-4.198554	-1.359204
54	1	0	-1.762395	-5.366833	-0.301713
55	1	0	1.034853	-2.769474	-2.301141
56	1	0	0.305393	-5.062413	-1.645567
57	6	0	-3.642158	-0.916792	1.443958
58	6	0	-5.035258	-0.818545	1.591389
59	6	0	-2.852033	-1.264036	2.557830
60	6	0	-5.626424	-1.070317	2.830690
61	1	0	-5.658459	-0.559220	0.741842
62	6	0	-3.450702	-1.515975	3.791075
63	1	0	-1.774885	-1.366120	2.454767
64	6	0	-4.838104	-1.416067	3.929863
65	1	0	-6.705360	-1.001493	2.933680
66	1	0	-2.835455	-1.795145	4.641415
67	1	0	-5.302902	-1.612347	4.891552
68	6	0	-4.083897	-0.276890	-1.407872
69	6	0	-4.385512	-1.262847	-2.358139
70	6	0	-4.767779	0.951487	-1.445709
71	6	0	-5.362403	-1.022616	-3.326337
72	1	0	-3.857197	-2.210688	-2.347703
73	6	0	-5.744430	1.185665	-2.412412
74	1	0	-4.548652	1.727184	-0.712365
75	6	0	-6.041056	0.197027	-3.354763
76	1	0	-5.590304	-1.790021	-4.060102
77	1	0	-6.269177	2.136206	-2.432917
78	1	0	-6.798322	0.379860	-4.111390
79	1	0	3.523422	3.731241	-2.832539



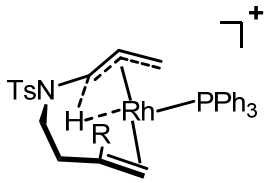
23

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.977382	1.529784	-1.540990
2	6	0	0.602424	2.060685	-1.162864
3	6	0	-0.465213	1.808689	-2.019502
4	6	0	2.469854	-0.980405	-1.827194
5	6	0	1.951198	-2.342491	-1.346832
6	6	0	0.446689	-2.464952	-1.094890
7	6	0	-0.438822	-1.868925	-1.972818
8	7	0	2.042076	0.144368	-0.941566
9	6	0	4.551290	0.343472	0.384615
10	6	0	5.327336	-0.810970	0.226146
11	6	0	6.694355	-0.677205	-0.001303
12	6	0	7.302982	0.586811	-0.063880
13	6	0	6.500911	1.725054	0.114961
14	6	0	5.131690	1.616938	0.343099
15	16	0	2.800189	0.198865	0.678453
16	8	0	2.510689	-1.096273	1.292774
17	8	0	2.309642	1.445684	1.263039
18	1	0	2.077637	1.417914	-2.624187
19	1	0	2.798480	2.160553	-1.194062
20	1	0	0.517934	2.740847	-0.321595
21	1	0	-1.415050	2.307371	-1.863996
22	1	0	-0.300569	1.425740	-3.024827
23	1	0	2.062595	-0.738908	-2.812548
24	1	0	3.562715	-1.006060	-1.930718
25	1	0	2.216649	-3.071870	-2.126538
26	1	0	2.503814	-2.641293	-0.460515
27	1	0	-1.483812	-2.151811	-1.970699
28	1	0	-0.089787	-1.410795	-2.895228
29	1	0	4.875683	-1.793734	0.309335
30	1	0	7.302148	-1.569847	-0.120904
31	1	0	6.957404	2.710651	0.087211

32	1	0	4.527837	2.500080	0.520916
33	45	0	-0.167242	0.049380	-0.673815
34	15	0	-2.321552	0.315726	0.074457
35	6	0	-2.464549	1.956421	0.910937
36	6	0	-1.951035	2.141889	2.205323
37	6	0	-3.002084	3.063118	0.230063
38	6	0	-1.980130	3.401511	2.803875
39	1	0	-1.538891	1.304480	2.757441
40	6	0	-3.028086	4.321746	0.833015
41	1	0	-3.426088	2.945164	-0.762380
42	6	0	-2.516385	4.494592	2.120123
43	1	0	-1.586987	3.525297	3.808752
44	1	0	-3.456188	5.164048	0.297049
45	1	0	-2.540749	5.473470	2.590013
46	6	0	-2.613387	-0.935510	1.390685
47	6	0	-3.848696	-1.574004	1.586009
48	6	0	-1.536780	-1.258071	2.237789
49	6	0	-4.007911	-2.495633	2.621982
50	1	0	-4.686503	-1.362475	0.931321
51	6	0	-1.704262	-2.174241	3.276536
52	1	0	-0.561543	-0.801422	2.086483
53	6	0	-2.940803	-2.791968	3.472433
54	1	0	-4.969176	-2.981283	2.763286
55	1	0	-0.865353	-2.408099	3.925288
56	1	0	-3.070938	-3.505965	4.280589
57	6	0	-3.756455	0.265464	-1.069862
58	6	0	-5.046558	0.623651	-0.634113
59	6	0	-3.574424	-0.120908	-2.406120
60	6	0	-6.127774	0.568674	-1.512841
61	1	0	-5.205135	0.959104	0.386553
62	6	0	-4.659150	-0.171782	-3.284477
63	1	0	-2.580358	-0.368385	-2.762271
64	6	0	-5.936580	0.167196	-2.837993
65	1	0	-7.118415	0.845901	-1.164388
66	1	0	-4.503608	-0.471651	-4.316828
67	1	0	-6.780417	0.127985	-3.520655
68	6	0	8.790367	0.717258	-0.276111
69	1	0	9.042540	1.650668	-0.788451
70	1	0	9.317487	0.720316	0.686876
71	1	0	9.187492	-0.116810	-0.862543
72	6	0	-0.012350	-3.486135	-0.116794
73	6	0	0.768242	-3.937765	0.882402
74	1	0	1.751594	-3.541766	1.104474
75	1	0	0.409175	-4.718351	1.546342

76	6	0	-1.397006	-4.068395	-0.305788
77	1	0	-1.515057	-4.502036	-1.306686
78	1	0	-1.586394	-4.853335	0.430460
79	1	0	-2.178872	-3.310931	-0.182035



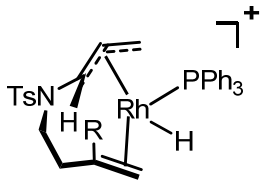
24-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.355494	-0.069923	-0.069787
2	1	0	0.843592	0.420286	-1.016448
3	6	0	1.903379	0.785173	0.108380
4	6	0	2.860669	-1.483678	0.297725
5	6	0	1.897891	-2.280089	-0.630871
6	6	0	0.384567	-2.223592	-0.439689
7	6	0	-0.227139	-3.037813	0.653211
8	6	0	-0.043086	1.648220	1.333333
9	6	0	-1.659944	-3.507179	0.500923
10	6	0	0.485250	-3.450520	1.720848
11	7	0	2.983736	-0.062991	-0.046582
12	6	0	5.684890	0.375666	-0.435744
13	6	0	6.001402	1.479017	0.365004
14	6	0	7.225976	1.498204	1.022603
15	6	0	8.143098	0.440599	0.888893
16	6	0	7.797308	-0.646365	0.073709
17	6	0	6.575028	-0.688927	-0.595640
18	16	0	4.138102	0.350379	-1.311073
19	8	0	3.762637	1.707412	-1.709420
20	8	0	4.149449	-0.762268	-2.260899
21	1	0	2.025595	1.728652	-0.423011
22	1	0	1.305791	0.135276	2.123896
23	1	0	-0.649087	1.671032	2.232586
24	1	0	-0.103232	2.525626	0.693697
25	1	0	3.858410	-1.921162	0.219140
26	1	0	2.575792	-1.549033	1.349679

27	1	0	2.141080	-1.995257	-1.657024
28	1	0	2.185804	-3.333496	-0.529323
29	1	0	-1.440574	-2.098289	-1.603082
30	1	0	0.063806	-1.471676	-2.434517
31	1	0	-2.370371	-2.687951	0.363111
32	1	0	-1.757890	-4.164162	-0.372172
33	1	0	-1.972312	-4.073790	1.381958
34	1	0	0.030289	-4.074813	2.484007
35	1	0	1.532767	-3.218580	1.871559
36	1	0	5.311522	2.311619	0.455415
37	1	0	7.482006	2.352398	1.643586
38	1	0	8.497366	-1.468043	-0.048917
39	1	0	6.322411	-1.518660	-1.246820
40	6	0	-0.413969	-1.771244	-1.505226
41	6	0	1.077413	0.802710	1.297341
42	6	0	9.481752	0.496227	1.581804
43	1	0	10.182306	1.125307	1.017518
44	1	0	9.395839	0.927453	2.584627
45	1	0	9.930631	-0.497161	1.671466
46	15	0	-2.823511	0.282650	0.010279
47	6	0	-3.165354	2.029801	-0.497335
48	6	0	-3.578402	2.362717	-1.796173
49	6	0	-2.956881	3.065901	0.431371
50	6	0	-3.770024	3.698033	-2.158054
51	1	0	-3.773324	1.588356	-2.528634
52	6	0	-3.154413	4.396984	0.067246
53	1	0	-2.665150	2.835094	1.450582
54	6	0	-3.555960	4.718278	-1.231695
55	1	0	-4.095724	3.935499	-3.166661
56	1	0	-3.000722	5.182524	0.801738
57	1	0	-3.708786	5.755382	-1.515330
58	6	0	-3.895375	-0.755257	-1.074876
59	6	0	-5.036369	-1.413228	-0.588982
60	6	0	-3.547646	-0.915395	-2.429656
61	6	0	-5.816134	-2.198225	-1.441443
62	1	0	-5.322752	-1.316976	0.452315
63	6	0	-4.336714	-1.689806	-3.280291
64	1	0	-2.657540	-0.433490	-2.825167
65	6	0	-5.472913	-2.335183	-2.786645
66	1	0	-6.695799	-2.700520	-1.049334
67	1	0	-4.059004	-1.794201	-4.325179
68	1	0	-6.083567	-2.944202	-3.446670
69	6	0	-3.548583	0.150470	1.694314
70	6	0	-4.763797	0.776784	2.023682

71	6	0	-2.883963	-0.606444	2.671647
72	6	0	-5.298465	0.643640	3.305063
73	1	0	-5.287353	1.373575	1.282888
74	6	0	-3.423373	-0.739358	3.952819
75	1	0	-1.942260	-1.093577	2.431153
76	6	0	-4.629824	-0.113822	4.270710
77	1	0	-6.236458	1.133470	3.549909
78	1	0	-2.899639	-1.327098	4.701327
79	1	0	-5.047752	-0.212691	5.268347



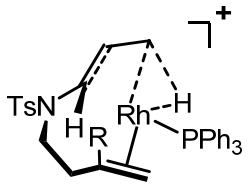
25

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.555093	0.365848	-0.282125
2	1	0	-0.305477	-0.994456	0.371392
3	6	0	-0.570652	1.719155	1.674690
4	6	0	2.959599	1.623819	0.346682
5	6	0	1.913948	1.993256	1.436302
6	6	0	0.494298	2.283918	0.995445
7	6	0	-0.025197	-0.428853	-2.191556
8	7	0	2.921979	0.203389	-0.014302
9	6	0	5.521650	-0.722450	0.293519
10	6	0	5.847832	-1.406048	-0.883846
11	6	0	7.128456	-1.263416	-1.405205
12	6	0	8.090260	-0.457984	-0.769764
13	6	0	7.732821	0.205859	0.412510
14	6	0	6.455080	0.079825	0.955249
15	16	0	3.895035	-0.905749	0.981999
16	8	0	3.363784	-2.231841	0.675787
17	8	0	3.873250	-0.341483	2.328929
18	1	0	1.863974	-1.414257	-0.673310
19	1	0	1.331954	1.314514	-2.050859
20	1	0	-0.599196	-0.004083	-3.012618
21	1	0	0.002927	-1.515846	-2.196599

22	1	0	3.962666	1.840025	0.718768
23	1	0	2.820058	2.215272	-0.561102
24	1	0	1.921040	1.213113	2.200516
25	1	0	2.294500	2.898574	1.927530
26	1	0	-1.563944	2.152120	1.624581
27	1	0	-0.382938	1.070410	2.523705
28	1	0	5.120942	-2.048943	-1.369122
29	1	0	7.392308	-1.792336	-2.317013
30	1	0	8.466605	0.823715	0.922348
31	1	0	6.192137	0.573367	1.884589
32	6	0	1.950174	-0.336500	-0.780325
33	6	0	1.128031	0.298440	-1.724260
34	6	0	9.483292	-0.340680	-1.335787
35	1	0	10.075902	-1.231417	-1.090455
36	1	0	9.464749	-0.255695	-2.427400
37	1	0	10.010793	0.528063	-0.931891
38	15	0	-2.769257	-0.359631	-0.034461
39	6	0	-3.233523	-1.834146	-1.038654
40	6	0	-4.486179	-1.952566	-1.661913
41	6	0	-2.340139	-2.915704	-1.097128
42	6	0	-4.827517	-3.124050	-2.340372
43	1	0	-5.198142	-1.134467	-1.625209
44	6	0	-2.688821	-4.088519	-1.766510
45	1	0	-1.371990	-2.844909	-0.609889
46	6	0	-3.931764	-4.192982	-2.394573
47	1	0	-5.797718	-3.200238	-2.822947
48	1	0	-1.988912	-4.918588	-1.798971
49	1	0	-4.201241	-5.103572	-2.921634
50	6	0	-3.354653	-0.817862	1.649590
51	6	0	-4.726972	-0.974464	1.915545
52	6	0	-2.428027	-1.115082	2.658597
53	6	0	-5.156488	-1.395798	3.172668
54	1	0	-5.462060	-0.769891	1.142899
55	6	0	-2.861061	-1.545198	3.914875
56	1	0	-1.366093	-1.020747	2.457372
57	6	0	-4.224672	-1.680507	4.175000
58	1	0	-6.219006	-1.508395	3.367962
59	1	0	-2.131821	-1.774553	4.686479
60	1	0	-4.562515	-2.012119	5.152532
61	6	0	-3.850333	1.009340	-0.611270
62	6	0	-3.948738	1.273176	-1.990149
63	6	0	-4.468692	1.887996	0.293827
64	6	0	-4.667287	2.376490	-2.450171
65	1	0	-3.477555	0.607119	-2.707861

66	6	0	-5.184576	2.993374	-0.172082
67	1	0	-4.407196	1.704272	1.361785
68	6	0	-5.286845	3.239520	-1.542264
69	1	0	-4.746946	2.559202	-3.518025
70	1	0	-5.667474	3.657464	0.539114
71	1	0	-5.848402	4.096807	-1.901760
72	6	0	0.276437	3.379448	0.006000
73	6	0	1.203175	4.324270	-0.235515
74	1	0	2.154932	4.373735	0.282527
75	1	0	1.009021	5.125187	-0.942787
76	6	0	-1.045653	3.420708	-0.728810
77	1	0	-1.258897	2.480315	-1.266746
78	1	0	-1.894364	3.587578	-0.056994
79	1	0	-1.048877	4.215075	-1.480006



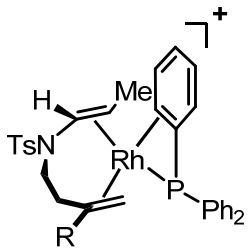
26-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.806810	1.082898	-0.834210
2	1	0	-1.581687	0.527108	-2.122017
3	6	0	-0.062619	0.953381	-2.963246
4	6	0	1.516961	2.369677	1.299628
5	6	0	0.171617	2.760042	0.711972
6	6	0	2.652310	1.940913	0.341472
7	7	0	2.418500	0.620413	-0.248858
8	6	0	4.765516	-0.780674	0.217161
9	6	0	5.177131	-1.285744	-1.022008
10	6	0	6.533850	-1.287993	-1.324199
11	6	0	7.486431	-0.803023	-0.410394
12	6	0	7.040246	-0.311423	0.824930
13	6	0	5.685337	-0.297399	1.151812
14	16	0	3.037749	-0.788641	0.626315
15	8	0	2.373896	-1.928698	-0.004392

16	8	0	2.874300	-0.482447	2.045941
17	1	0	1.319649	-0.634629	-1.440469
18	1	0	1.281087	2.440306	-2.068052
19	1	0	-0.508441	1.659270	-3.658077
20	1	0	-0.046216	-0.076795	-3.310250
21	1	0	3.591893	1.893489	0.895798
22	1	0	2.797192	2.653510	-0.473871
23	1	0	1.380117	1.566502	2.027180
24	1	0	1.894226	3.232633	1.863233
25	1	0	-1.941956	2.562896	1.128926
26	1	0	-0.845623	1.364846	1.976858
27	1	0	4.452956	-1.684530	-1.724715
28	1	0	6.863610	-1.680833	-2.282107
29	1	0	7.763172	0.058177	1.546695
30	1	0	5.347928	0.059369	2.118983
31	6	0	1.489847	0.412630	-1.212512
32	6	0	0.958147	1.405278	-2.082867
33	6	0	8.956601	-0.843846	-0.744127
34	1	0	9.359386	-1.852761	-0.587004
35	1	0	9.136025	-0.583699	-1.792457
36	1	0	9.531582	-0.157835	-0.115708
37	15	0	-2.413433	-0.465859	-0.001198
38	6	0	-2.397770	-2.066411	-0.929422
39	6	0	-2.225806	-3.304389	-0.292818
40	6	0	-2.615641	-2.044781	-2.317975
41	6	0	-2.256855	-4.490142	-1.032706
42	1	0	-2.068866	-3.353455	0.778604
43	6	0	-2.657260	-3.228720	-3.051108
44	1	0	-2.773818	-1.099203	-2.831090
45	6	0	-2.470447	-4.456803	-2.409762
46	1	0	-2.116854	-5.439883	-0.524477
47	1	0	-2.836211	-3.193389	-4.122066
48	1	0	-2.495306	-5.379835	-2.981665
49	6	0	-2.090667	-0.933737	1.749447
50	6	0	-3.029998	-0.724798	2.769156
51	6	0	-0.819508	-1.437731	2.082740
52	6	0	-2.706133	-1.024162	4.095920
53	1	0	-4.013640	-0.331195	2.536485
54	6	0	-0.502160	-1.736191	3.406747
55	1	0	-0.076982	-1.605646	1.307730
56	6	0	-1.446078	-1.528409	4.417391
57	1	0	-3.443734	-0.859991	4.876303
58	1	0	0.484925	-2.120692	3.645701
59	1	0	-1.197645	-1.757034	5.449772

60	6	0	-4.176561	0.048089	-0.075241
61	6	0	-5.213029	-0.877274	0.138946
62	6	0	-4.500249	1.381685	-0.362156
63	6	0	-6.544036	-0.466535	0.079960
64	1	0	-4.980063	-1.918294	0.343581
65	6	0	-5.834166	1.790782	-0.421475
66	1	0	-3.705222	2.097667	-0.552470
67	6	0	-6.856271	0.867523	-0.198238
68	1	0	-7.338266	-1.188817	0.245189
69	1	0	-6.072948	2.826196	-0.647028
70	1	0	-7.894483	1.182990	-0.247163
71	6	0	-0.959146	2.107665	1.196404
72	6	0	0.058051	4.032345	-0.054237
73	6	0	1.104869	4.863336	-0.223751
74	1	0	2.090419	4.680697	0.189769
75	1	0	0.987154	5.801381	-0.757736
76	6	0	-1.297652	4.422658	-0.606049
77	1	0	-2.013556	4.624422	0.200656
78	1	0	-1.222043	5.327271	-1.214860
79	1	0	-1.728027	3.626869	-1.228518



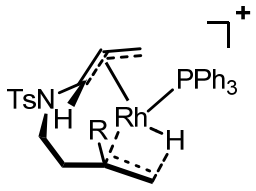
27

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.613151	-0.687871	-0.792859
2	6	0	0.264242	-3.626154	-0.992837
3	6	0	1.631888	1.215052	-2.243266
4	6	0	0.115653	1.019846	-2.165356
5	6	0	2.610514	0.060892	-1.968023
6	7	0	2.497525	-0.551413	-0.639250
7	6	0	4.881119	0.220519	0.465066
8	6	0	5.536266	-0.999187	0.672502

9	6	0	6.912154	-1.060063	0.486708
10	6	0	7.648124	0.076011	0.103792
11	6	0	6.963071	1.283058	-0.088430
12	6	0	5.582351	1.368414	0.091860
13	16	0	3.122981	0.319046	0.726572
14	8	0	2.737016	-0.479198	1.892892
15	8	0	2.713772	1.723878	0.617621
16	1	0	1.486004	-1.811648	0.652733
17	1	0	1.131809	-2.169640	-2.392373
18	1	0	0.972014	-4.435044	-1.224368
19	1	0	0.013893	-3.697329	0.069531
20	1	0	3.627992	0.451098	-2.070328
21	1	0	2.524593	-0.746588	-2.699430
22	1	0	1.924062	2.037136	-1.596010
23	1	0	1.838024	1.557678	-3.269356
24	1	0	-1.528357	0.032973	-3.184350
25	1	0	0.091168	-0.756390	-3.409294
26	1	0	4.980350	-1.877794	0.983260
27	1	0	7.428941	-2.002682	0.646275
28	1	0	7.515979	2.172426	-0.377582
29	1	0	5.057820	2.308411	-0.040076
30	6	0	1.542908	-1.526813	-0.392890
31	6	0	0.878194	-2.289192	-1.344214
32	6	0	9.144167	-0.006991	-0.071769
33	1	0	9.645265	-0.096651	0.900363
34	1	0	9.427646	-0.885065	-0.662465
35	1	0	9.541281	0.882321	-0.569109
36	15	0	-2.581782	0.134854	0.184960
37	6	0	-1.975912	-1.173166	1.347734
38	6	0	-0.865401	-0.920194	2.186153
39	6	0	-2.509245	-2.483745	1.313015
40	6	0	-0.328238	-1.936834	2.982636
41	1	0	-0.441493	0.073990	2.257516
42	6	0	-1.979698	-3.483184	2.124177
43	1	0	-3.353523	-2.707388	0.670172
44	6	0	-0.889906	-3.212799	2.961430
45	1	0	0.523838	-1.717066	3.618169
46	1	0	-2.418515	-4.476658	2.105945
47	1	0	-0.483868	-3.996941	3.593907
48	6	0	-2.802889	1.709475	1.100911
49	6	0	-4.067949	2.287177	1.300549
50	6	0	-1.664765	2.378708	1.589081
51	6	0	-4.192350	3.483979	2.007326
52	1	0	-4.958746	1.811899	0.906770

53	6	0	-1.797748	3.565125	2.309585
54	1	0	-0.671137	1.989568	1.394619
55	6	0	-3.061593	4.118918	2.523155
56	1	0	-5.177329	3.917022	2.155470
57	1	0	-0.910677	4.061769	2.691802
58	1	0	-3.163259	5.046437	3.079009
59	6	0	-4.237316	-0.424837	-0.357836
60	6	0	-5.260419	-0.709444	0.566725
61	6	0	-4.485933	-0.603733	-1.727302
62	6	0	-6.506390	-1.149826	0.122416
63	1	0	-5.081746	-0.593006	1.631896
64	6	0	-5.736565	-1.041582	-2.168372
65	1	0	-3.700655	-0.410126	-2.451067
66	6	0	-6.746859	-1.312754	-1.245218
67	1	0	-7.288736	-1.367635	0.843590
68	1	0	-5.917784	-1.173231	-3.231010
69	1	0	-7.718913	-1.655149	-1.587863
70	6	0	-0.510793	-0.069500	-2.819823
71	1	0	-0.643489	-3.816818	-1.575254
72	6	0	-0.643838	2.285755	-1.921797
73	6	0	-0.168369	3.267672	-1.133044
74	1	0	0.754492	3.189306	-0.568606
75	1	0	-0.728841	4.188388	-1.003330
76	6	0	-1.962348	2.485757	-2.638084
77	1	0	-2.723562	1.764219	-2.316953
78	1	0	-2.358819	3.484246	-2.438144
79	1	0	-1.850610	2.374909	-3.723661



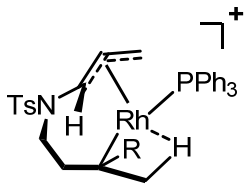
28-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.821990	1.299349	0.077949
2	1	0	1.446171	1.320371	-1.427131
3	6	0	0.524510	2.710792	-1.771689

4	6	0	-2.743412	2.006828	-0.059083
5	6	0	-1.891027	2.701611	-1.143961
6	6	0	-0.452413	3.109891	-0.831713
7	6	0	0.771852	1.162049	2.307382
8	7	0	-2.278287	0.661325	0.306801
9	6	0	-4.575128	-0.784569	-0.199728
10	6	0	-4.925803	-1.327012	1.042354
11	6	0	-6.271945	-1.410894	1.378310
12	6	0	-7.274012	-0.972176	0.494371
13	6	0	-6.888489	-0.441444	-0.744862
14	6	0	-5.544974	-0.345260	-1.104531
15	16	0	-2.860389	-0.697294	-0.656820
16	8	0	-2.135470	-1.852606	-0.128909
17	8	0	-2.754796	-0.292420	-2.058572
18	1	0	-0.865659	-0.570165	1.162340
19	1	0	-0.901248	2.480597	1.890020
20	1	0	1.340392	1.934204	2.819059
21	1	0	1.030759	0.140304	2.560397
22	1	0	-3.766627	1.905409	-0.429233
23	1	0	-2.803275	2.592598	0.861081
24	1	0	-1.895478	2.049671	-2.020774
25	1	0	-2.440627	3.608069	-1.431763
26	1	0	1.439369	3.284118	-1.886917
27	1	0	0.194888	2.212635	-2.679234
28	1	0	-4.161964	-1.686708	1.723920
29	1	0	-6.554198	-1.830490	2.340101
30	1	0	-7.649328	-0.104193	-1.443153
31	1	0	-5.251883	0.045875	-2.072807
32	6	0	-1.130214	0.470587	1.012866
33	6	0	-0.499227	1.477618	1.803346
34	6	0	-8.730385	-1.100137	0.864852
35	1	0	-9.078383	-2.129720	0.710966
36	1	0	-8.897514	-0.856541	1.919204
37	1	0	-9.359942	-0.444942	0.256132
38	15	0	2.301035	-0.571743	-0.025227
39	6	0	2.258210	-1.722897	1.414937
40	6	0	3.257519	-1.726333	2.399066
41	6	0	1.145884	-2.573364	1.563972
42	6	0	3.151168	-2.570149	3.508212
43	1	0	4.125723	-1.082834	2.298385
44	6	0	1.045987	-3.412190	2.674111
45	1	0	0.368602	-2.601278	0.803975
46	6	0	2.047519	-3.412046	3.649053
47	1	0	3.937471	-2.571080	4.257713

48	1	0	0.188752	-4.072271	2.772015
49	1	0	1.969196	-4.068625	4.510696
50	6	0	2.027415	-1.712241	-1.442197
51	6	0	2.637781	-2.981205	-1.452048
52	6	0	1.205998	-1.348848	-2.518890
53	6	0	2.449387	-3.847436	-2.527706
54	1	0	3.253214	-3.297278	-0.615206
55	6	0	1.013593	-2.221678	-3.591844
56	1	0	0.695899	-0.392039	-2.512487
57	6	0	1.638302	-3.468444	-3.600808
58	1	0	2.930163	-4.821406	-2.523871
59	1	0	0.366228	-1.928270	-4.412956
60	1	0	1.486474	-4.148206	-4.434243
61	6	0	4.043127	0.017311	-0.133053
62	6	0	4.402485	1.149698	0.618491
63	6	0	5.012930	-0.601710	-0.935483
64	6	0	5.707681	1.640799	0.583745
65	1	0	3.654976	1.647332	1.231890
66	6	0	6.315560	-0.100242	-0.977248
67	1	0	4.755962	-1.466553	-1.537361
68	6	0	6.666832	1.016262	-0.216942
69	1	0	5.972932	2.513108	1.174441
70	1	0	7.055564	-0.584759	-1.607710
71	1	0	7.681511	1.402053	-0.252103
72	6	0	-0.195721	4.279389	0.053894
73	6	0	-1.194795	4.959704	0.648937
74	1	0	-2.244443	4.725062	0.511104
75	1	0	-0.983636	5.823863	1.271304
76	6	0	1.236060	4.739222	0.245216
77	1	0	1.641728	5.177582	-0.675530
78	1	0	1.293872	5.504585	1.023255
79	1	0	1.902135	3.914100	0.528596



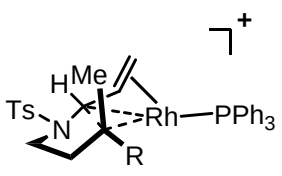
29

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	45	0	0.644668	1.029537	0.288961
2	6	0	0.658175	2.566895	-1.538799
3	6	0	-2.850754	2.001061	-0.026535
4	6	0	-1.798959	2.640772	-0.958945
5	6	0	-0.362042	2.808331	-0.459231
6	6	0	0.398355	0.318426	2.276073
7	7	0	-2.614772	0.563464	0.158273
8	6	0	-5.030929	-0.694781	-0.332520
9	6	0	-5.259502	-1.540468	0.759375
10	6	0	-6.553800	-1.659929	1.251855
11	6	0	-7.624071	-0.957433	0.670141
12	6	0	-7.361248	-0.124882	-0.427184
13	6	0	-6.071958	0.012621	-0.939162
14	16	0	-3.385119	-0.542851	-0.982465
15	8	0	-2.659683	-1.802431	-0.817751
16	8	0	-3.432327	0.165996	-2.259814
17	1	0	-1.324756	-0.936461	0.732472
18	1	0	-1.170758	1.850508	2.154123
19	1	0	0.988102	0.856602	3.013816
20	1	0	0.516128	-0.760512	2.310490
21	1	0	-3.842086	2.121095	-0.467725
22	1	0	-2.881408	2.469361	0.959933
23	1	0	-1.800981	2.047097	-1.877101
24	1	0	-2.183226	3.630961	-1.239923
25	1	0	1.526472	3.225261	-1.525303
26	1	0	0.218084	2.539328	-2.539853
27	1	0	-4.444818	-2.104317	1.201605
28	1	0	-6.741750	-2.315673	2.097688
29	1	0	-8.177708	0.418183	-0.894822
30	1	0	-5.878161	0.638244	-1.803740
31	6	0	-1.525309	0.124261	0.839049
32	6	0	-0.828877	0.876618	1.821417
33	6	0	-9.026376	-1.125198	1.199436
34	1	0	-9.472482	-2.054610	0.822442
35	1	0	-9.036724	-1.182048	2.292855
36	1	0	-9.674831	-0.300079	0.891454
37	15	0	2.533954	-0.557372	0.029862
38	6	0	3.374805	-1.205419	1.538642
39	6	0	4.554420	-0.631817	2.036261
40	6	0	2.778047	-2.260126	2.253139
41	6	0	5.122196	-1.101959	3.222391
42	1	0	5.045699	0.169570	1.494309

43	6	0	3.350179	-2.727379	3.436454
44	1	0	1.881748	-2.741673	1.871171
45	6	0	4.522338	-2.147047	3.926198
46	1	0	6.041280	-0.654054	3.589410
47	1	0	2.883098	-3.549790	3.970844
48	1	0	4.968935	-2.512615	4.846208
49	6	0	2.074642	-2.069447	-0.905741
50	6	0	2.921486	-3.192046	-0.955608
51	6	0	0.852432	-2.105820	-1.593313
52	6	0	2.551221	-4.317878	-1.690271
53	1	0	3.863625	-3.189703	-0.415640
54	6	0	0.481381	-3.237221	-2.322520
55	1	0	0.181662	-1.253153	-1.547988
56	6	0	1.331732	-4.342175	-2.373901
57	1	0	3.212676	-5.178837	-1.724528
58	1	0	-0.475601	-3.253604	-2.835037
59	1	0	1.044118	-5.224501	-2.938420
60	6	0	3.858534	0.274683	-0.949310
61	6	0	4.227369	1.585415	-0.594970
62	6	0	4.488947	-0.333267	-2.044977
63	6	0	5.219347	2.262431	-1.304763
64	1	0	3.743150	2.078077	0.245229
65	6	0	5.472380	0.352431	-2.761697
66	1	0	4.213327	-1.338201	-2.345327
67	6	0	5.842561	1.646335	-2.392752
68	1	0	5.501542	3.269843	-1.011878
69	1	0	5.950078	-0.129697	-3.609766
70	1	0	6.609560	2.174430	-2.951676
71	1	0	1.123002	1.500359	-1.496597
72	6	0	-0.099133	3.910195	0.515886
73	6	0	-1.084909	4.662839	1.043021
74	1	0	-0.861095	5.446002	1.761050
75	1	0	-2.128212	4.566929	0.764983
76	6	0	1.335025	4.188511	0.928362
77	1	0	1.923414	4.603097	0.100225
78	1	0	1.367106	4.914477	1.745088
79	1	0	1.847584	3.279175	1.267766

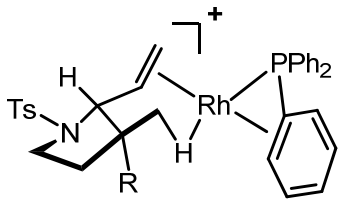


30-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.750617	-0.825520	-0.669997
2	6	0	0.859650	-3.007851	-1.017149
3	6	0	1.776679	-1.071536	-1.254986
4	6	0	2.220874	-3.566736	-1.459891
5	6	0	-0.200635	-3.341282	-2.067052
6	6	0	0.086997	0.545181	-2.029163
7	7	0	2.935454	-1.421181	-0.556042
8	6	0	4.560580	0.579711	0.429876
9	6	0	5.834699	0.251743	-0.047903
10	6	0	6.690546	1.274421	-0.440381
11	6	0	6.302687	2.623360	-0.356907
12	6	0	5.026897	2.919932	0.139388
13	6	0	4.150995	1.908838	0.536455
14	16	0	3.461105	-0.733041	0.934582
15	8	0	4.251058	-1.778468	1.581072
16	8	0	2.294250	-0.131854	1.588077
17	1	0	1.878657	-1.295053	-2.317276
18	1	0	1.339606	0.852409	-0.251904
19	1	0	-0.305778	1.555252	-2.019923
20	1	0	0.115176	0.082731	-3.016909
21	1	0	4.148929	-2.602079	-1.812347
22	1	0	3.982022	-3.189487	-0.155069
23	1	0	2.233943	-3.617605	-2.552648
24	1	0	2.311925	-4.597832	-1.101383
25	1	0	-0.339581	-4.431863	-2.116533
26	1	0	0.117484	-3.008881	-3.060638
27	1	0	6.156096	-0.783705	-0.092864
28	1	0	7.681860	1.024982	-0.809711
29	1	0	4.714482	3.956980	0.226195
30	1	0	3.176178	2.149257	0.946234
31	6	0	3.443515	-2.731991	-0.982948
32	6	0	1.035685	0.170293	-1.034988
33	6	0	7.253425	3.718666	-0.773075
34	1	0	8.112004	3.771174	-0.092164
35	1	0	7.651110	3.538341	-1.778341
36	1	0	6.765851	4.697582	-0.770933
37	15	0	-2.393443	0.598806	0.010565
38	6	0	-2.168547	1.140336	1.746986

39	6	0	-3.260195	1.605814	2.504306
40	6	0	-0.895668	1.081920	2.336265
41	6	0	-3.072053	2.019812	3.822008
42	1	0	-4.254926	1.638061	2.069084
43	6	0	-0.715725	1.494788	3.658615
44	1	0	-0.048431	0.695765	1.778752
45	6	0	-1.799650	1.966126	4.399842
46	1	0	-3.919243	2.378024	4.399635
47	1	0	0.272465	1.437478	4.105273
48	1	0	-1.658220	2.284312	5.428751
49	6	0	-2.767128	2.095152	-0.987067
50	6	0	-2.949437	3.353169	-0.393250
51	6	0	-2.877793	1.977554	-2.385117
52	6	0	-3.254754	4.465436	-1.181259
53	1	0	-2.854715	3.471284	0.680404
54	6	0	-3.193127	3.088540	-3.165831
55	1	0	-2.707315	1.017057	-2.864534
56	6	0	-3.383156	4.335639	-2.564116
57	1	0	-3.392649	5.433639	-0.708882
58	1	0	-3.282113	2.982399	-4.243127
59	1	0	-3.623059	5.202285	-3.173090
60	6	0	-3.935848	-0.413407	0.029919
61	6	0	-4.114778	-1.350524	1.065731
62	6	0	-4.900771	-0.334101	-0.987808
63	6	0	-5.230315	-2.186623	1.079080
64	1	0	-3.396729	-1.410752	1.878281
65	6	0	-6.015136	-1.173871	-0.969290
66	1	0	-4.800107	0.393399	-1.785506
67	6	0	-6.181216	-2.103356	0.058962
68	1	0	-5.360567	-2.896432	1.890912
69	1	0	-6.758511	-1.093647	-1.757102
70	1	0	-7.051248	-2.753254	0.070989
71	1	0	-1.194599	-2.912383	-1.882213
72	6	0	0.509743	-3.282774	0.410732
73	6	0	1.403543	-3.732005	1.311197
74	1	0	1.111026	-3.906129	2.342452
75	1	0	2.439277	-3.942804	1.083776
76	6	0	-0.908472	-3.019539	0.882630
77	1	0	-1.678906	-3.466299	0.247437
78	1	0	-1.053964	-3.404205	1.896717
79	1	0	-1.128995	-1.929200	1.012491



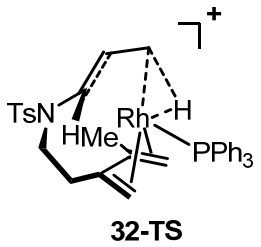
31

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.962917	-0.182090	0.994016
2	6	0	-1.608100	-2.473823	1.065780
3	6	0	-1.901144	-1.091873	0.370473
4	6	0	-3.052594	-3.029809	1.234143
5	6	0	-0.986135	-2.209453	2.449321
6	6	0	-0.465027	0.957617	-0.100733
7	7	0	-2.994138	-1.448752	-0.554998
8	6	0	-4.782989	0.711475	-0.678344
9	6	0	-6.116436	0.344310	-0.462622
10	6	0	-6.935186	1.172996	0.300532
11	6	0	-6.450997	2.371185	0.849015
12	6	0	-5.115699	2.722391	0.605230
13	6	0	-4.279719	1.904803	-0.154622
14	16	0	-3.717968	-0.366648	-1.636945
15	8	0	-4.575083	-1.204002	-2.474235
16	8	0	-2.636761	0.447820	-2.199120
17	1	0	-2.271227	-0.412331	1.159351
18	1	0	-0.427055	-0.873921	-1.257755
19	1	0	-0.003111	1.562894	-0.873507
20	1	0	-1.072936	1.517326	0.610633
21	1	0	-4.801588	-1.960858	0.475541
22	1	0	-4.200751	-3.176409	-0.659364
23	1	0	-3.460761	-2.700808	2.195566
24	1	0	-3.059997	-4.121677	1.230766
25	1	0	-0.816431	-3.136223	3.006956
26	1	0	-1.638642	-1.569575	3.051497
27	1	0	-6.508428	-0.559927	-0.915645
28	1	0	-7.972751	0.891577	0.462039
29	1	0	-4.729370	3.657335	1.003094
30	1	0	-3.261260	2.206175	-0.374543
31	6	0	-3.894163	-2.438762	0.084573
32	6	0	-0.737464	-0.405699	-0.328702

33	6	0	-7.360411	3.269142	1.652441
34	1	0	-8.116363	3.736690	1.009176
35	1	0	-7.898650	2.705091	2.422598
36	1	0	-6.802390	4.070610	2.145285
37	15	0	2.709946	0.532977	-0.154191
38	6	0	3.490070	-0.616080	-1.327570
39	6	0	4.823424	-1.027578	-1.163872
40	6	0	2.744017	-1.080294	-2.424944
41	6	0	5.399794	-1.896367	-2.091523
42	1	0	5.409780	-0.671544	-0.322199
43	6	0	3.330110	-1.943673	-3.349135
44	1	0	1.711711	-0.769886	-2.560703
45	6	0	4.655721	-2.354004	-3.181207
46	1	0	6.430570	-2.212764	-1.962674
47	1	0	2.751076	-2.298437	-4.196352
48	1	0	5.108336	-3.030208	-3.900393
49	6	0	2.828195	2.215012	-0.831769
50	6	0	3.588472	2.477572	-1.983767
51	6	0	2.158709	3.269775	-0.183361
52	6	0	3.684843	3.781639	-2.470633
53	1	0	4.102810	1.672727	-2.497936
54	6	0	2.266279	4.569514	-0.672923
55	1	0	1.554367	3.069300	0.697099
56	6	0	3.027619	4.825736	-1.817586
57	1	0	4.273126	3.979344	-3.361521
58	1	0	1.749833	5.380531	-0.168232
59	1	0	3.102878	5.838555	-2.202113
60	6	0	3.536274	0.438265	1.467490
61	6	0	3.431755	-0.805584	2.139042
62	6	0	4.038418	1.557320	2.160010
63	6	0	3.823075	-0.914778	3.480218
64	1	0	3.138577	-1.700049	1.592706
65	6	0	4.443785	1.427679	3.484375
66	1	0	4.118902	2.515573	1.657437
67	6	0	4.326873	0.198280	4.148703
68	1	0	3.753309	-1.873776	3.984702
69	1	0	4.853577	2.287156	4.006579
70	1	0	4.641413	0.112474	5.184467
71	1	0	0.002340	-1.709655	2.392233
72	6	0	-0.737973	-3.401618	0.190656
73	6	0	-1.224357	-4.041972	-0.880325
74	1	0	-0.584474	-4.686314	-1.477628
75	1	0	-2.251225	-3.960469	-1.215009
76	6	0	0.719276	-3.588043	0.552073

77	1	0	0.855354	-3.988059	1.564366
78	1	0	1.204645	-4.274636	-0.147068
79	1	0	1.265676	-2.631182	0.503048



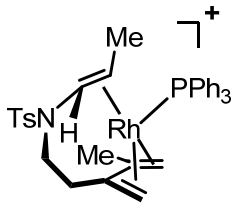
32-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.929761	1.510716	-0.486118
2	1	0	-1.988031	1.548825	-1.710937
3	6	0	-0.583218	1.087657	-2.717160
4	6	0	1.799335	2.834830	0.995137
5	6	0	0.280736	2.794066	0.912448
6	6	0	-0.503414	3.668322	0.058684
7	6	0	2.668402	2.093352	-0.066860
8	6	0	0.133996	4.714440	-0.822744
9	6	0	-1.910004	3.480762	0.075117
10	7	0	2.295815	0.706036	-0.358847
11	6	0	4.631537	-0.630703	0.252243
12	6	0	4.984110	-1.270427	-0.942289
13	6	0	6.329996	-1.371016	-1.273980
14	6	0	7.330671	-0.851797	-0.432634
15	6	0	6.943616	-0.223551	0.758967
16	6	0	5.599696	-0.109588	1.113627
17	16	0	2.916593	-0.519273	0.708199
18	8	0	2.209539	-1.742679	0.321626
19	8	0	2.822530	0.013100	2.070327
20	1	0	0.886251	-0.640280	-1.116989
21	1	0	1.155771	2.252699	-2.248168
22	1	0	-0.879890	1.804514	-3.477214
23	1	0	-0.947107	0.076007	-2.869305
24	1	0	3.700868	2.089962	0.291660
25	1	0	2.684516	2.638486	-1.012079
26	1	0	2.083357	2.439090	1.971366

27	1	0	2.123785	3.882176	0.969400
28	1	0	-1.378640	2.001830	2.116463
29	1	0	0.178465	1.056105	2.168700
30	1	0	0.305219	5.632145	-0.243867
31	1	0	1.100080	4.409124	-1.235201
32	1	0	-0.526056	4.978222	-1.654371
33	1	0	-2.498483	4.019525	-0.662935
34	1	0	-2.444555	3.242688	0.988092
35	1	0	4.221839	-1.691728	-1.589620
36	1	0	6.613760	-1.867317	-2.198164
37	1	0	7.703172	0.176533	1.424708
38	1	0	5.305304	0.357390	2.047222
39	6	0	1.174933	0.404068	-1.118454
40	6	0	0.666796	1.301069	-2.075497
41	6	0	8.786873	-0.995923	-0.798525
42	1	0	9.127419	-2.025983	-0.632803
43	1	0	8.957041	-0.766098	-1.855835
44	1	0	9.420297	-0.337145	-0.197927
45	15	0	-2.262543	-0.465837	0.042116
46	6	0	-1.905235	-1.884663	-1.096535
47	6	0	-1.030597	-2.931045	-0.765543
48	6	0	-2.477854	-1.867047	-2.383427
49	6	0	-0.738738	-3.932211	-1.696569
50	1	0	-0.584513	-2.988511	0.220009
51	6	0	-2.183995	-2.868892	-3.308666
52	1	0	-3.181377	-1.085012	-2.656306
53	6	0	-1.310064	-3.904599	-2.968439
54	1	0	-0.067054	-4.738545	-1.416373
55	1	0	-2.646836	-2.844801	-4.291299
56	1	0	-1.084249	-4.686858	-3.687247
57	6	0	-2.067800	-1.120504	1.758874
58	6	0	-3.161538	-1.232001	2.631610
59	6	0	-0.789406	-1.468707	2.231562
60	6	0	-2.981404	-1.699923	3.935958
61	1	0	-4.157096	-0.957777	2.302964
62	6	0	-0.616670	-1.948179	3.529463
63	1	0	0.081786	-1.368319	1.593441
64	6	0	-1.713466	-2.065333	4.386638
65	1	0	-3.839805	-1.778779	4.597013
66	1	0	0.378728	-2.218857	3.869307
67	1	0	-1.578212	-2.432135	5.399976
68	6	0	-4.084286	-0.267673	-0.168253
69	6	0	-4.921903	-1.398853	-0.188901
70	6	0	-4.659616	1.003755	-0.290475

71	6	0	-6.300992	-1.253104	-0.328068
72	1	0	-4.495385	-2.393572	-0.101110
73	6	0	-6.042763	1.147653	-0.428611
74	1	0	-4.021879	1.880435	-0.288288
75	6	0	-6.864298	0.020952	-0.447925
76	1	0	-6.935843	-2.134299	-0.346003
77	1	0	-6.474601	2.139818	-0.524717
78	1	0	-7.939137	0.131728	-0.558837
79	6	0	-0.412483	1.812609	1.663226



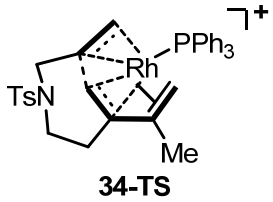
33

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.769385	-1.116696	-0.546018
2	6	0	-0.093326	1.135649	-2.702905
3	6	0	-2.058433	-2.983804	-0.043794
4	6	0	-0.580287	-2.759349	0.187960
5	6	0	0.477917	-3.359787	-0.538273
6	6	0	-2.838149	-1.844685	-0.757163
7	6	0	0.262720	-4.249687	-1.734586
8	6	0	1.816689	-2.922378	-0.169570
9	7	0	-2.556913	-0.487677	-0.280663
10	6	0	-5.080968	0.415537	0.455906
11	6	0	-5.317315	1.596939	-0.256291
12	6	0	-6.598863	1.845506	-0.734728
13	6	0	-7.650979	0.940550	-0.508872
14	6	0	-7.382495	-0.230171	0.213879
15	6	0	-6.105275	-0.501723	0.702995
16	16	0	-3.450065	0.091869	1.090936
17	8	0	-2.802061	1.349762	1.460609
18	8	0	-3.524316	-1.042188	2.013328
19	1	0	-1.471476	1.272638	-0.332891
20	1	0	-1.048140	-0.846903	-2.536408

21	1	0	-0.666751	1.440675	-3.589405
22	1	0	0.061550	2.019429	-2.079314
23	1	0	-3.909074	-2.035480	-0.643098
24	1	0	-2.636371	-1.858172	-1.830913
25	1	0	-2.520936	-3.140168	0.935256
26	1	0	-2.224392	-3.896179	-0.625391
27	1	0	0.625544	-2.081317	1.911296
28	1	0	-0.894532	-1.142805	1.612480
29	1	0	0.307416	-5.301118	-1.419777
30	1	0	-0.699847	-4.090384	-2.227584
31	1	0	1.057484	-4.107033	-2.473536
32	1	0	2.617801	-3.190673	-0.857719
33	1	0	2.135628	-2.953700	0.870489
34	1	0	-4.519052	2.314682	-0.414372
35	1	0	-6.791830	2.762368	-1.285299
36	1	0	-8.185248	-0.936515	0.406561
37	1	0	-5.908647	-1.395069	1.285789
38	6	0	-1.581312	0.319068	-0.840295
39	6	0	-0.835248	0.051242	-1.957952
40	6	0	-9.042448	1.244457	-1.005934
41	1	0	-9.545716	1.953849	-0.336328
42	1	0	-9.021351	1.699268	-2.001817
43	1	0	-9.659239	0.342394	-1.053175
44	15	0	2.504053	0.421960	0.082294
45	6	0	2.073573	2.208907	0.321446
46	6	0	1.638972	2.707748	1.559234
47	6	0	2.113929	3.084104	-0.779141
48	6	0	1.252244	4.042710	1.691541
49	1	0	1.618237	2.071132	2.435494
50	6	0	1.729898	4.418563	-0.642152
51	1	0	2.466191	2.733410	-1.743492
52	6	0	1.293338	4.901557	0.592909
53	1	0	0.925601	4.409590	2.660212
54	1	0	1.780557	5.081180	-1.501635
55	1	0	0.995950	5.940643	0.699534
56	6	0	3.288753	-0.120773	1.663068
57	6	0	4.657241	-0.420203	1.748088
58	6	0	2.489366	-0.293254	2.808741
59	6	0	5.212299	-0.863266	2.951097
60	1	0	5.297782	-0.310403	0.880397
61	6	0	3.049827	-0.724217	4.011561
62	1	0	1.424238	-0.087687	2.769770
63	6	0	4.414425	-1.011676	4.085524
64	1	0	6.273815	-1.089034	2.997578

65	1	0	2.418376	-0.838569	4.888053
66	1	0	4.850520	-1.352058	5.020065
67	6	0	3.864299	0.473525	-1.154982
68	6	0	4.898265	1.424073	-1.072908
69	6	0	3.880483	-0.453348	-2.208545
70	6	0	5.920825	1.438308	-2.020656
71	1	0	4.900460	2.156788	-0.271594
72	6	0	4.903087	-0.435641	-3.159757
73	1	0	3.093166	-1.199572	-2.285226
74	6	0	5.924523	0.509875	-3.065812
75	1	0	6.714140	2.176266	-1.944737
76	1	0	4.899856	-1.157848	-3.971089
77	1	0	6.720496	0.526261	-3.804578
78	6	0	-0.137630	-1.797950	1.189442
79	1	0	0.885452	0.796828	-3.063483



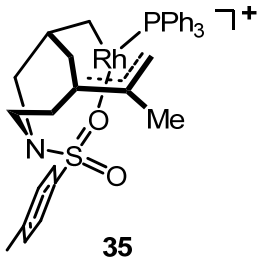
34-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.781954	-1.166842	-0.678563
2	6	0	0.842946	-1.244861	-2.531331
3	6	0	0.408179	-2.955679	-1.663166
4	6	0	2.674205	-2.410773	0.046783
5	6	0	1.447878	-3.092517	0.677651
6	6	0	0.207184	-3.075107	-0.198445
7	6	0	-1.101380	-3.189012	0.352529
8	6	0	-0.127823	-0.162643	-2.382865
9	6	0	-1.364561	-3.503986	1.803426
10	6	0	-2.163467	-2.795303	-0.528090
11	7	0	2.360162	-1.091096	-0.541727
12	6	0	4.538274	0.525625	0.245291
13	6	0	5.379970	-0.046218	1.204386
14	6	0	6.757936	0.119738	1.080153
15	6	0	7.311012	0.853003	0.019894
16	6	0	6.439919	1.426118	-0.920563

17	6	0	5.060135	1.272684	-0.816480
18	16	0	2.773370	0.283904	0.371847
19	8	0	2.460158	-0.089528	1.754065
20	8	0	2.107478	1.402051	-0.306657
21	1	0	2.968023	-1.692330	-2.464557
22	1	0	2.570221	0.019937	-2.307773
23	1	0	0.822214	-1.730609	-3.507724
24	1	0	-0.895041	-0.071135	-3.150023
25	1	0	0.261833	0.793840	-2.037704
26	1	0	3.118993	-3.031882	-0.738412
27	1	0	3.440147	-2.301293	0.818945
28	1	0	1.708575	-4.132200	0.928453
29	1	0	1.236428	-2.586716	1.623207
30	1	0	-0.367849	-3.383402	-2.292298
31	1	0	1.380595	-3.341845	-1.956588
32	1	0	-1.374921	-4.592589	1.947569
33	1	0	-0.612146	-3.092450	2.480973
34	1	0	-2.344588	-3.125822	2.106498
35	1	0	-3.141207	-2.621700	-0.089135
36	1	0	-2.211102	-3.152805	-1.555195
37	1	0	4.960728	-0.582609	2.048707
38	1	0	7.414314	-0.318820	1.827009
39	1	0	6.848331	2.011002	-1.740493
40	1	0	4.397046	1.750940	-1.529435
41	6	0	2.267176	-0.984170	-2.004458
42	15	0	-2.230597	0.522290	0.032441
43	6	0	8.802226	1.056752	-0.086585
44	1	0	9.126287	1.109684	-1.130807
45	1	0	9.099963	1.997415	0.394716
46	1	0	9.354368	0.249544	0.404058
47	6	0	-2.199569	2.129924	-0.872686
48	6	0	-0.991809	2.852251	-0.876219
49	6	0	-3.318396	2.664760	-1.527220
50	6	0	-0.910975	4.081689	-1.528268
51	1	0	-0.114571	2.465289	-0.364524
52	6	0	-3.228456	3.896673	-2.181395
53	1	0	-4.265039	2.135988	-1.522206
54	6	0	-2.027635	4.605619	-2.185641
55	1	0	0.025839	4.631486	-1.518823
56	1	0	-4.103809	4.301460	-2.681430
57	1	0	-1.962079	5.563834	-2.693022
58	6	0	-3.984331	-0.036192	-0.015805
59	6	0	-4.774089	-0.134216	1.138390
60	6	0	-4.529394	-0.435910	-1.250180

61	6	0	-6.086135	-0.610557	1.056782
62	1	0	-4.373219	0.161284	2.101899
63	6	0	-5.841619	-0.899194	-1.329140
64	1	0	-3.924544	-0.385834	-2.152172
65	6	0	-6.623496	-0.988848	-0.173260
66	1	0	-6.686734	-0.680702	1.959162
67	1	0	-6.252424	-1.194532	-2.290442
68	1	0	-7.644326	-1.354687	-0.233618
69	6	0	-1.878989	1.030846	1.762117
70	6	0	-0.892792	0.371249	2.507170
71	6	0	-2.562948	2.118138	2.336384
72	6	0	-0.601273	0.778936	3.810830
73	1	0	-0.328009	-0.438749	2.057343
74	6	0	-2.279603	2.512606	3.642421
75	1	0	-3.308632	2.659949	1.761650
76	6	0	-1.299072	1.842863	4.381508
77	1	0	0.180487	0.273185	4.369486
78	1	0	-2.815679	3.349867	4.079931
79	1	0	-1.073100	2.160864	5.395286



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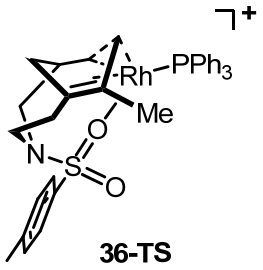
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.600579	-1.188674	-0.047023
2	6	0	0.927508	-2.003919	-2.397075
3	6	0	0.493185	-3.404976	-1.898952
4	6	0	2.873877	-3.303466	-0.139744
5	6	0	1.563227	-3.934628	0.376496
6	6	0	0.334186	-3.475985	-0.384985
7	6	0	-0.913974	-3.393283	0.245118
8	6	0	-0.153657	-0.990585	-2.029951
9	6	0	-1.101338	-3.800065	1.698120
10	6	0	-2.007764	-2.706029	-0.414858

11	7	0	2.743679	-1.898614	-0.566184
12	6	0	3.886405	0.463506	0.327584
13	6	0	5.106622	0.251123	0.977465
14	6	0	6.149431	1.146574	0.759721
15	6	0	5.997807	2.249777	-0.095624
16	6	0	4.761140	2.435523	-0.731210
17	6	0	3.700117	1.555544	-0.524976
18	16	0	2.579622	-0.718150	0.594160
19	8	0	2.760087	-1.371293	1.891604
20	8	0	1.306210	0.028344	0.320810
21	1	0	3.076980	-2.185736	-2.579145
22	1	0	2.547576	-0.565287	-2.172591
23	1	0	0.968570	-2.039064	-3.499404
24	1	0	-1.053573	-1.151869	-2.630450
25	1	0	0.175237	0.047343	-2.142019
26	1	0	3.252144	-3.834012	-1.018752
27	1	0	3.641499	-3.374909	0.633279
28	1	0	1.658588	-5.029354	0.296042
29	1	0	1.467617	-3.708303	1.439428
30	1	0	-0.446281	-3.667904	-2.394650
31	1	0	1.225631	-4.158645	-2.215199
32	1	0	-1.022903	-4.890431	1.790855
33	1	0	-0.355065	-3.366926	2.372451
34	1	0	-2.093277	-3.513361	2.057579
35	1	0	-2.951739	-2.650692	0.124099
36	1	0	-2.150532	-2.813309	-1.488190
37	1	0	5.228033	-0.588236	1.653737
38	1	0	7.097421	0.989091	1.266924
39	1	0	4.623737	3.285869	-1.393881
40	1	0	2.741226	1.727246	-1.001720
41	6	0	2.364588	-1.623622	-1.963752
42	15	0	-1.977507	0.717137	0.020490
43	6	0	7.127882	3.228644	-0.297939
44	1	0	7.048298	3.741478	-1.261192
45	1	0	7.119020	3.997480	0.485676
46	1	0	8.101714	2.731122	-0.252871
47	6	0	-1.392551	2.227584	-0.850131
48	6	0	-0.147517	2.779599	-0.493587
49	6	0	-2.140270	2.831065	-1.872320
50	6	0	0.325757	3.919854	-1.141773
51	1	0	0.444413	2.324992	0.293794
52	6	0	-1.653594	3.966475	-2.525425
53	1	0	-3.105458	2.426424	-2.157307
54	6	0	-0.423646	4.513991	-2.161663

55	1	0	1.278899	4.349036	-0.844749
56	1	0	-2.244463	4.425447	-3.312813
57	1	0	-0.051923	5.401768	-2.665199
58	6	0	-3.719563	0.487431	-0.519044
59	6	0	-4.790691	0.983646	0.240271
60	6	0	-3.990103	-0.178480	-1.726452
61	6	0	-6.104441	0.814295	-0.201316
62	1	0	-4.604058	1.500489	1.175830
63	6	0	-5.303184	-0.336487	-2.169247
64	1	0	-3.174798	-0.571950	-2.325731
65	6	0	-6.363406	0.156782	-1.404792
66	1	0	-6.924757	1.199233	0.397527
67	1	0	-5.498273	-0.849184	-3.106841
68	1	0	-7.386407	0.027219	-1.745765
69	6	0	-2.067033	1.167153	1.798808
70	6	0	-2.110830	0.124569	2.741295
71	6	0	-2.087606	2.495697	2.250538
72	6	0	-2.169413	0.403204	4.106584
73	1	0	-2.114905	-0.911978	2.409213
74	6	0	-2.148990	2.770977	3.617939
75	1	0	-2.054451	3.314441	1.539301
76	6	0	-2.186663	1.728623	4.546331
77	1	0	-2.200881	-0.411399	4.824249
78	1	0	-2.166985	3.802796	3.956767
79	1	0	-2.230304	1.947946	5.609097



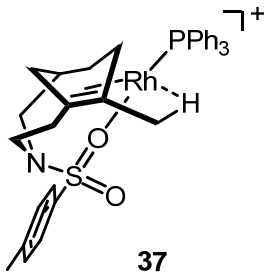
36-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.463439	-0.951510	-0.004183
2	6	0	-1.528799	-2.879492	-0.799370
3	6	0	-0.525639	-1.828603	-2.108331
4	6	0	2.905611	-3.079107	0.252739

5	6	0	1.803417	-4.091177	0.681120
6	6	0	0.604454	-3.865308	-0.196025
7	6	0	0.896017	-2.411562	-2.217900
8	6	0	0.899251	-3.865208	-1.680542
9	6	0	-1.114660	-3.548398	1.667870
10	6	0	-0.619957	-3.440525	0.239148
11	7	0	2.320263	-1.780087	-0.147981
12	6	0	3.812234	0.577324	0.392563
13	6	0	5.076750	0.385061	0.961089
14	6	0	6.134092	1.183443	0.535826
15	6	0	5.954721	2.170673	-0.446722
16	6	0	4.674576	2.340422	-0.994964
17	6	0	3.599171	1.555696	-0.583505
18	16	0	2.488360	-0.491078	0.921754
19	8	0	2.827625	-1.075003	2.218326
20	8	0	1.225421	0.304935	0.782586
21	1	0	2.980154	-1.813505	-2.140263
22	1	0	1.859263	-0.504177	-1.760987
23	1	0	1.128477	-2.442775	-3.293614
24	1	0	-1.153996	-2.195477	-2.921205
25	1	0	-0.521368	-0.735375	-2.234678
26	1	0	3.474605	-3.456179	-0.603212
27	1	0	3.604619	-2.928767	1.075305
28	1	0	2.209985	-5.106029	0.573035
29	1	0	1.568060	-3.943038	1.737016
30	1	0	0.149590	-4.442834	-2.235431
31	1	0	1.861866	-4.343921	-1.886825
32	1	0	-1.521485	-4.552404	1.849947
33	1	0	-0.324764	-3.377539	2.405113
34	1	0	-1.917635	-2.832593	1.864129
35	1	0	-2.471467	-2.480455	-0.421681
36	1	0	-1.770426	-3.576942	-1.598683
37	1	0	5.219691	-0.359184	1.736846
38	1	0	7.115704	1.042136	0.980114
39	1	0	4.514679	3.104555	-1.750783
40	1	0	2.610969	1.718979	-0.999433
41	6	0	2.057539	-1.565837	-1.597027
42	15	0	-1.945999	0.742435	0.016001
43	6	0	7.107128	3.044125	-0.876177
44	1	0	6.899456	3.548721	-1.824136
45	1	0	7.307189	3.818843	-0.124911
46	1	0	8.027251	2.461704	-0.991759
47	6	0	-1.560507	2.158673	-1.092309
48	6	0	-0.301729	2.773290	-0.950190

49	6	0	-2.460311	2.654678	-2.047161
50	6	0	0.044022	3.859334	-1.752008
51	1	0	0.394667	2.410284	-0.200090
52	6	0	-2.102721	3.738097	-2.854638
53	1	0	-3.442851	2.209510	-2.158997
54	6	0	-0.853053	4.340177	-2.711136
55	1	0	1.011327	4.337608	-1.623976
56	1	0	-2.808787	4.114393	-3.589303
57	1	0	-0.580912	5.185701	-3.336319
58	6	0	-3.654482	0.211171	-0.399243
59	6	0	-4.699212	0.310683	0.532677
60	6	0	-3.918552	-0.348032	-1.663443
61	6	0	-5.980894	-0.136603	0.203570
62	1	0	-4.517545	0.740210	1.512059
63	6	0	-5.201259	-0.785009	-1.990298
64	1	0	-3.122961	-0.433420	-2.398620
65	6	0	-6.235115	-0.682694	-1.054868
66	1	0	-6.780909	-0.052788	0.933370
67	1	0	-5.394256	-1.205427	-2.973183
68	1	0	-7.233529	-1.027007	-1.308120
69	6	0	-2.019999	1.467315	1.697410
70	6	0	-1.721430	0.657995	2.805667
71	6	0	-2.384889	2.808660	1.901049
72	6	0	-1.788604	1.180728	4.097423
73	1	0	-1.427760	-0.377464	2.654083
74	6	0	-2.454388	3.325019	3.194934
75	1	0	-2.613408	3.447852	1.053957
76	6	0	-2.155190	2.513882	4.292538
77	1	0	-1.549860	0.549226	4.948152
78	1	0	-2.739060	4.362382	3.345166
79	1	0	-2.205337	2.921697	5.298034



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Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	45	0	-0.562976	1.052714	0.038083
2	6	0	-0.021932	3.715880	1.760504
3	6	0	1.260969	2.956756	2.206365
4	6	0	2.499051	2.451437	-1.834849
5	6	0	1.226906	3.359699	-1.887311
6	6	0	0.921682	3.803978	-0.485636
7	6	0	2.503445	3.296772	1.325581
8	6	0	2.097810	4.361877	0.283243
9	6	0	-1.538900	3.187446	-0.298830
10	6	0	-0.194031	3.550262	0.258625
11	7	0	2.554009	1.599438	-0.629465
12	6	0	3.558206	-0.998189	-0.244788
13	6	0	4.569977	-1.240644	-1.181890
14	6	0	5.666918	-2.006243	-0.802026
15	6	0	5.774011	-2.536143	0.495317
16	6	0	4.738989	-2.283231	1.406666
17	6	0	3.629442	-1.518239	1.050064
18	16	0	2.167112	-0.016307	-0.767201
19	8	0	1.876558	-0.273962	-2.177045
20	8	0	1.097345	-0.293831	0.263435
21	1	0	4.216607	2.402258	0.349519
22	1	0	3.282632	1.263344	1.311566
23	1	0	3.284893	3.720278	1.968835
24	1	0	1.474951	3.188138	3.255448
25	1	0	1.042984	1.882697	2.158694
26	1	0	3.409470	3.059422	-1.838888
27	1	0	2.523770	1.813008	-2.718172
28	1	0	1.454887	4.209079	-2.546212
29	1	0	0.396118	2.802360	-2.329619
30	1	0	1.814968	5.285479	0.801165
31	1	0	2.935013	4.617646	-0.372711
32	1	0	-2.321651	3.816372	0.147236
33	1	0	-1.616414	3.259437	-1.383778
34	1	0	-1.988545	2.168157	0.040856
35	1	0	-0.890078	3.319217	2.296252
36	1	0	0.054434	4.777288	2.036846
37	1	0	4.486384	-0.859517	-2.194245
38	1	0	6.450151	-2.206479	-1.528184
39	1	0	4.795927	-2.698014	2.409143
40	1	0	2.824439	-1.347234	1.755538
41	6	0	3.193911	2.100906	0.615228
42	15	0	-2.053350	-0.638500	0.023699

43	6	0	6.979147	-3.352052	0.891833
44	1	0	6.810328	-3.891769	1.827812
45	1	0	7.236780	-4.082282	0.117239
46	1	0	7.856330	-2.707601	1.032591
47	6	0	-2.219650	-1.484638	1.647787
48	6	0	-1.076180	-1.663460	2.444385
49	6	0	-3.453130	-1.984183	2.097938
50	6	0	-1.167820	-2.327571	3.667513
51	1	0	-0.118525	-1.285505	2.102365
52	6	0	-3.538535	-2.647136	3.323762
53	1	0	-4.347586	-1.855907	1.496980
54	6	0	-2.398404	-2.817731	4.110758
55	1	0	-0.278570	-2.459395	4.277605
56	1	0	-4.497810	-3.027963	3.662359
57	1	0	-2.468544	-3.330185	5.065931
58	6	0	-3.747194	-0.039494	-0.374021
59	6	0	-4.401123	-0.393614	-1.562953
60	6	0	-4.384719	0.838676	0.522297
61	6	0	-5.665985	0.125757	-1.851587
62	1	0	-3.930154	-1.075527	-2.263113
63	6	0	-5.648354	1.349676	0.232502
64	1	0	-3.899056	1.110940	1.456564
65	6	0	-6.290482	0.996711	-0.958642
66	1	0	-6.162709	-0.157072	-2.775216
67	1	0	-6.134451	2.018746	0.937004
68	1	0	-7.274693	1.396417	-1.185074
69	6	0	-1.683342	-1.956002	-1.196412
70	6	0	-1.136048	-1.596026	-2.438479
71	6	0	-1.962748	-3.306549	-0.931432
72	6	0	-0.885327	-2.570174	-3.404772
73	1	0	-0.892952	-0.557337	-2.639976
74	6	0	-1.705267	-4.277162	-1.900152
75	1	0	-2.378186	-3.602326	0.026440
76	6	0	-1.169508	-3.911037	-3.136881
77	1	0	-0.458259	-2.281923	-4.360826
78	1	0	-1.923384	-5.319743	-1.687050
79	1	0	-0.969125	-4.669802	-3.888042

$[Rh(PPh_3)_3]^+$

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	45	0	-0.068340	0.440790	0.052082
2	15	0	2.343188	0.681014	0.023362
3	15	0	-0.252048	-1.806979	0.041057
4	15	0	-2.290472	1.070505	0.043036
5	6	0	0.673264	-2.497851	-1.398712
6	6	0	1.558358	-3.579697	-1.299948
7	6	0	0.462574	-1.906025	-2.657346
8	6	0	2.204048	-4.068871	-2.438298
9	6	0	1.097399	-2.405621	-3.793600
10	1	0	-0.206457	-1.053891	-2.743167
11	6	0	1.970630	-3.491112	-3.685820
12	1	0	0.914887	-1.945581	-4.760935
13	1	0	2.470864	-3.878209	-4.568928
14	6	0	0.368356	-2.669387	1.549947
15	6	0	0.188959	-4.055435	1.714135
16	6	0	0.986308	-1.940699	2.575611
17	6	0	0.647467	-4.694700	2.865645
18	1	0	-0.319116	-4.634704	0.949005
19	6	0	1.438682	-2.581991	3.731972
20	6	0	1.275153	-3.960011	3.875839
21	1	0	0.506388	-5.765925	2.977965
22	1	0	1.913095	-2.001477	4.518298
23	1	0	1.625033	-4.460362	4.774333
24	6	0	-1.938349	-2.559202	-0.123268
25	6	0	-2.418320	-3.071614	-1.337460
26	6	0	-2.765265	-2.625423	1.011983
27	6	0	-3.692356	-3.639456	-1.411813
28	1	0	-1.798389	-3.048841	-2.226213
29	6	0	-4.035702	-3.193717	0.934634
30	1	0	-2.411165	-2.253444	1.967637
31	6	0	-4.503146	-3.703843	-0.279037
32	1	0	-4.044246	-4.038621	-2.358810
33	1	0	-4.655200	-3.247102	1.825578
34	1	0	-5.489986	-4.154181	-0.337944
35	6	0	3.620465	-0.555706	-0.476003
36	6	0	4.215572	-0.529563	-1.745367
37	6	0	4.001080	-1.558629	0.433085
38	6	0	5.176289	-1.481275	-2.094881
39	1	0	3.944260	0.239206	-2.461104
40	6	0	4.965001	-2.502819	0.081772
41	1	0	3.559311	-1.597641	1.424150
42	6	0	5.555832	-2.466958	-1.183689

43	1	0	5.635158	-1.441573	-3.078859
44	1	0	5.258057	-3.263194	0.800506
45	6	0	2.989665	1.305316	1.636511
46	6	0	4.365483	1.413753	1.903436
47	6	0	2.076932	1.712167	2.622646
48	6	0	4.810710	1.929371	3.121541
49	1	0	5.090474	1.088382	1.163781
50	6	0	2.523119	2.226485	3.841602
51	1	0	1.010335	1.604674	2.437649
52	6	0	3.891916	2.338318	4.091334
53	1	0	5.876954	2.007875	3.314122
54	1	0	1.803288	2.533257	4.595465
55	1	0	4.242476	2.736040	5.039445
56	6	0	2.579360	2.080962	-1.160061
57	6	0	3.454939	3.151946	-0.923632
58	6	0	1.838404	2.059645	-2.355289
59	6	0	3.593354	4.170703	-1.867571
60	1	0	4.029391	3.195487	-0.004502
61	6	0	1.984244	3.076916	-3.299983
62	1	0	1.151068	1.238855	-2.543522
63	6	0	2.862668	4.134416	-3.057199
64	1	0	4.276214	4.993015	-1.672981
65	1	0	2.976137	4.928052	-3.790295
66	6	0	-3.480171	0.540824	-1.248302
67	6	0	-4.790453	0.134656	-0.960323
68	6	0	-3.029263	0.491836	-2.580460
69	6	0	-5.638798	-0.286760	-1.987030
70	1	0	-5.152299	0.139173	0.061701
71	6	0	-3.882595	0.082558	-3.603548
72	1	0	-2.008692	0.782910	-2.815975
73	6	0	-5.192082	-0.306266	-3.308134
74	1	0	-6.652082	-0.597799	-1.749453
75	1	0	-3.525591	0.063240	-4.629503
76	1	0	-5.857419	-0.627470	-4.104433
77	6	0	-3.211505	1.200438	1.627325
78	6	0	-4.345252	2.023338	1.747921
79	6	0	-2.727524	0.532960	2.761838
80	6	0	-4.993447	2.151354	2.975667
81	1	0	-4.717210	2.569726	0.885730
82	6	0	-3.377524	0.665425	3.991201
83	1	0	-1.832477	-0.077219	2.681277
84	6	0	-4.512626	1.469910	4.097732
85	1	0	-5.869314	2.788419	3.058812
86	1	0	-2.994812	0.143051	4.863541

87	1	0	-5.018293	1.574099	5.053462
88	6	0	-1.834122	2.815928	-0.336029
89	6	0	-0.930335	3.423199	0.560296
90	6	0	-2.241503	3.527332	-1.476599
91	6	0	-0.437242	4.706764	0.313212
92	1	0	-0.648307	2.910037	1.476649
93	6	0	-1.756399	4.813502	-1.709575
94	1	0	-2.945805	3.085385	-2.173290
95	6	0	-0.848874	5.402315	-0.823049
96	1	0	0.256025	5.162075	1.014372
97	1	0	-2.092616	5.362031	-2.585079
98	1	0	-0.474418	6.403681	-1.014272
99	1	0	1.411035	3.044002	-4.222375
100	1	0	1.103637	-0.867473	2.470273
101	1	0	1.758604	-4.038943	-0.338882
102	1	0	6.311589	-3.199029	-1.454147
103	1	0	2.894607	-4.901889	-2.343747

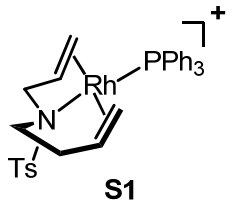
$[Rh(PPh_3)_2]^+$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.000054	-0.425348	-0.000119
2	15	0	2.304408	-0.153716	-0.097705
3	15	0	-2.304504	-0.153738	0.097568
4	6	0	1.523300	0.135757	-1.720123
5	6	0	1.430555	1.395004	-2.368274
6	6	0	0.755522	-0.961420	-2.214585
7	6	0	0.639055	1.536555	-3.494728
8	1	0	2.004305	2.234878	-1.988436
9	6	0	-0.055760	-0.781086	-3.361911
10	1	0	0.947248	-1.972995	-1.860597
11	6	0	-0.110293	0.448626	-3.992446
12	1	0	0.600105	2.493589	-4.007435
13	1	0	-0.604540	-1.629845	-3.759856
14	6	0	3.527005	-1.497343	-0.257937
15	6	0	4.241219	-1.715101	-1.448226
16	6	0	3.758791	-2.328219	0.850781
17	6	0	5.176259	-2.748652	-1.521789
18	1	0	4.068535	-1.081559	-2.313391

19	6	0	4.700049	-3.354170	0.773040
20	1	0	3.203722	-2.173458	1.772314
21	6	0	5.407512	-3.565889	-0.412943
22	1	0	5.724569	-2.913531	-2.444736
23	1	0	4.876407	-3.991556	1.634493
24	1	0	6.136183	-4.368941	-0.473791
25	6	0	3.177919	1.346596	0.454882
26	6	0	4.569544	1.486291	0.324718
27	6	0	2.426947	2.382252	1.036974
28	6	0	5.195204	2.656330	0.754742
29	1	0	5.161941	0.685508	-0.106614
30	6	0	3.059343	3.551197	1.459885
31	1	0	1.353649	2.265297	1.161449
32	6	0	4.442407	3.689091	1.318930
33	1	0	6.271189	2.760290	0.650153
34	1	0	4.934381	4.597384	1.654734
35	6	0	-3.177963	1.346720	-0.454723
36	6	0	-4.569717	1.486049	-0.325581
37	6	0	-2.426776	2.382844	-1.035711
38	6	0	-5.195297	2.656182	-0.755474
39	1	0	-5.162286	0.684926	0.104877
40	6	0	-3.059091	3.551883	-1.458479
41	1	0	-1.353361	2.266184	-1.159448
42	6	0	-4.442293	3.689409	-1.318522
43	1	0	-6.271385	2.759848	-0.651660
44	1	0	-2.474551	4.351065	-1.905221
45	1	0	-4.934205	4.597773	-1.654229
46	6	0	-3.527043	-1.497412	0.257795
47	6	0	-4.242464	-1.714039	1.447577
48	6	0	-3.757538	-2.329479	-0.850288
49	6	0	-5.177440	-2.747630	1.521238
50	1	0	-4.070703	-1.079619	2.312285
51	6	0	-4.698736	-3.355488	-0.772462
52	1	0	-3.201489	-2.175599	-1.771373
53	6	0	-5.407419	-3.566053	0.412990
54	1	0	-5.726679	-2.911648	2.443786
55	1	0	-4.874088	-3.993815	-1.633424
56	1	0	-6.136043	-4.369143	0.473915
57	6	0	-1.523282	0.135435	1.719999
58	6	0	-0.755564	-0.961921	2.214173
59	6	0	-1.430477	1.394495	2.368494
60	6	0	0.055729	-0.781940	3.361545
61	1	0	-0.947402	-1.973399	1.859959
62	6	0	-0.638990	1.535694	3.495008

63	1	0	-2.004192	2.234504	1.988902
64	6	0	0.110307	0.447595	3.992427
65	1	0	0.604467	-1.630832	3.759262
66	1	0	-0.600021	2.492583	4.007984
67	1	0	0.719428	0.577139	4.882062
68	1	0	2.474986	4.350025	1.907500
69	1	0	-0.719423	0.578455	-4.882033



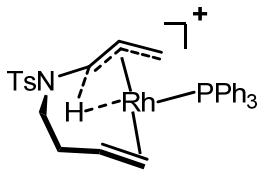
S1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.181320	-1.034869	-1.637910
2	6	0	-1.021699	-1.912568	-1.193964
3	6	0	0.137817	-1.993804	-1.898839
4	6	0	-2.369289	1.544269	-1.545537
5	6	0	-1.495370	2.666456	-0.968613
6	6	0	-0.018335	2.295388	-0.877827
7	6	0	0.648279	1.698504	-1.966122
8	7	0	-2.076488	0.246492	-0.851096
9	6	0	-4.613349	-0.044388	0.427142
10	6	0	-5.392094	1.117618	0.356065
11	6	0	-6.757907	0.997664	0.115948
12	6	0	-7.363361	-0.259613	-0.042927
13	6	0	-6.559212	-1.406416	0.052220
14	6	0	-5.190402	-1.312636	0.290590
15	16	0	-2.868428	0.095951	0.754504
16	8	0	-2.608510	1.354637	1.445667
17	8	0	-2.372951	-1.181725	1.271864
18	1	0	-2.078139	-0.766241	-2.692355
19	1	0	-3.157501	-1.515223	-1.510970
20	1	0	-1.167756	-2.509804	-0.300179
21	1	0	0.936502	-2.657296	-1.584904
22	1	0	0.253672	-1.528742	-2.874001
23	1	0	-2.135462	1.373849	-2.600245
24	1	0	-3.436788	1.789669	-1.494033

25	1	0	-1.608940	3.547251	-1.618890
26	1	0	-1.863537	2.950208	0.017156
27	1	0	1.722144	1.822728	-2.067488
28	1	0	0.130780	1.505309	-2.905461
29	1	0	-4.942250	2.091086	0.519056
30	1	0	-7.367838	1.895346	0.064259
31	1	0	-7.013620	-2.388114	-0.048974
32	1	0	-4.585656	-2.205839	0.404280
33	45	0	0.130788	0.131495	-0.580729
34	15	0	2.329204	-0.085923	0.074151
35	6	0	2.296364	-0.758264	1.782189
36	6	0	3.380019	-0.574827	2.659478
37	6	0	1.165086	-1.460394	2.229548
38	6	0	3.332213	-1.095445	3.952277
39	1	0	4.256565	-0.022105	2.336005
40	6	0	1.117305	-1.969267	3.528581
41	1	0	0.308940	-1.603987	1.576304
42	6	0	2.201197	-1.790754	4.389080
43	1	0	4.176170	-0.951844	4.620734
44	1	0	0.230942	-2.498633	3.865122
45	1	0	2.164634	-2.187422	5.399525
46	6	0	3.290772	1.476356	0.222930
47	6	0	4.402446	1.759447	-0.584172
48	6	0	2.868267	2.432203	1.165882
49	6	0	5.074503	2.978218	-0.454506
50	1	0	4.757670	1.030512	-1.305008
51	6	0	3.545861	3.643125	1.294894
52	1	0	2.019859	2.222209	1.811927
53	6	0	4.648573	3.920505	0.481175
54	1	0	5.936471	3.183425	-1.082733
55	1	0	3.215549	4.368660	2.032692
56	1	0	5.175373	4.864872	0.582290
57	6	0	3.383332	-1.215956	-0.924739
58	6	0	4.152430	-2.229177	-0.332793
59	6	0	3.418797	-1.060872	-2.322590
60	6	0	4.943261	-3.066332	-1.123738
61	1	0	4.135433	-2.371113	0.742524
62	6	0	4.218714	-1.891266	-3.106899
63	1	0	2.819619	-0.291175	-2.801432
64	6	0	4.981199	-2.898036	-2.508161
65	1	0	5.530752	-3.849332	-0.653130
66	1	0	4.242968	-1.756145	-4.184506
67	1	0	5.599015	-3.549016	-3.119778
68	6	0	-8.850134	-0.375269	-0.267023

69	1	0	-9.105075	-1.290409	-0.809686
70	1	0	-9.382484	-0.404057	0.692655
71	1	0	-9.238875	0.479482	-0.829022
72	1	0	0.565538	2.871927	-0.165653



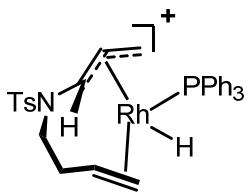
S2-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.382856	-0.311654	0.311866
2	1	0	-0.562470	-1.090187	1.261218
3	6	0	-1.935992	0.423664	0.712868
4	6	0	-2.718820	-0.706554	-1.350751
5	6	0	-1.789634	-1.944871	-1.389984
6	6	0	-0.305001	-1.697251	-1.301067
7	6	0	0.064253	1.801888	0.968936
8	7	0	-2.930731	-0.196822	0.014794
9	6	0	-5.673143	-0.216456	0.359527
10	6	0	-6.013208	1.061421	0.819960
11	6	0	-7.181722	1.650423	0.352081
12	6	0	-8.020177	0.985420	-0.560940
13	6	0	-7.654561	-0.296356	-0.994775
14	6	0	-6.487304	-0.908795	-0.540114
15	16	0	-4.196806	-0.995675	0.966200
16	8	0	-3.930633	-0.576502	2.341122
17	8	0	-4.199813	-2.401001	0.564805
18	1	0	-2.069978	0.396571	1.790788
19	1	0	-1.106197	1.694930	-0.857503
20	1	0	0.744933	2.548345	0.575395
21	1	0	0.004228	1.734513	2.053747
22	1	0	-3.698475	-0.966746	-1.756521
23	1	0	-2.330754	0.108430	-1.969765
24	1	0	-2.115893	-2.650491	-0.621811
25	1	0	-1.968219	-2.431523	-2.360010
26	1	0	1.597238	-2.545874	-0.740657
27	1	0	0.151470	-3.132441	0.236715

28	1	0	-5.385921	1.572704	1.542748
29	1	0	-7.456659	2.640020	0.707094
30	1	0	-8.296328	-0.829553	-1.690453
31	1	0	-6.223431	-1.912072	-0.856680
32	6	0	0.558107	-2.408278	-0.464990
33	6	0	-1.011053	1.364577	0.173595
34	6	0	-9.296433	1.633761	-1.036210
35	1	0	-10.042913	1.655392	-0.232239
36	1	0	-9.124984	2.671062	-1.344322
37	1	0	-9.733080	1.093236	-1.880508
38	15	0	2.877796	0.132048	-0.041136
39	6	0	3.743267	0.175035	1.575944
40	6	0	5.147493	0.153369	1.653763
41	6	0	2.994330	0.213969	2.761992
42	6	0	5.782405	0.190398	2.894711
43	1	0	5.742979	0.098053	0.747334
44	6	0	3.633006	0.245967	4.003001
45	1	0	1.908308	0.208817	2.715627
46	6	0	5.026846	0.238093	4.069760
47	1	0	6.867281	0.175648	2.944516
48	1	0	3.042345	0.270216	4.914136
49	1	0	5.524963	0.260914	5.034633
50	6	0	3.868371	-1.061220	-1.037772
51	6	0	4.308961	-0.772778	-2.337916
52	6	0	4.141365	-2.328170	-0.488848
53	6	0	5.011708	-1.731545	-3.071837
54	1	0	4.122093	0.201794	-2.776227
55	6	0	4.845508	-3.280129	-1.225177
56	1	0	3.821349	-2.565712	0.522608
57	6	0	5.280144	-2.984512	-2.520042
58	1	0	5.355451	-1.492001	-4.074025
59	1	0	5.057670	-4.250564	-0.785806
60	1	0	5.828956	-3.726432	-3.092611
61	6	0	3.138269	1.769286	-0.844726
62	6	0	4.038262	2.725810	-0.353195
63	6	0	2.371371	2.078168	-1.983229
64	6	0	4.174939	3.959403	-0.994879
65	1	0	4.631250	2.515448	0.530451
66	6	0	2.519939	3.305453	-2.629034
67	1	0	1.659310	1.352977	-2.372988
68	6	0	3.422172	4.250423	-2.133105
69	1	0	4.874171	4.691979	-0.602224
70	1	0	1.929584	3.525984	-3.513926
71	1	0	3.533784	5.209491	-2.630247

72	1	0	0.128063	-1.198335	-2.170890

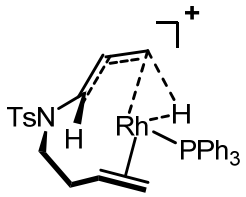


S3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.518252	-0.085728	-0.261841
2	1	0	0.446905	0.416171	1.180740
3	6	0	0.609448	-2.397137	0.284300
4	6	0	-2.864752	-1.452661	-0.971038
5	6	0	-1.847854	-2.477851	-0.405391
6	6	0	-0.381288	-2.248529	-0.659626
7	6	0	0.021094	1.875829	-0.925290
8	7	0	-2.945694	-0.238035	-0.150313
9	6	0	-5.609547	0.107461	0.538569
10	6	0	-5.925753	1.444811	0.271540
11	6	0	-7.169299	1.740368	-0.274727
12	6	0	-8.104623	0.727461	-0.551965
13	6	0	-7.758730	-0.600519	-0.264328
14	6	0	-6.517744	-0.923017	0.282759
15	16	0	-4.032178	-0.286194	1.254138
16	8	0	-3.577392	0.811518	2.104362
17	8	0	-4.041189	-1.676356	1.702892
18	1	0	-1.943508	1.312150	0.745778
19	1	0	-1.283813	0.645829	-2.212053
20	1	0	0.615071	2.241201	-1.760252
21	1	0	-0.036638	2.576180	-0.095130
22	1	0	-3.858701	-1.902922	-0.995962
23	1	0	-2.622217	-1.164856	-1.998347
24	1	0	-2.041756	-2.608256	0.662491
25	1	0	-2.096877	-3.435272	-0.886119
26	1	0	1.623245	-2.646439	-0.008239
27	1	0	0.351056	-2.564809	1.326385
28	1	0	-5.221351	2.236358	0.505033
29	1	0	-7.425454	2.775862	-0.482063
30	1	0	-8.473335	-1.394667	-0.461305

31	1	0	-6.266084	-1.948741	0.529713
32	6	0	-1.975046	0.708855	-0.157340
33	6	0	-1.122474	1.050637	-1.215836
34	6	0	-9.460149	1.072526	-1.116199
35	1	0	-10.112080	1.480371	-0.333067
36	1	0	-9.384266	1.832626	-1.901008
37	1	0	-9.957702	0.193705	-1.535854
38	15	0	2.813191	0.149696	0.046270
39	6	0	3.478963	1.861202	-0.013761
40	6	0	4.573017	2.216897	-0.817751
41	6	0	2.909831	2.825075	0.835009
42	6	0	5.081593	3.517135	-0.775315
43	1	0	5.030730	1.487798	-1.478578
44	6	0	3.427249	4.118660	0.880654
45	1	0	2.064739	2.562642	1.465792
46	6	0	4.512038	4.468123	0.072130
47	1	0	5.926341	3.782807	-1.404365
48	1	0	2.981893	4.854106	1.544381
49	1	0	4.911069	5.477731	0.103679
50	6	0	3.639566	-0.591715	1.506014
51	6	0	5.043836	-0.617224	1.587077
52	6	0	2.882200	-1.076408	2.581296
53	6	0	5.671653	-1.140901	2.715452
54	1	0	5.646954	-0.223294	0.774082
55	6	0	3.515448	-1.592109	3.714323
56	1	0	1.798620	-1.041130	2.534954
57	6	0	4.908323	-1.629658	3.780105
58	1	0	6.756301	-1.160078	2.767839
59	1	0	2.919096	-1.961049	4.543688
60	1	0	5.400623	-2.031883	4.660719
61	6	0	3.440218	-0.711354	-1.447392
62	6	0	3.132397	-0.167676	-2.710783
63	6	0	4.085875	-1.957187	-1.381263
64	6	0	3.477887	-0.850208	-3.877516
65	1	0	2.647402	0.802449	-2.782901
66	6	0	4.426342	-2.636165	-2.552935
67	1	0	4.336596	-2.391692	-0.418868
68	6	0	4.123396	-2.086976	-3.800519
69	1	0	3.248661	-0.413169	-4.845192
70	1	0	4.934612	-3.593883	-2.488261
71	1	0	4.393476	-2.617315	-4.708919
72	1	0	-0.084171	-2.268619	-1.713577

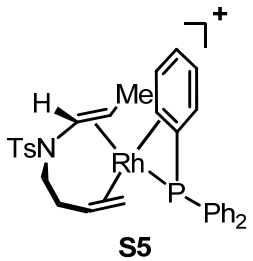


S4-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.789511	-0.383349	-1.463759
2	1	0	1.683755	0.707141	-2.208042
3	6	0	0.042777	1.371609	-2.628184
4	6	0	-1.497642	-2.774264	-0.899128
5	6	0	-0.134567	-2.520777	-1.488969
6	6	0	-2.657505	-1.854095	-1.340133
7	7	0	-2.532709	-0.514979	-0.752811
8	6	0	-4.935521	0.141389	0.474922
9	6	0	-5.261111	1.447182	0.088321
10	6	0	-6.586996	1.744941	-0.203312
11	6	0	-7.593140	0.766704	-0.110050
12	6	0	-7.233247	-0.528584	0.288874
13	6	0	-5.910734	-0.853381	0.586103
14	16	0	-3.248606	-0.257014	0.855866
15	8	0	-2.555557	0.921715	1.375703
16	8	0	-3.191648	-1.554870	1.521923
17	1	0	-1.430785	1.190434	-0.487308
18	1	0	-1.347192	-0.197487	-3.280409
19	1	0	0.431945	1.530433	-3.629706
20	1	0	0.087699	2.245659	-1.983056
21	1	0	-3.609161	-2.276585	-1.013724
22	1	0	-2.707785	-1.752275	-2.428460
23	1	0	-1.451759	-2.773286	0.193547
24	1	0	-1.789113	-3.791039	-1.200903
25	1	0	1.974773	-2.816833	-1.175638
26	1	0	0.965003	-2.620849	0.349857
27	1	0	-4.497122	2.215798	0.036657
28	1	0	-6.850684	2.756299	-0.500618
29	1	0	-7.999188	-1.293787	0.377252
30	1	0	-5.643064	-1.850046	0.919945
31	6	0	-1.607991	0.371271	-1.177700
32	6	0	-1.014317	0.427906	-2.459312
33	6	0	-9.029587	1.118563	-0.405004

34	1	0	-9.464935	1.691454	0.423725
35	1	0	-9.111659	1.738776	-1.303979
36	1	0	-9.642844	0.224476	-0.547489
37	15	0	2.506618	0.124484	0.051854
38	6	0	2.634171	1.941215	0.369134
39	6	0	2.529819	2.489910	1.656286
40	6	0	2.893541	2.799258	-0.713827
41	6	0	2.671854	3.866959	1.850809
42	1	0	2.342295	1.851435	2.512162
43	6	0	3.044949	4.169850	-0.514933
44	1	0	2.995240	2.395410	-1.718194
45	6	0	2.928046	4.708986	0.769762
46	1	0	2.585729	4.275889	2.853438
47	1	0	3.254660	4.817104	-1.361815
48	1	0	3.039584	5.778262	0.924167
49	6	0	2.159041	-0.623443	1.694948
50	6	0	3.050100	-1.504726	2.324492
51	6	0	0.913599	-0.363668	2.297902
52	6	0	2.706745	-2.103302	3.540135
53	1	0	4.010401	-1.729378	1.873230
54	6	0	0.578554	-0.959617	3.512638
55	1	0	0.201189	0.305507	1.823405
56	6	0	1.475207	-1.832437	4.136427
57	1	0	3.406901	-2.782588	4.017898
58	1	0	-0.384908	-0.745805	3.965860
59	1	0	1.211978	-2.300156	5.080676
60	6	0	4.222159	-0.348876	-0.398199
61	6	0	5.315978	0.073406	0.378375
62	6	0	4.455843	-1.117189	-1.547508
63	6	0	6.613388	-0.286703	0.017662
64	1	0	5.155450	0.689419	1.258619
65	6	0	5.757066	-1.474371	-1.907708
66	1	0	3.618138	-1.420218	-2.169570
67	6	0	6.835359	-1.063206	-1.123615
68	1	0	7.452079	0.044502	0.623153
69	1	0	5.926300	-2.067785	-2.801580
70	1	0	7.847918	-1.338953	-1.403670
71	6	0	1.024886	-2.538570	-0.730657
72	1	0	-0.048128	-2.686807	-2.564605

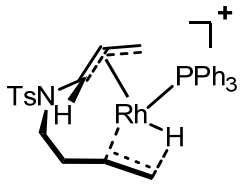


S5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.810693	-1.003062	-0.823698
2	6	0	0.215080	-3.931100	-0.750474
3	6	0	1.295030	0.814878	-2.437103
4	6	0	-0.174025	0.445824	-2.334066
5	6	0	2.377320	-0.210851	-2.051706
6	7	0	2.288502	-0.722551	-0.676431
7	6	0	4.595975	0.346263	0.345231
8	6	0	5.360679	-0.773815	0.691890
9	6	0	6.736897	-0.729864	0.501883
10	6	0	7.365390	0.414027	-0.021971
11	6	0	6.571671	1.520754	-0.353058
12	6	0	5.188975	1.500250	-0.170881
13	16	0	2.836609	0.309100	0.613538
14	8	0	2.528126	-0.423955	1.842356
15	8	0	2.299500	1.657544	0.391448
16	1	0	1.338560	-1.910004	0.723894
17	1	0	1.006536	-2.558246	-2.277122
18	1	0	0.932468	-4.732511	-0.975009
19	1	0	0.035552	-3.941152	0.328802
20	1	0	3.359635	0.256319	-2.168862
21	1	0	2.374778	-1.080489	-2.715051
22	1	0	1.461211	1.714680	-1.841379
23	1	0	1.488515	1.096725	-3.484034
24	1	0	-1.847587	-0.582979	-3.241755
25	1	0	-0.239984	-1.412884	-3.471944
26	1	0	4.887705	-1.655003	1.112762
27	1	0	7.338090	-1.594677	0.769612
28	1	0	7.040573	2.415346	-0.753303
29	1	0	4.580941	2.366010	-0.409565
30	6	0	1.388289	-1.723836	-0.345490
31	6	0	0.760982	-2.599574	-1.220646
32	6	0	8.863465	0.451303	-0.195246

33	1	0	9.361750	0.593308	0.772281
34	1	0	9.239864	-0.486675	-0.617319
35	1	0	9.173071	1.270743	-0.850049
36	15	0	-2.551802	0.301221	0.009097
37	6	0	-1.936318	-0.482222	1.544701
38	6	0	-1.295007	0.205746	2.593408
39	6	0	-1.939013	-1.899230	1.548425
40	6	0	-0.700057	-0.504975	3.630626
41	1	0	-1.270711	1.290323	2.595967
42	6	0	-1.335163	-2.602138	2.601010
43	1	0	-2.496092	-2.447092	0.788925
44	6	0	-0.717091	-1.906695	3.636872
45	1	0	-0.217503	0.033245	4.440668
46	1	0	-1.370300	-3.687697	2.612681
47	1	0	-0.251883	-2.449035	4.454488
48	6	0	-2.459848	2.115773	0.171397
49	6	0	-3.615104	2.914154	0.157573
50	6	0	-1.195394	2.726034	0.281340
51	6	0	-3.506559	4.301357	0.264606
52	1	0	-4.595494	2.458467	0.065692
53	6	0	-1.098544	4.112157	0.399659
54	1	0	-0.288420	2.127078	0.287150
55	6	0	-2.251951	4.901058	0.388284
56	1	0	-4.404666	4.911878	0.253242
57	1	0	-0.119888	4.573037	0.495887
58	1	0	-2.172396	5.980981	0.472742
59	6	0	-4.305605	-0.162856	-0.188968
60	6	0	-5.158280	-0.299900	0.919747
61	6	0	-4.811666	-0.372573	-1.482033
62	6	0	-6.498026	-0.639513	0.731311
63	1	0	-4.777740	-0.143628	1.924944
64	6	0	-6.154177	-0.705690	-1.664398
65	1	0	-4.159184	-0.277456	-2.345769
66	6	0	-6.996433	-0.840681	-0.558564
67	1	0	-7.152263	-0.746556	1.591555
68	1	0	-6.539463	-0.865498	-2.667048
69	1	0	-8.040040	-1.105477	-0.700993
70	6	0	-0.809627	-0.664799	-2.926743
71	1	0	-0.720365	-4.188140	-1.260326
72	1	0	-0.794520	1.324470	-2.173559

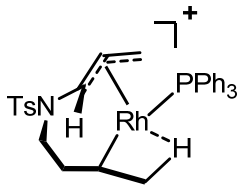


S6-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.492649	0.479653	-0.355238
2	1	0	-0.802862	1.021479	1.092415
3	6	0	-0.423621	2.639799	0.386281
4	6	0	2.991247	1.656813	-1.003836
5	6	0	1.996398	2.675483	-0.397974
6	6	0	0.522620	2.462215	-0.642105
7	6	0	-0.125030	-1.385915	-1.407136
8	7	0	2.944570	0.373325	-0.296241
9	6	0	5.558323	-0.181423	0.450301
10	6	0	5.831016	-1.494031	0.046138
11	6	0	7.086235	-1.783695	-0.475428
12	6	0	8.074032	-0.789730	-0.597351
13	6	0	7.771626	0.511152	-0.170612
14	6	0	6.520193	0.827684	0.355683
15	16	0	3.972182	0.200831	1.149203
16	8	0	3.426743	-0.965444	1.839266
17	8	0	4.019704	1.525892	1.761761
18	1	0	1.811152	-1.197722	0.379311
19	1	0	1.243168	-0.031132	-2.453442
20	1	0	-0.753085	-1.559997	-2.274730
21	1	0	-0.126116	-2.186794	-0.670741
22	1	0	4.007925	2.047054	-0.928842
23	1	0	2.796589	1.477595	-2.065285
24	1	0	2.204653	2.755977	0.672506
25	1	0	2.254911	3.647345	-0.843012
26	1	0	-1.419467	3.012652	0.171843
27	1	0	-0.062611	2.844886	1.392144
28	1	0	5.085401	-2.273802	0.161037
29	1	0	7.311035	-2.801287	-0.783273
30	1	0	8.529142	1.286742	-0.238571
31	1	0	6.301611	1.828250	0.712723
32	6	0	1.893446	-0.466481	-0.419958
33	6	0	1.038068	-0.578087	-1.537942

34	6	0	9.425060	-1.123622	-1.178384
35	1	0	9.820893	-2.052896	-0.754638
36	1	0	9.356401	-1.267497	-2.264290
37	1	0	10.151093	-0.327130	-0.993789
38	15	0	-2.784454	-0.168619	0.003387
39	6	0	-3.544245	-1.230878	-1.302585
40	6	0	-4.383858	-0.712009	-2.298859
41	6	0	-3.236426	-2.603817	-1.320480
42	6	0	-4.898990	-1.546901	-3.293839
43	1	0	-4.655689	0.337671	-2.296841
44	6	0	-3.756570	-3.433561	-2.312564
45	1	0	-2.607159	-3.032782	-0.545832
46	6	0	-4.586585	-2.906034	-3.305388
47	1	0	-5.553696	-1.130816	-4.054231
48	1	0	-3.517791	-4.493275	-2.306393
49	1	0	-4.992176	-3.553150	-4.077579
50	6	0	-3.108297	-1.099020	1.553285
51	6	0	-4.335195	-1.760614	1.748161
52	6	0	-2.137252	-1.152219	2.564608
53	6	0	-4.584147	-2.444773	2.937097
54	1	0	-5.092295	-1.745939	0.969909
55	6	0	-2.389957	-1.839840	3.753506
56	1	0	-1.178148	-0.663872	2.417850
57	6	0	-3.612957	-2.484372	3.941691
58	1	0	-5.535285	-2.950079	3.077633
59	1	0	-1.628305	-1.875045	4.526952
60	1	0	-3.808497	-3.021965	4.865008
61	6	0	-3.842321	1.339748	0.065147
62	6	0	-3.687161	2.311549	-0.941040
63	6	0	-4.774268	1.567301	1.087528
64	6	0	-4.462775	3.471116	-0.935777
65	1	0	-2.958740	2.159867	-1.734826
66	6	0	-5.540807	2.735594	1.096077
67	1	0	-4.905121	0.839629	1.880843
68	6	0	-5.391803	3.685788	0.085733
69	1	0	-4.338498	4.207116	-1.725096
70	1	0	-6.256875	2.898788	1.896328
71	1	0	-5.991733	4.591010	0.094758
72	1	0	0.191697	2.640515	-1.666614

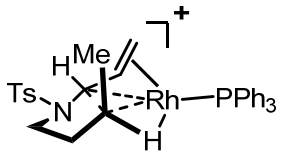


S7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.553988	-0.881997	-0.561488
2	6	0	0.534528	-2.985107	0.596564
3	6	0	-2.973234	-1.930829	-0.743841
4	6	0	-1.944090	-2.821511	-0.020483
5	6	0	-0.493262	-2.703008	-0.452589
6	6	0	0.319823	0.546780	-2.096009
7	7	0	-2.789069	-0.513810	-0.402720
8	6	0	-5.299626	0.338439	0.390532
9	6	0	-5.581350	1.470747	-0.382666
10	6	0	-6.876691	1.651868	-0.853305
11	6	0	-7.896230	0.728915	-0.559893
12	6	0	-7.581207	-0.390453	0.223963
13	6	0	-6.289950	-0.595239	0.707198
14	16	0	-3.655296	0.103460	1.017865
15	8	0	-3.025201	1.393570	1.289178
16	8	0	-3.660472	-0.984722	1.993367
17	1	0	-1.520039	1.101222	-0.292928
18	1	0	-1.220440	-0.918874	-2.656907
19	1	0	0.934484	0.361990	-2.973270
20	1	0	0.410047	1.551827	-1.691625
21	1	0	-3.984997	-2.217381	-0.450428
22	1	0	-2.917885	-2.035322	-1.831718
23	1	0	-2.042082	-2.631162	1.052914
24	1	0	-2.264758	-3.861284	-0.184505
25	1	0	1.323099	-3.677298	0.294938
26	1	0	0.110425	-3.265175	1.565375
27	1	0	-4.807403	2.200586	-0.596194
28	1	0	-7.105939	2.528970	-1.452324
29	1	0	-8.358343	-1.109173	0.468331
30	1	0	-6.056924	-1.449029	1.334269
31	6	0	-1.688707	0.161173	-0.808845
32	6	0	-0.908004	-0.161650	-1.945957
33	6	0	-9.302806	0.960252	-1.052465

34	1	0	-9.825058	1.676302	-0.404780
35	1	0	-9.308509	1.376293	-2.065223
36	1	0	-9.885514	0.034697	-1.056784
37	15	0	2.676907	0.244538	0.004559
38	6	0	3.292081	1.626968	-1.045770
39	6	0	4.274010	1.438451	-2.028745
40	6	0	2.708906	2.898117	-0.895700
41	6	0	4.667995	2.503538	-2.842689
42	1	0	4.744709	0.468782	-2.154572
43	6	0	3.107386	3.957984	-1.709687
44	1	0	1.960163	3.068858	-0.126176
45	6	0	4.086869	3.762390	-2.686893
46	1	0	5.436940	2.346919	-3.593810
47	1	0	2.656706	4.937364	-1.576392
48	1	0	4.398121	4.588835	-3.319076
49	6	0	2.727913	0.932636	1.704918
50	6	0	3.794947	1.740468	2.138924
51	6	0	1.678806	0.651923	2.593294
52	6	0	3.816044	2.234520	3.442632
53	1	0	4.601798	1.991070	1.456454
54	6	0	1.701752	1.150439	3.897350
55	1	0	0.832841	0.058415	2.256497
56	6	0	2.771757	1.938130	4.323555
57	1	0	4.644825	2.855923	3.769378
58	1	0	0.880609	0.930834	4.573389
59	1	0	2.789291	2.329139	5.336737
60	6	0	3.969542	-1.065454	-0.089525
61	6	0	3.913249	-1.961975	-1.172693
62	6	0	4.979361	-1.222610	0.871090
63	6	0	4.858821	-2.979700	-1.302454
64	1	0	3.128258	-1.858990	-1.919500
65	6	0	5.917281	-2.249565	0.743743
66	1	0	5.033767	-0.553141	1.722894
67	6	0	5.862344	-3.125730	-0.341611
68	1	0	4.808931	-3.659206	-2.148587
69	1	0	6.692519	-2.362811	1.496091
70	1	0	6.595239	-3.921609	-0.436720
71	1	0	1.128788	-2.025982	0.882947
72	1	0	-0.292658	-3.174709	-1.418929



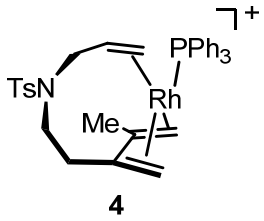
S8-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.778157	-1.063309	-0.411709
2	6	0	1.327183	-1.514174	-1.627463
3	6	0	0.737655	-2.956535	-0.058621
4	6	0	3.157879	-2.276203	-0.388160
5	6	0	2.105144	-2.837112	0.591169
6	6	0	-0.933367	-1.157184	-2.521307
7	6	0	0.480560	-4.214922	-0.872940
8	7	0	2.570465	-1.126287	-1.107650
9	6	0	4.464408	0.571005	-0.095154
10	6	0	5.020138	0.526502	1.184870
11	6	0	6.395288	0.711152	1.325426
12	6	0	7.215373	0.941816	0.212081
13	6	0	6.621850	0.985434	-1.062287
14	6	0	5.252866	0.809601	-1.227196
15	16	0	2.701571	0.421358	-0.288702
16	8	0	2.074964	0.319159	1.039958
17	8	0	2.230290	1.421146	-1.247907
18	1	0	1.427638	-2.426246	-2.209555
19	1	0	0.533867	0.459841	-2.222071
20	1	0	-1.669851	-0.514993	-2.994737
21	1	0	-1.003049	-2.206793	-2.804238
22	1	0	3.426972	-3.016924	-1.149464
23	1	0	4.078163	-1.975406	0.113427
24	1	0	2.443656	-3.823069	0.937481
25	1	0	2.048288	-2.179309	1.461638
26	1	0	0.447272	-5.087443	-0.205892
27	1	0	1.264010	-4.415119	-1.614334
28	1	0	4.385616	0.361647	2.048937
29	1	0	6.836127	0.680478	2.317845
30	1	0	7.242888	1.168313	-1.935147
31	1	0	4.801253	0.863037	-2.212163
32	6	0	0.305626	-0.592484	-2.106954
33	1	0	-0.480429	-4.175071	-1.396858
34	6	0	8.699368	1.161543	0.369740

35	1	0	8.957743	2.212273	0.187167
36	1	0	9.040573	0.905616	1.376684
37	1	0	9.268657	0.560840	-0.348154
38	15	0	-2.444360	0.419932	0.031348
39	6	0	-2.462568	-0.255224	1.733289
40	6	0	-3.566720	-0.914018	2.302011
41	6	0	-1.218885	-0.267968	2.409720
42	6	0	-3.436247	-1.553226	3.533536
43	1	0	-4.521788	-0.918009	1.785979
44	6	0	-1.099855	-0.923796	3.639477
45	1	0	-0.362354	0.270488	2.004853
46	6	0	-2.205605	-1.563241	4.200753
47	1	0	-4.297323	-2.044455	3.977442
48	1	0	-0.146777	-0.917612	4.160245
49	1	0	-2.114504	-2.064936	5.159698
50	6	0	-4.111977	0.247333	-0.689911
51	6	0	-5.024701	1.314274	-0.710101
52	6	0	-4.485772	-0.993661	-1.234095
53	6	0	-6.295360	1.134993	-1.258010
54	1	0	-4.744552	2.281111	-0.304327
55	6	0	-5.758915	-1.168082	-1.775129
56	1	0	-3.776252	-1.817435	-1.234923
57	6	0	-6.663840	-0.103348	-1.788267
58	1	0	-6.996386	1.964342	-1.271977
59	1	0	-6.041558	-2.129975	-2.192940
60	1	0	-7.653005	-0.237527	-2.216341
61	6	0	-2.077196	2.203952	0.139826
62	6	0	-2.385516	2.948097	1.290311
63	6	0	-1.490654	2.844933	-0.963350
64	6	0	-2.112143	4.316068	1.330164
65	1	0	-2.834068	2.463103	2.152155
66	6	0	-1.224462	4.212605	-0.918982
67	1	0	-1.238392	2.278980	-1.855657
68	6	0	-1.533285	4.948271	0.227697
69	1	0	-2.351206	4.886243	2.223123
70	1	0	-0.767762	4.700696	-1.774705
71	1	0	-1.319451	6.012504	0.263123
72	1	0	-0.039612	-2.867798	0.713883

11.Computed Coordinates of All Stationary Points Using M06 Method



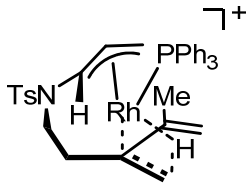
4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.828060	0.318159	-1.982430
2	6	0	0.391740	0.730754	-1.815690
3	6	0	-0.572242	0.443837	-2.751607
4	6	0	2.717861	-1.950638	-1.285622
5	6	0	1.803894	-3.031982	-0.718937
6	6	0	0.338374	-2.928328	-1.064553
7	6	0	-0.651717	-2.964475	0.012380
8	6	0	-0.074543	-2.713373	-2.375554
9	6	0	-0.208623	-3.025825	1.440921
10	6	0	-2.004813	-2.798336	-0.288716
11	7	0	2.317609	-0.588450	-0.947160
12	6	0	4.513680	0.413183	0.379238
13	6	0	5.446277	-0.566706	0.718570
14	6	0	6.796313	-0.297855	0.543283
15	6	0	7.228870	0.933795	0.041886
16	6	0	6.271005	1.900947	-0.279950
17	6	0	4.915821	1.653052	-0.114607
18	16	0	2.788757	0.056358	0.518839
19	8	0	2.625617	-1.004636	1.506532
20	8	0	2.061597	1.315374	0.636213
21	1	0	1.964122	-0.189640	-2.946678
22	1	0	2.448868	1.228077	-2.018897
23	1	0	0.207682	1.478975	-1.043553
24	1	0	-1.516443	0.992248	-2.763713
25	1	0	-0.322838	-0.103184	-3.662462
26	1	0	2.773408	-2.007922	-2.380289
27	1	0	3.742967	-2.141361	-0.931435
28	1	0	2.160352	-4.003819	-1.096785
29	1	0	1.944260	-3.051902	0.364191
30	1	0	-1.043503	-3.028626	-2.761591
31	1	0	0.682916	-2.561842	-3.145389

32	1	0	0.228300	-4.013903	1.647946
33	1	0	0.551276	-2.270521	1.675833
34	1	0	-1.055490	-2.889093	2.121177
35	1	0	-2.710897	-2.704684	0.536542
36	1	0	-2.448093	-3.117128	-1.233064
37	1	0	5.113532	-1.512343	1.142602
38	1	0	7.534564	-1.053330	0.810948
39	1	0	6.599177	2.869380	-0.656530
40	1	0	4.175381	2.420752	-0.331419
41	45	0	-0.939031	-1.044925	-1.121168
42	15	0	-2.274090	0.408320	0.180676
43	6	0	-2.000725	2.208249	-0.018770
44	6	0	-1.146996	2.938415	0.813676
45	6	0	-2.598306	2.847274	-1.114472
46	6	0	-0.898400	4.282459	0.553392
47	1	0	-0.676620	2.468364	1.674910
48	6	0	-2.345701	4.189455	-1.369543
49	1	0	-3.288300	2.300177	-1.759098
50	6	0	-1.492594	4.908719	-0.536989
51	1	0	-0.239398	4.842633	1.213567
52	1	0	-2.824706	4.677620	-2.216115
53	1	0	-1.296677	5.960620	-0.735503
54	6	0	-1.992475	0.016954	1.938783
55	6	0	-3.007450	-0.450405	2.779503
56	6	0	-0.678449	0.090034	2.421852
57	6	0	-2.711624	-0.817016	4.089742
58	1	0	-4.030311	-0.534816	2.414463
59	6	0	-0.392788	-0.262887	3.734884
60	1	0	0.137491	0.404223	1.767724
61	6	0	-1.409333	-0.718235	4.570599
62	1	0	-3.506826	-1.179587	4.738396
63	1	0	0.633491	-0.201349	4.092430
64	1	0	-1.185215	-1.003955	5.596507
65	6	0	-4.056416	0.239421	-0.157743
66	6	0	-4.998710	0.983509	0.564932
67	6	0	-4.486109	-0.574137	-1.208493
68	6	0	-6.349431	0.882105	0.258692
69	1	0	-4.671740	1.648936	1.364864
70	6	0	-5.839577	-0.666415	-1.520588
71	1	0	-3.747129	-1.125830	-1.793462
72	6	0	-6.770192	0.055807	-0.782196
73	1	0	-7.077607	1.456489	0.827718
74	1	0	-6.165647	-1.298690	-2.344077
75	1	0	-7.828973	-0.015600	-1.023160

76	6	0	8.689589	1.225600	-0.108958
77	1	0	8.873162	1.984401	-0.878320
78	1	0	9.109086	1.608440	0.831800
79	1	0	9.257414	0.325433	-0.372395



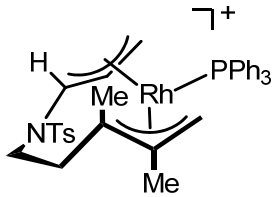
12-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.590692	-0.980048	-0.372462
2	1	0	0.153787	-0.092296	0.909041
3	6	0	-0.042895	-1.745823	1.612459
4	6	0	-2.830234	-1.888063	-0.575970
5	6	0	-2.046965	-2.759293	0.437547
6	6	0	-0.548954	-2.593085	0.566911
7	6	0	0.395871	-3.285785	-0.287531
8	6	0	0.664790	-0.324543	-2.534041
9	6	0	-0.080885	-4.155973	-1.411995
10	6	0	1.759373	-3.033006	-0.128341
11	7	0	-2.516642	-0.462615	-0.621182
12	6	0	-4.868393	0.531351	0.291196
13	6	0	-5.309497	1.281786	-0.799044
14	6	0	-6.665800	1.317978	-1.073976
15	6	0	-7.585521	0.624750	-0.274738
16	6	0	-7.110885	-0.115886	0.810313
17	6	0	-5.754327	-0.168101	1.105230
18	16	0	-3.147564	0.503362	0.661079
19	8	0	-2.560495	1.819275	0.464750
20	8	0	-2.943069	-0.225833	1.906378
21	1	0	-1.143988	1.048840	-1.060590
22	1	0	-1.009785	-1.682032	-2.565972
23	1	0	1.224627	-0.923335	-3.251531
24	1	0	0.948456	0.727807	-2.480989
25	1	0	-3.900189	-1.980704	-0.347207

26	1	0	-2.718356	-2.270980	-1.597296
27	1	0	-2.487836	-2.591510	1.425636
28	1	0	-2.272396	-3.803137	0.175449
29	1	0	0.888759	-1.966433	2.134526
30	1	0	-0.795336	-1.256595	2.233241
31	1	0	-0.215170	-5.187806	-1.057482
32	1	0	-1.039130	-3.836927	-1.837869
33	1	0	0.659524	-4.185921	-2.220593
34	1	0	2.453609	-3.429495	-0.869045
35	1	0	2.203149	-2.792778	0.835402
36	1	0	-4.598344	1.833471	-1.411701
37	1	0	-7.028224	1.899667	-1.921021
38	1	0	-7.818070	-0.656005	1.438503
39	1	0	-5.382208	-0.729998	1.959609
40	6	0	-1.326546	-0.018249	-1.186234
41	6	0	-0.638793	-0.726843	-2.197660
42	6	0	-9.050648	0.703813	-0.569283
43	1	0	-9.467967	1.653428	-0.206752
44	1	0	-9.247768	0.658181	-1.647161
45	1	0	-9.606728	-0.105401	-0.083190
46	15	0	2.445395	0.450202	0.023824
47	6	0	2.009086	2.186766	-0.354182
48	6	0	2.794857	2.991138	-1.185193
49	6	0	0.798844	2.698909	0.136141
50	6	0	2.387852	4.285380	-1.499203
51	1	0	3.728626	2.611273	-1.595886
52	6	0	0.400395	3.993306	-0.171733
53	1	0	0.147081	2.082385	0.757388
54	6	0	1.196044	4.789817	-0.991662
55	1	0	3.009589	4.900222	-2.147172
56	1	0	-0.541955	4.369939	0.221684
57	1	0	0.881734	5.801214	-1.241607
58	6	0	4.011308	0.114946	-0.849753
59	6	0	5.175003	0.799168	-0.470200
60	6	0	4.077217	-0.828429	-1.875593
61	6	0	6.374461	0.553813	-1.125152
62	1	0	5.139701	1.521005	0.346756
63	6	0	5.282199	-1.076300	-2.527777
64	1	0	3.180155	-1.382756	-2.149933
65	6	0	6.428040	-0.383040	-2.155837
66	1	0	7.272929	1.090508	-0.827130
67	1	0	5.326288	-1.815844	-3.324972
68	1	0	7.370704	-0.576709	-2.663992
69	6	0	2.944361	0.379254	1.782313

70	6	0	2.482729	1.294387	2.730004
71	6	0	3.722391	-0.708585	2.198992
72	6	0	2.793003	1.121389	4.075906
73	1	0	1.889714	2.154461	2.421097
74	6	0	4.028234	-0.877579	3.544333
75	1	0	4.113090	-1.413787	1.463251
76	6	0	3.559417	0.035262	4.485480
77	1	0	2.435805	1.844613	4.806485
78	1	0	4.640580	-1.721211	3.857341
79	1	0	3.798734	-0.097025	5.538720



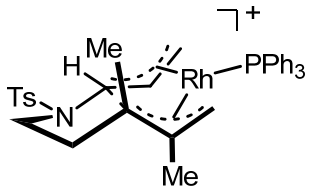
14

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.324350	-0.302815	-1.843319
2	6	0	0.425015	0.783042	-1.860767
3	6	0	-0.774652	0.537681	-2.552645
4	6	0	3.008414	-1.851523	-1.174097
5	6	0	2.120529	-2.854071	-0.414700
6	6	0	0.660107	-2.870067	-0.775157
7	6	0	-0.307579	-2.817535	0.260158
8	6	0	0.363318	-3.489824	-2.122285
9	6	0	0.075068	-2.750483	1.714046
10	6	0	-1.669760	-2.655885	-0.095676
11	7	0	2.520431	-0.470150	-1.152575
12	6	0	4.615597	0.563484	0.188820
13	6	0	5.409381	-0.094734	1.123417
14	6	0	6.787211	0.069474	1.058281
15	6	0	7.372062	0.879498	0.081389
16	6	0	6.543547	1.525666	-0.846023
17	6	0	5.167446	1.379188	-0.799013
18	16	0	2.862725	0.422448	0.284153

19	8	0	2.513863	-0.389792	1.444669
20	8	0	2.243111	1.723619	0.099565
21	1	0	1.289101	-0.960120	-2.716662
22	1	0	0.555839	1.663574	-1.238465
23	1	0	-1.538568	1.312353	-2.572188
24	1	0	-0.798212	-0.167094	-3.388652
25	1	0	3.109434	-2.127932	-2.232648
26	1	0	4.020991	-1.869206	-0.753228
27	1	0	2.539671	-3.849428	-0.637484
28	1	0	2.257922	-2.684610	0.656071
29	1	0	0.458644	-4.584526	-2.047118
30	1	0	1.089437	-3.169359	-2.881139
31	1	0	0.507150	-3.714461	2.020010
32	1	0	0.810351	-1.969488	1.937002
33	1	0	-0.804976	-2.570101	2.340017
34	1	0	-2.402747	-2.572514	0.707939
35	1	0	-2.065694	-3.080162	-1.018749
36	1	0	4.948661	-0.714469	1.890042
37	1	0	7.423740	-0.436725	1.782914
38	1	0	6.992248	2.158905	-1.610692
39	1	0	4.523095	1.891430	-1.511478
40	45	0	-0.689782	-0.887399	-0.909695
41	1	0	-0.633831	-3.271840	-2.517273
42	15	0	-2.398172	0.327244	0.112232
43	6	0	8.854540	1.079334	0.037223
44	1	0	9.223885	1.133725	-0.993831
45	1	0	9.132859	2.022129	0.528207
46	1	0	9.388671	0.272815	0.551829
47	6	0	-2.404696	2.137063	-0.196873
48	6	0	-1.620709	3.027635	0.542324
49	6	0	-3.172055	2.629824	-1.262343
50	6	0	-1.606299	4.382048	0.221525
51	1	0	-1.030906	2.679427	1.387957
52	6	0	-3.151582	3.982319	-1.580322
53	1	0	-3.806249	1.953866	-1.838302
54	6	0	-2.365954	4.861338	-0.839694
55	1	0	-0.999054	5.064488	0.812784
56	1	0	-3.758515	4.350949	-2.404985
57	1	0	-2.352414	5.920932	-1.086816
58	6	0	-2.063269	0.130206	1.897034
59	6	0	-3.010688	-0.360186	2.800140
60	6	0	-0.762709	0.400650	2.347737
61	6	0	-2.668134	-0.551987	4.136108
62	1	0	-4.018007	-0.602761	2.464585

63	6	0	-0.430757	0.221824	3.684609
64	1	0	0.008517	0.729403	1.648304
65	6	0	-1.383586	-0.254886	4.581162
66	1	0	-3.411760	-0.935915	4.831903
67	1	0	0.583239	0.436916	4.016825
68	1	0	-1.122510	-0.404061	5.627069
69	6	0	-4.136368	-0.118092	-0.199546
70	6	0	-5.177029	0.529428	0.481140
71	6	0	-4.442380	-1.043786	-1.198491
72	6	0	-6.498522	0.218729	0.189829
73	1	0	-4.951130	1.288596	1.230665
74	6	0	-5.768201	-1.347551	-1.494743
75	1	0	-3.630980	-1.513010	-1.756009
76	6	0	-6.794138	-0.722813	-0.794716
77	1	0	-7.302923	0.719923	0.724488
78	1	0	-5.998378	-2.069153	-2.276017
79	1	0	-7.831328	-0.960064	-1.023584



16-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.952801	-0.751816	-0.967221
2	6	0	1.612431	-0.642900	-1.344853
3	6	0	0.963520	-2.388989	-0.856749
4	6	0	3.426661	-2.023306	-0.936835
5	6	0	2.324351	-2.918060	-0.381500
6	6	0	-0.168458	0.858022	-2.217848
7	6	0	-0.086360	-2.364875	0.210950
8	6	0	0.564099	-3.050921	-2.171838
9	6	0	0.290865	-2.051565	1.625367
10	6	0	-1.419473	-2.706406	-0.081658
11	7	0	2.924301	-0.658060	-0.782518
12	6	0	5.077116	0.489292	0.309079

13	6	0	6.102887	-0.166645	0.984244
14	6	0	7.416266	0.174772	0.691609
15	6	0	7.712710	1.161458	-0.253122
16	6	0	6.657316	1.805051	-0.910696
17	6	0	5.338750	1.479526	-0.635781
18	16	0	3.401637	0.093501	0.689885
19	8	0	3.392082	-0.899091	1.757205
20	8	0	2.612078	1.308438	0.820727
21	1	0	1.719753	-0.889299	-2.411213
22	1	0	0.888400	1.203511	-0.352146
23	1	0	-0.690235	1.812611	-2.182415
24	1	0	-0.065631	0.412537	-3.211195
25	1	0	3.604374	-2.196011	-2.008379
26	1	0	4.383790	-2.151462	-0.420739
27	1	0	2.436617	-3.957816	-0.718849
28	1	0	2.398797	-2.907901	0.709537
29	1	0	0.252639	-4.090005	-1.998353
30	1	0	1.419905	-3.077851	-2.858900
31	1	0	0.722397	-2.941492	2.108526
32	1	0	1.038172	-1.252968	1.711389
33	1	0	-0.596506	-1.767030	2.201907
34	1	0	-2.126554	-2.767031	0.746532
35	1	0	-1.675424	-3.308670	-0.955025
36	1	0	5.867570	-0.924578	1.728690
37	1	0	8.231189	-0.330911	1.208775
38	1	0	6.879419	2.575244	-1.648406
39	1	0	4.519010	1.984452	-1.144516
40	6	0	0.725351	0.531919	-1.188854
41	1	0	-0.258601	-2.544131	-2.700688
42	6	0	9.133294	1.538428	-0.537025
43	1	0	9.500319	2.260042	0.205938
44	1	0	9.797755	0.667224	-0.494271
45	1	0	9.240706	2.003529	-1.523557
46	15	0	-2.643356	0.331672	0.044657
47	6	0	-2.357622	0.274533	1.840367
48	6	0	-3.163668	-0.486127	2.692495
49	6	0	-1.229451	0.924485	2.361014
50	6	0	-2.855315	-0.576444	4.047567
51	1	0	-4.036136	-1.008569	2.301812
52	6	0	-0.934297	0.843358	3.715308
53	1	0	-0.568869	1.490869	1.702956
54	6	0	-1.747800	0.091085	4.560470
55	1	0	-3.488426	-1.170084	4.704093
56	1	0	-0.058901	1.356488	4.107986

57	1	0	-1.513000	0.021196	5.620655
58	6	0	-4.295903	-0.370308	-0.270257
59	6	0	-5.423440	0.236334	0.299502
60	6	0	-4.457826	-1.463982	-1.121919
61	6	0	-6.689683	-0.271033	0.041319
62	1	0	-5.309840	1.108188	0.945190
63	6	0	-5.729662	-1.963198	-1.387040
64	1	0	-3.581263	-1.916466	-1.587163
65	6	0	-6.842592	-1.371652	-0.800341
66	1	0	-7.562229	0.197602	0.491998
67	1	0	-5.850202	-2.813191	-2.055549
68	1	0	-7.837088	-1.763839	-1.003923
69	6	0	-2.871016	2.087523	-0.401179
70	6	0	-2.796286	3.136653	0.517154
71	6	0	-3.190921	2.362564	-1.737648
72	6	0	-3.022416	4.445835	0.097565
73	1	0	-2.577372	2.938251	1.564984
74	6	0	-3.418439	3.667544	-2.149898
75	1	0	-3.270109	1.544752	-2.456894
76	6	0	-3.328283	4.712631	-1.231327
77	1	0	-2.962920	5.258150	0.819188
78	1	0	-3.669952	3.872676	-3.188570
79	1	0	-3.505001	5.736647	-1.554173
