Supporting Information

Density Functional Theory Study of the Mechanisms and Stereochemistry of the Rh(I)-Catalyzed Intramolecular [3+2] Cycloadditions of 1-Ene- and 1-Yne-Vinylcyclopropanes

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Contents

1. Computational Details

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 criteria (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.[2d] The keyword "5D" in Gaussian 03 pragram was used to specify that five (instead of six) d-type STO 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 reactions of carbonyl rhodium(I) complexes and other Rh-catalyzed cycloadditions. 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 approach, where simple united atom topological model (UA0) was used to define the atomic radii. Solvation calculations were carried out at the optimized gas-phase geometry. The reported energies are the zero-point energy-corrected enthalpies (ΔH_{gas}), Gibbs free energies ($\Delta G_{gas\ 298K}$), both in the gas phase, and the Gibbs free energies in 1,2-dichloroethane solution ($\Delta G_{sol\ 298K}$). Unless specifically mentioned, all discussed relative energies in the paper are referred to the $\Delta G_{sol\ 298K}$.

(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.

(2) Other related computational references: (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785. (c) Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, 1986. (d) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299.

2. Comparison of DFT methods of M06 and B3LYP

We compared the computed energy profiles of the key alkene-insertion steps obtained from the M06//B3LYP and the B3LYP calculations. The M06 method is proved to perform better than B3LYP in calculating the energy barriers of several model catalytic reactions.[3] The M06 calculations were performed using Gaussian 09.[4] Single-point energies based on the structures obtained at the B3LYP level using the same basic set were obtained. Both cis-insertion (**17** → **20-TS**) and trans-insertion (**18** → **21-TS**) steps were calculated, and the results are shown in Figure S1.

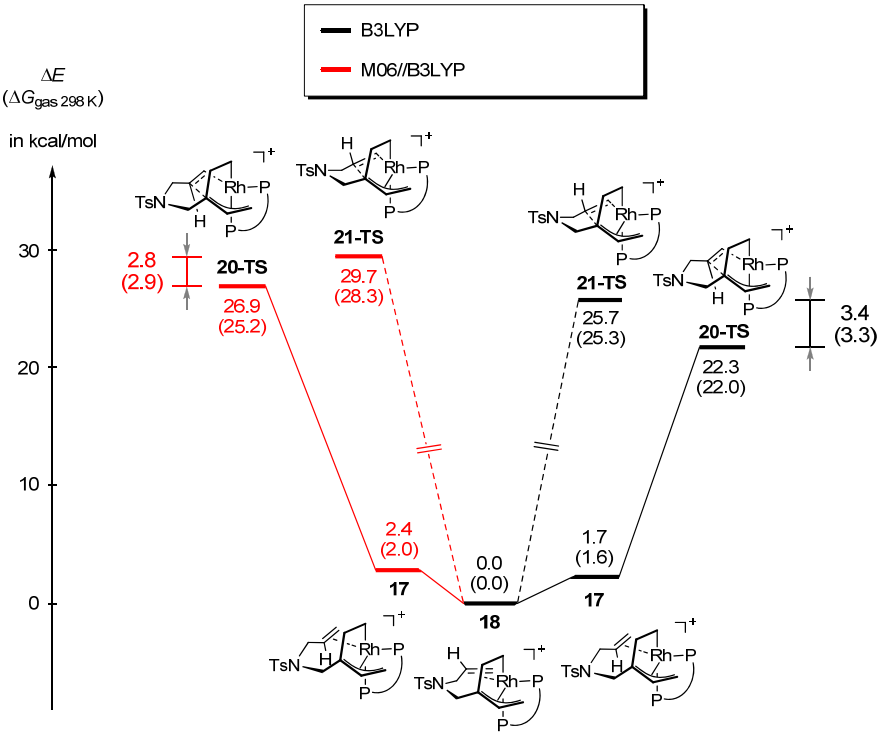


Figure S1. Comparison of the energy profiles for the key alkene-insertion steps computed by the M06 and B3LYP methods. Electronic energies (ΔE) and Gibbs free energies ($\Delta G_{\text{gas 298K}}$), both in the gas phase, are reported and compared.

The results indicate that, M06 method gives relatively higher activation energy barriers for the rate-determining alkene-insertion steps. The activation barriers computed by the M06 method are ca. 4 kcal/mol higher than those computed by the B3LYP method. The computed energy difference of the diastereomeric transition states of M06 method is very close to that obtained from the B3LYP (2.8 kcal/mol of M06 vs. 3.4 kcal/mol of B3LYP), indicating that both the B3LYP and

(3) Yang, K.; Zheng, J.; Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2010**, *132*, 164117.
(4) Full citation of Gaussian 09: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A. Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C. ; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, Revision A.02; Gaussian Inc.: Wallingford CT, 2009.

M06 methods can give the correct stereochemistry of the present [3+2] reactions. Because we here concern about the reaction mechanisms and stereochemistry, but not the absolute activation energies of these reactions, we regard that B3LYP is suitable for studying the mechanisms and stereochemistry of the Rh-catalyzed cycloadditions of vinylcyclopropanes.

3. Discussion on the Catalytic Species of the [3+2] Reactions

The optimal Rh(I)-catalyst used in the [3+2] cycloaddition reactions was prepared by treatment of $[Rh(CO)_2Cl]_2$ with $AgSbF_6$ and then with phosphine ligand dppp. Initially, cationic rhodium(I) species $[Rh(dppp)(CO)_m(solvent)_n]^+$ could be generated. Subsequently, this species binds the substrate. Then the resulting complex will undergo the ring-opening, insertion, reductive elimination, and ligand exchange reactions (Figure S2). Since the catalytic cycle proceeds through a coordinatively saturated 18-e intermediate **IN2**, it is clear that dissociation of CO from the rhodium center must occur prior to the formation of **IN2**.

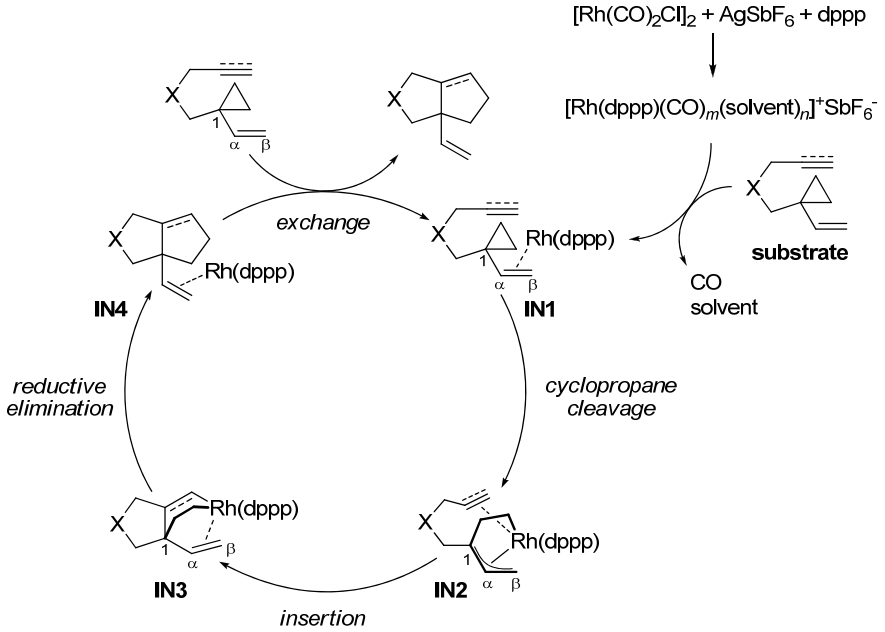
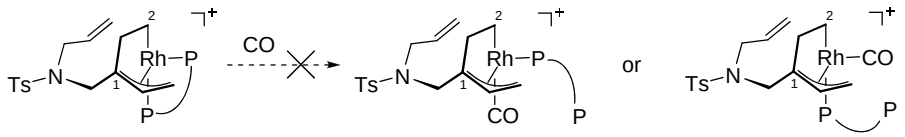


Figure S2. The [3+2] cycloaddition cycle.

Meanwhile, DFT calculations show that CO complexation to the rhodium center in **IN2** to replace one phosphine ligand of dppp (this makes dppp act as a monodentate ligand) is energetically much disfavored (Scheme S1). This suggests that CO is not involved in the catalytic cycle. Thus, it is reasonable to conclude that the catalytic species is $Rh(dppp)^+$ cation, and the CO ligand is not involved in the catalytic species.

Scheme S1[a]



	16	**S1**	**S2**
$\Delta G_{sol\ 298K}$	-7.2	1.5	8.3
($\Delta G_{gas\ 298K}$)	(-11.3)	(0.9)	(4.1)
[ΔH_{gas}]	[-9.8]	[-5.8]	[-0.5]

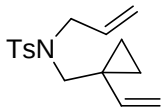
[a] Energies are reported in kcal/mol.

4. 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 (ΔH, ΔG, and ΔG_{sol}) at 298 K are reported in kcal/mol.

Structure	*E*	*H*	*G*	TCGFE	E_{sol}	G_{sol}	ΔH	ΔG	ΔG_{sol}
Potential energy surface for [3+2] reaction of 1-ene-VCP **1**									
1	−1225.224285	−1225.202396	−1225.276323	0.289757	−1225.562171	−1225.272414	0.0	0.0	0.0
2	−1225.287802	−1225.267954	−1225.336872	0.297924	−1225.635629	−1225.337705	–	–	–
12	−2294.689412	−2294.651381	−2294.761163	0.513158	−2295.305343	−2294.792185	−6.0	−6.8	−5.0
13	−2294.684078	−2294.647362	−2294.752364	0.518200	−2295.304470	−2294.786270	−3.5	−1.3	−1.3
14-TS	−2294.684185	−2294.646604	−2294.755504	0.512660	−2295.295053	−2294.782393	−3.0	−3.2	1.1
15-TS	−2294.669051	−2294.632846	−2294.735908	0.519042	−2295.289180	−2294.770138	5.6	9.1	8.8
16	−2294.695450	−2294.657314	−2294.768386	0.511626	−2295.307313	−2294.795687	−9.8	−11.3	−7.2
CO	−113.301878	−113.298573	−113.321016	−0.014102	−113.304047	−113.318149	–	–	–
S1	−2407.990993	−2407.949534	−2408.069955	0.512485	−2408.612399	−2408.099914	−5.8	0.9	1.5
S2	−2407.983041	−2407.941106	−2408.064790	0.508886	−2408.597963	−2408.089077	−0.5	4.1	8.3
17	−2294.704213	−2294.667889	−2294.770670	0.521040	−2295.328097	−2294.807057	−16.4	−12.7	−14.4
17'	−2294.701961	−2294.665969	−2294.766799	0.524334	−2295.325427	−2294.801093	−15.2	−10.3	−10.6
18	−2294.706943	−2294.670688	−2294.773233	0.521763	−2295.330849	−2294.809086	−18.2	−14.3	−15.6
19	−2294.710789	−2294.673564	−2294.778711	0.517821	−2295.315902	−2294.798081	−20.0	−17.8	−8.7
20-TS	−2294.671380	−2294.635410	−2294.738127	0.519064	−2295.292868	−2294.773804	4.0	7.7	6.5
20-TS'	−2294.624864	−2294.589494	−2294.688944	0.522904	−2295.248827	−2294.725923	32.8	38.5	36.5
21-TS	−2294.665964	−2294.630168	−2294.732826	0.519507	−2295.286322	−2294.766815	7.3	11.0	10.9
22	−2294.702732	−2294.666495	−2294.771528	0.519802	−2295.328428	−2294.808626	−15.5	−13.3	−15.4
23-TS	−2294.677531	−2294.641911	−2294.744238	0.521482	−2295.307307	−2294.785825	−0.1	3.8	−1.0
24	−2294.743138	−2294.707302	−2294.810918	0.522608	−2295.372056	−2294.849448	−41.1	−38.0	−41.0
27-TS	−2294.662650	−2294.625061	−2294.733393	0.509002	−2295.268688	−2294.759686	10.5	10.7	15.4
31	−2294.690726	−2294.653951	−2294.760030	0.516694	−2295.308215	−2294.791521	−7.7	−6.1	−4.6
29-TS	−2294.682937	−2294.646493	−2294.751048	0.514672	−2295.296756	−2294.782084	−3.0	−0.4	1.3
30	−2294.688971	−2294.652197	−2294.758054	0.515678	−2295.305313	−2294.789635	−6.6	−4.8	−3.4
32-TS	−2294.676167	−2294.639581	−2294.744969	0.514651	−2295.291796	−2294.777145	1.4	3.4	4.4
33	−2294.719611	−2294.682187	−2294.790432	0.515939	−2295.338409	−2294.822470	−25.4	−25.1	−24.0
Alkene insertion transition states for 6,5-ring formation									
25-TS	−2333.949438	−2333.912489	−2334.017249	0.547657	−2334.598587	−2334.050930	3.7	2.3	0.5
26-TS	−2333.954979	−2333.918342	−2334.020979	0.550324	−2334.602025	−2334.051701	0.0	0.0	0.0
Potential energy surface for β-hydride elimination pathway of 1-ene-VCP **1**									
34	−1908.346925	−1908.321450	−1908.404242	0.299727	−1908.704349	−1908.404622	0.0	0.0	0.0
35	−1908.338250	−1908.312601	−1908.396059	0.298132	−1908.693677	−1908.395545	5.6	5.1	5.7
36-TS	−1908.317525	−1908.292497	−1908.373832	0.298986	−1908.674172	−1908.375186	18.2	19.1	18.5
38	−1908.318810	−1908.292604	−1908.377053	0.294796	−1908.670796	−1908.376000	18.1	17.1	18.0
39-TS	−1908.315886	−1908.289929	−1908.373600	0.292515	−1908.666594	−1908.374079	19.8	19.2	19.2
40	−1908.324445	−1908.298042	−1908.383575	0.292909	−1908.675267	−1908.382358	14.7	13.0	14.0
41-TS	−1908.317019	−1908.290580	−1908.376939	0.290432	−1908.665013	−1908.374581	19.4	17.1	18.9
Potential energy surface for [3+2] reaction of 1-ene-VCP **10**									
10	−1223.988571	−1223.966730	−1224.041430	0.264320	−1224.304726	−1224.040406	0.0	0.0	0.0
11	−1224.073947	−1224.054181	−1224.123269	0.272970	−1224.413228	−1224.140258	–	–	–
43	−2293.464504	−2293.427689	−2293.533941	0.492778	−2294.059281	−2293.566503	−3.9	−2.0	−11.1
44-TS	−2293.442159	−2293.405676	−2293.510122	0.492063	−2294.036847	−2293.544784	9.9	13.0	2.5
45	−2293.454908	−2293.417120	−2293.525863	0.489778	−2294.048682	−2293.558904	2.7	3.1	−6.4
46-TS	−2293.449738	−2293.412340	−2293.520258	0.488964	−2294.037565	−2293.548601	5.7	6.6	0.1
47	−2293.459902	−2293.422015	−2293.532366	0.488007	−2294.049457	−2293.561450	−0.4	−1.0	−8.0
48	−2293.477306	−2293.440630	−2293.544548	0.494651	−2294.076312	−2293.581661	−12.1	−8.6	−20.6
49-TS	−2293.447811	−2293.411990	−2293.513352	0.495751	−2294.047413	−2293.551662	5.9	10.9	−1.8
50	−2293.501700	−2293.465591	−2293.571444	0.494206	−2294.100009	−2293.605803	−27.7	−25.5	−35.8
51-TS	−2293.484760	−2293.449453	−2293.550786	0.497845	−2294.087832	−2293.589987	−17.6	−12.6	−25.9
52	−2293.544745	−2293.508856	−2293.612614	0.498386	−2294.146996	−2293.648610	−54.9	−51.4	−62.7
Alkyne insertion transition states for substrate ***6***									
53-TS	−1764.776976	−1764.744777	−1764.837109	0.479617	−1765.349593	−1764.869976	0.0	0.0	0.0
54-TS	−1764.768530	−1764.736570	−1764.827801	0.480936	−1765.340304	−1764.859368	5.1	5.8	6.7
Alkyne insertion transition states for substrate **8**									
55-TS	−2563.701584	−2563.659551	−2563.774137	0.598444	−2564.399959	−2563.801515	−0.4	−2.5	0.4
56-TS	−2563.702541	−2563.660149	−2563.778184	0.594942	−2564.397055	−2563.802113	0.0	0.0	0.0

5. Coordinates of All Stationary Points

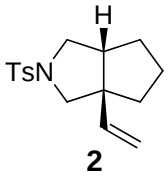


1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.434247	-3.374911	-0.056271
2	6	0	3.078390	-2.596162	-0.472353
3	6	0	4.055950	-2.954908	-1.307103
4	6	0	2.746034	-1.206853	-0.030892
5	1	0	4.230464	-3.997288	-1.560073
6	1	0	4.722373	-2.226176	-1.761649
7	6	0	3.806726	-0.133592	-0.036266
8	6	0	3.342236	-0.720445	1.274651
9	6	0	1.281044	-0.870770	-0.343288
10	1	0	3.507489	0.884803	-0.261562
11	1	0	4.798826	-0.397365	-0.391169
12	1	0	4.011703	-1.397945	1.797594
13	1	0	2.710855	-0.113135	1.915678
14	1	0	1.091181	-1.043924	-1.410805
15	1	0	0.649909	-1.577454	0.204681
16	6	0	0.831458	1.505135	-1.107743
17	1	0	-0.210745	1.764623	-1.345240
18	1	0	1.239020	1.014291	-1.996147
19	6	0	1.614649	2.759813	-0.814198
20	1	0	1.363074	3.262270	0.116010
21	6	0	2.528926	3.267239	-1.642004
22	1	0	3.048254	4.195053	-1.417885
23	1	0	2.792709	2.778995	-2.578819
24	7	0	0.859612	0.502939	-0.011258
25	16	0	-0.305725	0.686642	1.196914
26	8	0	0.056197	-0.243086	2.269089
27	8	0	-0.424438	2.130325	1.422542
28	6	0	-1.872090	0.130346	0.513473
29	6	0	-2.700791	1.040428	-0.149133
30	6	0	-2.248800	-1.210249	0.642462
31	6	0	-3.898534	0.592993	-0.705613
32	1	0	-2.425914	2.088796	-0.192611
33	6	0	-3.449673	-1.638428	0.081294

34	1	0	-1.625097	-1.895079	1.206790
35	6	0	-4.288349	-0.749950	-0.608663
36	1	0	-4.547681	1.303036	-1.212052
37	1	0	-3.747789	-2.678186	0.192456
38	6	0	-5.575381	-1.232426	-1.234499
39	1	0	-6.047391	-2.013082	-0.628513
40	1	0	-6.293263	-0.415190	-1.356566
41	1	0	-5.392738	-1.659901	-2.229451

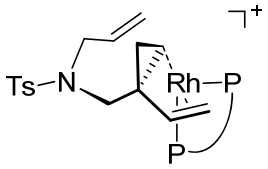


2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.463034	0.796575	-0.184937
2	6	0	2.317323	0.213562	1.290754
3	6	0	0.955609	-0.506197	1.313086
4	6	0	1.145835	0.366905	-0.882916
5	6	0	3.698332	0.055569	-0.756278
6	6	0	4.574913	-0.250802	0.465132
7	6	0	3.540501	-0.712087	1.503425
8	1	0	3.364634	-0.889120	-1.202879
9	1	0	4.208968	0.619959	-1.542238
10	1	0	5.082473	0.659930	0.807434
11	1	0	5.344263	-1.004297	0.263893
12	1	0	3.911233	-0.677525	2.533702
13	1	0	3.254202	-1.750397	1.292846
14	1	0	0.958008	-1.428134	1.897979
15	1	0	0.165789	0.156726	1.703955
16	1	0	1.285712	0.103161	-1.932553
17	1	0	0.390645	1.168334	-0.819259
18	6	0	2.577967	2.304609	-0.161356
19	6	0	3.562169	3.070407	-0.634855
20	1	0	4.443068	2.666807	-1.125760
21	1	0	3.519824	4.152193	-0.542005
22	1	0	2.323574	1.025357	2.025127
23	1	0	1.732612	2.800840	0.321205
24	7	0	0.734983	-0.815580	-0.109968

25	16	0	-0.644312	-1.662755	-0.564476
26	6	0	-2.044220	-0.589440	-0.225167
27	8	0	-0.557084	-1.826584	-2.017207
28	8	0	-0.735978	-2.804131	0.348697
29	6	0	-2.483400	0.305468	-1.204763
30	6	0	-2.664509	-0.635392	1.026768
31	6	0	-3.546405	1.161105	-0.919634
32	1	0	-2.011518	0.309177	-2.181637
33	6	0	-3.725667	0.227635	1.294061
34	1	0	-2.332115	-1.355818	1.766665
35	6	0	-4.183269	1.137372	0.329488
36	1	0	-3.892173	1.853940	-1.683023
37	1	0	-4.212135	0.189016	2.265834
38	6	0	-5.357129	2.043000	0.617861
39	1	0	-6.305821	1.543338	0.380797
40	1	0	-5.395290	2.326222	1.675035
41	1	0	-5.313869	2.959402	0.020330



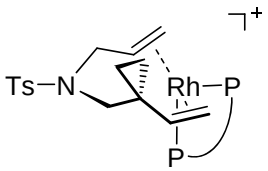
12

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.369354	-2.022831	-1.012994
2	6	0	-0.699223	-1.128479	-1.538716
3	6	0	-1.783108	-1.222597	-2.396526
4	6	0	0.180212	0.066845	-1.404965
5	1	0	-2.252529	-2.185328	-2.570249
6	1	0	-1.995232	-0.470896	-3.153555
7	6	0	-0.529304	1.470614	-1.479606
8	6	0	0.381892	0.983431	-2.571941
9	6	0	1.310299	-0.143700	-0.377237
10	1	0	-0.160190	2.241312	-0.810558
11	1	0	-1.591213	1.561216	-1.747162
12	1	0	-0.055083	0.696169	-3.523553
13	1	0	1.351950	1.460886	-2.643535
14	1	0	0.871449	-0.244014	0.622804
15	1	0	1.775706	-1.104947	-0.620119

16	6	0	2.416698	1.825262	0.814338
17	1	0	3.443394	1.822229	1.201735
18	1	0	1.785748	1.433581	1.620497
19	6	0	2.021171	3.238593	0.468340
20	1	0	2.506357	3.648821	-0.415002
21	6	0	1.190407	3.983237	1.200721
22	1	0	0.977217	5.017938	0.947027
23	1	0	0.721909	3.599198	2.105729
24	7	0	2.337135	0.891381	-0.330482
25	16	0	3.781099	0.623030	-1.194545
26	8	0	3.397604	-0.240008	-2.314494
27	8	0	4.363509	1.951978	-1.385332
28	6	0	4.873593	-0.304763	-0.123687
29	6	0	5.789333	0.373794	0.686449
30	6	0	4.802667	-1.701992	-0.110172
31	6	0	6.619507	-0.359394	1.532765
32	1	0	5.870989	1.453879	0.627813
33	6	0	5.641890	-2.415408	0.741754
34	1	0	4.127319	-2.219980	-0.782817
35	6	0	6.560122	-1.759856	1.577151
36	1	0	7.335858	0.165552	2.159275
37	1	0	5.595276	-3.501425	0.747950
38	6	0	7.491915	-2.546529	2.466500
39	1	0	8.407920	-2.817406	1.925430
40	1	0	7.792038	-1.968335	3.345890
41	1	0	7.029755	-3.477992	2.808908
42	1	0	-4.328462	2.880180	-0.728662
43	6	0	-4.774003	2.343913	0.114523
44	15	0	-3.482388	1.325955	0.959788
45	1	0	-5.570951	1.705466	-0.277134
46	1	0	-5.209639	3.072615	0.807535
47	6	0	-4.365218	0.660507	2.448794
48	45	0	-2.411279	-0.165446	-0.509726
49	6	0	-2.374034	2.601953	1.702344
50	6	0	-5.276923	-0.547484	2.176072
51	1	0	-3.597565	0.385105	3.183365
52	1	0	-4.948222	1.479156	2.888942
53	1	0	-1.622920	2.116574	2.332093
54	1	0	-2.949309	3.306873	2.312686
55	1	0	-1.854769	3.157958	0.916692
56	1	0	-6.030628	-0.297230	1.418223
57	1	0	-5.841404	-0.757970	3.092123
58	6	0	-4.521171	-1.827914	1.782974
59	15	0	-3.761717	-1.851823	0.089675

60	1	0	-3.713247	-2.019256	2.500655
61	1	0	-5.200178	-2.688759	1.833159
62	6	0	-5.212786	-2.089219	-1.028104
63	6	0	-2.947266	-3.509487	0.088654
64	1	0	-5.793419	-2.969541	-0.730091
65	1	0	-5.860624	-1.208833	-0.999963
66	1	0	-4.868769	-2.219562	-2.057671
67	1	0	-2.549457	-3.745088	-0.902026
68	1	0	-2.120814	-3.516882	0.805478
69	1	0	-3.666243	-4.287245	0.368952



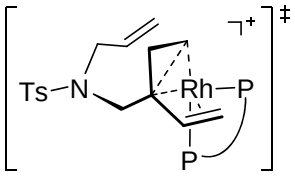
13

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.725081	0.019975	0.038826
2	1	0	-1.300349	1.571155	-2.259908
3	6	0	-1.238747	1.863810	-1.212127
4	6	0	-2.433744	2.070757	-0.516903
5	6	0	0.092895	2.424357	-0.831825
6	1	0	-3.385865	2.028151	-1.033863
7	1	0	-2.447613	2.668855	0.390763
8	6	0	0.265330	3.230707	0.447145
9	6	0	0.215766	3.956801	-0.857569
10	1	0	1.217358	3.148927	0.962643
11	1	0	-0.582458	3.331720	1.119217
12	1	0	-0.678355	4.524429	-1.098568
13	1	0	1.140200	4.367501	-1.254492
14	1	0	-0.505928	-1.783780	1.691008
15	6	0	-0.639425	-1.783339	0.609670
16	6	0	0.208779	-0.984618	-0.196881
17	1	0	-1.024306	-2.723492	0.221929
18	6	0	1.198597	-0.080132	0.499126
19	1	0	0.469165	-1.302152	-1.201905
20	1	0	0.670721	0.525492	1.267762
21	1	0	1.898267	-0.706646	1.069136
22	7	0	1.984409	0.753778	-0.402250

23	6	0	1.290456	1.626360	-1.366652
24	16	0	3.404505	1.394157	0.331913
25	1	0	0.949995	0.997109	-2.198107
26	1	0	2.051563	2.293394	-1.770805
27	8	0	3.870323	2.456772	-0.563720
28	8	0	3.127617	1.673748	1.748779
29	6	0	4.536553	0.014649	0.253796
30	6	0	4.932114	-0.619228	1.431704
31	6	0	5.052071	-0.375582	-0.987024
32	6	0	5.847947	-1.670438	1.358024
33	1	0	4.541595	-0.281730	2.385721
34	6	0	5.963461	-1.423778	-1.038182
35	1	0	4.753347	0.143090	-1.892172
36	6	0	6.377369	-2.087734	0.130368
37	1	0	6.161961	-2.166284	2.272614
38	1	0	6.370534	-1.729248	-1.998732
39	6	0	7.391471	-3.203146	0.056478
40	1	0	7.176018	-3.884862	-0.773616
41	1	0	8.399557	-2.801992	-0.109102
42	1	0	7.416598	-3.787007	0.981196
43	1	0	-5.548650	-1.128265	-0.374229
44	6	0	-5.008581	-2.013634	-0.014422
45	6	0	-4.534709	-1.802822	1.434569
46	1	0	-5.746711	-2.824264	-0.013097
47	6	0	-3.905771	-2.410724	-1.014414
48	15	0	-3.546048	-0.250992	1.706109
49	1	0	-3.908775	-2.648465	1.746910
50	1	0	-5.402017	-1.785269	2.106203
51	15	0	-2.761680	-1.077423	-1.607562
52	1	0	-3.282995	-3.208013	-0.591851
53	1	0	-4.367375	-2.819727	-1.923019
54	6	0	-4.863641	1.041296	1.851664
55	6	0	-3.002984	-0.439948	3.465742
56	6	0	-3.821788	-0.047807	-2.708767
57	6	0	-1.685018	-1.975012	-2.803123
58	1	0	-4.412463	1.999307	2.127984
59	1	0	-5.374872	1.177431	0.893382
60	1	0	-5.604223	0.770367	2.612361
61	1	0	-2.286685	-1.262626	3.550766
62	1	0	-3.855338	-0.642893	4.123837
63	1	0	-2.511529	0.477934	3.803833
64	1	0	-4.247290	-0.682332	-3.494012
65	1	0	-4.639612	0.410639	-2.147565
66	1	0	-3.234698	0.744472	-3.180646

67	1	0	-1.028761	-1.269044	-3.319611
68	1	0	-1.067264	-2.716242	-2.289823
69	1	0	-2.305064	-2.490181	-3.545237

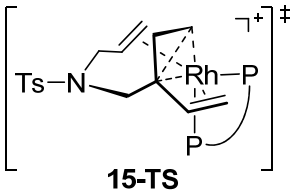


14-TS Imaginary frequency: −193.5 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	2.141477	-0.132047	-0.580840
2	1	0	-0.091265	1.245051	-1.521963
3	6	0	0.411340	0.329115	-1.813525
4	6	0	1.492623	0.368536	-2.691118
5	6	0	-0.063894	-0.901660	-1.223103
6	1	0	1.787154	1.319181	-3.121698
7	1	0	1.832721	-0.506196	-3.238491
8	6	0	1.410318	-2.232770	-1.035075
9	6	0	0.161895	-2.223327	-1.875168
10	1	0	1.331079	-2.814300	-0.122593
11	1	0	2.358627	-2.340311	-1.570303
12	1	0	0.318754	-2.174769	-2.952118
13	1	0	-0.592032	-2.969172	-1.630894
14	1	0	-1.850075	-3.380655	2.898739
15	6	0	-1.720416	-3.979067	1.998705
16	6	0	-2.207078	-3.585875	0.819324
17	1	0	-1.211382	-4.931587	2.117527
18	6	0	-2.985692	-2.316016	0.608098
19	1	0	-2.088857	-4.215947	-0.061574
20	1	0	-3.976504	-2.570398	0.220194
21	1	0	-3.119150	-1.782505	1.561174
22	7	0	-2.349921	-1.447899	-0.409459
23	6	0	-1.055982	-0.846878	-0.063963
24	16	0	-3.396696	-0.507974	-1.372658
25	1	0	-0.669105	-1.440030	0.767665
26	1	0	-1.152580	0.186273	0.295763
27	8	0	-2.490796	0.266903	-2.230563
28	8	0	-4.390299	-1.433306	-1.910754

29	6	0	-4.237197	0.635443	-0.281567
30	6	0	-5.435496	0.248652	0.328582
31	6	0	-3.689707	1.899752	-0.044356
32	6	0	-6.071736	1.133240	1.195420
33	1	0	-5.875572	-0.716813	0.103096
34	6	0	-4.343184	2.771289	0.825354
35	1	0	-2.788378	2.207173	-0.563523
36	6	0	-5.539150	2.404952	1.459822
37	1	0	-7.006050	0.836814	1.665014
38	1	0	-3.925674	3.758957	1.003442
39	6	0	-6.260839	3.366422	2.372109
40	1	0	-5.584234	4.127879	2.771802
41	1	0	-7.060499	3.888768	1.831140
42	1	0	-6.727563	2.845584	3.214545
43	1	0	5.473145	0.798066	1.462744
44	6	0	4.708365	1.337149	2.038066
45	6	0	3.711120	0.350440	2.669337
46	1	0	5.250861	1.833186	2.851723
47	6	0	4.049661	2.426632	1.175078
48	15	0	2.943180	-0.882089	1.509402
49	1	0	2.890117	0.907770	3.138965
50	1	0	4.202871	-0.218012	3.468795
51	15	0	3.372954	1.861362	-0.460798
52	1	0	3.219876	2.882962	1.730221
53	1	0	4.770191	3.228697	0.971124
54	6	0	4.266259	-2.165137	1.336339
55	6	0	1.732106	-1.703038	2.640149
56	6	0	4.881914	1.816402	-1.531655
57	6	0	2.516116	3.398682	-1.028277
58	1	0	3.889109	-3.011650	0.754607
59	1	0	5.129055	-1.751310	0.805838
60	1	0	4.593665	-2.528372	2.316693
61	1	0	0.949424	-0.990852	2.918835
62	1	0	2.232158	-2.050687	3.550964
63	1	0	1.260036	-2.561031	2.153343
64	1	0	5.403345	2.780070	-1.522120
65	1	0	5.567985	1.038801	-1.182568
66	1	0	4.597050	1.575284	-2.559829
67	1	0	2.193476	3.300603	-2.068450
68	1	0	1.632215	3.579861	-0.409211
69	1	0	3.184799	4.263114	-0.952090

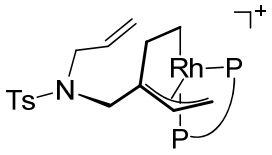


15-TS Imaginary frequency: –298.2 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.738537	-0.051669	-0.247545
2	1	0	0.997834	0.456009	-2.872174
3	6	0	1.166353	-0.435644	-2.275199
4	6	0	2.467316	-0.973758	-2.095061
5	6	0	-0.000766	-1.118413	-1.744788
6	1	0	3.299271	-0.504184	-2.607020
7	1	0	2.605509	-2.038546	-1.926794
8	6	0	0.406248	-2.146146	-0.251366
9	6	0	-0.122699	-2.583081	-1.597874
10	1	0	-0.324798	-2.076466	0.542627
11	1	0	1.351818	-2.598385	0.018098
12	1	0	0.554703	-3.191984	-2.193811
13	1	0	-1.144417	-2.959028	-1.607906
14	1	0	0.720422	0.187773	2.390727
15	6	0	0.868576	0.926467	1.607710
16	6	0	-0.107802	1.081005	0.625145
17	1	0	1.526034	1.746160	1.878519
18	6	0	-1.404903	0.317441	0.782534
19	1	0	-0.162861	2.008555	0.063956
20	1	0	-1.266556	-0.476724	1.521931
21	1	0	-2.128219	1.024282	1.218188
22	7	0	-2.007073	-0.239269	-0.442692
23	6	0	-1.276138	-0.269170	-1.698636
24	16	0	-3.300801	-1.317690	-0.197167
25	1	0	-1.014811	0.759692	-1.968075
26	1	0	-1.960089	-0.655348	-2.458846
27	8	0	-3.501612	-1.990649	-1.485997
28	8	0	-3.008544	-2.083695	1.021506
29	6	0	-4.705933	-0.269409	0.137132
30	6	0	-5.143592	-0.103930	1.451885
31	6	0	-5.361514	0.356999	-0.928627
32	6	0	-6.248235	0.712428	1.697754
33	1	0	-4.641975	-0.623166	2.261239
34	6	0	-6.460906	1.165160	-0.661169

35	1	0	-5.028812	0.195279	-1.948680
36	6	0	-6.922905	1.356880	0.652748
37	1	0	-6.596819	0.840160	2.719032
38	1	0	-6.978411	1.648963	-1.485585
39	6	0	-8.136902	2.212572	0.920108
40	1	0	-8.102748	3.145749	0.347148
41	1	0	-9.054983	1.687588	0.626898
42	1	0	-8.225371	2.465476	1.980618
43	1	0	5.671866	0.820270	0.330724
44	6	0	5.175034	1.269288	1.201190
45	6	0	4.569735	0.175059	2.099812
46	1	0	5.972737	1.764398	1.767685
47	6	0	4.184510	2.361318	0.753665
48	15	0	3.455175	-1.037228	1.234655
49	1	0	3.983843	0.640378	2.903202
50	1	0	5.374704	-0.390575	2.585370
51	15	0	2.979175	1.910038	-0.591972
52	1	0	3.601997	2.706683	1.617240
53	1	0	4.739784	3.234552	0.388133
54	6	0	4.668530	-2.173444	0.418822
55	6	0	2.875410	-2.079149	2.652122
56	6	0	4.036671	1.983015	-2.104600
57	6	0	2.013041	3.479506	-0.743779
58	1	0	4.141459	-3.019135	-0.034414
59	1	0	5.203383	-1.647723	-0.377640
60	1	0	5.394926	-2.564350	1.139732
61	1	0	2.260917	-1.482483	3.333309
62	1	0	3.720672	-2.493279	3.213057
63	1	0	2.264073	-2.910049	2.285248
64	1	0	4.522817	2.962087	-2.170814
65	1	0	4.809345	1.210076	-2.075428
66	1	0	3.431695	1.835216	-3.003927
67	1	0	1.337307	3.421269	-1.602524
68	1	0	1.416422	3.654615	0.156091
69	1	0	2.686712	4.331860	-0.883590

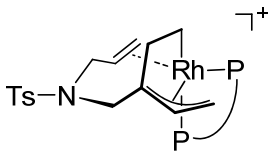


16

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.371685	-0.707002	-0.380152
2	6	0	-2.334796	-2.683437	2.650718
3	6	0	-3.247781	-1.880664	1.764906
4	6	0	-1.476933	-0.520944	0.639783
5	6	0	0.103984	-2.115772	-0.713564
6	6	0	1.626261	-2.197723	-0.533567
7	6	0	-2.000719	-2.332878	3.894439
8	45	0	2.204113	-0.245434	-0.026073
9	1	0	-0.423021	-2.827674	-0.072670
10	1	0	-0.218153	-2.341676	-1.737030
11	1	0	2.124775	-2.633207	-1.404651
12	1	0	1.904813	-2.786307	0.351966
13	1	0	-1.370923	-2.963241	4.515871
14	1	0	-2.371447	-1.416456	4.350036
15	1	0	-4.102648	-2.497282	1.473065
16	1	0	-3.626662	-0.997386	2.301142
17	1	0	-1.840101	0.519085	0.631667
18	1	0	-1.052970	-0.704101	1.635682
19	6	0	0.195195	0.393803	-0.986650
20	6	0	1.357739	0.280605	-1.851494
21	1	0	1.401558	-0.552349	-2.551143
22	1	0	1.746236	1.205749	-2.272992
23	15	0	2.719109	2.037071	0.806074
24	6	0	2.464004	3.434806	-0.383462
25	6	0	1.785094	2.625434	2.293449
26	1	0	0.715696	2.672504	2.064977
27	1	0	2.708544	4.396072	0.081496
28	6	0	5.550717	1.777014	0.368351
29	6	0	5.720171	0.246168	0.360698
30	1	0	5.774550	-0.123740	1.393082
31	1	0	6.673981	-0.016872	-0.114510
32	1	0	5.362131	2.148986	-0.647814
33	1	0	6.513606	2.211324	0.662450
34	15	0	4.405515	-0.746598	-0.501403

35	6	0	4.944587	-2.471023	-0.129871
36	1	0	4.833757	-2.673356	0.939985
37	6	0	4.804255	-0.545270	-2.290002
38	1	0	4.156434	-1.197293	-2.882812
39	1	0	-1.965440	-3.614139	2.221738
40	1	0	5.993452	-2.616615	-0.409988
41	1	0	4.327790	-3.185902	-0.679862
42	1	0	4.628779	0.487592	-2.604067
43	1	0	5.849690	-0.805929	-2.487631
44	1	0	3.095600	3.303264	-1.267578
45	1	0	1.421146	3.464344	-0.714038
46	1	0	1.924644	1.925577	3.123564
47	1	0	2.121257	3.619233	2.609481
48	1	0	-0.195143	1.380644	-0.746096
49	6	0	4.481316	2.303209	1.344479
50	1	0	4.602888	1.815331	2.320669
51	1	0	4.627243	3.377855	1.511344
52	1	0	-7.924097	3.534442	-0.841035
53	6	0	-7.168604	3.497307	-0.045521
54	1	0	-7.705082	3.447491	0.907607
55	6	0	-6.258483	2.307704	-0.230508
56	1	0	-6.612642	4.439240	-0.077843
57	6	0	-5.024720	2.437760	-0.884640
58	6	0	-6.646915	1.033720	0.213792
59	6	0	-4.196818	1.335752	-1.092905
60	1	0	-4.715238	3.413275	-1.250945
61	6	0	-5.835485	-0.080101	0.014636
62	1	0	-7.605824	0.909954	0.710290
63	6	0	-4.606156	0.080305	-0.634033
64	1	0	-3.264210	1.435262	-1.637874
65	1	0	-6.162470	-1.065502	0.328943
66	16	0	-3.547446	-1.340830	-0.880879
67	7	0	-2.564209	-1.494137	0.507413
68	8	0	-2.600881	-1.012424	-1.954714
69	8	0	-4.384581	-2.537718	-0.910585

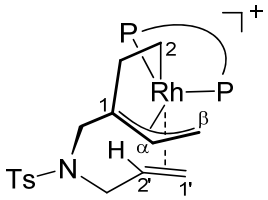


17

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.122701	-1.329853	-1.496933
2	6	0	-0.246917	0.667543	0.738531
3	6	0	-1.463929	-0.216572	0.739363
4	6	0	-1.188877	-0.639997	-1.769519
5	6	0	0.159819	-2.598757	-0.645873
6	6	0	1.144897	-2.293016	0.489812
7	6	0	0.698004	0.621395	1.744188
8	1	0	-0.839295	-2.840921	-0.274922
9	1	0	0.474506	-3.445444	-1.268664
10	1	0	1.976396	-3.000776	0.537545
11	1	0	0.666227	-2.246881	1.469551
12	1	0	1.287287	1.500745	1.981671
13	1	0	0.620900	-0.127046	2.527956
14	1	0	-1.259208	-1.150145	1.273995
15	1	0	-2.229524	0.313844	1.324485
16	1	0	-1.767520	-1.235713	-2.485838
17	1	0	-1.003919	0.332887	-2.243151
18	6	0	1.274260	-0.919850	-2.179381
19	6	0	2.570157	-1.407380	-1.819601
20	1	0	2.701866	-2.449186	-1.543770
21	1	0	3.425787	-0.977388	-2.331372
22	1	0	-0.319912	1.560225	0.123387
23	1	0	1.191043	-0.075700	-2.861412
24	7	0	-2.050077	-0.455316	-0.590852
25	16	0	-3.485594	-1.403593	-0.525433
26	6	0	-4.711883	-0.227845	0.022021
27	8	0	-3.762266	-1.789960	-1.912147
28	8	0	-3.326119	-2.418904	0.525066
29	6	0	-5.171401	0.746612	-0.870526
30	6	0	-5.225000	-0.323132	1.316265
31	6	0	-6.147562	1.640974	-0.445676
32	1	0	-4.781278	0.791192	-1.882093
33	6	0	-6.203615	0.585047	1.722291
34	1	0	-4.874701	-1.104447	1.982108

35	6	0	-6.680152	1.576038	0.853964
36	1	0	-6.511896	2.398398	-1.134919
37	1	0	-6.608908	0.514339	2.728087
38	6	0	-7.762806	2.534067	1.287055
39	1	0	-8.738883	2.219329	0.895878
40	1	0	-7.845420	2.581935	2.376846
41	1	0	-7.575998	3.546001	0.912005
42	1	0	5.463329	1.595545	0.067911
43	6	0	4.866002	2.044203	0.872488
44	6	0	4.488225	0.979844	1.918171
45	1	0	5.533662	2.763014	1.362344
46	6	0	3.679760	2.834397	0.288759
47	1	0	3.814719	1.417403	2.666319
48	1	0	5.388278	0.662350	2.459734
49	15	0	3.677689	-0.570170	1.288686
50	15	0	2.596423	1.904500	-0.908294
51	1	0	3.038334	3.191530	1.105638
52	1	0	4.052197	3.728742	-0.226506
53	45	0	1.776160	-0.341311	-0.083598
54	6	0	3.420731	-1.502458	2.860156
55	6	0	5.078561	-1.490113	0.515026
56	6	0	3.657295	1.875690	-2.428075
57	6	0	1.368939	3.219689	-1.357074
58	1	0	2.729352	-0.961125	3.512061
59	1	0	4.372417	-1.629580	3.387092
60	1	0	2.997858	-2.488655	2.651601
61	1	0	4.738584	-2.484985	0.213818
62	1	0	5.436003	-0.968889	-0.377335
63	1	0	5.909867	-1.600565	1.219839
64	1	0	3.987479	2.886463	-2.691097
65	1	0	4.541227	1.250044	-2.271944
66	1	0	3.099066	1.464915	-3.275192
67	1	0	0.697502	2.855582	-2.141278
68	1	0	0.763410	3.492284	-0.486859
69	1	0	1.874172	4.121173	-1.720545

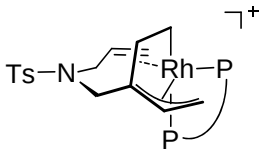


17'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.030978	-1.243819	1.511144
2	6	0	0.002763	-0.476163	-1.806417
3	6	0	-1.370460	-0.702456	-1.208835
4	6	0	-1.401726	-0.753066	1.313672
5	6	0	0.865023	-0.780852	2.716870
6	6	0	2.263284	-0.468700	2.168335
7	6	0	0.871911	-1.435535	-2.206452
8	1	0	0.408010	0.115019	3.145588
9	1	0	0.872088	-1.544761	3.507140
10	1	0	3.033407	-1.188406	2.453007
11	1	0	2.616725	0.528046	2.433242
12	1	0	1.710511	-1.188813	-2.846315
13	1	0	0.674268	-2.493690	-2.060565
14	1	0	-2.088661	-0.327081	-1.944697
15	1	0	-1.586488	-1.769667	-1.083923
16	1	0	-1.679973	-0.090814	2.133475
17	1	0	-2.088003	-1.615505	1.327959
18	6	0	0.432334	-2.387669	0.795312
19	6	0	1.759518	-2.858777	0.702699
20	1	0	2.420627	-2.878605	1.560485
21	1	0	1.962320	-3.629798	-0.036238
22	1	0	0.183892	0.546582	-2.112131
23	1	0	-0.271143	-2.786104	0.069345
24	7	0	-1.583372	0.013444	0.062245
25	16	0	-2.762622	1.242984	0.044616
26	6	0	-4.374881	0.487095	-0.094945
27	8	0	-2.661554	1.882638	1.360929
28	8	0	-2.494745	1.981646	-1.196057
29	6	0	-5.021024	0.029969	1.059205
30	6	0	-4.964548	0.345205	-1.354451
31	6	0	-6.262140	-0.588616	0.937911
32	1	0	-4.573066	0.183327	2.035303

33	6	0	-6.207906	-0.276963	-1.452291
34	1	0	-4.471731	0.743055	-2.235030
35	6	0	-6.875140	-0.754571	-0.314823
36	1	0	-6.770588	-0.938739	1.832410
37	1	0	-6.672908	-0.382697	-2.428785
38	6	0	-8.236197	-1.396358	-0.426563
39	1	0	-9.028020	-0.663775	-0.223289
40	1	0	-8.410575	-1.797445	-1.429417
41	1	0	-8.355929	-2.210999	0.295111
42	1	0	4.199646	2.162657	-1.503135
43	6	0	4.489812	2.117075	-0.444707
44	6	0	5.059252	0.731241	-0.096945
45	1	0	5.299794	2.847811	-0.333087
46	6	0	3.328886	2.564080	0.457647
47	1	0	5.215344	0.655820	0.986811
48	1	0	6.043656	0.600467	-0.563861
49	15	0	4.016457	-0.715546	-0.608857
50	15	0	1.664572	1.770995	0.171779
51	1	0	3.598888	2.398950	1.507949
52	1	0	3.172576	3.644339	0.349346
53	45	0	1.764917	-0.662719	0.129240
54	6	0	5.012562	-2.125364	0.046656
55	6	0	4.362138	-0.823990	-2.423194
56	6	0	1.059860	2.713429	-1.302773
57	6	0	0.706794	2.577867	1.529848
58	1	0	4.966272	-2.141875	1.139567
59	1	0	6.060281	-2.033507	-0.259501
60	1	0	4.615082	-3.071570	-0.330294
61	1	0	3.962070	-1.759079	-2.825529
62	1	0	3.899098	0.010294	-2.958445
63	1	0	5.441995	-0.802047	-2.606259
64	1	0	1.260230	3.779906	-1.153320
65	1	0	1.563044	2.392804	-2.220475
66	1	0	-0.020493	2.583673	-1.417689
67	1	0	-0.357825	2.345638	1.454588
68	1	0	1.074581	2.248392	2.505553
69	1	0	0.833701	3.664335	1.465511

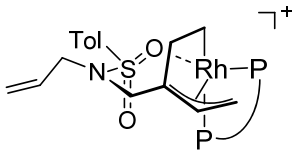


18

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.059784	-0.952446	1.621157
2	6	0	0.051691	-0.366420	-1.393905
3	6	0	1.256639	0.387251	-0.872700
4	6	0	1.442816	-0.339604	1.524992
5	6	0	-0.158972	-2.400204	1.179324
6	6	0	-1.395693	-2.413312	0.268952
7	6	0	-1.040189	0.193199	-2.001664
8	45	0	-1.818438	-0.326898	0.220894
9	1	0	0.733372	-2.757038	0.659517
10	1	0	-0.271781	-3.037876	2.066634
11	1	0	-2.229153	-2.986168	0.683226
12	1	0	-1.185155	-2.787571	-0.735157
13	1	0	-1.659870	-0.408696	-2.657276
14	1	0	-1.128898	1.269017	-2.120861
15	1	0	1.937249	0.529869	-1.719016
16	1	0	0.983310	1.385377	-0.510517
17	1	0	2.125862	-0.931407	2.142558
18	1	0	1.426530	0.684019	1.925212
19	6	0	-0.941043	-0.259754	2.298451
20	6	0	-2.310690	-0.692494	2.298670
21	1	0	-2.539341	-1.747094	2.421495
22	1	0	-3.032432	-0.038307	2.780396
23	15	0	-2.368571	2.129126	0.388561
24	6	0	-3.160592	2.683770	1.969100
25	6	0	-1.021407	3.392009	0.211174
26	1	0	-0.274658	3.252183	0.999319
27	1	0	-3.381078	3.756195	1.938799
28	6	0	-4.894600	1.929491	-0.994259
29	6	0	-4.744156	0.557284	-1.676176
30	1	0	-4.174107	0.666198	-2.607440
31	1	0	-5.734834	0.179676	-1.959967
32	1	0	-5.372173	1.818802	-0.011944
33	1	0	-5.599188	2.518316	-1.593703
34	15	0	-3.925782	-0.786435	-0.685325

35	6	0	-3.992970	-2.205074	-1.863988
36	1	0	-3.357099	-2.016415	-2.733932
37	6	0	-5.220095	-1.246234	0.546245
38	1	0	-4.897956	-2.129867	1.104261
39	1	0	0.229463	-1.428943	-1.522292
40	1	0	-5.020098	-2.364670	-2.209454
41	1	0	-3.639716	-3.115772	-1.373358
42	1	0	-5.378182	-0.432316	1.258834
43	1	0	-6.167887	-1.472258	0.045884
44	1	0	-4.094415	2.139885	2.138468
45	1	0	-2.498556	2.491215	2.818860
46	1	0	-0.519976	3.288719	-0.756025
47	1	0	-1.422124	4.408947	0.286885
48	1	0	-0.701296	0.735456	2.670480
49	6	0	-3.594958	2.745848	-0.871341
50	1	0	-3.087311	2.778018	-1.844079
51	1	0	-3.838321	3.784547	-0.614381
52	1	0	9.154576	1.511315	-0.514207
53	6	0	8.292212	2.088755	-0.156787
54	1	0	8.198410	2.965215	-0.806613
55	6	0	7.038888	1.248091	-0.180229
56	1	0	8.525620	2.435084	0.854437
57	6	0	6.565529	0.625573	0.984787
58	6	0	6.337253	1.043143	-1.378196
59	6	0	5.425975	-0.175233	0.965086
60	1	0	7.103379	0.761129	1.919331
61	6	0	5.195705	0.245852	-1.420484
62	1	0	6.696267	1.505491	-2.294105
63	6	0	4.743223	-0.352338	-0.241106
64	1	0	5.086079	-0.675084	1.865948
65	1	0	4.677769	0.065795	-2.356393
66	16	0	3.263262	-1.352276	-0.271748
67	7	0	1.989218	-0.318460	0.171669
68	8	0	3.354777	-2.344332	0.803506
69	8	0	2.998960	-1.729198	-1.664124

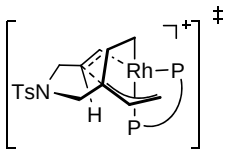


19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.400387	1.881093	-1.620192
2	6	0	-3.371206	3.292622	0.371686
3	6	0	-3.244423	2.193204	-0.651324
4	6	0	-0.790460	2.455420	-0.889202
5	6	0	0.166249	1.035622	-2.876161
6	6	0	0.820765	-0.313032	-2.563050
7	6	0	-3.651594	4.557808	0.055353
8	45	0	1.582583	0.149162	-0.648799
9	1	0	-0.907864	0.942514	-3.058248
10	1	0	0.603043	1.537178	-3.748673
11	1	0	1.575656	-0.615463	-3.293436
12	1	0	0.094980	-1.117929	-2.425613
13	1	0	-3.770263	5.323694	0.816471
14	1	0	-3.794225	4.874920	-0.976306
15	1	0	-4.007794	1.425739	-0.497106
16	1	0	-3.397661	2.590436	-1.660683
17	1	0	-1.220914	3.256360	-1.503719
18	1	0	-0.490611	2.920109	0.058304
19	6	0	1.690595	2.266949	-1.257656
20	6	0	2.835363	1.505715	-1.712764
21	1	0	2.902227	1.205454	-2.755676
22	1	0	3.798935	1.761556	-1.278531
23	15	0	2.406334	0.746084	1.641352
24	6	0	4.109576	1.474436	1.726490
25	6	0	1.454746	1.939136	2.688381
26	1	0	1.437653	2.922811	2.206988
27	1	0	4.423746	1.624403	2.765476
28	6	0	3.396620	-1.888263	2.276718
29	6	0	2.786869	-2.705508	1.122487
30	1	0	1.756473	-2.988145	1.374755
31	1	0	3.350865	-3.639219	0.999144
32	1	0	4.401005	-1.536774	2.006867
33	1	0	3.546982	-2.576003	3.117913
34	15	0	2.716311	-1.887602	-0.546006

35	6	0	2.000573	-3.240942	-1.575924
36	1	0	0.963698	-3.422906	-1.277812
37	6	0	4.478486	-1.852223	-1.095332
38	1	0	4.527479	-1.484805	-2.124683
39	1	0	-3.240109	3.003370	1.412660
40	1	0	2.575497	-4.164966	-1.452725
41	1	0	2.009421	-2.955543	-2.631111
42	1	0	5.063733	-1.174692	-0.467251
43	1	0	4.923781	-2.852263	-1.051572
44	1	0	4.837282	0.827249	1.228039
45	1	0	4.123471	2.445272	1.219939
46	1	0	0.423351	1.595533	2.802106
47	1	0	1.916454	2.046731	3.676445
48	1	0	1.811862	2.973975	-0.439027
49	6	0	2.537633	-0.715499	2.784024
50	1	0	1.513753	-1.059572	2.979442
51	1	0	2.939249	-0.357377	3.740634
52	1	0	-6.206719	-4.386224	0.293991
53	6	0	-6.520083	-3.348778	0.119657
54	1	0	-7.283319	-3.105169	0.864065
55	6	0	-5.339757	-2.413710	0.208714
56	1	0	-6.983670	-3.313494	-0.871806
57	6	0	-4.433997	-2.303880	-0.861607
58	6	0	-5.107718	-1.651111	1.361775
59	6	0	-3.326969	-1.465914	-0.788247
60	1	0	-4.600216	-2.886792	-1.763610
61	6	0	-4.008255	-0.798442	1.456803
62	1	0	-5.796716	-1.722202	2.198720
63	6	0	-3.130219	-0.712646	0.375067
64	1	0	-2.632645	-1.392254	-1.618541
65	1	0	-3.830772	-0.211413	2.351377
66	16	0	-1.690737	0.324667	0.527460
67	7	0	-1.916154	1.496151	-0.699188
68	8	0	-0.525362	-0.520429	0.139051
69	8	0	-1.658042	0.929968	1.869616

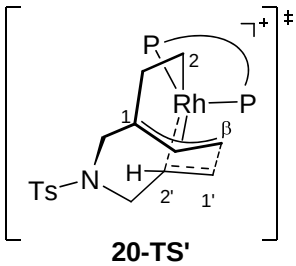


20-TS Imaginary frequency: –260.2 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.080911	-0.592115	1.321260
2	6	0	0.229160	0.529008	-0.388605
3	6	0	1.641881	0.043898	-0.669312
4	6	0	1.454237	-0.078059	1.752247
5	6	0	0.026012	-2.052880	0.848439
6	6	0	-1.205499	-2.219666	-0.053409
7	6	0	-0.782024	0.335498	-1.430050
8	45	0	-2.050458	-0.288285	0.113123
9	1	0	0.949193	-2.321212	0.328489
10	1	0	-0.008159	-2.696896	1.737223
11	1	0	-1.888565	-3.003982	0.288154
12	1	0	-0.926549	-2.434676	-1.087422
13	1	0	-1.189304	1.241032	-1.878134
14	1	0	-0.565238	-0.436105	-2.168891
15	1	0	1.631996	-0.902110	-1.222047
16	1	0	2.130596	0.794278	-1.304940
17	1	0	1.858024	-0.721115	2.539987
18	1	0	1.374172	0.936494	2.165302
19	6	0	-1.013066	-0.202583	2.232359
20	6	0	-2.074510	-0.989663	2.595208
21	1	0	-2.120043	-2.050265	2.380809
22	1	0	-2.822225	-0.602872	3.280572
23	15	0	-3.019687	1.989770	0.477445
24	6	0	-3.985766	2.201229	2.043355
25	6	0	-1.885106	3.455463	0.540282
26	1	0	-1.190102	3.359570	1.380747
27	1	0	-4.417565	3.205735	2.111624
28	6	0	-5.315025	1.513154	-1.189918
29	6	0	-4.805062	0.319268	-2.016555
30	1	0	-4.178460	0.679818	-2.843016
31	1	0	-5.656434	-0.200754	-2.474031
32	1	0	-5.840183	1.161783	-0.292065
33	1	0	-6.075479	2.028028	-1.789050
34	15	0	-3.827011	-0.979161	-1.119587

35	6	0	-3.453490	-2.159061	-2.485387
36	1	0	-2.742015	-1.710934	-3.185209
37	6	0	-5.096562	-1.885840	-0.131974
38	1	0	-4.625767	-2.743579	0.357020
39	1	0	0.220591	1.523302	0.055662
40	1	0	-4.370082	-2.415654	-3.026931
41	1	0	-3.012816	-3.074786	-2.083953
42	1	0	-5.514423	-1.238610	0.644366
43	1	0	-5.909035	-2.244866	-0.773807
44	1	0	-4.793175	1.464480	2.092994
45	1	0	-3.334386	2.042904	2.908634
46	1	0	-1.300812	3.524165	-0.383150
47	1	0	-2.448637	4.386852	0.663433
48	1	0	-0.958067	0.805554	2.643692
49	6	0	-4.235698	2.544604	-0.816191
50	1	0	-3.660189	2.813828	-1.711959
51	1	0	-4.710996	3.467657	-0.461092
52	7	0	2.364522	-0.080438	0.603979
53	16	0	3.670993	-1.201095	0.619597
54	6	0	5.025787	-0.238976	-0.026529
55	8	0	3.906935	-1.496728	2.035221
56	8	0	3.379495	-2.274849	-0.342091
57	6	0	5.667527	0.681804	0.807652
58	6	0	5.445303	-0.438972	-1.342579
59	6	0	6.735405	1.416281	0.302777
60	1	0	5.344698	0.807120	1.835914
61	6	0	6.517000	0.309533	-1.828933
62	1	0	4.952581	-1.178622	-1.964187
63	6	0	7.178262	1.243536	-1.019705
64	1	0	7.241276	2.130915	0.946750
65	1	0	6.850733	0.156609	-2.851822
66	6	0	8.360873	2.022484	-1.541562
67	1	0	9.302540	1.538659	-1.251288
68	1	0	8.349483	2.087817	-2.633744
69	1	0	8.381618	3.039643	-1.136710



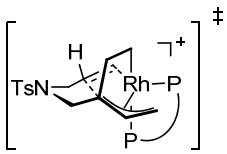
20-TS'

Imaginary frequency: –494.6 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.113663	-1.292683	1.611423
2	6	0	0.271829	-0.879007	-1.467484
3	6	0	-1.196515	-0.585615	-1.116169
4	6	0	-1.450908	-0.591498	1.438990
5	6	0	0.907474	-0.760091	2.659877
6	6	0	2.350198	-0.714300	2.161855
7	6	0	0.709428	-2.266381	-1.523191
8	1	0	0.582592	0.239232	2.956279
9	1	0	0.810410	-1.396575	3.551870
10	1	0	2.904896	-1.638673	2.355944
11	1	0	2.913424	0.129344	2.567793
12	1	0	1.559777	-2.481959	-2.168079
13	1	0	-0.066397	-3.022762	-1.643184
14	1	0	-1.616616	0.031464	-1.911338
15	1	0	-1.775337	-1.521443	-1.100563
16	1	0	-1.647287	0.128117	2.233811
17	1	0	-2.265805	-1.332699	1.435180
18	6	0	-0.018342	-2.483794	0.933370
19	6	0	1.144065	-3.027836	0.258129
20	1	0	2.119066	-2.881095	0.723679
21	1	0	1.076395	-4.051486	-0.102489
22	1	0	0.660936	-0.264812	-2.278718
23	1	0	-0.958763	-2.858866	0.526411
24	7	0	-1.444497	0.172184	0.150002
25	16	0	-2.665164	1.372269	0.041240
26	6	0	-4.254658	0.570808	-0.118707
27	8	0	-2.627050	2.062575	1.336520
28	8	0	-2.385943	2.090995	-1.209665
29	6	0	-4.965215	0.218545	1.033578
30	6	0	-4.765659	0.297141	-1.391260
31	6	0	-6.193245	-0.425267	0.900267
32	1	0	-4.576194	0.472747	2.013716

33	6	0	-5.996031	-0.346758	-1.501280
34	1	0	-4.223457	0.610889	-2.276714
35	6	0	-6.728703	-0.718435	-0.363601
36	1	0	-6.751780	-0.693606	1.793144
37	1	0	-6.400696	-0.553252	-2.488598
38	6	0	-8.078415	-1.380214	-0.495729
39	1	0	-8.879186	-0.629243	-0.497282
40	1	0	-8.159491	-1.945058	-1.429535
41	1	0	-8.274904	-2.062553	0.337296
42	1	0	4.253948	2.134336	-1.620002
43	6	0	4.513918	2.131523	-0.553621
44	6	0	5.068571	0.761484	-0.133924
45	1	0	5.318352	2.868373	-0.443945
46	6	0	3.325100	2.594511	0.297017
47	1	0	5.259619	0.747579	0.946286
48	1	0	6.027563	0.569321	-0.631304
49	15	0	3.960692	-0.663388	-0.525463
50	15	0	1.684105	1.746494	0.060447
51	1	0	3.577332	2.501746	1.360781
52	1	0	3.133682	3.659550	0.116682
53	45	0	1.764963	-0.563753	0.132266
54	6	0	4.916227	-2.112305	0.100550
55	6	0	4.125722	-0.828924	-2.358184
56	6	0	1.017725	2.507002	-1.478218
57	6	0	0.746844	2.582259	1.408180
58	1	0	4.993475	-2.071106	1.190599
59	1	0	5.924760	-2.115643	-0.327016
60	1	0	4.416675	-3.044766	-0.179411
61	1	0	3.641480	-1.747673	-2.700646
62	1	0	3.650423	0.015705	-2.864608
63	1	0	5.182918	-0.867243	-2.643987
64	1	0	1.146438	3.594400	-1.439579
65	1	0	1.537031	2.119823	-2.359951
66	1	0	-0.050413	2.287239	-1.561584
67	1	0	-0.308572	2.309628	1.400278
68	1	0	1.183813	2.325834	2.377534
69	1	0	0.828150	3.666340	1.268589

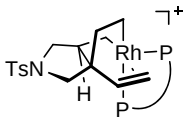


21-TS Imaginary frequency: –244.7 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.051424	-1.058365	1.256529
2	6	0	0.352712	-0.262748	-0.512268
3	6	0	1.554535	0.598919	-0.148232
4	6	0	1.473963	-0.729023	1.805815
5	6	0	-0.279600	-2.495122	0.815287
6	6	0	-1.522471	-2.392701	-0.097155
7	6	0	-0.746490	0.252161	-1.343940
8	45	0	-2.067486	-0.338965	0.154097
9	1	0	0.575006	-2.943146	0.297954
10	1	0	-0.457251	-3.118339	1.699883
11	1	0	-2.324821	-3.077491	0.195352
12	1	0	-1.274355	-2.582862	-1.144449
13	1	0	-0.903603	-0.301845	-2.269019
14	1	0	-0.777745	1.330976	-1.503774
15	1	0	2.134671	0.839459	-1.043942
16	1	0	1.265499	1.544310	0.327958
17	1	0	1.918070	-1.627005	2.242792
18	1	0	1.389161	0.021618	2.599810
19	6	0	-0.971773	-0.516837	2.197225
20	6	0	-2.122765	-1.141517	2.597186
21	1	0	-2.348812	-2.173446	2.359759
22	1	0	-2.772938	-0.659511	3.320570
23	15	0	-2.704496	2.011383	0.638920
24	6	0	-3.749433	2.250277	2.148414
25	6	0	-1.378086	3.279705	0.903616
26	1	0	-0.764275	3.005443	1.767626
27	1	0	-4.038808	3.300069	2.268312
28	6	0	-4.946310	2.030932	-1.163129
29	6	0	-4.617615	0.790345	-2.012067
30	1	0	-3.906029	1.058287	-2.803723
31	1	0	-5.527692	0.439562	-2.515648
32	1	0	-5.582594	1.755471	-0.311862
33	1	0	-5.559805	2.698025	-1.780457
34	15	0	-3.907220	-0.682066	-1.132527

35	6	0	-3.721253	-1.872428	-2.527316
36	1	0	-2.953703	-1.521246	-3.223506
37	6	0	-5.335498	-1.373467	-0.190619
38	1	0	-5.041303	-2.322116	0.267775
39	1	0	0.710092	-1.207797	-0.911393
40	1	0	-4.668272	-1.973165	-3.068308
41	1	0	-3.421937	-2.853450	-2.150444
42	1	0	-5.634897	-0.688422	0.607365
43	1	0	-6.191251	-1.548850	-0.852331
44	1	0	-4.654189	1.638656	2.085044
45	1	0	-3.195578	1.937244	3.038928
46	1	0	-0.726659	3.339609	0.026090
47	1	0	-1.807914	4.271139	1.084576
48	1	0	-0.751631	0.457678	2.631981
49	6	0	-3.721757	2.831072	-0.684709
50	1	0	-3.054787	3.026629	-1.534747
51	1	0	-4.043473	3.809786	-0.307052
52	7	0	2.368866	-0.178050	0.786865
53	16	0	3.491751	-1.281762	0.068261
54	6	0	4.907157	-0.234310	-0.208168
55	8	0	3.782447	-2.258764	1.120525
56	8	0	2.987310	-1.723266	-1.243225
57	6	0	5.628351	0.245910	0.890447
58	6	0	5.303337	0.048622	-1.515328
59	6	0	6.752742	1.030923	0.663840
60	1	0	5.317111	0.002134	1.900850
61	6	0	6.434870	0.839403	-1.719709
62	1	0	4.742680	-0.354605	-2.351539
63	6	0	7.175637	1.339874	-0.641323
64	1	0	7.318763	1.407183	1.512047
65	1	0	6.750315	1.062666	-2.735285
66	6	0	8.415997	2.169377	-0.866595
67	1	0	9.319698	1.577390	-0.673187
68	1	0	8.474647	2.534951	-1.895872
69	1	0	8.447071	3.033455	-0.193817

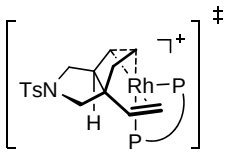


22

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.366698	-0.670613	-1.242448
2	6	0	0.379844	-0.485553	0.314848
3	6	0	1.791094	0.081947	0.591836
4	6	0	1.787134	-1.242751	-1.449645
5	6	0	0.159730	0.669222	-1.986531
6	6	0	-1.182033	1.356088	-1.645706
7	6	0	-0.805528	0.310326	0.841234
8	45	0	-2.380067	0.036529	-0.525020
9	1	0	0.998352	1.336387	-1.762984
10	1	0	0.227555	0.465170	-3.062315
11	1	0	-1.768002	1.589601	-2.546600
12	1	0	-1.002272	2.297622	-1.124322
13	1	0	-1.173627	-0.054179	1.804507
14	1	0	-0.582163	1.376440	0.917174
15	1	0	1.799538	1.176129	0.541466
16	1	0	2.162747	-0.221951	1.576334
17	1	0	2.161452	-1.119038	-2.466478
18	1	0	1.818299	-2.312461	-1.202115
19	6	0	-0.748311	-1.632891	-1.534705
20	6	0	-1.766644	-1.467492	-2.419010
21	1	0	-1.783244	-0.668369	-3.152563
22	1	0	-2.513042	-2.248004	-2.540954
23	15	0	-3.759075	-1.675255	0.677639
24	6	0	-5.274192	-2.300634	-0.188333
25	6	0	-2.907086	-3.253369	1.136761
26	1	0	-2.612853	-3.797631	0.234173
27	1	0	-5.789554	-3.059977	0.410097
28	6	0	-5.147238	0.227315	2.326250
29	6	0	-4.240371	1.457193	2.136080
30	1	0	-3.391924	1.410287	2.831567
31	1	0	-4.802016	2.364778	2.392083
32	1	0	-5.954621	0.231176	1.582764
33	1	0	-5.646041	0.341084	3.296071
34	15	0	-3.535575	1.749088	0.444336
35	6	0	-2.732619	3.394150	0.650682

36	1	0	-1.841774	3.314571	1.279963
37	6	0	-4.996119	2.130651	-0.618082
38	1	0	-4.651237	2.475696	-1.597457
39	1	0	0.337628	-1.494545	0.746370
40	1	0	-3.434021	4.090712	1.121770
41	1	0	-2.436727	3.795935	-0.321281
42	1	0	-5.617653	1.243216	-0.765996
43	1	0	-5.605711	2.918540	-0.161754
44	1	0	-5.970408	-1.480020	-0.388130
45	1	0	-4.994161	-2.743100	-1.149610
46	1	0	-2.006103	-3.038263	1.719721
47	1	0	-3.565279	-3.897073	1.730617
48	1	0	-0.731672	-2.555155	-0.952712
49	6	0	-4.423020	-1.130658	2.327482
50	1	0	-3.573289	-1.094628	3.022316
51	1	0	-5.099625	-1.909279	2.701475
52	7	0	2.627748	-0.494851	-0.486829
53	16	0	3.854000	0.517273	-1.126441
54	6	0	5.234723	0.210214	-0.037840
55	8	0	4.157203	-0.023145	-2.454874
56	8	0	3.451228	1.922826	-0.956952
57	6	0	6.012096	-0.936097	-0.231827
58	6	0	5.532566	1.121568	0.975394
59	6	0	7.091019	-1.169396	0.614095
60	1	0	5.781914	-1.621779	-1.040469
61	6	0	6.618205	0.867567	1.814339
62	1	0	4.936522	2.020367	1.090383
63	6	0	7.411994	-0.275006	1.649491
64	1	0	7.701547	-2.056501	0.465873
65	1	0	6.857601	1.575501	2.603460
66	6	0	8.603676	-0.531023	2.539973
67	1	0	9.539905	-0.306807	2.012869
68	1	0	8.574792	0.090376	3.439910
69	1	0	8.652520	-1.580546	2.850496

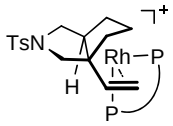


23-TS Imaginary frequency: –423.8 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.627260	-0.535447	-1.072742
2	6	0	-0.716541	-0.440476	0.476675
3	6	0	-2.021709	-1.189732	0.831671
4	6	0	-2.102201	-0.384828	-1.485437
5	6	0	-0.055772	-1.935483	-1.363698
6	6	0	1.261647	-2.083918	-0.608335
7	6	0	0.600441	-0.926070	1.055557
8	45	0	2.286878	-0.093928	-0.260003
9	1	0	-0.783678	-2.688590	-1.051127
10	1	0	0.090702	-2.074283	-2.441228
11	1	0	2.142088	-2.094227	-1.274315
12	1	0	1.331321	-2.967165	0.022079
13	1	0	1.076414	-0.183519	1.710671
14	1	0	0.546401	-1.866391	1.598596
15	1	0	-1.848899	-2.222701	1.152906
16	1	0	-2.565219	-0.676602	1.634806
17	1	0	-2.323402	-0.800379	-2.470550
18	1	0	-2.406290	0.674992	-1.475987
19	6	0	0.308681	0.553398	-1.537553
20	6	0	1.362441	0.405943	-2.399038
21	1	0	1.566298	-0.522713	-2.921129
22	1	0	1.856896	1.280592	-2.806607
23	15	0	3.585613	1.847781	-0.518387
24	6	0	4.751745	1.898916	-1.954345
25	6	0	2.577331	3.378843	-0.754901
26	1	0	1.975626	3.311663	-1.665559
27	1	0	5.254848	2.870450	-2.013988
28	6	0	5.657265	1.280359	1.394548
29	6	0	4.996127	0.103823	2.129973
30	1	0	4.364795	0.483297	2.944061
31	1	0	5.766899	-0.524235	2.594550
32	1	0	6.273597	0.914328	0.563514
33	1	0	6.356909	1.758504	2.090096
34	15	0	3.934439	-1.012295	1.096873

35	6	0	3.381770	-2.244107	2.355060
36	1	0	2.715094	-1.772342	3.082695
37	6	0	5.151059	-1.978252	0.095610
38	1	0	4.627503	-2.769483	-0.449442
39	1	0	-0.846950	0.616732	0.737734
40	1	0	4.248754	-2.652069	2.885127
41	1	0	2.846567	-3.068342	1.875309
42	1	0	5.646321	-1.335649	-0.637482
43	1	0	5.910039	-2.435078	0.741006
44	1	0	5.508158	1.115018	-1.857637
45	1	0	4.210690	1.724289	-2.888346
46	1	0	1.903148	3.510864	0.096537
47	1	0	3.226229	4.257996	-0.833735
48	1	0	0.039137	1.561488	-1.221554
49	6	0	4.671643	2.351715	0.901072
50	1	0	4.010329	2.657943	1.721917
51	1	0	5.222946	3.246844	0.587008
52	7	0	-2.764815	-1.173906	-0.441001
53	16	0	-4.395509	-1.561202	-0.506232
54	8	0	-4.698757	-1.710284	-1.929951
55	8	0	-4.569723	-2.639579	0.467143
56	6	0	-5.279786	-0.128032	0.101194
57	6	0	-5.604785	-0.040022	1.457843
58	6	0	-5.623358	0.897285	-0.785807
59	6	0	-6.269005	1.093339	1.924665
60	1	0	-5.368756	-0.862137	2.125224
61	6	0	-6.286830	2.021509	-0.299495
62	1	0	-5.402248	0.797049	-1.843408
63	6	0	-6.620537	2.139169	1.058788
64	1	0	-6.532206	1.159916	2.977302
65	1	0	-6.564619	2.815224	-0.988528
66	6	0	-7.378542	3.342449	1.565612
67	1	0	-8.461192	3.189558	1.467263
68	1	0	-7.171645	3.532095	2.623611
69	1	0	-7.126140	4.244719	0.999119

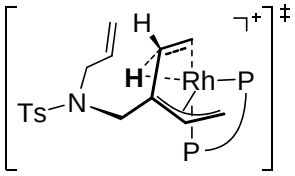


24

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.598849	-0.815623	-0.786018
2	6	0	-0.632744	-1.094033	0.778626
3	6	0	-2.132343	-1.109347	1.152346
4	6	0	-2.088013	-0.552614	-1.143865
5	6	0	-0.092082	-2.145836	-1.386636
6	6	0	0.883341	-2.662919	-0.332129
7	6	0	0.111432	-2.439643	0.976196
8	45	0	2.435030	-0.058184	-0.418949
9	1	0	-0.934436	-2.842525	-1.457997
10	1	0	0.333561	-2.050105	-2.389089
11	1	0	1.830941	-2.056291	-0.341859
12	1	0	1.216968	-3.694026	-0.489488
13	1	0	0.744101	-2.443973	1.869106
14	1	0	-0.613314	-3.255012	1.087335
15	1	0	-2.397049	-1.892039	1.865423
16	1	0	-2.440744	-0.136078	1.568833
17	1	0	-2.348017	-0.882555	-2.151185
18	1	0	-2.336518	0.518397	-1.044929
19	6	0	0.264151	0.383263	-1.128695
20	6	0	1.137319	0.490706	-2.192754
21	1	0	1.302314	-0.326523	-2.889607
22	1	0	1.442574	1.466033	-2.558144
23	15	0	3.252453	2.030502	-0.320092
24	6	0	4.312093	2.489163	-1.761894
25	6	0	1.976919	3.364521	-0.287252
26	1	0	1.341126	3.321363	-1.175539
27	1	0	4.652929	3.527219	-1.675700
28	6	0	5.520933	1.611241	1.423784
29	6	0	5.185273	0.202486	1.938684
30	1	0	4.537085	0.275463	2.821535
31	1	0	6.101836	-0.309700	2.257036
32	1	0	6.159098	1.552701	0.532849
33	1	0	6.127312	2.114039	2.186252
34	15	0	4.315911	-0.888633	0.719523
35	6	0	4.003378	-2.409635	1.719978

36	1	0	3.264902	-2.203139	2.499763
37	6	0	5.655434	-1.425638	-0.434942
38	1	0	5.257118	-2.163039	-1.138023
39	1	0	-0.116730	-0.295676	1.322988
40	1	0	4.931751	-2.750805	2.190895
41	1	0	3.619343	-3.208993	1.080460
42	1	0	6.029577	-0.577347	-1.015037
43	1	0	6.488241	-1.874687	0.118153
44	1	0	5.184219	1.832419	-1.820797
45	1	0	3.746502	2.377039	-2.690791
46	1	0	1.346639	3.253856	0.599818
47	1	0	2.463334	4.345551	-0.255685
48	1	0	-0.034383	1.298861	-0.618434
49	6	0	4.291065	2.491099	1.147746
50	1	0	3.627770	2.493856	2.022140
51	1	0	4.609344	3.529268	0.987327
52	7	0	-2.773087	-1.367480	-0.141689
53	16	0	-4.441572	-1.633751	-0.241983
54	6	0	-5.237398	-0.069751	0.114633
55	8	0	-4.688501	-1.958165	-1.646806
56	8	0	-4.741183	-2.555830	0.852800
57	6	0	-5.525967	0.811968	-0.931174
58	6	0	-5.559511	0.255608	1.436008
59	6	0	-6.135175	2.031726	-0.642024
60	1	0	-5.306028	0.528443	-1.955069
61	6	0	-6.167355	1.480298	1.704334
62	1	0	-5.366033	-0.455530	2.232182
63	6	0	-6.466616	2.385463	0.674512
64	1	0	-6.371513	2.714316	-1.454397
65	1	0	-6.428418	1.731359	2.729341
66	6	0	-7.167291	3.688966	0.972790
67	1	0	-8.256478	3.551897	0.978649
68	1	0	-6.885079	4.081641	1.955072
69	1	0	-6.939363	4.450093	0.219925

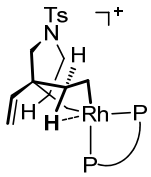


27-TS Imaginary frequency: –988.5 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.107356	1.456046	-0.334343
2	6	0	-2.156566	3.789114	0.320395
3	6	0	-3.041104	2.571646	0.340911
4	6	0	-1.331892	1.002315	-0.605218
5	6	0	0.937027	1.736386	-1.514960
6	6	0	2.243732	2.321908	-1.259502
7	6	0	-2.113229	4.658992	-0.690353
8	45	0	2.223197	0.354989	-0.306475
9	1	0	0.418909	1.842085	-2.470816
10	1	0	2.294549	3.149371	-0.559024
11	1	0	2.885505	2.442606	-2.127875
12	1	0	-1.496217	5.552021	-0.649035
13	1	0	-2.714870	4.525480	-1.587472
14	1	0	-3.705485	2.620357	1.208333
15	1	0	-3.659291	2.535308	-0.568733
16	1	0	-1.341112	-0.075617	-0.786480
17	1	0	-1.679574	1.484930	-1.526862
18	6	0	0.575761	1.419885	1.006940
19	6	0	1.863941	1.691208	1.530564
20	1	0	2.458532	2.545748	1.243567
21	1	0	2.038670	1.350181	2.548234
22	15	0	1.801088	-1.913085	0.352394
23	6	0	1.506838	-2.133789	2.162900
24	6	0	0.335140	-2.759935	-0.386286
25	1	0	-0.574884	-2.281538	-0.014819
26	1	0	1.411858	-3.195185	2.417726
27	6	0	4.575690	-2.706906	0.311191
28	6	0	5.137998	-1.646089	-0.649381
29	1	0	4.940159	-1.942797	-1.687548
30	1	0	6.228487	-1.583868	-0.541208
31	1	0	4.645133	-2.361943	1.351389
32	1	0	5.222705	-3.590176	0.250372
33	15	0	4.490237	0.079311	-0.438141

34	6	0	5.333721	0.953764	-1.828011
35	1	0	4.880014	0.668912	-2.781949
36	6	0	5.418465	0.692554	1.035853
37	1	0	5.211487	1.756645	1.180848
38	1	0	-1.557451	3.952558	1.215048
39	1	0	6.398902	0.698561	-1.849503
40	1	0	5.234510	2.035414	-1.704205
41	1	0	5.096798	0.158796	1.934385
42	1	0	6.497568	0.555044	0.903182
43	1	0	2.329292	-1.700044	2.739529
44	1	0	0.577150	-1.626452	2.437938
45	1	0	0.371531	-2.687870	-1.477722
46	1	0	0.314695	-3.817431	-0.099349
47	1	0	-0.126637	0.935082	1.680039
48	6	0	3.140622	-3.146349	-0.017960
49	1	0	3.067100	-3.390797	-1.085725
50	1	0	2.894704	-4.063657	0.531691
51	1	0	-7.813833	-1.306609	-2.850593
52	6	0	-7.562027	-2.040820	-2.074636
53	1	0	-7.313326	-2.980853	-2.575433
54	6	0	-6.421075	-1.548194	-1.218684
55	1	0	-8.466345	-2.201160	-1.477684
56	6	0	-5.136903	-2.099016	-1.335774
57	6	0	-6.622996	-0.522145	-0.281283
58	6	0	-4.077049	-1.636964	-0.557017
59	1	0	-4.966217	-2.911207	-2.037312
60	6	0	-5.579003	-0.046780	0.507054
61	1	0	-7.616144	-0.098254	-0.157570
62	6	0	-4.303902	-0.604260	0.356559
63	1	0	-3.097833	-2.096754	-0.633500
64	1	0	-5.753830	0.722277	1.251726
65	16	0	-2.956579	0.039325	1.340280
66	7	0	-2.251337	1.327144	0.482689
67	8	0	-1.894787	-0.980479	1.392787
68	8	0	-3.515573	0.627075	2.555119
69	1	0	1.415299	0.405564	-1.886275

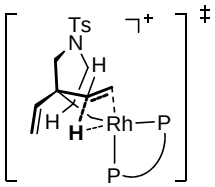


31

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.327290	2.219611	-0.052921
2	6	0	0.164504	1.178807	-1.219328
3	6	0	1.338137	0.172983	-1.085176
4	6	0	1.855151	2.137052	0.247386
5	6	0	-0.509656	1.802239	1.172979
6	6	0	-0.493267	0.346940	1.557167
7	6	0	-1.221951	0.545168	-1.367130
8	45	0	-2.214473	0.187300	0.432749
9	1	0	-0.336304	2.466993	2.029384
10	1	0	-1.599355	2.090828	0.912460
11	1	0	-0.784111	0.172273	2.601534
12	1	0	0.386586	-0.234167	1.310997
13	1	0	-1.908777	1.246206	-1.850556
14	1	0	-1.176121	-0.370165	-1.964776
15	1	0	1.007633	-0.808579	-0.743796
16	1	0	1.840479	0.039675	-2.052089
17	1	0	2.091348	2.354474	1.290266
18	1	0	2.397951	2.854257	-0.382677
19	6	0	-0.014347	3.620102	-0.523548
20	6	0	-0.811375	4.517979	0.059572
21	1	0	-1.341805	4.335001	0.990159
22	1	0	-0.948613	5.502852	-0.376962
23	15	0	-4.469262	0.517638	-0.527192
24	6	0	-5.780250	0.681647	0.772288
25	6	0	-4.820903	1.965163	-1.622875
26	1	0	-4.644577	2.894776	-1.073047
27	1	0	-5.783051	-0.193899	1.429511
28	6	0	-4.846967	-2.303671	-0.954217
29	6	0	-3.385458	-2.793810	-0.974835
30	1	0	-2.941955	-2.603903	-1.960828
31	1	0	-3.360983	-3.881737	-0.829116
32	1	0	-5.254669	-2.357058	0.063803
33	1	0	-5.436255	-3.019548	-1.539403
34	15	0	-2.227652	-2.076194	0.285790

35	6	0	-0.656987	-2.968692	-0.064798
36	1	0	-0.334456	-2.765901	-1.090390
37	6	0	-2.783855	-2.783566	1.897054
38	1	0	-2.037828	-2.561669	2.665852
39	1	0	0.320551	1.733111	-2.156806
40	1	0	-0.811511	-4.048270	0.042167
41	1	0	0.137168	-2.646441	0.614615
42	1	0	-3.740514	-2.353415	2.207708
43	1	0	-2.894751	-3.870726	1.816920
44	1	0	-5.580586	1.564270	1.388304
45	1	0	-6.773966	0.784937	0.322388
46	1	0	-4.155417	1.952030	-2.491845
47	1	0	-5.857983	1.952927	-1.975326
48	1	0	0.498039	3.910561	-1.442202
49	6	0	-5.082650	-0.905446	-1.556878
50	1	0	-4.586679	-0.836732	-2.533950
51	1	0	-6.154860	-0.758862	-1.739048
52	1	0	8.874715	-1.746632	-1.823731
53	6	0	8.644342	-0.714842	-1.541157
54	6	0	7.280484	-0.606402	-0.903610
55	1	0	9.430798	-0.361317	-0.866746
56	1	0	8.699139	-0.105010	-2.452619
57	6	0	6.985216	0.440059	-0.015875
58	6	0	6.274831	-1.541240	-1.190066
59	6	0	5.724489	0.563982	0.562171
60	1	0	7.757698	1.162116	0.235626
61	6	0	5.006488	-1.435924	-0.622231
62	1	0	6.490930	-2.371067	-1.857938
63	6	0	4.739762	-0.376201	0.247162
64	1	0	5.513000	1.360471	1.267601
65	1	0	4.242723	-2.178424	-0.826929
66	16	0	3.114726	-0.208741	0.967599
67	7	0	2.244206	0.765714	-0.094980
68	8	0	3.240560	0.542587	2.219928
69	8	0	2.474208	-1.535856	0.935735

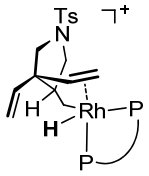


29-TS Imaginary frequency: −700.0 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.265815	2.224115	0.003682
2	6	0	0.161337	1.250533	-1.219613
3	6	0	1.315464	0.228377	-1.065789
4	6	0	1.792298	2.161950	0.334381
5	6	0	-0.548299	1.691848	1.184184
6	6	0	-0.432389	0.352060	1.651478
7	6	0	-1.231502	0.649054	-1.427259
8	45	0	-2.189202	0.258447	0.387110
9	1	0	-0.810059	2.436100	1.934682
10	1	0	-2.019904	1.898887	0.568476
11	1	0	-0.739589	0.159903	2.680315
12	1	0	0.341070	-0.311309	1.291225
13	1	0	-1.872264	1.360029	-1.950117
14	1	0	-1.195894	-0.288302	-1.989655
15	1	0	0.961964	-0.749931	-0.733910
16	1	0	1.834769	0.087457	-2.022015
17	1	0	2.008941	2.342803	1.388260
18	1	0	2.324734	2.916041	-0.260122
19	6	0	-0.114736	3.635407	-0.394407
20	6	0	-0.995547	4.459941	0.175325
21	1	0	-1.590852	4.200307	1.046011
22	1	0	-1.146162	5.461294	-0.217038
23	15	0	-4.326194	0.485747	-0.608441
24	6	0	-5.581062	0.761270	0.722460
25	6	0	-4.650355	1.881272	-1.769974
26	1	0	-4.394971	2.827096	-1.283397
27	1	0	-6.590005	0.827017	0.300175
28	6	0	-4.841902	-2.345294	-0.863776
29	6	0	-3.411213	-2.917154	-0.863589
30	1	0	-2.975165	-2.820417	-1.866790
31	1	0	-3.443275	-3.991624	-0.642576
32	1	0	-5.243986	-2.315180	0.157674
33	1	0	-5.480467	-3.053549	-1.404826

34	15	0	-2.213639	-2.142694	0.329286
35	6	0	-0.651319	-3.037920	-0.073538
36	1	0	-0.352583	-2.815990	-1.103083
37	6	0	-2.698326	-2.865002	1.961026
38	1	0	-1.957049	-2.588423	2.716887
39	1	0	0.372619	1.846272	-2.119049
40	1	0	-0.798873	-4.119779	0.018216
41	1	0	0.160662	-2.727848	0.590732
42	1	0	-3.672409	-2.482407	2.281223
43	1	0	-2.750534	-3.957695	1.902783
44	1	0	-5.560076	-0.053192	1.453135
45	1	0	-5.356280	1.694754	1.247222
46	1	0	-4.034663	1.780133	-2.668874
47	1	0	-5.703375	1.902569	-2.070093
48	1	0	0.443374	4.001624	-1.257200
49	6	0	-4.997645	-0.971447	-1.545327
50	1	0	-4.498978	-0.985903	-2.523554
51	1	0	-6.059799	-0.775253	-1.740258
52	1	0	9.368106	-0.391819	-0.941262
53	6	0	8.569491	-0.739771	-1.604180
54	1	0	8.786982	-1.773987	-1.887937
55	6	0	7.215605	-0.618369	-0.948171
56	1	0	8.616914	-0.131927	-2.517369
57	6	0	6.939909	0.435755	-0.062877
58	6	0	6.200169	-1.548608	-1.213895
59	6	0	5.688892	0.571255	0.532921
60	1	0	7.720515	1.154400	0.172711
61	6	0	4.941003	-1.432120	-0.627890
62	1	0	6.401170	-2.384116	-1.879349
63	6	0	4.694018	-0.365098	0.238351
64	1	0	5.493283	1.373536	1.236428
65	1	0	4.169938	-2.171425	-0.815826
66	16	0	3.083514	-0.186499	0.986337
67	7	0	2.209444	0.812529	-0.056563
68	8	0	3.231607	0.552184	2.243210
69	8	0	2.427543	-1.506195	0.950402



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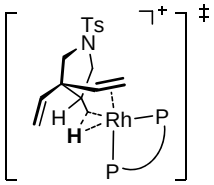
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.277403	2.250912	-0.117655
2	6	0	-0.171719	1.356834	1.163205
3	6	0	-1.268910	0.274234	1.019389
4	6	0	-1.806043	2.157769	-0.429489
5	6	0	0.524019	1.657331	-1.268604
6	6	0	0.445115	0.357335	-1.730265
7	6	0	1.241408	0.846867	1.442783
8	45	0	2.257724	0.393607	-0.324198
9	1	0	0.991499	2.378295	-1.931425
10	1	0	2.588883	1.949315	-0.279588
11	1	0	0.862886	0.131981	-2.710548
12	1	0	-0.261789	-0.367641	-1.350635
13	1	0	1.824990	1.616318	1.947857
14	1	0	1.244346	-0.068926	2.042556
15	1	0	-0.865276	-0.687346	0.695254
16	1	0	-1.781595	0.113012	1.975884
17	1	0	-2.037251	2.302818	-1.485313
18	1	0	-2.345713	2.917478	0.151606
19	6	0	0.096456	3.683745	0.202224
20	6	0	1.031825	4.458572	-0.349296
21	1	0	1.692988	4.133725	-1.146846
22	1	0	1.166023	5.481990	-0.011474
23	15	0	4.321051	0.352950	0.752354
24	6	0	5.633735	0.703153	-0.497545
25	6	0	4.623312	1.609865	2.062358
26	1	0	4.427539	2.608863	1.662934
27	1	0	6.624399	0.694030	-0.029765
28	6	0	4.724122	-2.504758	0.738413
29	6	0	3.284014	-3.040665	0.661804
30	1	0	2.844679	-3.053882	1.668098
31	1	0	3.295806	-4.081551	0.315055
32	1	0	5.141291	-2.372133	-0.268744
33	1	0	5.343273	-3.277161	1.209530

34	15	0	2.104524	-2.106769	-0.435626
35	6	0	0.534094	-3.013167	-0.081629
36	1	0	0.253591	-2.867340	0.966414
37	6	0	2.552300	-2.714893	-2.126433
38	1	0	1.819716	-2.353379	-2.854274
39	1	0	-0.450685	1.990386	2.017714
40	1	0	0.674901	-4.085877	-0.255730
41	1	0	-0.290109	-2.655470	-0.704344
42	1	0	3.538411	-2.343719	-2.423383
43	1	0	2.564553	-3.809859	-2.157573
44	1	0	5.616912	-0.044118	-1.296628
45	1	0	5.457849	1.686118	-0.943518
46	1	0	3.957775	1.439616	2.913624
47	1	0	5.659507	1.556004	2.412451
48	1	0	-0.516617	4.113463	0.995781
49	6	0	4.885024	-1.215293	1.565065
50	1	0	4.334142	-1.308042	2.510093
51	1	0	5.940203	-1.070855	1.830188
52	1	0	-8.667922	-1.713502	2.140637
53	6	0	-8.508339	-0.718258	1.715427
54	6	0	-7.165476	-0.614641	1.034216
55	1	0	-9.326677	-0.509603	1.018158
56	1	0	-8.588531	0.008137	2.534674
57	6	0	-6.907579	0.417144	0.116893
58	6	0	-6.145021	-1.537504	1.303260
59	6	0	-5.669029	0.537273	-0.506305
60	1	0	-7.692809	1.130071	-0.121086
61	6	0	-4.896975	-1.435828	0.689917
62	1	0	-6.332377	-2.355441	1.993925
63	6	0	-4.667498	-0.391455	-0.207353
64	1	0	-5.487515	1.321756	-1.233309
65	1	0	-4.121863	-2.169747	0.882208
66	16	0	-3.070709	-0.226333	-0.987315
67	7	0	-2.187107	0.810572	0.004333
68	8	0	-3.245597	0.466080	-2.266580
69	8	0	-2.402920	-1.538948	-0.918173

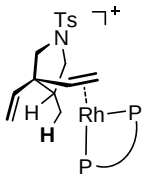


32-TS Imaginary frequency: –689.4 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.499242	-0.176623	1.767165
2	6	0	-0.555035	-1.543090	0.995895
3	6	0	-1.880735	-1.514089	0.171951
4	6	0	-2.013511	0.211545	1.847579
5	6	0	0.236083	0.889376	0.976683
6	6	0	0.170055	1.058972	-0.381399
7	6	0	0.717106	-1.857852	0.183975
8	45	0	2.108071	-0.190755	-0.084988
9	1	0	0.632700	1.711953	1.569209
10	1	0	1.915987	-1.046927	1.206301
11	1	0	0.470745	2.001550	-0.823817
12	1	0	-0.405354	0.410440	-1.033012
13	1	0	1.146076	-2.814858	0.483116
14	1	0	0.529022	-1.907547	-0.897142
15	1	0	-1.708497	-1.470792	-0.905707
16	1	0	-2.479503	-2.409193	0.379204
17	1	0	-2.183294	1.285002	1.937870
18	1	0	-2.470427	-0.286576	2.713922
19	6	0	0.067463	-0.383326	3.152826
20	6	0	1.202140	0.097994	3.667380
21	1	0	1.878499	0.738860	3.109832
22	1	0	1.493374	-0.136989	4.687011
23	15	0	3.921000	-1.603691	-0.457065
24	6	0	4.773743	-2.184858	1.070954
25	6	0	3.482895	-3.169883	-1.329500
26	1	0	2.780951	-3.758601	-0.734059
27	1	0	5.596357	-2.864440	0.823179
28	6	0	5.929106	0.371353	-1.117289
29	6	0	5.055348	1.599522	-1.423034
30	1	0	4.736772	1.575909	-2.473391
31	1	0	5.644997	2.515651	-1.293089
32	1	0	6.213582	0.357038	-0.057095
33	1	0	6.868764	0.482294	-1.671108

34	15	0	3.524040	1.766227	-0.385091
35	6	0	2.787053	3.313054	-1.082642
36	1	0	2.381973	3.125594	-2.081880
37	6	0	4.191556	2.353729	1.237298
38	1	0	3.365011	2.607099	1.907634
39	1	0	-0.663951	-2.321203	1.759078
40	1	0	3.546425	4.099422	-1.152002
41	1	0	1.976592	3.674496	-0.442522
42	1	0	4.785574	1.569882	1.715637
43	1	0	4.818296	3.242045	1.099285
44	1	0	5.168497	-1.333756	1.632551
45	1	0	4.057914	-2.707011	1.712091
46	1	0	3.012437	-2.941639	-2.290599
47	1	0	4.382077	-3.769497	-1.507918
48	1	0	-0.550571	-1.024904	3.782357
49	6	0	5.303182	-0.973301	-1.523836
50	1	0	4.917387	-0.911299	-2.549814
51	1	0	6.072874	-1.755564	-1.525377
52	1	0	-9.802937	0.016864	-1.014826
53	6	0	-9.225908	-0.713078	-0.432181
54	1	0	-9.412453	-1.699733	-0.867154
55	6	0	-7.756249	-0.369143	-0.447504
56	1	0	-9.628643	-0.705990	0.585942
57	6	0	-7.231906	0.572751	0.452056
58	6	0	-6.888409	-0.956916	-1.378951
59	6	0	-5.884274	0.921031	0.429494
60	1	0	-7.890889	1.045423	1.175806
61	6	0	-5.535735	-0.622621	-1.418645
62	1	0	-7.277601	-1.681910	-2.089017
63	6	0	-5.043694	0.312962	-0.506831
64	1	0	-5.491713	1.665542	1.113923
65	1	0	-4.874478	-1.065198	-2.155695
66	16	0	-3.308264	0.731603	-0.523945
67	7	0	-2.593129	-0.303136	0.610492
68	8	0	-3.155534	2.093399	0.000981
69	8	0	-2.771148	0.359822	-1.842345

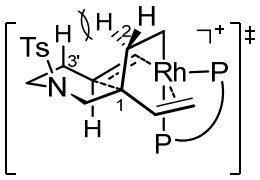


33

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.491662	-0.225096	1.718873
2	6	0	-0.678386	-1.677645	1.161301
3	6	0	-1.921237	-1.629874	0.231542
4	6	0	-1.988157	0.237829	1.763888
5	6	0	0.259057	0.747305	0.814035
6	6	0	0.200853	0.806606	-0.567049
7	6	0	0.577911	-2.294663	0.546863
8	45	0	2.170550	-0.161083	-0.067016
9	1	0	0.554345	1.654555	1.339839
10	1	0	0.400043	1.738311	-1.082329
11	1	0	-0.329700	0.076271	-1.168002
12	1	0	0.423306	-3.339002	0.251885
13	1	0	0.870992	-1.792366	-0.405918
14	1	0	-1.657784	-1.630494	-0.829663
15	1	0	-2.573290	-2.493097	0.411547
16	1	0	-2.110035	1.321094	1.745388
17	1	0	-2.459879	-0.151292	2.677099
18	6	0	0.097047	-0.289524	3.111976
19	6	0	1.335661	0.039325	3.484042
20	1	0	2.068584	0.418052	2.775460
21	1	0	1.660234	-0.070043	4.514902
22	15	0	4.086136	-1.453350	-0.528858
23	6	0	5.075086	-1.983249	0.939638
24	6	0	3.669971	-3.056186	-1.347962
25	1	0	3.028150	-3.655924	-0.695912
26	1	0	5.897309	-2.642387	0.639838
27	6	0	5.828696	0.678990	-1.318372
28	6	0	4.754192	1.771974	-1.449846
29	1	0	4.292409	1.726953	-2.444280
30	1	0	5.224063	2.759991	-1.361757
31	1	0	6.263095	0.689222	-0.310327
32	1	0	6.651790	0.937968	-1.994748
33	15	0	3.373154	1.732128	-0.211042

34	6	0	2.462345	3.280602	-0.636196
35	1	0	2.072664	3.227889	-1.656720
36	6	0	4.195146	2.187963	1.380655
37	1	0	3.434396	2.366817	2.146071
38	1	0	-0.939125	-2.297650	2.028041
39	1	0	3.143507	4.135388	-0.565268
40	1	0	1.626817	3.444927	0.049913
41	1	0	4.845831	1.382778	1.731335
42	1	0	4.791416	3.099205	1.256632
43	1	0	5.488859	-1.113805	1.458104
44	1	0	4.430856	-2.518306	1.643915
45	1	0	3.134434	-2.868393	-2.283255
46	1	0	4.579360	-3.626962	-1.566609
47	1	0	-0.584719	-0.684435	3.866422
48	6	0	5.348279	-0.736173	-1.681303
49	1	0	4.897493	-0.730161	-2.681954
50	1	0	6.202279	-1.424018	-1.719945
51	1	0	1.400983	-2.281659	1.271957
52	1	0	-9.848357	0.443948	-0.196994
53	6	0	-9.273446	-0.486230	-0.258055
54	1	0	-9.640714	-1.058481	-1.115115
55	6	0	-7.793078	-0.211970	-0.367486
56	1	0	-9.498224	-1.065580	0.646967
57	6	0	-7.195782	0.801913	0.398677
58	6	0	-6.980696	-0.963928	-1.227836
59	6	0	-5.829167	1.054667	0.322242
60	1	0	-7.812688	1.409196	1.056121
61	6	0	-5.609949	-0.726679	-1.320459
62	1	0	-7.428502	-1.739245	-1.843796
63	6	0	-5.044104	0.280025	-0.536468
64	1	0	-5.379762	1.856758	0.897874
65	1	0	-4.992612	-1.294535	-2.008147
66	16	0	-3.288487	0.590622	-0.632534
67	7	0	-2.601917	-0.372055	0.584830
68	8	0	-3.049856	1.986876	-0.248001
69	8	0	-2.806923	0.059889	-1.916225



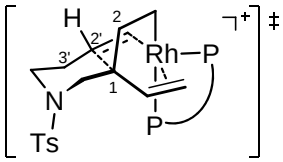
25-TS

Imaginary frequency: –282.3 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.191857	0.001829	0.820458
2	6	0	2.364744	0.527552	-1.393301
3	6	0	1.540833	0.757254	0.921395
4	6	0	0.222691	-1.528916	0.856952
5	6	0	-1.143540	-2.042905	0.377330
6	45	0	-2.192792	-0.218225	0.154572
7	1	0	1.035585	-1.914292	0.239433
8	1	0	0.467259	-1.844122	1.879957
9	1	0	-1.622130	-2.721658	1.090399
10	1	0	-1.070495	-2.555025	-0.585569
11	1	0	3.211779	0.124288	-1.953330
12	1	0	2.336707	1.608650	-1.593294
13	1	0	1.894087	0.622058	1.948302
14	1	0	1.370169	1.832965	0.772358
15	6	0	-0.762612	0.603951	1.775858
16	6	0	-1.608135	-0.077735	2.615244
17	1	0	-1.540834	-1.146696	2.772482
18	1	0	-2.241723	0.474122	3.302904
19	15	0	-3.362714	1.978387	0.006195
20	6	0	-4.078236	2.636212	1.583192
21	6	0	-2.424851	3.451674	-0.618325
22	1	0	-1.594714	3.684561	0.056226
23	1	0	-4.601532	3.584550	1.418621
24	6	0	-5.854161	0.866560	-0.909169
25	6	0	-5.379041	-0.533008	-1.338390
26	1	0	-4.967404	-0.490715	-2.355305
27	1	0	-6.239694	-1.213138	-1.378922
28	1	0	-6.189202	0.853632	0.136346
29	1	0	-6.748482	1.104323	-1.497652
30	15	0	-4.104603	-1.367321	-0.275056
31	6	0	-3.917530	-2.979489	-1.147695
32	1	0	-3.442293	-2.826799	-2.120726
33	6	0	-5.039878	-1.837835	1.245754

34	1	0	-4.406139	-2.465284	1.879464
35	1	0	-4.898210	-3.442824	-1.299329
36	1	0	-3.293111	-3.656924	-0.560752
37	1	0	-5.314618	-0.947107	1.817123
38	1	0	-5.947994	-2.395223	0.989625
39	1	0	-4.780618	1.915861	2.013447
40	1	0	-3.279704	2.801129	2.313073
41	1	0	-3.071344	4.333272	-0.688926
42	1	0	-0.755467	1.692711	1.835688
43	6	0	-4.832836	1.995996	-1.133398
44	1	0	-4.450506	1.946297	-2.161735
45	1	0	-5.330015	2.968976	-1.032361
46	6	0	1.067065	-0.123176	-1.871344
47	1	0	1.121570	-1.210121	-1.761939
48	1	0	0.974163	0.072566	-2.949365
49	6	0	-0.204741	0.439880	-1.234381
50	1	0	-0.181214	1.525725	-1.134048
51	6	0	-1.461108	-0.078811	-1.785844
52	1	0	-1.373801	-1.028219	-2.316329
53	1	0	-2.070497	0.640602	-2.333704
54	1	0	-2.012388	3.244314	-1.611117
55	1	0	9.617569	0.835941	-1.635580
56	6	0	9.223268	1.223608	-0.691833
57	6	0	7.832410	0.706531	-0.416788
58	1	0	9.240707	2.318147	-0.738064
59	1	0	9.915276	0.923409	0.105318
60	6	0	7.042461	1.288778	0.590710
61	6	0	7.305986	-0.372619	-1.137440
62	6	0	5.768246	0.811144	0.873541
63	1	0	7.437547	2.124237	1.162944
64	6	0	6.029142	-0.868303	-0.869044
65	1	0	7.903472	-0.838708	-1.916239
66	6	0	5.267742	-0.264981	0.132028
67	1	0	5.172965	1.259990	1.662103
68	1	0	5.629816	-1.714827	-1.416712
69	16	0	3.649602	-0.917037	0.511217
70	7	0	2.609821	0.348148	0.035390
71	8	0	3.476826	-1.022078	1.964043
72	8	0	3.425651	-2.079181	-0.361284



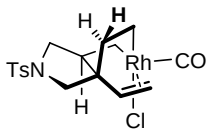
26-TS

Imaginary frequency: –278.5 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.020590	-1.783601	0.250262
2	6	0	1.478731	-2.124401	0.064724
3	6	0	-0.904794	-3.037798	0.248985
4	6	0	-2.356691	-2.603387	0.002733
5	45	0	-2.133789	-0.499091	-0.020490
6	1	0	-0.557197	-3.731532	-0.525612
7	1	0	-0.773943	-3.566044	1.203075
8	1	0	-3.043942	-2.945789	0.782522
9	1	0	-2.727041	-2.960700	-0.961126
10	1	0	1.552526	-2.916547	-0.691512
11	1	0	1.831319	-2.538806	1.014187
12	6	0	-0.293008	-0.853628	1.365556
13	6	0	-1.278360	-1.010097	2.308877
14	1	0	-1.833471	-1.931009	2.438153
15	1	0	-1.375861	-0.276268	3.102285
16	1	0	0.342550	0.024582	1.435032
17	6	0	0.773910	-0.059718	-1.973504
18	1	0	0.710658	0.213526	-3.037052
19	1	0	0.619702	0.856114	-1.401235
20	6	0	-0.345562	-1.056830	-1.691663
21	1	0	-0.123447	-2.074601	-2.014672
22	6	0	-1.707358	-0.643729	-2.055247
23	1	0	-1.792143	0.333900	-2.530375
24	1	0	-2.316557	-1.400652	-2.547480
25	1	0	9.256160	-0.233528	-1.279476
26	6	0	8.872898	0.641902	-0.744313
27	6	0	7.415209	0.476993	-0.391214
28	1	0	9.038448	1.524673	-1.368657
29	1	0	9.481206	0.758453	0.161849
30	6	0	6.514649	1.542044	-0.523537
31	6	0	6.935642	-0.748540	0.104313
32	6	0	5.171812	1.402266	-0.171439
33	1	0	6.867923	2.498066	-0.900276
34	6	0	5.601534	-0.910512	0.459189

35	1	0	7.621259	-1.584125	0.217850
36	6	0	4.726026	0.171147	0.310956
37	1	0	4.481419	2.234243	-0.255979
38	1	0	5.244853	-1.856467	0.853247
39	16	0	3.025712	-0.015630	0.812660
40	8	0	2.374548	1.303136	0.686578
41	8	0	2.944737	-0.747618	2.080394
42	6	0	2.189424	-0.581791	-1.712517
43	1	0	2.922627	0.202184	-1.919564
44	1	0	2.416743	-1.415050	-2.391765
45	7	0	2.391355	-1.073987	-0.349344
46	1	0	-2.905739	2.136829	2.452746
47	6	0	-2.018962	2.564885	1.976139
48	15	0	-1.883304	2.018538	0.209431
49	1	0	-2.071239	3.657179	2.044194
50	1	0	-1.138689	2.227520	2.532295
51	6	0	-3.234816	3.004946	-0.610069
52	6	0	-0.408642	2.999380	-0.337934
53	6	0	-4.677031	2.572426	-0.301872
54	1	0	-3.059172	2.953254	-1.693109
55	1	0	-3.098912	4.054946	-0.321921
56	15	0	-4.395187	-0.309779	-0.160498
57	1	0	0.506536	2.606858	0.114595
58	1	0	-0.308411	2.954341	-1.426976
59	1	0	-0.528139	4.049378	-0.047573
60	6	0	-5.095683	1.229958	-0.923424
61	1	0	-4.852062	2.563485	0.781694
62	1	0	-5.349506	3.342360	-0.699269
63	6	0	-5.249666	-0.415688	1.472274
64	6	0	-5.253731	-1.608706	-1.149496
65	1	0	-4.827014	1.210605	-1.987635
66	1	0	-6.187403	1.127176	-0.873263
67	1	0	-5.013033	-1.373948	1.943468
68	1	0	-4.904288	0.382321	2.134564
69	1	0	-6.336057	-0.337244	1.352050
70	1	0	-4.887153	-1.600993	-2.180317
71	1	0	-6.333325	-1.425057	-1.157130
72	1	0	-5.067112	-2.597230	-0.723397

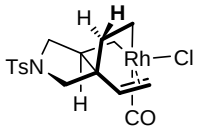


34

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.827413	1.033909	-0.395839
2	6	0	-0.527961	-0.499049	-0.448335
3	6	0	0.893356	-0.594980	0.130055
4	6	0	0.519233	1.602451	-0.886792
5	6	0	-1.167193	1.491619	1.042706
6	6	0	-2.427069	0.802140	1.612777
7	6	0	-1.617890	-1.335610	0.204854
8	45	0	-3.413290	-0.248096	0.070286
9	1	0	-0.298809	1.321597	1.688880
10	1	0	-1.307390	2.579901	1.021151
11	1	0	-3.177064	1.522712	1.960241
12	1	0	-2.183554	0.149428	2.453666
13	1	0	-1.859597	-2.243430	-0.353183
14	1	0	-1.398958	-1.584833	1.244896
15	1	0	0.877926	-0.632728	1.225587
16	1	0	1.435144	-1.471699	-0.239448
17	1	0	0.708425	2.619533	-0.539398
18	1	0	0.574584	1.605870	-1.982721
19	6	0	-1.995895	1.253254	-1.325069
20	6	0	-3.136776	1.937456	-1.058485
21	1	0	-3.264474	2.546542	-0.169334
22	1	0	-3.929997	1.973314	-1.798119
23	1	0	-0.476155	-0.770956	-1.510638
24	1	0	-1.918057	0.777489	-2.303122
25	7	0	1.536555	0.653143	-0.353050
26	16	0	2.777951	1.288084	0.609193
27	6	0	4.152375	0.225259	0.177334
28	8	0	3.025965	2.640992	0.099313
29	8	0	2.489431	1.074177	2.037157
30	6	0	4.699400	0.301739	-1.107360
31	6	0	4.677703	-0.644498	1.131428
32	6	0	5.776490	-0.515297	-1.433435
33	1	0	4.286374	0.992574	-1.835071
34	6	0	5.759020	-1.456967	0.785583

35	1	0	4.246135	-0.676237	2.125932
36	6	0	6.323812	-1.406545	-0.494646
37	1	0	6.203499	-0.461733	-2.431956
38	1	0	6.170286	-2.138782	1.525626
39	6	0	7.508845	-2.269318	-0.857704
40	1	0	8.438707	-1.685880	-0.841452
41	1	0	7.629952	-3.100976	-0.156813
42	1	0	7.406875	-2.685448	-1.866114
43	17	0	-4.897937	-0.885671	-1.765328
44	6	0	-4.176977	-1.487158	1.217472
45	8	0	-4.653188	-2.243582	1.936793

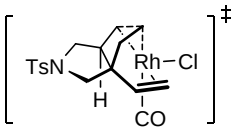


35

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.826093	-0.913887	-0.633973
2	6	0	0.552129	0.590231	-0.329092
3	6	0	-0.830796	0.556437	0.339323
4	6	0	-0.542486	-1.335592	-1.201571
5	6	0	1.200299	-1.710275	0.638648
6	6	0	2.513600	-1.209407	1.274237
7	6	0	1.718781	1.239591	0.390493
8	45	0	3.466254	0.107460	-0.024694
9	1	0	0.369112	-1.670354	1.351450
10	1	0	1.284837	-2.766393	0.351055
11	1	0	3.237790	-2.018672	1.438468
12	1	0	2.360829	-0.712876	2.233370
13	1	0	1.952771	2.245882	0.042618
14	1	0	1.641747	1.234333	1.476544
15	1	0	-0.758963	0.322070	1.407391
16	1	0	-1.376543	1.498920	0.225266
17	1	0	-0.743553	-2.403235	-1.102557
18	1	0	-0.638863	-1.069402	-2.262341
19	6	0	1.989353	-0.882069	-1.592766
20	6	0	3.139658	-1.627695	-1.515048
21	1	0	3.240003	-2.477106	-0.847897

22	1	0	3.886915	-1.544918	-2.299484
23	1	0	0.430533	1.083150	-1.303935
24	1	0	1.874422	-0.217550	-2.449436
25	7	0	-1.516640	-0.532257	-0.406352
26	16	0	-2.758266	-1.352123	0.401219
27	6	0	-4.153407	-0.252957	0.172687
28	8	0	-2.993894	-2.582226	-0.363228
29	8	0	-2.477142	-1.407223	1.844151
30	6	0	-4.805198	-0.226101	-1.063918
31	6	0	-4.582809	0.549768	1.228382
32	6	0	-5.891086	0.625397	-1.237955
33	1	0	-4.469605	-0.871944	-1.868671
34	6	0	-5.672852	1.400075	1.033997
35	1	0	-4.076483	0.496831	2.186165
36	6	0	-6.342118	1.451791	-0.194899
37	1	0	-6.402522	0.648268	-2.197292
38	1	0	-6.010539	2.028536	1.854223
39	6	0	-7.538360	2.352058	-0.393706
40	1	0	-8.472729	1.776413	-0.363763
41	1	0	-7.598444	3.118051	0.385492
42	1	0	-7.502010	2.856732	-1.365672
43	17	0	4.507860	1.172630	1.800150
44	6	0	4.346330	1.465705	-1.296361
45	8	0	4.763809	2.313723	-1.939451



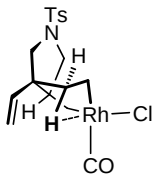
36-TS

Imaginary frequency: –406.7 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.577197	-0.765376	0.743038
2	6	0	-0.340871	-0.225582	-0.693820
3	6	0	0.862480	-1.042230	-1.206768
4	6	0	0.858445	-0.959104	1.253697
5	6	0	-1.358427	-2.087473	0.577733
6	6	0	-2.645538	-1.783337	-0.181219
7	6	0	-1.656220	-0.273007	-1.442220
8	45	0	-3.263534	0.317218	0.115732

9	1	0	-0.734960	-2.813977	0.048777
10	1	0	-1.569981	-2.522682	1.562050
11	1	0	-3.562806	-1.869411	0.430164
12	1	0	-2.828046	-2.358581	-1.083797
13	1	0	-1.974015	0.676399	-1.873474
14	1	0	-1.753145	-1.044792	-2.200160
15	1	0	0.564408	-1.922968	-1.785768
16	1	0	1.519388	-0.433702	-1.838109
17	1	0	0.942967	-1.686176	2.063947
18	1	0	1.282832	-0.002066	1.597305
19	6	0	-1.419087	0.275702	1.453534
20	6	0	-2.545661	0.021808	2.220559
21	1	0	-2.857014	-0.985255	2.478758
22	1	0	-2.957155	0.804158	2.850015
23	1	0	-0.027976	0.822410	-0.601377
24	1	0	-0.986502	1.275090	1.487532
25	7	0	1.535563	-1.465626	0.043942
26	16	0	3.173938	-1.794586	0.059949
27	8	0	3.455376	-2.351039	1.385083
28	8	0	3.450167	-2.520167	-1.181021
29	6	0	4.007708	-0.208799	-0.048942
30	6	0	4.362341	0.301672	-1.300763
31	6	0	4.266589	0.519116	1.116894
32	6	0	4.966165	1.556099	-1.379421
33	1	0	4.191138	-0.291795	-2.192609
34	6	0	4.869995	1.771227	1.018162
35	1	0	4.023738	0.093715	2.084989
36	6	0	5.227599	2.310438	-0.226951
37	1	0	5.247396	1.951475	-2.352401
38	1	0	5.076710	2.335917	1.924140
39	6	0	5.913522	3.652875	-0.318266
40	1	0	5.562636	4.336747	0.461798
41	1	0	6.999340	3.547428	-0.193437
42	1	0	5.741682	4.126431	-1.290163
43	6	0	-3.956370	2.053410	0.543468
44	8	0	-4.332173	3.118621	0.747672
45	17	0	-4.833726	0.233861	-1.672887

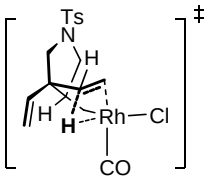


38

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.515451	1.400882	-0.689021
2	6	0	0.461251	0.705607	0.718881
3	6	0	-0.395157	-0.572732	0.546210
4	6	0	-0.812211	0.925871	-1.334792
5	6	0	1.742003	0.902547	-1.483809
6	6	0	2.004265	-0.563941	-1.504856
7	6	0	1.817077	0.500882	1.387466
8	45	0	3.279704	-0.090075	0.045455
9	1	0	1.829104	1.379561	-2.468559
10	1	0	2.668652	1.428893	-0.960902
11	1	0	2.629370	-0.909424	-2.333944
12	1	0	1.188647	-1.246764	-1.301475
13	1	0	2.183850	1.437204	1.815425
14	1	0	1.794014	-0.277133	2.153535
15	1	0	0.202230	-1.487908	0.582741
16	1	0	-1.152031	-0.631125	1.339131
17	1	0	-0.764612	0.888554	-2.425233
18	1	0	-1.628740	1.608969	-1.050602
19	6	0	0.498635	2.909290	-0.545907
20	6	0	1.332657	3.802207	-1.082060
21	1	0	2.170113	3.533362	-1.719413
22	1	0	1.198179	4.864622	-0.900441
23	1	0	-0.098989	1.383723	1.380430
24	1	0	-0.321721	3.279535	0.071427
25	1	0	-7.384397	0.425863	2.763394
26	6	0	-6.826159	1.182251	2.201319
27	6	0	-5.748965	0.553657	1.349511
28	1	0	-7.538269	1.749383	1.593696
29	1	0	-6.393649	1.876379	2.934206
30	6	0	-5.444926	1.063844	0.079153
31	6	0	-5.022649	-0.552740	1.814709
32	6	0	-4.437239	0.501626	-0.703310
33	1	0	-6.014111	1.904933	-0.308971
34	6	0	-4.011936	-1.128576	1.047054

35	1	0	-5.260271	-0.978155	2.786818
36	6	0	-3.717989	-0.590951	-0.210055
37	1	0	-4.231466	0.878230	-1.699795
38	1	0	-3.477176	-2.005420	1.396582
39	16	0	-2.384271	-1.290420	-1.187019
40	7	0	-1.008942	-0.421248	-0.787114
41	8	0	-2.654530	-0.979194	-2.592448
42	8	0	-2.155851	-2.652751	-0.706062
43	17	0	3.495493	-2.317843	0.764066
44	6	0	4.720990	0.588265	1.264157
45	8	0	5.629324	0.904563	1.884958

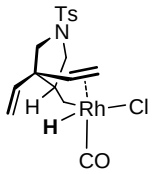


39-TS Imaginary frequency: –724.3 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.505199	1.259995	-0.815518
2	6	0	0.439675	0.750069	0.666307
3	6	0	-0.389718	-0.556317	0.641113
4	6	0	-0.823449	0.707200	-1.402259
5	6	0	1.704331	0.637983	-1.543513
6	6	0	1.966468	-0.758481	-1.505147
7	6	0	1.800770	0.658991	1.351971
8	45	0	3.264797	-0.014019	0.043074
9	1	0	2.018069	1.165237	-2.444535
10	1	0	2.864589	1.350564	-0.795838
11	1	0	2.608834	-1.178927	-2.277618
12	1	0	1.272152	-1.460046	-1.064058
13	1	0	2.117670	1.638421	1.713918
14	1	0	1.820560	-0.069665	2.165633
15	1	0	0.224233	-1.451433	0.777060
16	1	0	-1.141362	-0.543538	1.440409
17	1	0	-0.777779	0.541306	-2.480696
18	1	0	-1.639086	1.418659	-1.196562
19	6	0	0.500429	2.773763	-0.863483
20	6	0	1.382515	3.595506	-1.434382

21	1	0	2.267295	3.255237	-1.964385
22	1	0	1.245165	4.671839	-1.385946
23	1	0	-0.144192	1.493183	1.228773
24	1	0	-0.356664	3.216291	-0.353481
25	1	0	-7.208116	0.964283	2.810574
26	6	0	-6.830141	1.526807	1.951274
27	1	0	-6.445980	2.484011	2.328278
28	6	0	-5.753100	0.761739	1.219299
29	1	0	-7.676279	1.754612	1.294110
30	6	0	-5.437458	1.068180	-0.113468
31	6	0	-5.040581	-0.265507	1.853429
32	6	0	-4.431619	0.384482	-0.793016
33	1	0	-5.996783	1.844307	-0.630464
34	6	0	-4.030511	-0.961569	1.189725
35	1	0	-5.287467	-0.534140	2.877506
36	6	0	-3.724679	-0.625434	-0.131866
37	1	0	-4.216109	0.601101	-1.834025
38	1	0	-3.506135	-1.779031	1.673295
39	16	0	-2.390293	-1.476455	-0.978813
40	7	0	-1.009795	-0.565343	-0.698296
41	8	0	-2.644592	-1.378458	-2.417468
42	8	0	-2.174349	-2.750813	-0.294616
43	17	0	3.672725	-2.235771	0.874080
44	6	0	4.621331	0.760061	1.201190
45	8	0	5.464151	1.195839	1.842022

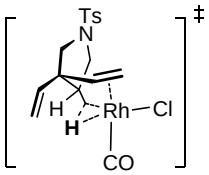


40

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.121997	1.937453	-0.394787
2	6	0	-0.815185	0.728054	-1.341887
3	6	0	0.396689	0.013776	-0.714017
4	6	0	0.310033	2.337555	0.074943
5	6	0	-1.982808	1.505859	0.789050
6	6	0	-1.701094	0.511710	1.690802

7	6	0	-2.030642	-0.135266	-1.637242
8	45	0	-3.052182	-0.541165	0.128232
9	1	0	-2.792919	2.181838	1.042397
10	1	0	-3.976336	0.665916	-0.299321
11	1	0	-2.317128	0.425537	2.584617
12	1	0	-0.793919	-0.079389	1.701293
13	1	0	-2.720544	0.370747	-2.313322
14	1	0	-1.755075	-1.115035	-2.036278
15	1	0	0.093628	-0.788121	-0.031966
16	1	0	1.035373	-0.427430	-1.487542
17	1	0	0.324240	2.754000	1.083412
18	1	0	0.725422	3.095359	-0.601289
19	6	0	-1.748028	3.064461	-1.193105
20	6	0	-2.999374	3.525162	-1.158591
21	1	0	-3.767918	3.131915	-0.500130
22	1	0	-3.306179	4.331408	-1.818855
23	1	0	-0.485369	1.148431	-2.305246
24	1	0	-1.057788	3.516097	-1.907136
25	1	0	7.168022	-2.644477	-1.389127
26	6	0	6.972099	-1.608601	-1.682360
27	6	0	5.784444	-1.039386	-0.943169
28	1	0	7.878981	-1.023681	-1.492696
29	1	0	6.802447	-1.598918	-2.767127
30	6	0	5.567557	0.348361	-0.903128
31	6	0	4.870096	-1.877096	-0.292513
32	6	0	4.467351	0.886476	-0.243581
33	1	0	6.276337	1.014437	-1.389344
34	6	0	3.761233	-1.356198	0.376462
35	1	0	5.028816	-2.952415	-0.300584
36	6	0	3.565983	0.024459	0.388343
37	1	0	4.313972	1.959847	-0.200422
38	1	0	3.063343	-2.004081	0.895914
39	16	0	2.155286	0.709743	1.251275
40	7	0	1.112051	1.100270	-0.014454
41	8	0	2.530638	1.992046	1.857665
42	8	0	1.585598	-0.367846	2.073844
43	17	0	-1.913777	-2.584505	0.927566
44	6	0	-4.220786	-1.675121	-0.836004
45	8	0	-4.938410	-2.359287	-1.406610

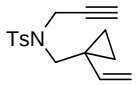


41-TS Imaginary frequency: –749.8 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.751830	1.594588	-0.030798
2	6	0	0.542561	0.836790	1.329812
3	6	0	-0.749988	-0.003162	1.147672
4	6	0	-0.714298	1.755071	-0.536954
5	6	0	1.552222	0.771354	-1.030461
6	6	0	1.432274	-0.570177	-1.252824
7	6	0	1.767867	0.026907	1.802903
8	45	0	3.255453	-0.340430	0.236970
9	1	0	2.117262	1.343771	-1.762997
10	1	0	2.961636	0.926215	1.113989
11	1	0	1.919563	-1.017910	-2.111975
12	1	0	0.752994	-1.211862	-0.702548
13	1	0	2.136880	0.370788	2.770978
14	1	0	1.549056	-1.041596	1.903155
15	1	0	-0.536140	-1.062859	0.983856
16	1	0	-1.394725	0.071827	2.032335
17	1	0	-0.791741	1.818914	-1.622895
18	1	0	-1.157012	2.664261	-0.106298
19	6	0	1.365738	2.954738	0.227637
20	6	0	2.569062	3.407244	-0.133140
21	1	0	3.285989	2.817297	-0.696120
22	1	0	2.884366	4.410457	0.140093
23	1	0	0.329769	1.607452	2.079645
24	1	0	0.719396	3.616971	0.806260
25	1	0	-8.684831	-0.508323	0.546199
26	6	0	-7.941352	-0.241725	1.308598
27	1	0	-8.057153	-0.942506	2.141062
28	6	0	-6.543287	-0.284074	0.738984
29	1	0	-8.196082	0.760991	1.669961
30	6	0	-6.094612	0.727241	-0.126440
31	6	0	-5.673431	-1.340589	1.036729
32	6	0	-4.817930	0.689684	-0.678699
33	1	0	-6.758814	1.551462	-0.375299

34	6	0	-4.390086	-1.396399	0.491605
35	1	0	-6.005556	-2.136765	1.698197
36	6	0	-3.969686	-0.374756	-0.359589
37	1	0	-4.484745	1.463972	-1.361971
38	1	0	-3.727582	-2.227860	0.706302
39	16	0	-2.318223	-0.421342	-1.052543
40	7	0	-1.414765	0.567818	-0.036099
41	8	0	-2.351244	0.244894	-2.358020
42	8	0	-1.832715	-1.800474	-0.904913
43	17	0	4.569765	-1.302495	-1.521172
44	6	0	4.703304	-0.721007	1.383747
45	8	0	5.585197	-0.948990	2.078561

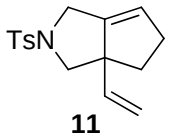


10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.582620	-3.313140	0.289375
2	6	0	3.157038	-2.583524	-0.286927
3	6	0	4.072332	-3.028528	-1.150128
4	1	0	4.266056	-4.090829	-1.272550
5	1	0	4.667245	-2.352496	-1.759267
6	6	0	3.833106	-0.068861	-0.230422
7	6	0	3.458991	-0.480785	1.172883
8	6	0	1.315130	-0.900392	-0.276203
9	1	0	3.500031	0.907516	-0.567544
10	1	0	4.810414	-0.360066	-0.604201
11	1	0	4.176265	-1.063269	1.744677
12	1	0	2.846375	0.197810	1.758677
13	1	0	1.059207	-1.238923	-1.289885
14	1	0	0.741379	-1.521937	0.417452
15	6	0	0.841096	1.344667	-1.331684
16	1	0	-0.196506	1.583064	-1.604207
17	1	0	1.237859	0.734564	-2.150398
18	7	0	0.881052	0.498025	-0.119184
19	16	0	-0.267263	0.847239	1.073932
20	8	0	0.119336	0.068518	2.252001
21	8	0	-0.389415	2.304635	1.095511
22	6	0	-1.834345	0.191909	0.485509

23	6	0	-2.679423	1.006392	-0.273704
24	6	0	-2.194835	-1.126037	0.782762
25	6	0	-3.877889	0.482615	-0.757550
26	1	0	-2.415954	2.044345	-0.447356
27	6	0	-3.396580	-1.631250	0.291795
28	1	0	-1.557631	-1.731023	1.418861
29	6	0	-4.251610	-0.842116	-0.492641
30	1	0	-4.539891	1.118926	-1.339684
31	1	0	-3.682249	-2.652470	0.532275
32	6	0	-5.538497	-1.410732	-1.041609
33	1	0	-6.004151	-2.104682	-0.333747
34	1	0	-6.261030	-0.620874	-1.269971
35	1	0	-5.357400	-1.967916	-1.970483
36	6	0	2.806493	-1.155195	-0.016704
37	6	0	1.620058	2.582182	-1.237390
38	6	0	2.264589	3.602162	-1.222825
39	1	0	2.822915	4.509145	-1.171712

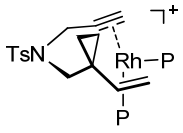


11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.398716	0.144506	1.132206
2	6	0	2.813919	0.344329	-0.327257
3	6	0	4.320117	0.000847	-0.264511
4	6	0	4.736235	0.338482	1.196150
5	6	0	3.441047	0.138872	1.962706
6	6	0	0.942433	-0.210717	1.217579
7	7	0	0.613658	-0.482828	-0.213057
8	6	0	1.855588	-0.653569	-1.020598
9	6	0	2.488994	1.758429	-0.778431
10	6	0	3.345191	2.724026	-1.117075
11	6	0	-2.085327	-0.502561	-0.179754
12	6	0	-2.421573	0.526389	-1.065797
13	6	0	-3.535034	1.314720	-0.797138
14	6	0	-4.325516	1.092456	0.343769
15	6	0	-3.971282	0.049725	1.207606
16	6	0	-2.856650	-0.752511	0.953510

17	6	0	-5.525752	1.965577	0.623713
18	16	0	-0.664283	-1.535868	-0.533027
19	8	0	-0.682895	-2.648448	0.428997
20	8	0	-0.604357	-1.799235	-1.974368
21	1	0	4.921320	0.513588	-1.020048
22	1	0	4.443551	-1.076223	-0.425807
23	1	0	5.540469	-0.313336	1.558282
24	1	0	5.103534	1.371585	1.287254
25	1	0	0.304187	0.602603	1.585366
26	1	0	0.775748	-1.092570	1.848064
27	1	0	1.639264	-0.426344	-2.065465
28	1	0	2.256152	-1.674497	-0.951833
29	1	0	1.421314	1.977633	-0.805601
30	1	0	2.986459	3.705592	-1.415481
31	1	0	4.423133	2.590025	-1.117141
32	1	0	-1.822809	0.693441	-1.955144
33	1	0	-3.802238	2.113330	-1.485216
34	1	0	-4.577003	-0.143610	2.089420
35	1	0	-2.591483	-1.570480	1.614757
36	1	0	-6.195688	2.011307	-0.243049
37	1	0	-6.101881	1.593525	1.476163
38	1	0	-5.221940	2.995649	0.849894
39	1	0	3.402224	-0.010062	3.038308



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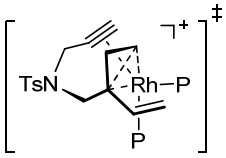
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.728069	-0.075596	-0.064315
2	15	0	-3.036900	-1.445446	-1.235116
3	6	0	-4.218906	-0.674462	-2.423439
4	6	0	-2.055274	-2.568213	-2.314125
5	1	0	-1.431436	-1.975339	-2.988825
6	1	0	-4.786541	-1.459821	-2.935818
7	6	0	-5.085430	-1.990217	0.737421
8	6	0	-4.457381	-1.259033	1.937777
9	1	0	-3.760002	-1.927611	2.457621

10	1	0	-5.239527	-0.988447	2.657690
11	1	0	-5.769144	-1.321422	0.198913
12	1	0	-5.713090	-2.802487	1.122066
13	15	0	-3.512581	0.267342	1.473446
14	6	0	-2.752184	0.811694	3.064417
15	1	0	-2.015502	0.073913	3.394646
16	6	0	-4.852637	1.515791	1.212385
17	1	0	-4.412537	2.502086	1.040069
18	1	0	-3.514863	0.937370	3.841059
19	1	0	-2.235000	1.765290	2.919772
20	1	0	-5.458919	1.260456	0.337774
21	1	0	-5.507495	1.573047	2.088929
22	1	0	-4.918956	-0.004788	-1.917763
23	1	0	-3.668447	-0.099341	-3.173402
24	1	0	-1.403953	-3.195539	-1.701753
25	1	0	-2.723945	-3.200559	-2.908521
26	6	0	-4.072865	-2.615328	-0.240905
27	1	0	-3.372739	-3.260994	0.303470
28	1	0	-4.603741	-3.251447	-0.961159
29	1	0	-0.848966	1.151398	-2.509550
30	6	0	-0.963053	1.713953	-1.583010
31	6	0	-2.239653	1.992562	-1.154967
32	6	0	0.281046	2.393697	-1.107846
33	1	0	-3.097243	1.745758	-1.768713
34	1	0	-2.418005	2.735285	-0.382851
35	6	0	0.251826	3.258211	0.138184
36	6	0	0.248452	3.930010	-1.199054
37	6	0	1.615045	1.754058	-1.507135
38	1	0	1.163028	3.296039	0.725955
39	1	0	-0.661123	3.280564	0.727644
40	1	0	-0.671802	4.382777	-1.555641
41	1	0	1.155512	4.430898	-1.527200
42	1	0	1.554311	1.409795	-2.549304
43	1	0	2.394556	2.515779	-1.467371
44	6	0	1.506816	-0.707798	-0.881957
45	1	0	2.224222	-1.458034	-0.526605
46	1	0	1.383457	-0.880983	-1.959163
47	6	0	0.196812	-0.904493	-0.192137
48	6	0	-0.494190	-1.545852	0.675746
49	1	0	-0.533011	-2.352384	1.392476
50	1	0	5.997163	-2.902198	1.543520
51	6	0	5.843724	-1.985686	0.980223
52	6	0	6.831550	-1.551093	0.088279
53	6	0	4.668806	-1.255682	1.171134

54	6	0	8.109043	-2.331121	-0.105517
55	6	0	6.616098	-0.353588	-0.617399
56	6	0	4.479852	-0.077086	0.449664
57	1	0	3.916988	-1.580350	1.882353
58	1	0	8.092136	-3.275495	0.445962
59	1	0	8.976248	-1.756082	0.241747
60	1	0	8.278386	-2.559247	-1.164411
61	6	0	5.452635	0.386456	-0.443646
62	1	0	7.377346	0.005390	-1.305426
63	16	0	2.992224	0.884439	0.698760
64	1	0	5.305969	1.319300	-0.978168
65	8	0	3.340621	2.309861	0.674554
66	8	0	2.268390	0.299547	1.833886
67	7	0	2.106219	0.613403	-0.724719



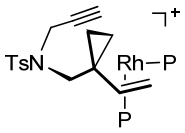
44-TS Imaginary frequency: –355.3 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.741088	-0.071510	0.266860
2	15	0	-2.701051	2.062545	0.241082
3	6	0	-3.457377	2.676256	1.811048
4	6	0	-1.560309	3.445326	-0.200689
5	1	0	-0.780757	3.533869	0.562337
6	1	0	-3.836028	3.695009	1.675096
7	6	0	-5.235899	1.280424	-0.921610
8	6	0	-4.931026	-0.105931	-1.518385
9	1	0	-4.472708	0.013648	-2.508652
10	1	0	-5.868612	-0.654529	-1.673746
11	1	0	-5.597912	1.180887	0.110330
12	1	0	-6.075085	1.706818	-1.484036
13	15	0	-3.798593	-1.184865	-0.509027
14	6	0	-3.612030	-2.656120	-1.616809
15	1	0	-3.049236	-2.385873	-2.515806
16	6	0	-4.941034	-1.844510	0.790429
17	1	0	-4.423390	-2.597818	1.392656
18	1	0	-4.588077	-3.053408	-1.916284

19	1	0	-3.059786	-3.449052	-1.102027
20	1	0	-5.258708	-1.040872	1.461651
21	1	0	-5.828295	-2.306726	0.343544
22	1	0	-4.285809	2.033440	2.121322
23	1	0	-2.712860	2.687431	2.612831
24	1	0	-1.084748	3.238250	-1.162953
25	1	0	-2.101648	4.395609	-0.264840
26	6	0	-4.074428	2.291056	-0.990776
27	1	0	-3.620585	2.269565	-1.989637
28	1	0	-4.462614	3.307594	-0.846237
29	1	0	-0.473047	0.999548	2.501633
30	6	0	-0.779226	0.005191	2.189931
31	6	0	-2.116588	-0.440245	2.374366
32	6	0	0.248815	-0.869282	1.662052
33	1	0	-2.812463	0.216395	2.885197
34	1	0	-2.326745	-1.497234	2.516497
35	6	0	-0.448693	-2.158740	0.479402
36	6	0	0.267582	-2.344361	1.791325
37	6	0	1.561838	-0.169259	1.261831
38	1	0	0.155087	-2.217610	-0.417507
39	1	0	-1.428832	-2.615522	0.430849
40	1	0	-0.332460	-2.771705	2.593676
41	1	0	1.256363	-2.793694	1.716598
42	1	0	1.505525	0.870436	1.610681
43	1	0	2.377494	-0.654582	1.803591
44	6	0	1.252810	0.846819	-1.003485
45	1	0	1.777194	0.863240	-1.963492
46	1	0	1.341423	1.841542	-0.543734
47	6	0	-0.166956	0.517667	-1.264789
48	6	0	-1.186807	0.148882	-1.878535
49	1	0	-1.732457	-0.085498	-2.773148
50	1	0	6.754462	2.017534	-1.707768
51	6	0	6.363371	1.283849	-1.007692
52	6	0	7.082290	0.994989	0.163880
53	6	0	5.167980	0.634010	-1.301082
54	6	0	8.366255	1.723177	0.477893
55	6	0	6.574907	0.018628	1.033071
56	6	0	4.678164	-0.322476	-0.405676
57	1	0	4.640551	0.838789	-2.226864
58	1	0	8.951130	1.911087	-0.428344
59	1	0	8.989524	1.156091	1.175575
60	1	0	8.159280	2.698024	0.938698
61	6	0	5.379705	-0.644429	0.758804
62	1	0	7.129978	-0.238593	1.931213

63	16	0	3.131607	-1.144592	-0.758549
64	1	0	5.013807	-1.424732	1.417281
65	8	0	3.071440	-2.357928	0.062131
66	8	0	2.930717	-1.159871	-2.207861
67	7	0	1.897377	-0.149185	-0.152872



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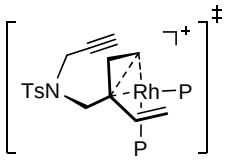
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.415345	-2.130807	-1.092395
2	6	0	-0.742111	-1.232615	-1.614155
3	6	0	-1.868822	-1.298954	-2.418281
4	6	0	0.176444	-0.063129	-1.539203
5	1	0	-2.374550	-2.248935	-2.555966
6	1	0	-2.088316	-0.551954	-3.177649
7	6	0	-0.480492	1.367708	-1.636118
8	6	0	0.373789	0.813662	-2.740148
9	6	0	1.346608	-0.290231	-0.565389
10	1	0	-0.057722	2.147906	-1.013094
11	1	0	-1.547630	1.482311	-1.864225
12	1	0	-0.107368	0.515046	-3.666736
13	1	0	1.363520	1.241524	-2.856551
14	1	0	0.945760	-0.622218	0.401095
15	1	0	1.937231	-1.119446	-0.967992
16	6	0	2.088180	1.648921	0.892825
17	1	0	3.038978	1.657472	1.440318
18	1	0	1.373235	1.126858	1.540146
19	6	0	1.643897	3.031274	0.681662
20	6	0	1.273434	4.172783	0.544917
21	1	0	1.007193	5.196594	0.402037
22	1	0	7.419277	-2.333986	3.388354
23	6	0	7.286091	-2.741274	2.381345
24	6	0	6.401329	-1.855928	1.537926
25	1	0	8.283380	-2.833806	1.931922
26	1	0	6.875365	-3.752068	2.470783
27	6	0	5.661967	-2.388243	0.469909

28	6	0	6.331317	-0.475089	1.774345
29	6	0	4.870100	-1.575576	-0.337808
30	1	0	5.720113	-3.452912	0.258600
31	6	0	5.546588	0.356370	0.977426
32	1	0	6.911607	-0.041073	2.584355
33	6	0	4.807484	-0.204073	-0.069611
34	1	0	4.336719	-1.989957	-1.186746
35	1	0	5.533962	1.429118	1.138893
36	16	0	3.770412	0.852220	-1.074037
37	8	0	3.571374	0.198656	-2.369441
38	8	0	4.255759	2.222845	-0.937846
39	7	0	2.222361	0.858422	-0.346867
40	1	0	-5.915299	-0.442107	2.989489
41	6	0	-5.259941	-0.298907	2.122386
42	6	0	-4.213347	0.765941	2.486227
43	1	0	-5.912467	0.059914	1.315185
44	6	0	-4.647890	-1.661550	1.758134
45	1	0	-3.532966	0.365694	3.248831
46	1	0	-4.702338	1.642759	2.928298
47	15	0	-3.162282	1.353700	1.073877
48	15	0	-3.826599	-1.768949	0.097627
49	1	0	-3.902462	-1.948486	2.510755
50	1	0	-5.424650	-2.436747	1.770747
51	45	0	-2.352814	-0.191510	-0.511717
52	6	0	-1.842944	2.297809	1.951538
53	6	0	-4.191173	2.673957	0.290230
54	6	0	-5.258498	-1.912406	-1.060986
55	6	0	-3.137667	-3.481714	0.150592
56	1	0	-1.243559	1.607415	2.553009
57	1	0	-2.284118	3.050652	2.614424
58	1	0	-1.178366	2.797597	1.241552
59	1	0	-3.618785	3.169478	-0.499766
60	1	0	-5.084368	2.236013	-0.164606
61	1	0	-4.496447	3.422910	1.029437
62	1	0	-5.915263	-2.738988	-0.766808
63	1	0	-5.833946	-0.982469	-1.060009
64	1	0	-4.901750	-2.085717	-2.079508
65	1	0	-2.729142	-3.766355	-0.822603
66	1	0	-2.335833	-3.534423	0.892953
67	1	0	-3.920002	-4.199017	0.422536

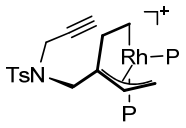


46-TS Imaginary frequency: –194.2 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.078581	0.904517	-1.787385
2	6	0	0.440965	-0.042956	-1.880647
3	6	0	1.548527	-0.160422	-2.717806
4	1	0	1.849248	0.692641	-3.315753
5	1	0	1.911681	-1.120440	-3.074168
6	6	0	1.433920	-2.402415	-0.602268
7	6	0	0.203077	-2.564896	-1.451909
8	6	0	-1.058148	-0.871996	0.029544
9	1	0	1.333224	-2.800648	0.402012
10	1	0	2.396198	-2.599089	-1.084577
11	1	0	0.381416	-2.725462	-2.514738
12	1	0	-0.549252	-3.255931	-1.075129
13	1	0	-0.705594	-1.319704	0.960734
14	1	0	-1.149117	0.206989	0.204386
15	6	0	-3.000699	-2.294417	0.799145
16	1	0	-3.907689	-2.725895	0.364947
17	1	0	-3.305907	-1.658176	1.645687
18	6	0	-2.140613	-3.373884	1.285047
19	6	0	-1.443991	-4.260976	1.717359
20	1	0	-0.870682	-5.081203	2.089074
21	1	0	-6.981609	4.082878	1.470203
22	6	0	-6.238090	3.553825	2.080417
23	6	0	-5.522733	2.508693	1.259918
24	1	0	-5.543660	4.303941	2.471414
25	1	0	-6.771145	3.105791	2.924900
26	6	0	-4.333584	2.815446	0.581198
27	6	0	-6.053377	1.216582	1.123585
28	6	0	-3.686190	1.867459	-0.208638
29	1	0	-3.917345	3.816497	0.659910
30	6	0	-5.422709	0.254641	0.338027
31	1	0	-6.981977	0.963636	1.628342
32	6	0	-4.232244	0.584611	-0.318672
33	1	0	-2.791610	2.126805	-0.764496
34	1	0	-5.862476	-0.728702	0.209271

35	16	0	-3.403562	-0.654154	-1.308842
36	8	0	-2.501714	0.035626	-2.238151
37	8	0	-4.400678	-1.626724	-1.746819
38	7	0	-2.351013	-1.502271	-0.267852
39	6	0	-0.037635	-1.141449	-1.072459
40	1	0	4.432747	-2.043201	2.889284
41	6	0	4.164370	-1.868801	1.841367
42	15	0	2.837480	-0.586076	1.699939
43	1	0	3.820413	-2.810439	1.403068
44	1	0	5.057783	-1.550828	1.295653
45	6	0	3.551650	0.846687	2.643197
46	45	0	2.133077	-0.247197	-0.528878
47	6	0	1.568803	-1.187682	2.904322
48	6	0	4.565746	1.716964	1.880652
49	1	0	2.710475	1.469065	2.974804
50	1	0	4.016442	0.438586	3.549696
51	1	0	0.775296	-0.441158	3.005362
52	1	0	2.023299	-1.352363	3.887561
53	1	0	1.118244	-2.125833	2.568529
54	1	0	5.360636	1.095216	1.446961
55	1	0	5.066754	2.364521	2.610048
56	6	0	3.935346	2.616161	0.803528
57	15	0	3.351281	1.748816	-0.732152
58	1	0	3.071552	3.146246	1.225394
59	1	0	4.653715	3.384426	0.490648
60	6	0	4.913617	1.532453	-1.699832
61	6	0	2.515791	3.141594	-1.616552
62	1	0	5.431652	2.488619	-1.833939
63	1	0	5.582438	0.835709	-1.185599
64	1	0	4.682528	1.111439	-2.682609
65	1	0	2.250234	2.847540	-2.635557
66	1	0	1.599053	3.420759	-1.088278
67	1	0	3.174144	4.015831	-1.667908



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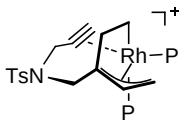
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.349131	-0.807729	-0.376495
2	6	0	-3.228787	-1.996246	1.704155
3	6	0	-1.477182	-0.566157	0.605509
4	6	0	0.155515	-2.233140	-0.570491
5	6	0	1.677373	-2.256308	-0.368111
6	45	0	2.167899	-0.248129	-0.001233
7	1	0	-0.359051	-2.889513	0.136521
8	1	0	-0.149512	-2.566191	-1.570461
9	1	0	2.205794	-2.728703	-1.201528
10	1	0	1.960641	-2.773905	0.558593
11	1	0	-3.986392	-2.726507	1.405906
12	1	0	-3.744975	-1.164404	2.210598
13	1	0	-1.835027	0.473234	0.548170
14	1	0	-1.081085	-0.717554	1.617195
15	6	0	0.192483	0.243337	-1.084879
16	6	0	1.383979	0.083335	-1.900693
17	1	0	1.474472	-0.808840	-2.518185
18	1	0	1.765265	0.976436	-2.392044
19	15	0	2.559003	2.117028	0.651491
20	6	0	2.308802	3.393652	-0.667883
21	6	0	1.529008	2.783828	2.038339
22	1	0	0.472002	2.767693	1.754350
23	1	0	2.497909	4.401129	-0.281403
24	6	0	5.412590	1.932489	0.360588
25	6	0	5.641391	0.415194	0.497701
26	1	0	5.662315	0.139399	1.560357
27	1	0	6.625726	0.152376	0.089222
28	1	0	5.253364	2.203043	-0.691896
29	1	0	6.344458	2.431633	0.651408
30	15	0	4.406866	-0.703354	-0.329028
31	6	0	4.984355	-2.365744	0.225155
32	1	0	4.815298	-2.483413	1.299882
33	6	0	4.892662	-0.658548	-2.107817
34	1	0	4.266781	-1.354172	-2.674108
35	1	0	6.053338	-2.487208	0.019435

36	1	0	4.431448	-3.150433	-0.297385
37	1	0	4.746829	0.344199	-2.519342
38	1	0	5.943294	-0.943895	-2.229617
39	1	0	2.984523	3.208213	-1.508659
40	1	0	1.282158	3.352350	-1.045070
41	1	0	1.651157	2.156967	2.927440
42	1	0	1.809935	3.812501	2.290301
43	1	0	-0.233114	1.235691	-0.951907
44	6	0	4.281983	2.499380	1.240829
45	1	0	4.374972	2.103827	2.260882
46	1	0	4.382270	3.589316	1.317810
47	6	0	-2.281858	-2.622726	2.625883
48	6	0	-1.512382	-3.143717	3.396744
49	1	0	-0.856957	-3.616517	4.093788
50	1	0	-6.775444	4.376562	-0.278603
51	6	0	-7.068764	3.503204	0.311105
52	6	0	-6.209376	2.304134	-0.007193
53	1	0	-8.126303	3.298118	0.112721
54	1	0	-6.986392	3.774194	1.371527
55	6	0	-5.014788	2.439780	-0.728490
56	6	0	-6.593013	1.019639	0.412230
57	6	0	-4.212450	1.335622	-1.015000
58	1	0	-4.716422	3.421683	-1.086513
59	6	0	-5.807695	-0.095883	0.135430
60	1	0	-7.528647	0.889849	0.949936
61	6	0	-4.610763	0.071679	-0.571088
62	1	0	-3.312281	1.441168	-1.611045
63	1	0	-6.132649	-1.087885	0.431028
64	16	0	-3.576756	-1.351140	-0.898630
65	8	0	-2.654616	-1.002582	-1.984429
66	8	0	-4.424235	-2.540213	-0.930662
67	7	0	-2.561145	-1.543371	0.462123



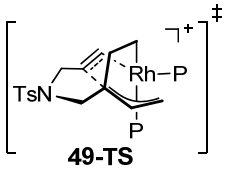
48

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.181695	-0.924092	1.483647

2	6	0	1.246446	0.065335	-1.304930
3	6	0	1.571130	-0.469519	1.107819
4	6	0	-0.167551	-2.395785	1.269718
5	6	0	-1.445147	-2.409177	0.428171
6	45	0	-1.796998	-0.319231	0.254158
7	1	0	0.662896	-2.891518	0.760960
8	1	0	-0.287817	-2.886864	2.244341
9	1	0	-2.272684	-2.941782	0.903200
10	1	0	-1.281778	-2.801530	-0.576710
11	1	0	1.749745	-0.138790	-2.255403
12	1	0	1.376371	1.133667	-1.069899
13	1	0	2.281689	-1.030275	1.725228
14	1	0	1.708806	0.602600	1.316455
15	6	0	-0.678816	-0.079262	2.186206
16	6	0	-2.051839	-0.426874	2.408503
17	1	0	-2.308998	-1.449553	2.670123
18	1	0	-2.681317	0.319029	2.886189
19	15	0	-2.154350	2.178596	0.106302
20	6	0	-2.691654	3.072816	1.638123
21	6	0	-0.744627	3.237561	-0.462818
22	1	0	0.085053	3.172612	0.248402
23	1	0	-2.830944	4.141588	1.441989
24	6	0	-4.838819	1.989942	-0.936406
25	6	0	-4.890420	0.517851	-1.383349
26	1	0	-4.458197	0.422657	-2.388105
27	1	0	-5.936981	0.197574	-1.466137
28	1	0	-5.191769	2.087786	0.098709
29	1	0	-5.567542	2.540301	-1.543528
30	15	0	-4.040826	-0.727841	-0.295960
31	6	0	-4.356827	-2.292808	-1.221377
32	1	0	-3.795836	-2.305211	-2.160490
33	6	0	-5.183880	-0.882685	1.143342
34	1	0	-4.838932	-1.687509	1.799044
35	1	0	-5.423954	-2.395082	-1.446091
36	1	0	-4.037577	-3.151841	-0.626117
37	1	0	-5.195388	0.044858	1.722363
38	1	0	-6.202174	-1.109115	0.809447
39	1	0	-3.634696	2.660817	2.009748
40	1	0	-1.941374	2.961208	2.427302
41	1	0	-0.392887	2.890833	-1.439148
42	1	0	-1.045542	4.287311	-0.551818
43	1	0	-0.342316	0.934409	2.398386
44	6	0	-3.472422	2.678630	-1.109685
45	1	0	-3.079406	2.473408	-2.114021

46	1	0	-3.599068	3.766326	-1.038318
47	6	0	-0.189420	-0.218534	-1.515248
48	6	0	-1.308073	-0.430778	-1.993104
49	1	0	-2.025180	-0.651941	-2.757168
50	1	0	7.689937	3.347747	-0.017612
51	6	0	7.806346	2.418111	0.548178
52	6	0	6.689014	1.446835	0.255589
53	1	0	8.776895	1.986703	0.270692
54	1	0	7.853914	2.667058	1.612959
55	6	0	6.287373	0.504366	1.214096
56	6	0	6.053037	1.438175	-0.995966
57	6	0	5.281158	-0.420407	0.942494
58	1	0	6.778557	0.484977	2.183416
59	6	0	5.045161	0.522570	-1.288540
60	1	0	6.361678	2.150018	-1.757094
61	6	0	4.658632	-0.398054	-0.309133
62	1	0	5.002196	-1.168738	1.676500
63	1	0	4.586859	0.501081	-2.271831
64	16	0	3.345754	-1.559493	-0.660575
65	8	0	3.435583	-2.648409	0.312151
66	8	0	3.291809	-1.782510	-2.105780
67	7	0	1.870877	-0.775258	-0.290277



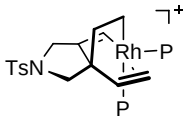
49-TS Imaginary frequency: –282.8 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.151366	-1.241503	1.007380
2	6	0	1.531151	-0.662924	-1.311057
3	6	0	1.672016	-1.114498	1.018775
4	6	0	-0.442186	-2.644427	0.840140
5	6	0	-1.884932	-2.484640	0.335560
6	45	0	-2.005817	-0.360376	0.226875
7	1	0	0.178746	-3.209615	0.140434
8	1	0	-0.383672	-3.167721	1.805018
9	1	0	-2.632490	-2.902898	1.015617
10	1	0	-2.024829	-2.924823	-0.652442

11	1	0	1.728849	-1.082302	-2.301542
12	1	0	1.896787	0.380354	-1.291059
13	1	0	2.075435	-1.811876	1.759897
14	1	0	1.967804	-0.090185	1.305825
15	6	0	-0.509831	-0.382594	2.004578
16	6	0	-1.655024	-0.683415	2.704967
17	1	0	-2.071340	-1.681259	2.749758
18	1	0	-2.043759	0.035008	3.420385
19	15	0	-2.026252	2.135541	0.128721
20	6	0	-2.517713	3.055208	1.660512
21	6	0	-0.428296	2.958217	-0.314164
22	1	0	0.325135	2.754642	0.453722
23	1	0	-2.501410	4.138990	1.500203
24	6	0	-4.619425	2.319538	-1.089706
25	6	0	-4.807310	0.854006	-1.522604
26	1	0	-4.310931	0.684051	-2.486909
27	1	0	-5.875136	0.655682	-1.681442
28	1	0	-5.038855	2.478905	-0.087872
29	1	0	-5.226705	2.938435	-1.760932
30	15	0	-4.200183	-0.464674	-0.364155
31	6	0	-4.733567	-1.996424	-1.236583
32	1	0	-4.155430	-2.125878	-2.156315
33	6	0	-5.364156	-0.371738	1.064993
34	1	0	-5.179208	-1.215107	1.736606
35	1	0	-5.797691	-1.938793	-1.488752
36	1	0	-4.566212	-2.869532	-0.601134
37	1	0	-5.206824	0.551574	1.629240
38	1	0	-6.405353	-0.410806	0.725252
39	1	0	-3.523192	2.761767	1.977438
40	1	0	-1.827366	2.813276	2.475023
41	1	0	-0.061760	2.563022	-1.266217
42	1	0	-0.550927	4.043133	-0.402628
43	1	0	-0.038912	0.582411	2.188099
44	6	0	-3.171867	2.839513	-1.153591
45	1	0	-2.738579	2.606261	-2.135061
46	1	0	-3.167706	3.932641	-1.058682
47	6	0	0.064646	-0.687432	-1.042061
48	6	0	-1.091765	-0.566948	-1.588181
49	1	0	-1.486108	-0.548015	-2.594986
50	1	0	5.882516	2.351585	-1.988715
51	6	0	5.657453	1.720059	-1.133129
52	6	0	6.065493	2.122314	0.148035
53	6	0	4.986760	0.515155	-1.333172
54	6	0	6.830883	3.407972	0.346212

55	6	0	5.780616	1.280648	1.234385
56	6	0	4.711915	-0.301359	-0.231096
57	1	0	4.708912	0.192342	-2.331086
58	1	0	7.909086	3.238161	0.229337
59	1	0	6.673618	3.820066	1.347889
60	1	0	6.540805	4.166401	-0.387928
61	6	0	5.111372	0.071531	1.056429
62	1	0	6.102715	1.568275	2.231859
63	16	0	3.835389	-1.842000	-0.471838
64	1	0	4.930449	-0.591827	1.895760
65	8	0	4.141937	-2.727469	0.648856
66	8	0	3.975372	-2.235653	-1.871788
67	7	0	2.174506	-1.484716	-0.294056



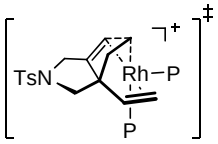
50

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.471320	0.431182	-1.083699
2	6	0	-1.551864	0.258238	1.162477
3	6	0	-1.949708	0.921793	-1.095143
4	6	0	-0.219490	-0.868248	-1.892398
5	6	0	1.168554	-1.465284	-1.586826
6	45	0	2.399110	-0.017711	-0.631343
7	1	0	-1.014698	-1.583466	-1.666350
8	1	0	-0.323008	-0.635439	-2.959674
9	1	0	1.715767	-1.737355	-2.501510
10	1	0	1.064491	-2.362144	-0.978261
11	1	0	-1.745998	-0.586909	1.824596
12	1	0	-1.588221	1.181730	1.757077
13	1	0	-2.482163	0.621799	-1.997724
14	1	0	-1.998389	2.015220	-1.006748
15	6	0	0.536459	1.487662	-1.470126
16	6	0	1.467041	1.415666	-2.458205
17	1	0	1.476624	0.622653	-3.199051
18	1	0	2.129574	2.256415	-2.644670
19	15	0	3.760308	1.801236	0.391441
20	6	0	5.229143	2.430158	-0.548369

21	6	0	2.847506	3.362886	0.775374
22	1	0	2.510388	3.837363	-0.151498
23	1	0	5.728733	3.240503	-0.005981
24	6	0	5.266163	0.048278	2.095414
25	6	0	4.400207	-1.222979	2.023150
26	1	0	3.583220	-1.161697	2.754145
27	1	0	5.005548	-2.092665	2.309489
28	1	0	6.038902	0.027872	1.316135
29	1	0	5.811695	0.013485	3.045889
30	15	0	3.634566	-1.651202	0.387694
31	6	0	2.830569	-3.264724	0.758159
32	1	0	1.925186	-3.106144	1.351093
33	6	0	5.057857	-2.102700	-0.695857
34	1	0	4.682449	-2.504291	-1.641917
35	1	0	3.519166	-3.906491	1.317622
36	1	0	2.550613	-3.771209	-0.168447
37	1	0	5.674742	-1.226239	-0.913718
38	1	0	5.680659	-2.864008	-0.213084
39	1	0	5.950994	1.625135	-0.718205
40	1	0	4.910870	2.806712	-1.525684
41	1	0	1.969048	3.136862	1.387186
42	1	0	3.485890	4.070770	1.314995
43	1	0	0.509089	2.391955	-0.862457
44	6	0	4.487306	1.374919	2.048062
45	1	0	3.657974	1.343104	2.766624
46	1	0	5.141849	2.198939	2.358662
47	6	0	-0.234225	0.147765	0.406356
48	6	0	0.995673	-0.139286	0.816629
49	1	0	1.280722	-0.414100	1.830275
50	1	0	-9.689753	0.776327	1.678609
51	6	0	-9.165523	1.305214	0.875819
52	6	0	-7.798321	0.715552	0.627739
53	1	0	-9.788765	1.266174	-0.022592
54	1	0	-9.088311	2.358123	1.177412
55	6	0	-7.277189	0.623910	-0.670645
56	6	0	-7.013661	0.253294	1.696505
57	6	0	-6.007465	0.098446	-0.905216
58	1	0	-7.877788	0.957092	-1.512887
59	6	0	-5.742953	-0.273851	1.484557
60	1	0	-7.409253	0.296470	2.708029
61	6	0	-5.247004	-0.340162	0.179856
62	1	0	-5.622056	0.005357	-1.914758
63	1	0	-5.153693	-0.652103	2.313072
64	16	0	-3.620206	-1.018656	-0.103333

65	8	0	-3.542581	-1.432796	-1.510529
66	8	0	-3.311183	-1.952076	0.986108
67	7	0	-2.571179	0.327398	0.100671

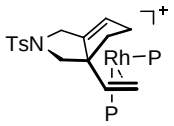


51-TS Imaginary frequency: –349.3 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.632467	-0.850387	-1.156772
2	6	0	-1.818481	-1.028697	1.023876
3	6	0	-2.165113	-0.817282	-1.347682
4	6	0	0.086771	-2.126642	-1.642745
5	6	0	1.436782	-2.201748	-0.908334
6	45	0	2.216760	-0.145306	-0.376232
7	1	0	-0.536240	-2.989867	-1.390096
8	1	0	0.220200	-2.129348	-2.730729
9	1	0	2.302997	-2.184485	-1.589021
10	1	0	1.542709	-3.076168	-0.268134
11	1	0	-1.869840	-1.758982	1.834139
12	1	0	-2.141334	-0.048301	1.418185
13	1	0	-2.504160	-1.375984	-2.221582
14	1	0	-2.526158	0.221699	-1.432532
15	6	0	0.100120	0.397907	-1.577196
16	6	0	1.168079	0.463029	-2.432908
17	1	0	1.478413	-0.381587	-3.038273
18	1	0	1.552176	1.428290	-2.745207
19	15	0	3.190884	2.033836	-0.329176
20	6	0	4.322477	2.503557	-1.715799
21	6	0	1.924127	3.377630	-0.355029
22	1	0	1.354751	3.352664	-1.288555
23	1	0	4.649640	3.544501	-1.615910
24	6	0	5.311746	1.504282	1.532777
25	6	0	4.836209	0.147617	2.076713
26	1	0	4.149345	0.304457	2.918432
27	1	0	5.693825	-0.413542	2.469065
28	1	0	5.977555	1.359647	0.672353
29	1	0	5.930732	1.974056	2.306138

30	15	0	3.972510	-0.970709	0.874839
31	6	0	3.664019	-2.451618	1.931876
32	1	0	2.996456	-2.199915	2.761033
33	6	0	5.322476	-1.550663	-0.245780
34	1	0	4.938348	-2.342513	-0.895577
35	1	0	4.610682	-2.812038	2.347594
36	1	0	3.208114	-3.256773	1.349726
37	1	0	5.676878	-0.735048	-0.882004
38	1	0	6.165529	-1.944577	0.333251
39	1	0	5.203628	1.855736	-1.722653
40	1	0	3.813089	2.384371	-2.676165
41	1	0	1.229199	3.245546	0.479440
42	1	0	2.404173	4.358394	-0.267661
43	1	0	-0.285506	1.324400	-1.153273
44	6	0	4.177397	2.479473	1.178012
45	1	0	3.472558	2.553418	2.016041
46	1	0	4.586941	3.484619	1.017409
47	6	0	-0.467149	-0.945786	0.364451
48	6	0	0.795745	-1.132073	0.763136
49	1	0	1.094933	-1.486534	1.743603
50	7	0	-2.642143	-1.469190	-0.117673
51	16	0	-4.297020	-1.754965	0.099754
52	6	0	-5.071613	-0.151458	0.283949
53	8	0	-4.749746	-2.332352	-1.164569
54	8	0	-4.389029	-2.455751	1.379972
55	6	0	-5.198809	0.413863	1.556807
56	6	0	-5.536898	0.522968	-0.849386
57	6	0	-5.788510	1.669988	1.685432
58	1	0	-4.872493	-0.139858	2.430916
59	6	0	-6.123748	1.777947	-0.699281
60	1	0	-5.469057	0.053514	-1.825188
61	1	0	-5.898996	2.107058	2.674619
62	6	0	-6.260302	2.370971	0.565032
63	1	0	-6.496401	2.299411	-1.577266
64	6	0	-6.937452	3.711250	0.720512
65	1	0	-6.542896	4.264409	1.578847
66	1	0	-8.015794	3.584809	0.882790
67	1	0	-6.814045	4.330214	-0.173830

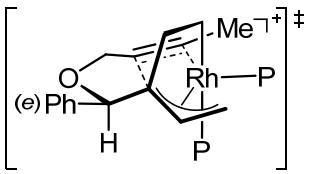


52

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.430435	-1.725746	-1.466890
2	6	0	-1.093842	-1.059205	0.831425
3	6	0	-1.965960	-1.534012	-1.378877
4	6	0	0.089402	-3.126645	-1.873060
5	6	0	1.316349	-3.403098	-0.952266
6	45	0	1.850922	-0.284824	-0.362468
7	1	0	-0.692156	-3.859961	-1.650502
8	1	0	0.317428	-3.203359	-2.940527
9	1	0	2.280222	-3.256715	-1.453067
10	1	0	1.318151	-4.437727	-0.588310
11	1	0	-1.108850	-1.436528	1.854305
12	1	0	-1.108680	0.043652	0.851414
13	1	0	-2.529067	-2.311440	-1.897730
14	1	0	-2.267816	-0.556673	-1.788457
15	6	0	0.299392	-0.571533	-2.138050
16	6	0	1.540680	-0.668667	-2.703964
17	1	0	2.043885	-1.618005	-2.848417
18	1	0	1.949564	0.161502	-3.267865
19	15	0	2.994333	1.664850	-1.015503
20	6	0	4.527834	1.348459	-1.999686
21	6	0	2.009225	2.801239	-2.093048
22	1	0	1.703119	2.307375	-3.018820
23	1	0	4.962253	2.289233	-2.355204
24	6	0	4.316177	2.230018	1.473551
25	6	0	3.382597	1.468652	2.425987
26	1	0	2.519956	2.098402	2.679630
27	1	0	3.902175	1.252211	3.367818
28	1	0	5.133276	1.580714	1.131868
29	1	0	4.797270	3.035366	2.040846
30	15	0	2.716513	-0.148828	1.800671
31	6	0	1.591977	-0.591514	3.200760
32	1	0	0.746551	0.102020	3.231846
33	6	0	4.151368	-1.292646	2.033154
34	1	0	3.859461	-2.318388	1.793033
35	1	0	2.135648	-0.525474	4.149549

36	1	0	1.201905	-1.606602	3.097233
37	1	0	4.968295	-1.011943	1.362124
38	1	0	4.512342	-1.257735	3.067158
39	1	0	5.266443	0.829181	-1.381715
40	1	0	4.305112	0.712142	-2.860263
41	1	0	1.108235	3.120853	-1.560451
42	1	0	2.599178	3.687347	-2.352048
43	1	0	-0.229465	0.378969	-2.187954
44	6	0	3.587201	2.858505	0.276485
45	1	0	2.711739	3.418096	0.630022
46	1	0	4.240792	3.580870	-0.228224
47	6	0	0.036501	-1.603134	-0.006909
48	6	0	1.096198	-2.454405	0.218722
49	1	0	1.456983	-2.714706	1.207807
50	1	0	-6.470908	4.483795	0.084614
51	6	0	-5.436064	4.335941	-0.250467
52	6	0	-5.005149	2.905381	-0.034442
53	1	0	-5.396215	4.612661	-1.308958
54	1	0	-4.809487	5.035346	0.312009
55	6	0	-5.266576	1.923845	-1.002711
56	6	0	-4.372722	2.515972	1.156142
57	6	0	-4.913221	0.591820	-0.795809
58	1	0	-5.769493	2.203363	-1.924994
59	6	0	-4.011374	1.189005	1.382367
60	1	0	-4.178185	3.259266	1.925282
61	6	0	-4.279812	0.232481	0.398270
62	1	0	-5.153973	-0.168249	-1.531691
63	1	0	-3.561491	0.887438	2.322566
64	16	0	-3.800523	-1.472175	0.666035
65	8	0	-4.616965	-2.312878	-0.206592
66	8	0	-3.678680	-1.689039	2.107639
67	7	0	-2.223332	-1.624813	0.071511



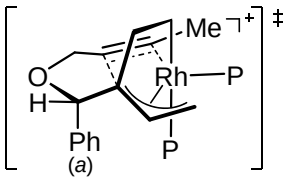
53-TS Imaginary frequency: –253.9 cm^{-1}

Standard orientation:

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

1	6	0	-1.607745	-0.039572	0.079673
2	6	0	-0.514937	0.413093	1.807278
3	6	0	-2.789147	0.850252	0.550507
4	6	0	-1.709015	-1.552122	0.306175
5	6	0	-0.277079	-2.106277	0.294635
6	45	0	0.811448	-0.305831	-0.039674
7	1	0	-2.212421	-1.737732	1.258445
8	1	0	-2.345083	-1.988157	-0.474101
9	1	0	-0.105335	-2.843703	-0.494842
10	1	0	0.001736	-2.550181	1.251968
11	1	0	-1.598194	1.019365	3.541004
12	1	0	-1.430297	2.288341	2.297449
13	1	0	-2.592451	1.880549	0.205954
14	6	0	-1.037949	0.375349	-1.210261
15	6	0	-0.477251	-0.454449	-2.158925
16	1	0	-0.624726	-1.526529	-2.159415
17	1	0	-0.087014	-0.021580	-3.074941
18	15	0	2.005331	1.853446	-0.430923
19	6	0	2.059976	2.494858	-2.168766
20	6	0	1.386845	3.331003	0.496098
21	1	0	0.364192	3.565074	0.183299
22	1	0	2.635722	3.424823	-2.234063
23	6	0	4.628647	0.683373	-0.532155
24	6	0	4.339983	-0.690767	0.099285
25	1	0	4.370044	-0.610121	1.193378
26	1	0	5.132646	-1.395584	-0.183172
27	1	0	4.515527	0.634454	-1.623218
28	1	0	5.688291	0.906756	-0.359702
29	15	0	2.732431	-1.510498	-0.339289
30	6	0	2.867710	-3.091486	0.600450
31	1	0	2.824368	-2.897721	1.675868
32	6	0	2.991783	-2.062723	-2.082651
33	1	0	2.143267	-2.677662	-2.396796
34	1	0	3.815047	-3.589663	0.368476
35	1	0	2.042879	-3.758267	0.337786
36	1	0	3.053098	-1.201195	-2.753262
37	1	0	3.910869	-2.652681	-2.173237
38	1	0	2.510592	1.753767	-2.835785
39	1	0	1.043768	2.691501	-2.525554
40	1	0	1.374390	3.116595	1.568869
41	1	0	2.015852	4.209514	0.315531
42	1	0	-1.044349	1.445968	-1.411037
43	6	0	3.803234	1.848853	0.042494

44	1	0	3.850562	1.828721	1.139365
45	1	0	4.242645	2.803548	-0.273039
46	6	0	-1.598917	1.210148	2.462775
47	6	0	0.669611	-0.048709	2.013797
48	8	0	-2.857143	0.832602	1.960064
49	6	0	-4.103035	0.366240	-0.036056
50	6	0	-4.465742	0.751221	-1.333173
51	6	0	-4.954627	-0.470550	0.695851
52	6	0	-5.657673	0.297294	-1.897728
53	1	0	-3.823799	1.420254	-1.902261
54	6	0	-6.149755	-0.918579	0.131072
55	1	0	-4.691965	-0.748263	1.710622
56	6	0	-6.501741	-0.541311	-1.166217
57	1	0	-5.931819	0.607221	-2.901998
58	1	0	-6.809235	-1.559230	0.709507
59	1	0	-7.433449	-0.890258	-1.601901
60	6	0	1.590846	-0.293756	3.156437
61	1	0	1.153771	0.050506	4.101710
62	1	0	1.801436	-1.364912	3.258646
63	1	0	2.550860	0.215562	3.014885



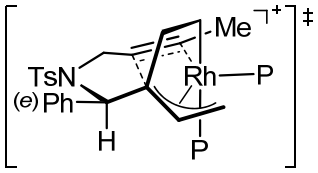
54-TS Imaginary frequency: –252.6 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.331805	-1.372694	-0.503280
2	6	0	-0.556042	-1.248712	1.450520
3	6	0	-2.801183	-1.536403	-0.002207
4	6	0	-0.641417	-2.694819	-0.874711
5	6	0	0.875126	-2.466513	-0.807365
6	45	0	0.894986	-0.415123	-0.231845
7	1	0	-0.970891	-3.472194	-0.179253
8	1	0	-0.983273	-3.002260	-1.873395
9	1	0	1.382236	-2.634360	-1.761636
10	1	0	1.351869	-3.084981	-0.045194
11	1	0	-1.738574	-2.019327	3.033524

12	1	0	-2.242273	-0.415794	2.450005
13	6	0	-1.052614	-0.244796	-1.402962
14	6	0	-0.153112	-0.245399	-2.451962
15	1	0	0.242416	-1.153884	-2.886999
16	1	0	-0.032321	0.660224	-3.038602
17	15	0	0.779002	1.988477	0.426180
18	6	0	0.461275	3.218403	-0.922743
19	6	0	-0.516252	2.434748	1.669551
20	1	0	-1.510856	2.204393	1.274097
21	1	0	0.443844	4.241829	-0.531821
22	6	0	3.622094	2.388472	0.451680
23	6	0	4.096986	0.924178	0.488006
24	1	0	4.083192	0.555448	1.521657
25	1	0	5.140424	0.871238	0.151517
26	1	0	3.539442	2.737907	-0.585884
27	1	0	4.413232	2.999907	0.901902
28	15	0	3.155611	-0.304685	-0.540197
29	6	0	4.097639	-1.855341	-0.215751
30	1	0	3.957789	-2.171228	0.821678
31	6	0	3.647898	0.112351	-2.269916
32	1	0	3.252653	-0.646525	-2.951625
33	1	0	5.165985	-1.698165	-0.398575
34	1	0	3.739424	-2.654580	-0.869344
35	1	0	3.230582	1.080232	-2.560713
36	1	0	4.738623	0.146669	-2.370173
37	1	0	1.235514	3.149439	-1.693273
38	1	0	-0.503675	3.012381	-1.396849
39	1	0	-0.367639	1.846111	2.580060
40	1	0	-0.476606	3.499330	1.924579
41	1	0	-1.590752	0.674433	-1.194702
42	6	0	2.317142	2.668541	1.219179
43	1	0	2.382825	2.239710	2.227704
44	1	0	2.188852	3.750816	1.346691
45	6	0	-1.868015	-1.401472	2.137964
46	6	0	0.704252	-1.146684	1.696987
47	8	0	-2.796550	-2.070805	1.311768
48	1	0	-3.187332	-2.355832	-0.625112
49	6	0	-3.758983	-0.356951	-0.177557
50	6	0	-4.102951	0.066435	-1.472195
51	6	0	-4.404166	0.242004	0.911227
52	6	0	-5.022427	1.095686	-1.670184
53	1	0	-3.663178	-0.424287	-2.337996
54	6	0	-5.324164	1.276064	0.714799
55	1	0	-4.230343	-0.127154	1.915218

56	6	0	-5.629203	1.713434	-0.573614
57	1	0	-5.277647	1.402567	-2.680529
58	1	0	-5.815919	1.724436	1.573450
59	1	0	-6.350212	2.511335	-0.725233
60	6	0	1.645709	-1.406124	2.819821
61	1	0	1.110988	-1.732800	3.719994
62	1	0	2.355659	-2.197713	2.551721
63	1	0	2.230060	-0.513648	3.070560



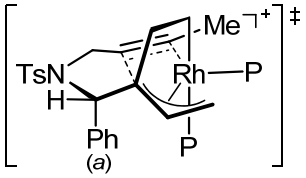
55-TS Imaginary frequency: –244.3 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.027699	0.689272	0.092818
2	6	0	0.567841	-1.168956	-0.686364
3	6	0	-1.321838	0.102911	0.707035
4	6	0	-0.081244	1.417917	-1.257880
5	6	0	1.345471	1.420272	-1.828988
6	45	0	2.349493	0.356553	-0.286225
7	1	0	-0.776793	0.895914	-1.919011
8	1	0	-0.482009	2.427458	-1.107426
9	1	0	1.750349	2.426027	-1.972673
10	1	0	1.412345	0.881008	-2.775596
11	1	0	-0.860914	-2.678143	-1.071635
12	1	0	-0.431133	-2.495968	0.635681
13	1	0	-1.069221	-0.276698	1.708815
14	6	0	0.824928	1.321229	1.116311
15	6	0	1.659201	2.404085	0.936962
16	1	0	1.588542	3.065253	0.083571
17	1	0	2.238158	2.766821	1.780844
18	15	0	3.414723	-0.924758	1.568570
19	6	0	3.895101	0.009577	3.094806
20	6	0	2.424476	-2.322744	2.268100
21	1	0	1.505837	-1.940342	2.724634
22	1	0	4.365270	-0.646801	3.835241
23	6	0	6.057005	-0.884974	0.446406

24	6	0	5.734255	-0.446764	-0.994212
25	1	0	5.457693	-1.322141	-1.595747
26	1	0	6.635892	-0.023453	-1.455314
27	1	0	6.260592	-0.008052	1.074790
28	1	0	6.999466	-1.444622	0.414026
29	15	0	4.389649	0.816323	-1.219023
30	6	0	4.425939	1.070726	-3.044632
31	1	0	4.092521	0.165583	-3.560049
32	6	0	5.151986	2.371984	-0.579604
33	1	0	4.485911	3.213657	-0.790561
34	1	0	5.441780	1.311985	-3.375305
35	1	0	3.758480	1.890145	-3.322686
36	1	0	5.287823	2.311424	0.503809
37	1	0	6.122926	2.559062	-1.052196
38	1	0	4.591732	0.815694	2.844949
39	1	0	3.007339	0.462641	3.547634
40	1	0	2.143128	-3.012135	1.466448
41	1	0	2.989927	-2.872533	3.028323
42	1	0	0.796190	0.862559	2.103175
43	6	0	4.997563	-1.783968	1.108819
44	1	0	4.731282	-2.604896	0.429998
45	1	0	5.416084	-2.245395	2.012104
46	6	0	-0.635436	-1.942223	-0.296100
47	6	0	1.690970	-1.322518	-1.298620
48	6	0	-2.341730	1.221717	0.887940
49	6	0	-2.534679	1.754647	2.169571
50	6	0	-3.055442	1.768088	-0.188263
51	6	0	-3.410882	2.821360	2.373120
52	1	0	-2.011636	1.319685	3.017566
53	6	0	-3.931632	2.834350	0.015067
54	1	0	-2.948328	1.343014	-1.180011
55	6	0	-4.107626	3.367820	1.293741
56	1	0	-3.554141	3.217932	3.374150
57	1	0	-4.483015	3.243302	-0.826711
58	1	0	-4.790907	4.197749	1.449631
59	7	0	-1.781081	-1.022403	-0.134788
60	16	0	-3.132706	-1.925623	0.531949
61	8	0	-2.992922	-3.253444	-0.073959
62	8	0	-3.128797	-1.763046	1.991684
63	6	0	-4.590431	-1.156069	-0.140689
64	6	0	-5.490484	-0.531290	0.721848
65	6	0	-4.857517	-1.280287	-1.507742
66	6	0	-6.671906	-0.009800	0.196589
67	1	0	-5.264846	-0.455992	1.779551

68	6	0	-6.037400	-0.743877	-2.012269
69	1	0	-4.159955	-1.795422	-2.159745
70	6	0	-6.964939	-0.105961	-1.170679
71	1	0	-7.378921	0.477473	0.862542
72	1	0	-6.251695	-0.832683	-3.074176
73	6	0	-8.261682	0.431154	-1.725605
74	1	0	-9.010202	-0.368024	-1.804270
75	1	0	-8.682106	1.210619	-1.082995
76	1	0	-8.127376	0.848052	-2.729227
77	6	0	2.307853	-2.258580	-2.276287
78	1	0	1.628347	-3.085047	-2.517702
79	1	0	2.544081	-1.737720	-3.211948
80	1	0	3.243237	-2.681251	-1.892239



56-TS Imaginary frequency: –261.0 cm^{-1}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.078960	0.369081	-1.306325
2	6	0	0.031312	-0.867653	0.398355
3	6	0	-1.399295	0.865704	-1.140337
4	6	0	0.275343	-0.759499	-2.333387
5	6	0	1.607106	-1.453483	-2.019562
6	45	0	2.214184	-0.306838	-0.334698
7	1	0	-0.558939	-1.462178	-2.275058
8	1	0	0.244057	-0.322785	-3.341636
9	1	0	2.330161	-1.398693	-2.838359
10	1	0	1.470730	-2.500391	-1.743578
11	1	0	-1.822438	-1.471100	1.222525
12	1	0	-1.360273	0.188903	1.616671
13	6	0	1.111028	1.417952	-1.330452
14	6	0	2.267113	1.408078	-2.088047
15	1	0	2.403441	0.761909	-2.945284
16	1	0	2.953275	2.245675	-2.004967
17	15	0	2.850010	1.108449	1.617056
18	6	0	3.668515	2.724474	1.227733

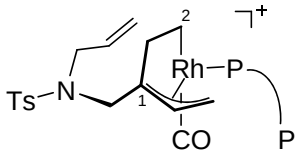
19	6	0	1.490443	1.633842	2.757847
20	1	0	0.746461	2.217075	2.205267
21	1	0	3.942461	3.268348	2.138685
22	6	0	5.329720	-0.242636	2.150280
23	6	0	5.119473	-1.508935	1.299284
24	1	0	4.543334	-2.248492	1.869937
25	1	0	6.093527	-1.968311	1.087098
26	1	0	5.841555	0.530559	1.562506
27	1	0	6.026639	-0.502969	2.956056
28	15	0	4.268853	-1.307917	-0.340444
29	6	0	4.344500	-3.026604	-1.003669
30	1	0	3.728184	-3.692860	-0.393865
31	6	0	5.522126	-0.426062	-1.371215
32	1	0	5.176637	-0.393188	-2.408728
33	1	0	5.376409	-3.393558	-0.996394
34	1	0	3.964994	-3.050546	-2.028282
35	1	0	5.646624	0.603036	-1.023145
36	1	0	6.490914	-0.937051	-1.334968
37	1	0	4.571333	2.557508	0.631978
38	1	0	2.990557	3.350712	0.638845
39	1	0	0.993891	0.750563	3.171703
40	1	0	1.872755	2.243260	3.584182
41	1	0	0.948486	2.261940	-0.667533
42	6	0	4.056138	0.331025	2.799368
43	1	0	3.520698	-0.467928	3.329002
44	1	0	4.332543	1.079020	3.553194
45	6	0	-1.369661	-0.561324	0.816488
46	6	0	1.020817	-1.621269	0.735477
47	7	0	-2.163346	-0.059948	-0.298575
48	16	0	-3.172809	-1.218224	-1.088280
49	8	0	-3.419966	-0.664663	-2.422685
50	8	0	-2.587900	-2.556651	-0.924911
51	1	0	-1.810392	0.774084	-2.152694
52	6	0	-1.588368	2.327396	-0.728462
53	6	0	-1.311579	3.328615	-1.673660
54	6	0	-2.081745	2.714242	0.523563
55	6	0	-1.484520	4.677278	-1.364960
56	1	0	-0.968007	3.049340	-2.667486
57	6	0	-2.255540	4.066085	0.836039
58	1	0	-2.378578	1.963442	1.247284
59	6	0	-1.950418	5.051981	-0.102281
60	1	0	-1.271960	5.433022	-2.115753
61	1	0	-2.645599	4.344262	1.811250
62	1	0	-2.092918	6.101213	0.139357

63	6	0	-4.663509	-1.144723	-0.111549
64	6	0	-5.113105	-2.299557	0.527878
65	6	0	-5.389689	0.050020	-0.049948
66	6	0	-6.306057	-2.248503	1.250817
67	1	0	-4.542270	-3.218567	0.452592
68	6	0	-6.574202	0.078609	0.676401
69	1	0	-5.032482	0.938621	-0.560307
70	6	0	-7.053519	-1.067405	1.336348
71	1	0	-6.662224	-3.144984	1.750979
72	1	0	-7.143098	1.003282	0.730162
73	6	0	-8.354626	-1.020761	2.099638
74	1	0	-8.400141	-0.145640	2.757604
75	1	0	-9.207355	-0.951717	1.412450
76	1	0	-8.494244	-1.915841	2.712497
77	6	0	1.263690	-2.863394	1.515991
78	1	0	0.337162	-3.234251	1.970872
79	1	0	1.650593	-3.655827	0.864177
80	1	0	2.000844	-2.702872	2.310747

CO (carbon monoxide)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.650137
2	8	0	0.000000	0.000000	0.487603



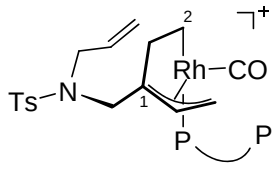
S1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.474181	-0.307131	-0.381083

2	6	0	-3.494046	-3.123414	1.872623
3	6	0	-4.388332	-2.115106	1.204573
4	6	0	-2.598895	-0.472026	0.617176
5	6	0	-0.961188	-1.514231	-1.153295
6	6	0	0.519687	-1.723082	-0.820880
7	6	0	-3.226448	-3.134160	3.180246
8	1	0	-1.568929	-2.388751	-0.904973
9	1	0	-1.128961	-1.325208	-2.219472
10	1	0	1.098418	-2.045240	-1.690280
11	1	0	0.653263	-2.470643	-0.022671
12	1	0	-2.606265	-3.904586	3.629594
13	1	0	-3.643405	-2.390260	3.856515
14	1	0	-5.206149	-2.635223	0.697194
15	1	0	-4.823526	-1.431111	1.948612
16	1	0	-2.981843	0.511524	0.932325
17	1	0	-2.184097	-0.954084	1.513400
18	6	0	-0.870084	0.926527	-0.541951
19	6	0	0.298107	1.101484	-1.381345
20	1	0	0.375189	0.522375	-2.298771
21	1	0	0.698750	2.108383	-1.471156
22	15	0	8.919282	1.042295	0.571019
23	6	0	9.071563	1.152940	-1.286603
24	6	0	9.169491	-0.792027	0.808448
25	1	0	10.228391	-1.019363	0.646267
26	1	0	8.478892	0.410119	-1.834026
27	6	0	6.111071	0.274472	0.029559
28	6	0	4.637830	0.558521	0.384867
29	1	0	4.381073	1.597038	0.137875
30	1	0	4.485692	0.455049	1.467358
31	1	0	6.265158	0.406784	-1.047502
32	1	0	6.350717	-0.769474	0.260498
33	15	0	3.347009	-0.503442	-0.420603
34	6	0	3.822809	-2.240366	-0.025993
35	1	0	3.838238	-2.383560	1.059125
36	6	0	3.633817	-0.338764	-2.231249
37	1	0	2.947921	-0.991340	-2.777947
38	1	0	-3.078329	-3.888488	1.217787
39	1	0	4.813151	-2.476557	-0.427190
40	1	0	3.095021	-2.932976	-0.457273
41	1	0	3.452174	0.694646	-2.541090
42	1	0	4.661581	-0.611997	-2.488732
43	1	0	8.782835	2.155606	-1.620574
44	1	0	10.123737	1.011526	-1.555525
45	1	0	8.932949	-1.065793	1.842581

46	1	0	8.580209	-1.419421	0.129136
47	1	0	-1.254395	1.778213	0.015137
48	6	0	7.055973	1.205145	0.808436
49	1	0	6.816599	2.252832	0.580490
50	1	0	6.882665	1.087476	1.886967
51	1	0	-9.196701	3.636368	0.196866
52	6	0	-8.449318	3.392996	0.963018
53	1	0	-8.993571	3.032032	1.841923
54	6	0	-7.479582	2.356448	0.450935
55	1	0	-7.940071	4.322981	1.232641
56	6	0	-6.222749	2.727627	-0.048566
57	6	0	-7.831565	0.997036	0.430094
58	6	0	-5.335369	1.777995	-0.552449
59	1	0	-5.939922	3.776969	-0.056019
60	6	0	-6.961523	0.032436	-0.070177
61	1	0	-8.806939	0.691573	0.799677
62	6	0	-5.709855	0.430949	-0.553148
63	1	0	-4.382213	2.077655	-0.974535
64	1	0	-7.257190	-1.010319	-0.113877
65	16	0	-4.575134	-0.803232	-1.171762
66	7	0	-3.654844	-1.369538	0.153448
67	8	0	-3.578283	-0.121482	-2.012234
68	8	0	-5.346072	-1.950419	-1.642724
69	45	0	1.142223	0.001008	0.192640
70	6	0	1.575114	1.592157	1.355193
71	8	0	1.810301	2.484027	2.030969



S2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.724211	-0.809609	-0.585406
2	6	0	-2.961089	-3.294574	1.729461
3	6	0	-3.783550	-2.230655	1.055770
4	6	0	-1.884262	-0.730666	0.397775
5	6	0	-0.256531	-2.178141	-1.036724

6	6	0	1.035801	-2.161836	-0.253311
7	6	0	-2.662217	-3.295671	3.030480
8	1	0	-0.960000	-2.956393	-0.737031
9	1	0	-0.132395	-2.227611	-2.120881
10	1	0	1.966630	-2.288030	-0.815816
11	1	0	1.013297	-2.755088	0.657216
12	1	0	-2.099512	-4.105303	3.486384
13	1	0	-2.997287	-2.502191	3.695883
14	1	0	-4.648097	-2.695095	0.572720
15	1	0	-4.151067	-1.501513	1.792816
16	1	0	-2.165060	0.318402	0.574192
17	1	0	-1.565630	-1.144501	1.358679
18	6	0	-0.273981	0.370407	-1.258464
19	6	0	0.911027	0.414453	-1.981597
20	1	0	1.356938	-0.475831	-2.417538
21	1	0	1.243938	1.358417	-2.397300
22	15	0	2.598090	2.024595	0.653221
23	6	0	2.738481	3.254599	-0.717259
24	6	0	1.971937	3.044207	2.060057
25	1	0	0.957148	3.392901	1.845542
26	1	0	3.331877	4.117168	-0.394588
27	6	0	5.111037	0.773893	0.114881
28	6	0	6.542572	0.469023	0.582183
29	1	0	6.513847	-0.012815	1.569191
30	1	0	7.092253	1.409100	0.726907
31	1	0	4.554390	-0.163924	-0.020214
32	1	0	5.137688	1.267373	-0.864426
33	15	0	7.657067	-0.613877	-0.485384
34	6	0	7.522626	0.234229	-2.142970
35	1	0	7.969591	1.232726	-2.084900
36	6	0	6.553080	-2.088139	-0.797634
37	1	0	7.080329	-2.782129	-1.460700
38	1	0	-2.632665	-4.111797	1.088105
39	1	0	6.495992	0.324156	-2.518454
40	1	0	8.102530	-0.339055	-2.873968
41	1	0	6.365159	-2.616599	0.143677
42	1	0	5.593042	-1.834898	-1.264894
43	1	0	3.221699	2.801983	-1.587663
44	1	0	1.745042	3.605265	-1.014095
45	1	0	1.942310	2.443087	2.973592
46	1	0	2.617432	3.913219	2.227466
47	1	0	-0.807347	1.295927	-1.059831
48	6	0	4.357470	1.662649	1.122277
49	1	0	4.326865	1.172571	2.104154

50	1	0	4.876640	2.620459	1.260524
51	1	0	-8.706046	3.166548	0.329977
52	6	0	-7.675930	3.343964	0.656443
53	1	0	-7.683006	3.358271	1.754072
54	6	0	-6.744930	2.274981	0.139172
55	1	0	-7.376371	4.338919	0.314558
56	6	0	-5.478063	2.600763	-0.365972
57	6	0	-7.130774	0.924575	0.151881
58	6	0	-4.609713	1.614581	-0.831776
59	1	0	-5.173861	3.643104	-0.411896
60	6	0	-6.279884	-0.075378	-0.310169
61	1	0	-8.119197	0.654442	0.514103
62	6	0	-5.013929	0.277110	-0.792125
63	1	0	-3.651038	1.879847	-1.264188
64	1	0	-6.603955	-1.110336	-0.331545
65	16	0	-3.906979	-1.003724	-1.368812
66	7	0	-3.016529	-1.559187	-0.022409
67	8	0	-2.887793	-0.373261	-2.222192
68	8	0	-4.709442	-2.138229	-1.815661
69	45	0	1.334571	-0.079503	0.235283
70	6	0	1.376635	-0.537105	2.082911
71	8	0	1.330059	-0.794258	3.200783
