Electronic and Steric Control of Regioselectivities in Rh(I)-Catalyzed (5+2) Cycloadditions: Experiment and Theory

Supporting Information

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Included in this PDF: Complete reference for Gaussian 03, discussions on determining the regioselectivity-determining transition state, structures of cyclopropyl C–C bond cleavage transition states, theoretical investigations of regioselectivities of internal alkynes, Cartesian coordinates and energies of all calculated species. Complete experimental details and characterization data for Table 1, 2, and 3 compounds and preparation of vinylcyclopropanes **1a**, **2a**, and **3a** (Pg = TBS). can be found in accompanying Supporting Information documents.

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Computational Details

All geometry optimizations and frequency calculations were performed with the B3LYP[1,2] functional implemented in Gaussian 03.[3] The SDD basis set was used on rhodium and the 6-31G(d) basis set for other atoms. All free energies reported involve solvation free energy correction, computed using the CPCM[4,5] polarizable conductor calculation model as implemented in Gaussian 03. 1,2-Dichloroethane (CH_2ClCH_2Cl) was specified as solvent. UAHF radii was used in the CPCM calculation. Figures for the transition state structures in the supporting information are prepared with CYLview.[6] Experimental free energy difference is calculated by $\Delta\Delta G^{\ddagger}(\text{exp}) = -RT \ln K$, where K is experimental regioselectivity.

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(6) CYLview, version 1.0b, Legault, C. Y., UCLA, **2007**.

Why alkyne insertion is the regioselectivity-determining transition state

The catalytic cycle of Rh-catalyzed (5+2) cycloaddition of propyne and VCP 1 is shown in Figure S1. All energies are Gibbs free energies with respect to the catalyst resting state, the Rh-product complex **11a**.The rate-determining step is alkyne insertion (**TS3a** and **TS3b**). The major conformer (**TS3a**, distal) requires 22.4 kcal/mol, much higher than the activation energies for cleavage of the cyclopropyl ring (**TS1**, $\Delta G^{\ddagger}$ = 11.5 kcal/mol), isomerization of the Rh-allyl complex (**TS2**, $\Delta G^{\ddagger}$ = 17.3 kcal/mol), or the subsequent reductive elimination (**TS4a**, $\Delta G^{\ddagger}$ = 16.4 kcal/mol). This suggests that all steps prior to the alkyne insertion are reversible. Under these Curtin–Hammett conditions, the ratio of the cycloadduct **5a** and **5b** is determined by the energy difference of **TS3a** and **TS3b**.

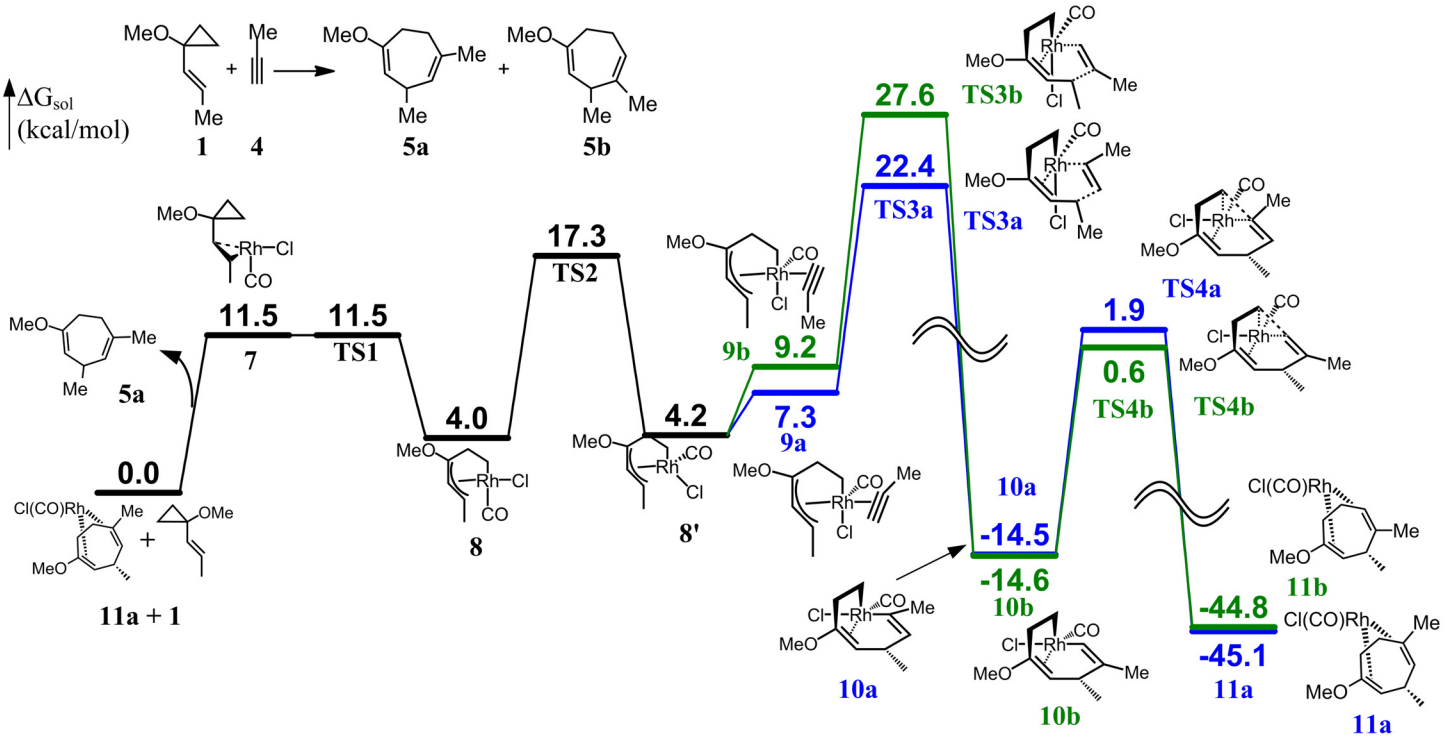
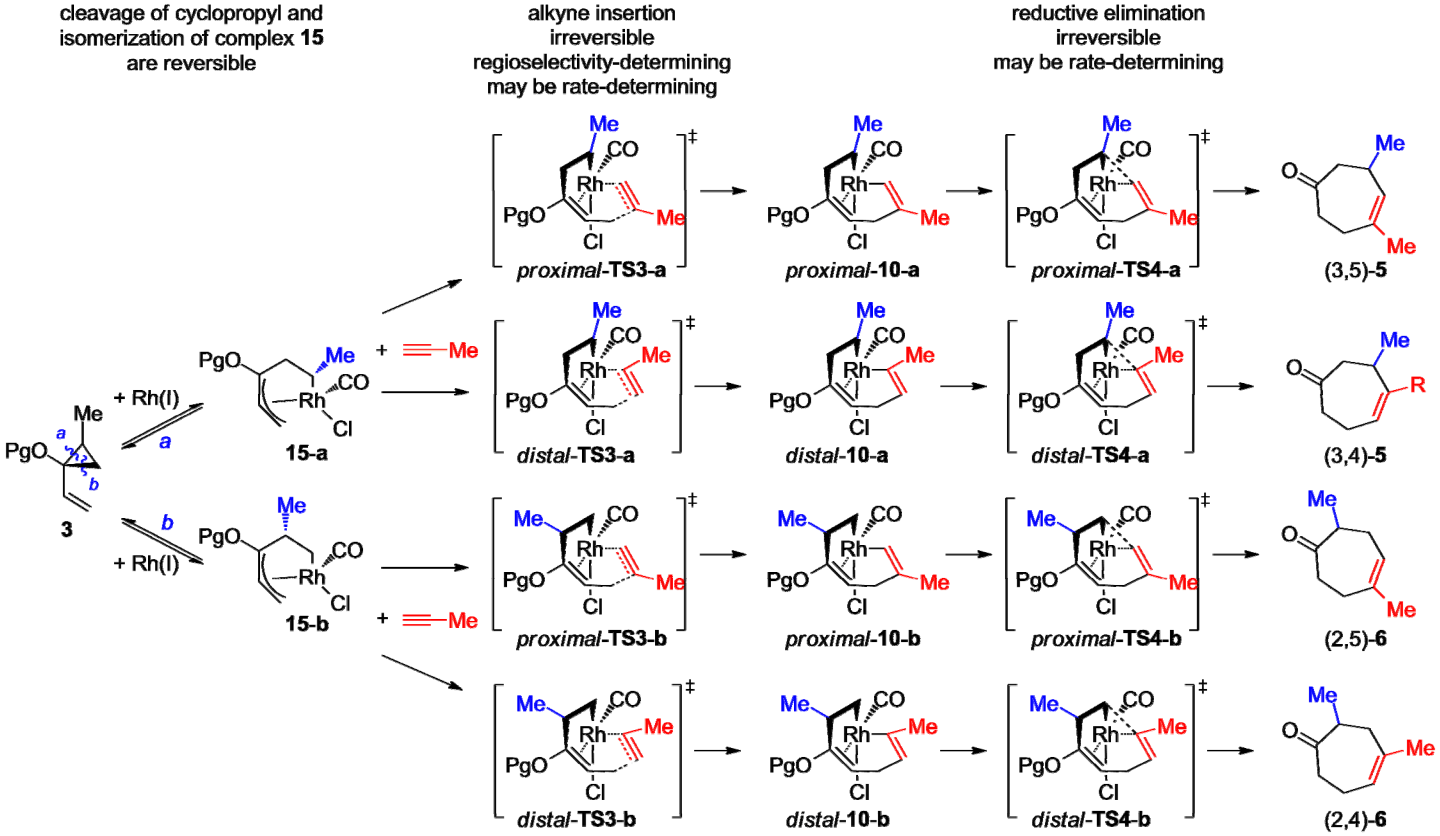


Figure S1. Free energy profile of Rh-catalyzed (5+2) cycloaddition of propyne and VCP **1**.

The cleavage of the cyclopropane ring of VCP **1** is very facile; **TS1** has about the same energy as the Rh-VCP π complex **7**. For reactions with VCP **3**, the cleavage of the cyclopropyl ring requires only slightly higher activation energies: 2.1 kcal/mol higher than the Rh-VCP π complex **7** for cleavage of the more substituted cyclopropyl C–C bond, and 0.4 kcal/mol higher than **7** for cleavage of the less substituted bond. These barriers are also much lower than the subsequent alkyne insertion step. Thus, the cleavage of cyclopropyl C–C bonds is reversible. We also investigated the barriers for reductive elimination with VCP **3**. The activation

barriers of alkyne insertion and reductive elimination for all four possible pathways are calculated and given in Table S1. The overall barrier of alkyne insertion ($\Delta G^{\ddagger}_{ins}$) is determined by the energy difference between the alkyne insertion transition state **TS3** and the catalyst resting state, the Rh-product complex **11**. $\Delta G^{\ddagger}_{ins}$ could be calculated by the sum of the energy of **TS3** with respect to the Rh-VCP π complex **7** ($\Delta G^{\ddagger}$(**TS3**)) and the ligand exchange energy ($\Delta G^{\ddagger}_{ex}$) to liberate the product from complex **11** and coordinate with VCP to regenerate complex **7**. For this reaction, $\Delta G^{\ddagger}_{ex}$ is 11.0 kcal/mol. The activation barrier for reductive elimination ($\Delta G^{\ddagger}_{elim}$) is calculated by the energy difference between the **TS4** and the rhodacycle intermediate **10**.

Table S1. Activation barriers for alkyne insertion and reductive elimination in the reaction of VCP **3** with propyne.

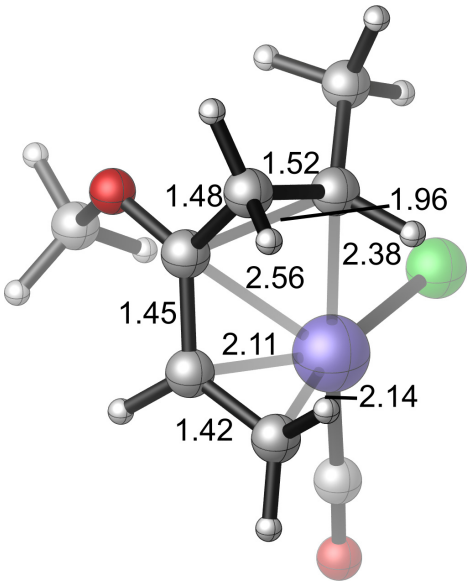


Pathway	$\Delta G^{\ddagger}$(**TS3**)^b	ΔG(**10**)^b	$\Delta G^{\ddagger}$(**TS4**)^b	barrier for alkyne insertion $\Delta G^{\ddagger}_{ins}$	reverse barrier for alkyne insertion $\Delta G^{\ddagger}_{ins\text{-}rev}$	barrier for reductive elimination $\Delta G^{\ddagger}_{elim}$
proximal-a	11.8	–29.0	–8.6	22.8	40.8	20.4
distal-a	10.9	–27.5	–5.1	21.9	38.4	22.4
proximal-b	10.9	–27.8	–13.4	21.9	38.7	14.4
distal-b	10.0	–26.6	–10.4	21.0	36.6	16.2

[a] Energies are in kcal/mol. [b] Energies are with respect to the Rh-VCP π complex **7**.

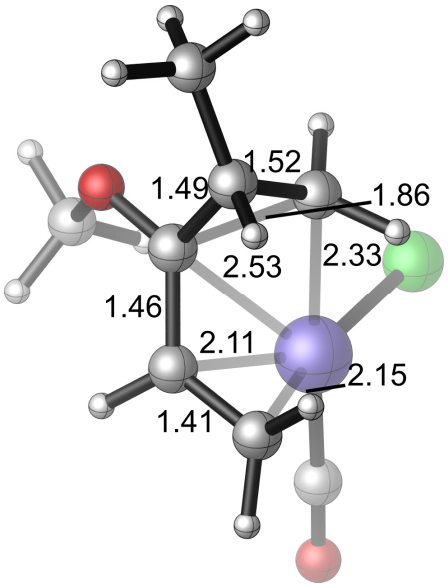
The regioselectivity is determined in the alkyne insertion step, since alkyne insertion is irreversible. The reverse barriers for alkyne insertion are higher than 36 kcal/mol for all pathways. For all pathways except *distal*-a, alkyne insertion has the highest barrier and thus is rate-determining. For pathway *distal*-a, which leads to the not observed product (3,4)-**5**, reductive elimination requires slightly higher activation barrier than alkyne insertion, and thus, reductive elimination is the rate-determining step in this case. The high activation barrier for reductive elimination in pathway *distal*-a is obviously due to the steric repulsion of the two methyl groups attached to the two carbons involved in the bond formation. For the reaction of VCP 3 with trimethylsilylacetylene, the reductive elimination of pathway *distal*-a requires 24.7 kcal/mol, also slightly higher than the alkyne insertion step. For other three pathways in the reaction with trimethylsilylacetylene, the rate-determining step is alkyne insertion. In these cases, the *distal*-a pathway is not productive, due to repulsions of the methyl group on VCP and alkyne substituent in both alkyne insertion and the reductive elimination steps.

Structures of cyclopropyl C–C bond cleavage transition states



$\Delta G^{\ddagger}$(**TS4-a**) = 2.1 kcal/mol

cleavage of the more-substituted bond



$\Delta G^{\ddagger}$(**TS4-b**) = 0.4 kcal/mol

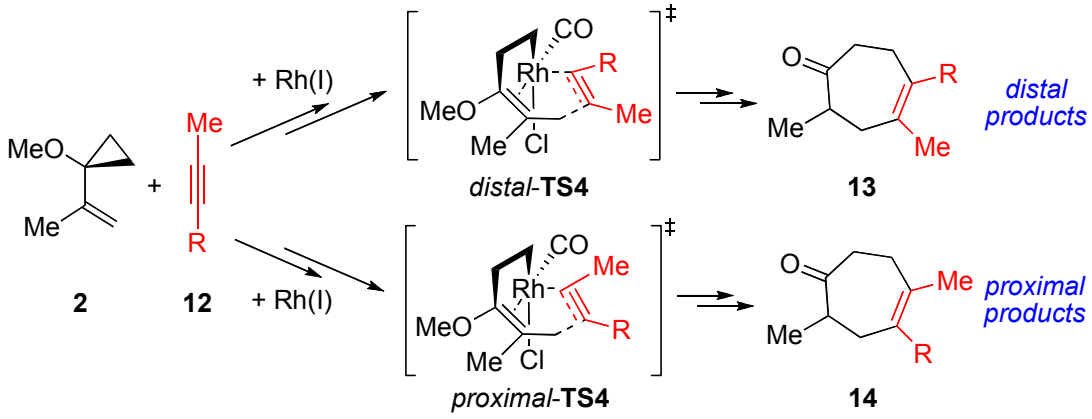
cleavage of the less-substituted bond

Figure S2. Structures of transition states of cleavage of the cyclopropyl C–C bond in VCP **3**.

Theoretical investigations of regioselectivities of internal alkynes

We also briefly investigated the reactions of VCP **2b** with internal alkynes. The results of these theoretical calculations are shown in Table S2. Here, *distal* is defined as variable alkyne substituent R positioned away from the forming C–C bond in the alkyne insertion transition state, and *proximal* is defined as R oriented towards the forming C–C bond. When the two substituents of the internal alkyne have similar sizes, electronic effects dominate the regioselectivity. For the internal alkynes studied, a strong energetic preference was found for the *proximal* pathway, in which the electron-withdrawing substituent R is closer to the forming C–C bond and the relatively electron-rich methyl group of the alkyne is oriented α to the metal, leading to products **14**.

Table S2. B3LYP/SDD-6-31G*/CPCM(DCE) free energies of activation for (5+2) cycloadditions between VCP **2** (Pg = Me) and internal alkynes.



entry	alkyne	R	$\Delta G^{\ddagger}$(**TS4**)[a,b]		$\Delta\Delta G^{\ddagger}$	ratio[c]
			distal-	*proximal-*	(*prox–dis*)[b]	
1	**12a**	CO_2Me	15.5	13.9	–1.6	1:14
2	**12b**	COMe	17.8	14.5	–3.2	< 1:20
3	**12c**	CH=O	15.6	12.5	–3.1	< 1:20

[a] Relative to the Rh(CO)Cl-VCP π-complex. [b] Energies in kcal/mol. [c] Predicted ratio of *distal* and *proximal* products at 298K.

The Cartesian coordinates (Å), total SCF energies, enthalpies at 298K, Gibbs free energies at 298K, and free energies in solution at 298K for the optimized structures. For transition state structures, one imaginary frequency was observed and given below. For all minimum structures, no imaginary frequency was observed.

Note: **CPX1** and **TS1** are the Rh-VCP complex and the alkyne insertion transition state for the reaction with VCP **1**; **CPX2** and **TS2** are for the reaction with VCP **2**; **CPX3** and **TS3** are for the reaction with VCP **3**. **CPX2'**, *distal*-**TS2k'**, and *proximal*-**TS2k'** are for the reaction with 1-TMSO-VCP **2**.

4a

Total SCF energy: -195.27710075 a.u.
Enthalpy at 298K: -195.156216 a.u.
Gibbs free energy at 298K: -195.192612 a.u.
Free energy in solution: -195.191720 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.645365	0.264225	0.000000
H	-3.699925	0.108836	0.000000
C	-1.450594	0.441712	0.000000
C	0.000000	0.636496	0.000000
C	0.793170	-0.688146	0.000000
H	0.288518	1.232556	0.877800
H	0.288518	1.232556	-0.877800
C	2.306694	-0.458221	0.000000
H	0.500859	-1.276577	0.878299
H	0.500859	-1.276577	-0.878299
H	2.849465	-1.409913	0.000000
H	2.624138	0.106364	-0.885414
H	2.624138	0.106364	0.885414

4b

Total SCF energy: -191.84496830 a.u.
Enthalpy at 298K: -191.778422 a.u.
Gibbs free energy at 298K: -191.810883 a.u.
Free energy in solution: -191.815297 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.944298	-0.206910	0.000000
H	-2.966317	-0.510667	0.000000
C	-0.785392	0.128413	0.000000
C	0.610168	0.565864	0.000000
H	0.785199	1.199448	-0.885642
H	0.785199	1.199448	0.885643
O	1.466785	-0.571417	0.000000
H	2.378776	-0.241096	-0.000003

4c

Total SCF energy: -270.48167231 a.u.
Enthalpy at 298K: -270.356429 a.u.
Gibbs free energy at 298K: -270.394877 a.u.
Free energy in solution: -270.397650 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.377150	0.000249	-0.033749
H	-3.442820	-0.000888	-0.066683
C	-1.171847	-0.000002	0.023369
C	0.300893	0.000008	0.035256
O	0.692842	-0.000088	1.417704
H	1.664285	-0.000452	1.429500
C	0.828235	1.272067	-0.658142
H	1.926017	1.268963	-0.656617
H	0.488461	1.329291	-1.697341
H	0.478816	2.159406	-0.123274
C	0.828133	-1.272011	-0.658297
H	0.477974	-2.159423	-0.124032
H	0.489028	-1.328657	-1.697745
H	1.925918	-1.269397	-0.656058

4d

Total SCF energy: -486.01939716 a.u.
Enthalpy at 298K: -485.877829 a.u.
Gibbs free energy at 298K: -485.921092 a.u.
Free energy in solution: -485.915530 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.000000	0.000000	-1.546347
C	0.000000	0.000000	-2.761908
H	0.000000	0.000000	-3.829597
Si	0.000000	0.000000	0.299096
C	0.000000	1.791531	0.901193
H	-0.885110	2.331538	0.546225
H	0.000000	1.832383	1.997650
H	0.885110	2.331538	0.546225
C	1.551511	-0.895766	0.901193
H	1.586891	-0.916192	1.997650
H	1.576616	-1.932297	0.546225
H	2.461726	-0.399241	0.546225
C	-1.551511	-0.895766	0.901193
H	-1.586891	-0.916192	1.997650
H	-2.461726	-0.399241	0.546225
H	-1.576616	-1.932297	0.546225

4e

Total SCF energy: -305.19514144 a.u.
Enthalpy at 298K: -305.116337 a.u.
Gibbs free energy at 298K: -305.153854 a.u.
Free energy in solution: -305.154428 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.634132	-0.409148	0.000536
H	3.668704	-0.670591	0.000355
C	1.463245	-0.115142	-0.000490
C	0.076184	0.307017	-0.000247
O	-0.285338	1.464476	0.000071
O	-0.751525	-0.756207	-0.000425
C	-2.153337	-0.432285	0.000321
H	-2.412806	0.146604	-0.889920
H	-2.670529	-1.391726	0.000932
H	-2.411817	0.146906	0.890746

4f

Total SCF energy: -229.96817009 a.u.
Enthalpy at 298K: -229.896099 a.u.
Gibbs free energy at 298K: -229.931319 a.u.
Free energy in solution: -229.932052 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.191179	-0.168367	0.000015

H	3.250093	-0.301457	0.000048
C	0.994143	0.006174	-0.000024
C	-0.452168	0.202539	-0.000067
O	-0.934713	1.321076	0.000028
C	-1.286785	-1.061803	0.000006
H	-1.051523	-1.670623	-0.881466
H	-1.052525	-1.669820	0.882311
H	-2.346555	-0.797970	-0.000694

4g

Total SCF energy: -758.73871780 a.u.
Enthalpy at 298K: -758.601665 a.u.
Gibbs free energy at 298K: -758.654712 a.u.
Free energy in solution: -758.652736 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-4.569457	-1.612826	0.013338
H	-5.240480	-2.442997	0.016626
C	-3.824313	-0.660036	0.009824
C	-2.969596	0.520911	0.006076
O	-3.465494	1.639427	0.015979
C	-1.490476	0.305906	-0.009433
C	-0.923904	-0.975073	-0.021764
C	-0.657362	1.435524	-0.014368
C	0.460940	-1.128466	-0.035452
H	-1.568038	-1.848602	-0.022388
C	0.723360	1.284707	-0.029223
H	-1.115228	2.418893	-0.008827
C	1.283013	0.000576	-0.038586
H	0.902330	-2.118888	-0.050263
H	1.370296	2.155827	-0.040955
C	2.781944	-0.152884	0.003971
F	3.401047	0.796689	-0.730401
F	3.250226	-0.040375	1.267646
F	3.180970	-1.355167	-0.462615

4h

Total SCF energy: -308.38693697 a.u.
Enthalpy at 298K: -308.269961 a.u.
Gibbs free energy at 298K: -308.307814 a.u.
Free energy in solution: -308.307846 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.000078	3.234699	0.000000
H	0.001426	4.300741	0.000000
C	0.000076	2.024511	0.000000
C	-0.000053	0.594615	0.000000
C	-0.000058	-0.119882	1.213345
C	-0.000058	-0.119882	-1.213345
C	-0.000058	-1.512854	1.208886
H	-0.000073	0.428331	2.150378
C	-0.000058	-1.512854	-1.208886
H	-0.000073	0.428331	-2.150378
C	-0.000052	-2.213464	0.000000
H	-0.000072	-2.053334	2.151555
H	-0.000072	-2.053334	-2.151555
H	-0.000029	-3.300057	0.000000

4i

Total SCF energy: -77.32380182 a.u.
Enthalpy at 298K: -77.293271 a.u.
Gibbs free energy at 298K: -77.316163 a.u.
Free energy in solution: -77.314888 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.000000	0.000000	0.602487
H	0.000000	0.000000	1.669139
C	0.000000	0.000000	-0.602487
H	0.000000	0.000000	-1.669139

4j

Total SCF energy: -116.65068354 a.u.
Enthalpy at 298K: -116.590015 a.u.
Gibbs free energy at 298K: -116.618144 a.u.
Free energy in solution: -116.617172 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.000000	0.000000	1.426285
H	0.000000	0.000000	2.492198
C	0.000000	0.000000	0.219014
C	0.000000	0.000000	-1.241557
H	0.000000	1.022478	-1.638215
H	0.885492	-0.511239	-1.638215
H	-0.885492	-0.511239	-1.638215

4k

Total SCF energy: -234.59052353 a.u.
Enthalpy at 298K: -234.440760 a.u.
Gibbs free energy at 298K: -234.478671 a.u.
Free energy in solution: -234.477970 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.000000	0.000000	2.383115
H	0.000000	0.000000	3.449115
C	0.000000	0.000000	1.174725
C	0.000000	0.000000	-0.298797
C	0.000000	1.460426	-0.808377
C	1.264766	-0.730213	-0.808377
C	-1.264766	-0.730213	-0.808377
H	-0.886472	1.998365	-0.456330
H	0.886472	1.998365	-0.456330
H	0.000000	1.476018	-1.904870
H	1.287399	-1.766890	-0.456330
H	1.278269	-0.738009	-1.904870
H	2.173871	-0.231475	-0.456330
H	-1.278269	-0.738009	-1.904870
H	-1.287399	-1.766890	-0.456330
H	-2.173871	-0.231475	-0.456330

4l

Total SCF energy: -190.64146175 a.u.
Enthalpy at 298K: -190.599012 a.u.
Gibbs free energy at 298K: -190.630162 a.u.
Free energy in solution: -190.630704 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.381161	1.837659	0.000000
H	-0.735448	2.844606	0.000000
C	0.000000	0.689207	0.000000
C	0.505188	-0.668415	0.000000
H	1.610233	-0.747209	0.000000
O	-0.202368	-1.656013	0.000000

4m

Total SCF energy: -169.56775865 a.u.
Enthalpy at 298K: -169.536205 a.u.
Gibbs free energy at 298K: -169.560482 a.u.
Free energy in solution: -169.560657 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.843377	0.000127	0.000000
H	2.910826	0.001887	0.000000
C	0.633687	-0.000535	0.000000
C	-0.739039	-0.000541	0.000000
N	-1.905568	0.000544	0.000000

4n

Total SCF energy: -132.67527652 a.u.
Enthalpy at 298K: -132.626076 a.u.
Gibbs free energy at 298K: -132.655018 a.u.
Free energy in solution: -132.658699 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.027599	1.370823	0.000000
H	-0.082407	2.433721	0.000000
C	0.000000	0.161668	0.000000
N	0.109120	-1.192886	0.000000
H	-0.257917	-1.639231	0.835122
H	-0.257917	-1.639231	-0.835122

distal-TS1a

Total SCF energy: -1228.59991468 a.u.
Enthalpy at 298K: -1228.273834 a.u.
Gibbs free energy at 298K: -1228.345378 a.u.
Free energy in solution: -1228.344900 a.u.
Imaginary frequency: -209.1695 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.247867	1.509913	-0.480363
C	-0.767607	1.927040	-0.489419
C	-1.908174	1.070509	-0.080831
C	-2.502607	0.111653	-0.888787
C	-1.938153	-0.265912	-2.244342
C	-0.465193	-0.670274	-2.023855
C	1.777711	0.361051	-0.272879
Rh	-0.130350	-0.302343	0.037864
Cl	-0.044583	0.201429	2.486949
C	0.103878	-2.094880	0.383821
O	0.260702	-3.217327	0.601838
H	1.521882	2.537575	-0.645030
H	0.236100	-0.056059	-2.595428
H	-0.302892	-1.718619	-2.280254
H	-2.313777	1.266818	0.904502
H	-2.047386	0.578419	-2.938622
H	-2.541961	-1.085929	-2.643175
O	-3.618404	-0.557044	-0.571184
C	-4.179107	-0.399518	0.739290
H	-4.524073	0.628734	0.894997
H	-5.027257	-1.083085	0.777029
H	-3.440195	-0.667894	1.502048
C	-0.689410	3.189749	0.360715
H	0.084464	3.878702	0.009465
H	-1.649113	3.719362	0.316766
H	-0.481742	2.928508	1.403059
H	-0.729344	2.102468	-1.563990
C	3.078375	-0.351620	-0.167713
H	3.139874	-0.790300	0.837391
H	3.077023	-1.199223	-0.867740
C	4.302513	0.544453	-0.428274
H	4.288745	1.379172	0.284009
H	4.219606	0.983961	-1.431013
C	5.621233	-0.224777	-0.303642
H	6.479206	0.431237	-0.487883
H	5.737150	-0.652403	0.699487
H	5.671006	-1.049649	-1.025194

distal-TS1b

Total SCF energy: -1225.18035416 a.u.
Enthalpy at 298K: -1224.908306 a.u.
Gibbs free energy at 298K: -1224.974494 a.u.
Free energy in solution: -1224.976773 a.u.
Imaginary frequency: -223.8594 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.185255	1.780305	-0.924080
C	-0.819772	1.914551	-0.465834
C	-1.699343	0.916660	0.192770
C	-2.337124	-0.123985	-0.469617
C	-2.059814	-0.437779	-1.926468
C	-0.537163	-0.647777	-2.057872
C	1.904894	0.727680	-0.794532
Rh	0.220441	-0.202559	-0.132076
Cl	0.917902	0.347472	2.226436
C	0.754289	-1.956044	0.102758
O	1.048711	-3.060185	0.245239
H	1.272125	2.828781	-1.152994
H	-0.067768	0.037716	-2.768586
H	-0.305876	-1.672021	-2.354522
H	-1.886413	1.076559	1.248416
H	-2.432429	0.379960	-2.558286
H	-2.629825	-1.331950	-2.193823
O	-3.248291	-0.929773	0.087432
C	-3.503266	-0.831069	1.495304
H	-3.934929	0.144186	1.746065
H	-4.220935	-1.620623	1.717355
H	-2.577708	-0.989980	2.059357
C	-0.710133	3.190192	0.361339
H	-0.144907	3.972183	-0.154092
H	-1.714776	3.584054	0.558785
H	-0.223927	2.978030	1.318760
H	-1.066441	2.074672	-1.514455
C	3.311909	0.220164	-0.774929
H	3.991991	1.087429	-0.751655
H	3.519805	-0.339554	-1.694373
O	3.559223	-0.659723	0.301072
H	3.082284	-0.321223	1.085073

distal-TS1c

Total SCF energy: -1303.81662508 a.u.
Enthalpy at 298K: -1303.485968 a.u.
Gibbs free energy at 298K: -1303.557756 a.u.
Free energy in solution: -1303.557342 a.u.
Imaginary frequency: -204.0983 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.047934	1.587959	-0.854792
C	-0.983491	1.872093	-0.716361
C	-2.010435	1.005823	-0.084237
C	-2.616598	-0.076895	-0.706716
C	-2.164638	-0.583414	-2.062103
C	-0.651166	-0.863454	-1.957824
C	1.678695	0.525525	-0.509950
Rh	-0.140786	-0.238538	-0.003127
Cl	0.243559	0.553117	2.359889
C	0.231140	-1.976828	0.499950
O	0.423406	-3.070032	0.807625
H	1.233350	2.595207	-1.186567
H	-0.055253	-0.276684	-2.661931
H	-0.435498	-1.921617	-2.114560
H	-2.408863	0.158185	-2.835011
H	-2.739969	-1.484324	-2.293117
O	-3.648538	-0.760647	-0.197570
C	-4.095982	-0.466285	1.132639
H	-4.491134	0.553756	1.194068
H	-4.890919	-1.183113	1.337704
H	-3.275185	-0.596085	1.846400
H	-1.071429	1.914351	-1.801347

C	3.056681	-0.026994	-0.238798
O	3.046378	-0.771784	0.975354
H	2.468091	-0.311789	1.617332
C	3.473418	-1.010025	-1.340548
H	3.580065	-0.501035	-2.303927
H	4.433703	-1.459762	-1.067958
H	2.734931	-1.810682	-1.439645
C	4.058735	1.139602	-0.125453
H	5.053273	0.738042	0.093601
H	4.108557	1.717030	-1.055993
H	3.768517	1.811234	0.688603
C	-0.913051	3.234346	-0.035880
H	-0.233529	3.920187	-0.550146
H	-1.909194	3.693843	-0.036259
H	-0.580944	3.122351	1.001010
H	-2.331131	1.303112	0.907489

distal-TS1d

Total SCF energy: -1519.33988556 a.u.
Enthalpy at 298K: -1518.993127 a.u.
Gibbs free energy at 298K: -1519.071920 a.u.
Free energy in solution: -1519.076605 a.u.
Imaginary frequency: -207.8010 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.792231	1.703238	-0.675967
C	-1.207955	1.896069	-0.662254
C	-2.245795	0.961590	-0.150676
C	-2.756139	-0.114470	-0.862240
C	-2.177078	-0.547923	-2.194198
C	-0.676618	-0.818011	-1.958119
C	1.473738	0.651976	-0.388904
Rh	-0.348671	-0.222585	0.051463
Cl	-0.313360	0.510805	2.445142
C	0.086706	-1.934774	0.547762
O	0.347753	-3.014268	0.865475
H	0.972698	2.728474	-0.957952
H	-0.026433	-0.217132	-2.599044
H	-0.439212	-1.872616	-2.106923
H	-2.655115	1.201989	0.823095
H	-2.354006	0.232920	-2.946022
H	-2.718230	-1.438714	-2.525466
O	-3.790975	-0.863285	-0.460934
C	-4.339456	-0.654257	0.847992
H	-4.787862	0.342257	0.927993
H	-5.109933	-1.416198	0.965520
H	-3.561394	-0.778932	1.608867
C	-1.267686	3.232307	0.072632
H	-0.581748	3.969727	-0.355423
H	-2.281982	3.644174	0.005460
H	-1.017227	3.090124	1.128572
H	-1.225953	1.983000	-1.748999
C	3.522990	-0.359299	1.622705
C	3.407203	-1.552758	-1.253797
C	4.408456	1.346817	-0.823372
H	3.403062	0.545749	2.227705
H	2.809368	-1.096350	2.004938
H	4.537413	-0.747718	1.779014
H	3.178235	-1.356216	-2.307774
H	4.436760	-1.928563	-1.200736
H	2.744572	-2.353617	-0.907723
H	5.450005	1.015546	-0.726225
H	4.232176	1.582447	-1.879528
H	4.300941	2.273359	-0.247418
Si	3.223814	0.006164	-0.200780

distal-TS1e

Total SCF energy: -1338.52197461 a.u.
Enthalpy at 298K: -1338.237908 a.u.
Gibbs free energy at 298K: -1338.310143 a.u.
Free energy in solution: -1338.312247 a.u.
Imaginary frequency: -189.1156 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.113520	1.588925	-0.557589
C	-0.956244	1.923531	-0.598208
C	-2.042622	1.032747	-0.135091
C	-2.585024	-0.008571	-0.879486
C	-2.012098	-0.432635	-2.217653
C	-0.519139	-0.744351	-1.985978
C	1.659590	0.453200	-0.317584
Rh	-0.200559	-0.242860	0.047918
Cl	-0.164521	0.407691	2.461927
C	0.103054	-2.009097	0.503665
O	0.277752	-3.106363	0.800526
H	1.355638	2.617098	-0.766941
H	0.146339	-0.131309	-2.599710
H	-0.297983	-1.795593	-2.175186
H	-2.454466	1.263720	0.840009
H	-2.171620	0.363109	-2.957840
H	-2.573439	-1.305717	-2.561850
O	-3.655949	-0.717956	-0.507946
C	-4.208650	-0.522508	0.802304
H	-4.619348	0.487996	0.904580
H	-5.008601	-1.257135	0.892283
H	-3.442810	-0.697742	1.565531
C	-0.922814	3.234933	0.174380
H	-0.172147	3.928582	-0.215685
H	-1.899901	3.727182	0.094251
H	-0.713985	3.044358	1.231741
H	-0.907821	2.029024	-1.681418
C	2.987064	-0.186774	-0.274087
O	3.176892	-1.384152	-0.253863
O	3.969224	0.738237	-0.267994
C	5.305351	0.206811	-0.208624
H	5.506780	-0.420956	-1.080769
H	5.961891	1.076940	-0.199484
H	5.438191	-0.387006	0.699312

distal-TS1f

Total SCF energy: -1263.29500527 a.u.
Enthalpy at 298K: -1263.017710 a.u.
Gibbs free energy at 298K: -1263.088125 a.u.
Free energy in solution: -1263.089878 a.u.
Imaginary frequency: -203.9405 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.311082	1.560872	-0.723681
C	-0.740782	1.883437	-0.695404
C	-1.806797	1.016477	-0.141563
C	-2.378051	-0.059684	-0.810279
C	-1.850229	-0.557000	-2.141219
C	-0.353840	-0.871881	-1.937838
C	1.881944	0.447381	-0.428859
Rh	0.043155	-0.247783	0.048063
Cl	0.190677	0.554948	2.412927
C	0.393636	-1.980903	0.582021
O	0.592978	-3.058762	0.931312
H	1.540830	2.570522	-1.022037
H	0.297665	-0.308887	-2.611468
H	-0.149951	-1.935542	-2.065874
H	-2.182020	1.300232	0.834355
H	-2.023647	0.202903	-2.915156
H	-2.429622	-1.439814	-2.425637
O	-3.435312	-0.745716	-0.363710
C	-3.943230	-0.476826	0.951456
H	-4.347854	0.539445	1.012117
H	-4.741366	-1.202134	1.108240
H	-3.152589	-0.613501	1.697074
C	-0.689800	3.235369	0.004081
H	0.041236	3.911350	-0.449589

H	-1.672602	3.717444	-0.066080
H	-0.441229	3.102092	1.061678
H	-0.744332	1.932319	-1.783699
C	3.224274	-0.188994	-0.397112
O	3.357334	-1.391906	-0.517815
C	4.396466	0.749984	-0.189134
H	5.331275	0.190821	-0.265836
H	4.381259	1.560371	-0.927384
H	4.321417	1.210168	0.803595

distal-TS1g

Total SCF energy: -1792.06660047 a.u.
Enthalpy at 298K: -1791.724112 a.u.
Gibbs free energy at 298K: -1791.811083 a.u.
Free energy in solution: -1791.808485 a.u.
Imaginary frequency: -188.5413 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.132729	1.155982	1.783255
C	-2.982871	0.301256	1.824490
C	-3.645052	-0.542013	0.799276
C	-4.312966	-0.043626	-0.315293
C	-4.276356	1.425379	-0.682933
C	-2.791008	1.792175	-0.869614
C	-0.359228	1.231150	0.762823
Rh	-1.741667	0.070745	-0.203255
Cl	-0.828818	-2.141041	0.573561
C	-1.039820	-0.214431	-1.884471
O	-0.597651	-0.404054	-2.931036
H	-1.158768	1.457971	2.817125
H	-2.471582	2.642973	-0.264475
H	-2.563799	1.999208	-1.915988
H	-3.427750	1.292142	1.910289
H	-4.758747	2.014403	0.107778
H	-4.865551	1.566391	-1.593317
O	-5.035701	-0.788426	-1.154071
C	-5.045723	-2.216902	-1.001778
H	-5.508136	-2.502132	-0.050847
H	-5.644151	-2.591901	-1.831581
H	-4.025506	-2.610749	-1.059348
C	0.844008	1.941368	0.262572
O	0.732006	3.109910	-0.083437
C	2.139866	1.207056	0.189520
C	2.249362	-0.149736	0.524400
C	3.277843	1.922586	-0.219622
C	3.488748	-0.785115	0.446045
H	1.374105	-0.720566	0.822406
C	4.511588	1.290123	-0.289670
H	3.170568	2.972033	-0.472629
C	4.616206	-0.067219	0.043553
H	3.574847	-1.835751	0.700474
H	5.394901	1.841724	-0.594844
C	5.949739	-0.756045	-0.090669
F	6.191067	-1.117147	-1.371617
F	6.021878	-1.875769	0.659028
F	6.966809	0.052084	0.285461
C	-2.823819	-0.439097	3.147557
H	-2.421016	0.204773	3.934763
H	-3.803693	-0.799899	3.482933
H	-2.159348	-1.299127	3.019593
H	-3.655165	-1.606589	0.999475

distal-TS1h

Total SCF energy: -1341.70808576 a.u.
Enthalpy at 298K: -1341.385926 a.u.
Gibbs free energy at 298K: -1341.458913 a.u.
Free energy in solution: -1341.457893 a.u.
Imaginary frequency: -192.3850 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.577786	1.890093	0.069031
C	-1.485512	1.960826	0.066216
C	-2.454070	0.843203	0.155446
C	-2.860898	0.066718	-0.921861
C	-2.233947	0.197806	-2.296183
C	-0.711303	0.021950	-2.117037
C	1.315362	0.841909	-0.028389
Rh	-0.462330	-0.181918	-0.021170
Cl	-0.479301	-0.427355	2.471437
C	0.018054	-1.952288	-0.205259
O	0.315625	-3.060785	-0.318567
H	0.672163	2.940333	0.285611
H	-0.136803	0.893337	-2.442223
H	-0.348544	-0.855699	-2.654437
H	-2.894661	0.677798	1.131534
H	-2.502395	1.168865	-2.734319
H	-2.670441	-0.572447	-2.938253
O	-3.837668	-0.846408	-0.866765
C	-4.430982	-1.163804	0.400213
H	-4.961753	-0.297016	0.809342
H	-5.138491	-1.967434	0.196376
H	-3.663743	-1.502601	1.104625
C	-1.630723	2.924457	1.237616
H	-0.991121	3.805491	1.130692
H	-2.668688	3.274799	1.293823
H	-1.381743	2.418915	2.175879
H	-1.469638	2.437843	-0.912876
C	2.705200	0.416192	-0.097565
C	3.166718	-0.654095	0.689072
C	3.609006	1.092673	-0.937099
C	4.507448	-1.029119	0.640742
H	2.469875	-1.162560	1.348494
C	4.946446	0.702941	-0.988352
H	3.252479	1.916093	-1.549293
C	5.399568	-0.357070	-0.199729
H	4.856455	-1.850745	1.260079
H	5.634874	1.228620	-1.644665
H	6.442577	-0.659045	-0.240670

distal-TS1j

Total SCF energy: -1149.97274889 a.u.
Enthalpy at 298K: -1149.706737 a.u.
Gibbs free energy at 298K: -1149.771277 a.u.
Free energy in solution: -1149.772122 a.u.
Imaginary frequency: -222.8285 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.587096	1.574371	-0.832643
C	-0.435650	1.899808	-0.560504
C	-1.459999	1.008577	0.034705
C	-2.107366	-0.010953	-0.649224
C	-1.708811	-0.418496	-2.053073
C	-0.205836	-0.765754	-2.012696
C	2.203913	0.467388	-0.646737
Rh	0.394879	-0.265844	-0.040533
Cl	0.801766	0.362364	2.347017
C	0.769915	-2.024521	0.355817
O	1.018226	-3.123946	0.603392
H	1.773514	2.602482	-1.091216
H	0.388034	-0.172225	-2.713142
H	-0.044270	-1.824072	-2.225179
H	-1.738212	1.229615	1.058359
H	-1.935143	0.398810	-2.751146
H	-2.329214	-1.269798	-2.347401
O	-3.133601	-0.716701	-0.159258
C	-3.536084	-0.515874	1.202668
H	-3.908451	0.503642	1.352139
H	-4.339394	-1.231659	1.376873
H	-2.698534	-0.713379	1.880319
C	-0.299493	3.199379	0.223415
H	0.381047	3.906147	-0.260403

H	-1.280876	3.684074	0.298468
H	0.066703	2.993333	1.233942
H	-0.555610	2.031162	-1.635250
C	3.540468	-0.174991	-0.685354
H	4.307013	0.521404	-1.045399
H	3.815263	-0.510169	0.320822
H	3.532629	-1.055021	-1.338405

distal-TS1k

Total SCF energy: -1267.91224043 a.u.
Enthalpy at 298K: -1267.557133 a.u.
Gibbs free energy at 298K: -1267.630049 a.u.
Free energy in solution: -1267.628280 a.u.
Imaginary frequency: -194.8245 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.092479	1.621889	-0.618280
C	-0.941381	1.907678	-0.624017
C	-2.012603	1.005590	-0.136059
C	-2.545252	-0.050093	-0.862354
C	-1.973832	-0.483517	-2.198155
C	-0.473595	-0.767043	-1.975749
C	1.723954	0.537390	-0.347232
Rh	-0.141744	-0.229020	0.046961
Cl	-0.099739	0.457889	2.459115
C	0.156859	-1.979291	0.528818
O	0.334229	-3.077881	0.836741
H	1.289159	2.650895	-0.865205
H	0.176266	-0.147654	-2.599202
H	-0.239387	-1.816884	-2.160404
H	-2.419835	1.242851	0.839404
H	-2.151645	0.299048	-2.948253
H	-2.523086	-1.370329	-2.526741
O	-3.603106	-0.773807	-0.475389
C	-4.153932	-0.563979	0.832436
H	-4.575728	0.443412	0.920647
H	-4.945421	-1.305995	0.937076
H	-3.384283	-0.717970	1.596488
C	-0.939771	3.230978	0.131464
H	-0.217030	3.941962	-0.279768
H	-1.933175	3.691335	0.062306
H	-0.705911	3.060004	1.186866
H	-0.928944	2.008422	-1.708855
C	3.123221	-0.007386	-0.257633
C	3.416549	-0.447085	1.193466
C	3.283601	-1.210360	-1.211627
C	4.112273	1.108362	-0.667681
H	3.289859	0.385481	1.891523
H	2.742656	-1.246550	1.512594
H	4.448074	-0.813318	1.262707
H	3.088259	-0.923934	-2.251236
H	4.308188	-1.595568	-1.150772
H	2.599973	-2.022340	-0.946013
H	5.142397	0.737870	-0.609782
H	3.928514	1.442321	-1.695273
H	4.024769	1.973452	-0.001494

distal-TS1l

Total SCF energy: -1223.96944568 a.u.
Enthalpy at 298K: -1223.721876 a.u.
Gibbs free energy at 298K: -1223.787974 a.u.
Free energy in solution: -1223.791432 a.u.
Imaginary frequency: -209.8409 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.302990	1.781951	-0.759181
C	-0.789903	1.847579	-0.672252
C	-1.715133	0.849597	-0.094665
C	-2.165767	-0.287164	-0.757062
C	-1.625580	-0.701660	-2.111362
C	-0.096161	-0.833694	-1.959626
C	2.011897	0.735745	-0.518891
Rh	0.286225	-0.171133	0.019153
Cl	0.398722	0.624540	2.383352
C	0.857669	-1.851918	0.534923
O	1.188589	-2.900667	0.871429
H	1.394933	2.821817	-1.026686
H	0.459163	-0.198677	-2.655437
H	0.227424	-1.866126	-2.097656
H	-2.091086	1.077700	0.895415
H	-1.915256	0.040776	-2.867147
H	-2.103018	-1.644879	-2.390993
O	-3.111294	-1.105365	-0.286216
C	-3.615293	-0.909605	1.043856
H	-4.142133	0.047619	1.122515
H	-4.312131	-1.730141	1.213181
H	-2.795877	-0.950495	1.769271
C	-0.880611	3.192192	0.035646
H	-0.260234	3.956555	-0.441710
H	-1.918483	3.546088	0.008194
H	-0.575500	3.088904	1.081640
H	-0.822097	1.898420	-1.759939
C	3.414861	0.298084	-0.556827
O	3.779676	-0.849044	-0.409339
H	4.146323	1.110196	-0.743874

distal-TS1m

Total SCF energy: -1202.88866996 a.u.
Enthalpy at 298K: -1202.651846 a.u.
Gibbs free energy at 298K: -1202.716864 a.u.
Free energy in solution: -1202.721087 a.u.
Imaginary frequency: -202.2011 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.474367	1.647929	-0.671546
C	-0.582914	1.902562	-0.594736
C	-1.595093	0.961669	-0.068507
C	-2.142557	-0.095101	-0.793306
C	-1.624968	-0.490101	-2.161846
C	-0.115156	-0.760070	-2.001572
C	2.118297	0.550314	-0.476848
Rh	0.294846	-0.227167	0.012602
Cl	0.446677	0.445033	2.408683
C	0.618056	-1.985451	0.485577
O	0.823953	-3.075841	0.788078
H	1.668351	2.684352	-0.892805
H	0.503257	-0.138659	-2.654379
H	0.122385	-1.808188	-2.188060
H	-1.965692	1.178056	0.926189
H	-1.840700	0.309319	-2.883032
H	-2.178164	-1.374258	-2.490163
O	-3.159368	-0.844967	-0.368739
C	-3.662950	-0.670451	0.966502
H	-4.104222	0.324557	1.086789
H	-4.431190	-1.433593	1.086859
H	-2.859444	-0.819913	1.695230
C	-0.565098	3.217607	0.172011
H	0.129622	3.942349	-0.262155
H	-1.566952	3.662890	0.143726
H	-0.289792	3.042574	1.216567
H	-0.602060	2.004921	-1.679298
C	3.407530	0.014884	-0.521907
N	4.465606	-0.473388	-0.568258

distal-TS1n

Total SCF energy: -1166.00610391 a.u.
Enthalpy at 298K: -1165.751391 a.u.
Gibbs free energy at 298K: -1165.815495 a.u.
Free energy in solution: -1165.819017 a.u.

Imaginary frequency: -222.0316 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.696419	1.575957	-0.673868
C	-0.357655	1.943084	-0.514997
C	-1.408590	1.063225	0.041787
C	-2.049476	0.056999	-0.669904
C	-1.647279	-0.321325	-2.083246
C	-0.127320	-0.579848	-2.070290
C	2.242573	0.400844	-0.548956
Rh	0.407537	-0.259484	-0.046912
Cl	0.734997	0.174838	2.401756
C	0.613942	-2.071810	0.236984
O	0.769598	-3.200277	0.422580
H	0.440908	0.131028	-2.675742
H	0.111589	-1.591671	-2.401324
H	-1.700750	1.263143	1.066060
H	-1.942809	0.474406	-2.781275
H	-2.215145	-1.214128	-2.359781
O	-3.091917	-0.646414	-0.208321
C	-3.505557	-0.474185	1.154153
H	-3.877011	0.542812	1.322831
H	-4.312450	-1.191199	1.305719
H	-2.674417	-0.688579	1.834605
C	-0.236538	3.240171	0.272691
H	0.462785	3.939435	-0.194465
H	-1.216448	3.731705	0.314600
H	0.091389	3.037220	1.297192
H	-0.424040	2.076957	-1.591711
H	1.978643	2.585407	-0.431805
N	3.414832	-0.262485	-0.720880
H	4.251499	0.305086	-0.812231
H	3.543764	-1.084806	-0.145523

distal-TS2a

Total SCF energy: -1228.59335021 a.u.
Enthalpy at 298K: -1228.267649 a.u.
Gibbs free energy at 298K: -1228.340334 a.u.
Free energy in solution: -1228.341944 a.u.
Imaginary frequency: -204.5112 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.365380	1.041348	-1.338080
C	-0.627918	1.395370	-1.531601
C	-1.810270	1.137206	-0.673629
C	-2.488136	-0.078584	-0.733510
C	-2.028332	-1.238383	-1.605100
C	-0.537094	-1.507423	-1.328482
C	1.863548	0.163142	-0.549780
Rh	-0.042060	-0.094834	0.153922
Cl	0.395867	1.602737	1.933135
C	0.159592	-1.403843	1.437475
O	0.301578	-2.225396	2.235079
H	0.098026	-1.328377	-2.200881
H	-0.377742	-2.535314	-0.995431
H	-2.235581	-0.993403	-2.658350
H	-2.624247	-2.126244	-1.383969
O	-3.675482	-0.115806	-0.091872
C	-4.287459	-1.360196	0.250716
H	-3.588775	-2.005269	0.795705
H	-5.121595	-1.098885	0.903424
H	-4.671825	-1.882126	-0.631931
H	-0.651180	0.931555	-2.515703
H	-0.420523	2.460775	-1.570799
C	-2.380350	2.295454	0.115637
H	-1.578617	2.947154	0.466893
H	-3.064602	2.875630	-0.519662
H	-2.938914	1.949636	0.986373
C	3.143974	-0.436633	-0.092048
H	3.232499	-0.238423	0.984576
H	3.084707	-1.529172	-0.196566
H	1.641698	1.814559	-2.033390
C	4.382234	0.098857	-0.833247
H	4.420743	1.189131	-0.715538
H	4.273055	-0.099371	-1.907700
C	5.681932	-0.526165	-0.317030
H	6.550434	-0.129992	-0.854807
H	5.825436	-0.316530	0.749700
H	5.678566	-1.615644	-0.445311

distal-TS2b

Total SCF energy: -1225.17494181 a.u.
Enthalpy at 298K: -1224.903117 a.u.
Gibbs free energy at 298K: -1224.969932 a.u.
Free energy in solution: -1224.974219 a.u.
Imaginary frequency: -215.5906 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.397652	-1.396802	1.532076
C	-0.578764	-1.760085	1.188241
C	-1.536188	-1.288060	0.158301
C	-2.274855	-0.120313	0.346910
C	-2.091781	0.783991	1.557990
C	-0.590652	1.084757	1.724327
C	2.016889	-0.375254	1.070536
Rh	0.291241	0.099300	0.091364
Cl	1.283775	-1.073583	-1.912926
C	0.673513	1.712785	-0.734060
O	0.870645	2.726553	-1.242902
H	1.553853	-2.316859	2.068459
H	-0.165529	0.668825	2.641974
H	-0.397582	2.159297	1.715281
H	-2.539465	0.297452	2.438470
H	-2.650550	1.710654	1.413474
O	-3.279848	0.081048	-0.530382
C	-3.873103	1.371765	-0.688102
H	-3.110002	2.133693	-0.884002
H	-4.525615	1.281802	-1.557538
H	-4.472286	1.653403	0.184015
H	-0.851241	-1.548294	2.220073
C	3.370601	0.245378	0.915482
H	4.127675	-0.518915	1.156575
H	3.485647	1.063587	1.636148
O	3.580537	0.797263	-0.364377
H	3.193955	0.183933	-1.023262
C	-1.829426	-2.206724	-1.008069
H	-2.591345	-2.944296	-0.719464
H	-2.204769	-1.652187	-1.869096
H	-0.922753	-2.732132	-1.314445
H	-0.333999	-2.805104	1.021185

distal-TS2c

Total SCF energy: -1303.81111103 a.u.
Enthalpy at 298K: -1303.480721 a.u.
Gibbs free energy at 298K: -1303.553160 a.u.
Free energy in solution: -1303.554658 a.u.
Imaginary frequency: -197.0554 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.208904	1.074838	-1.552917
C	-0.794777	1.411750	-1.587889
C	-1.887749	1.167616	-0.613821
C	-2.571992	-0.046577	-0.589597
C	-2.204720	-1.220416	-1.487445
C	-0.690168	-1.474190	-1.372802
C	1.775244	0.234430	-0.768129
Rh	-0.068710	-0.065504	0.057045
Cl	0.592931	1.631064	1.807126
C	0.211592	-1.394124	1.315771
O	0.345917	-2.232682	2.093473

H	1.428249	1.835482	-2.282147
H	-0.146686	-1.276539	-2.300819
H	-0.481059	-2.501107	-1.066641
H	-2.534669	-1.002032	-2.515045
H	-2.761584	-2.107419	-1.178617
O	-3.692135	-0.069003	0.163559
C	-4.264626	-1.306026	0.592963
H	-3.514751	-1.935150	1.086144
H	-5.034978	-1.029556	1.314091
H	-4.727382	-1.850542	-0.236746
H	-0.912942	0.935019	-2.558694
C	3.124153	-0.252709	-0.293878
O	3.106439	-0.437389	1.115908
H	2.605756	0.304144	1.516483
C	-2.363617	2.336496	0.221369
H	-3.091378	2.930395	-0.349289
H	-2.847464	2.000888	1.139437
H	-1.521897	2.974608	0.497289
H	-0.594153	2.476687	-1.663046
C	3.439901	-1.625425	-0.902772
H	3.541787	-1.560668	-1.990825
H	4.380171	-1.992445	-0.478555
H	2.650260	-2.342187	-0.659757
C	4.199201	0.786461	-0.672618
H	5.173946	0.439557	-0.315026
H	4.252420	0.931041	-1.758031
H	3.978655	1.749296	-0.201318

distal-TS2d

Total SCF energy: -1519.33320152 a.u.
Enthalpy at 298K: -1518.986703 a.u.
Gibbs free energy at 298K: -1519.066346 a.u.
Free energy in solution: -1519.062840 a.u.
Imaginary frequency: -201.5407 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.946266	1.072675	-1.587990
C	-1.024044	1.237692	-1.728273
C	-2.148557	1.007310	-0.781449
C	-2.741579	-0.246790	-0.655915
C	-2.241787	-1.477095	-1.399819
C	-0.725928	-1.608559	-1.165369
C	1.568288	0.325433	-0.747905
Rh	-0.283292	-0.000068	0.120610
Cl	0.045378	1.931493	1.668576
C	0.076729	-1.131221	1.522509
O	0.296433	-1.846131	2.402527
H	-0.137376	-1.487702	-2.078905
H	-0.475597	-2.575514	-0.724106
H	-2.511741	-1.384083	-2.463195
H	-2.763173	-2.365476	-1.037455
O	-3.894975	-0.276097	0.045923
C	-4.398525	-1.501755	0.579632
H	-3.631271	-2.017534	1.168524
H	-5.222108	-1.212252	1.233797
H	-4.778798	-2.163005	-0.206066
H	-1.064621	0.647724	-2.643084
H	-0.930389	2.302412	-1.924364
C	-2.773122	2.215757	-0.118526
H	-2.019143	2.983433	0.061064
H	-3.560781	2.626901	-0.765910
H	-3.222931	1.958845	0.841335
H	1.164776	1.771256	-2.379773
Si	3.289899	-0.224643	-0.243471
C	3.431347	-2.076903	-0.601347
H	2.692143	-2.653230	-0.033290
H	3.281869	-2.293139	-1.665621
H	4.425915	-2.446405	-0.321507
C	3.544261	0.138191	1.586563
H	2.939513	-0.523272	2.215826
H	4.597218	-0.002492	1.861990
H	3.253878	1.166313	1.826082
C	4.532958	0.736854	-1.300064
H	4.447306	1.816010	-1.128310
H	5.559996	0.441295	-1.051286
H	4.383947	0.550922	-2.370300

distal-TS2e

Total SCF energy: -1338.51505051 a.u.
Enthalpy at 298K: -1338.231296 a.u.
Gibbs free energy at 298K: -1338.304791 a.u.
Free energy in solution: -1338.308759 a.u.
Imaginary frequency: -186.2425 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.240787	1.230964	-1.289997
C	-0.800878	1.529838	-1.443316
C	-1.947901	1.164631	-0.583965
C	-2.571489	-0.078458	-0.710682
C	-2.085433	-1.149743	-1.676914
C	-0.584669	-1.388789	-1.429760
C	1.744398	0.281790	-0.592311
Rh	-0.119563	-0.045755	0.125768
Cl	0.261942	1.571038	1.983393
C	0.136751	-1.423784	1.337673
O	0.287974	-2.274386	2.096581
H	1.491717	2.060160	-1.928966
H	0.035072	-1.150695	-2.299189
H	-0.387335	-2.423611	-1.144403
H	-2.307952	-0.823270	-2.704236
H	-2.652731	-2.070737	-1.528285
O	-3.732570	-0.213518	-0.040413
C	-4.294278	-1.504167	0.210027
H	-3.557474	-2.169139	0.674243
H	-5.113551	-1.328080	0.908223
H	-4.690805	-1.958354	-0.703786
H	-0.805578	1.122444	-2.452357
C	3.041852	-0.357001	-0.305039
O	3.175222	-1.449187	0.204170
O	4.064747	0.431123	-0.693009
C	5.376284	-0.100771	-0.431222
H	5.523978	-1.038829	-0.973109
H	6.071955	0.661401	-0.782347
H	5.506601	-0.279591	0.639037
C	-2.554438	2.238877	0.292423
H	-3.309253	2.798101	-0.278262
H	-3.041152	1.810955	1.169684
H	-1.782984	2.927361	0.640349
H	-0.622096	2.600642	-1.413994

distal-TS2f

Total SCF energy: -1263.28941622 a.u.
Enthalpy at 298K: -1263.012420 a.u.
Gibbs free energy at 298K: -1263.083329 a.u.
Free energy in solution: -1263.085369 a.u.
Imaginary frequency: -196.0762 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.352292	0.766873	-1.784912
C	-0.631306	1.093656	-1.807043
C	-1.689395	1.025701	-0.767509
C	-2.368135	-0.168720	-0.510155
C	-2.019265	-1.479738	-1.199778
C	-0.505877	-1.716317	-1.050034
C	1.933841	0.032444	-0.911420
Rh	0.141335	-0.055935	0.072798
Cl	0.772181	1.938657	1.445217
C	0.463235	-1.099514	1.561288
O	0.664827	-1.747200	2.492350
H	1.566122	1.366164	-2.653803
H	0.031338	-1.711012	-2.001682

H	-0.294728	-2.659547	-0.543776
H	-0.453056	2.127992	-2.087310
H	-0.775022	0.438983	-2.664443
H	-2.350755	-1.429239	-2.248133
H	-2.582212	-2.298879	-0.748072
O	-3.453963	-0.056690	0.277785
C	-4.047280	-1.205478	0.889181
H	-3.301062	-1.780814	1.448307
H	-4.790489	-0.807563	1.581087
H	-4.544843	-1.844856	0.153095
C	3.234609	-0.548064	-0.494799
O	3.527635	-1.690464	-0.796127
C	-2.168302	2.324258	-0.156020
H	-1.342961	3.032955	-0.074191
H	-2.957116	2.759191	-0.785887
H	-2.578581	2.170336	0.842733
C	4.113616	0.365136	0.329068
H	4.963843	-0.199273	0.718960
H	4.474431	1.189129	-0.299861
H	3.531761	0.819749	1.139128

distal-TS2g

Total SCF energy: -1792.05970347 a.u.
Enthalpy at 298K: -1791.717548 a.u.
Gibbs free energy at 298K: -1791.805110 a.u.
Free energy in solution: -1791.804759 a.u.
Imaginary frequency: -191.7898 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.930813	0.774697	-2.059412
C	2.804301	0.072610	-2.026651
C	3.590979	-0.708785	-1.038721
C	4.300589	-0.069242	-0.018104
C	4.249633	1.434764	0.204242
C	2.774391	1.862064	0.291929
C	0.245197	1.029636	-1.005625
Rh	1.718635	0.056852	0.039928
Cl	0.654139	-2.193978	-0.232570
C	1.153850	0.063148	1.797497
O	0.797442	0.063285	2.892640
H	0.863851	0.849790	-3.132087
H	2.472085	2.548173	-0.502341
H	2.548670	2.330908	1.250971
H	2.600180	-0.535532	-2.903270
H	3.209734	1.051951	-2.275080
H	4.796090	1.931173	-0.611840
H	4.781943	1.695217	1.121089
O	5.152313	-0.852962	0.667352
C	5.712987	-0.430415	1.913825
H	4.926697	-0.129225	2.614701
H	6.229957	-1.307560	2.304486
H	6.432683	0.383136	1.778841
C	-0.924428	1.819006	-0.544597
O	-0.770541	3.014369	-0.331052
C	3.805149	-2.183497	-1.302430
H	2.946287	-2.607162	-1.823925
H	4.704771	-2.318347	-1.919472
H	3.943418	-2.742866	-0.376401
C	-2.235146	1.135420	-0.355394
C	-2.384164	-0.248985	-0.516288
C	-3.345304	1.926571	-0.014692
C	-3.635907	-0.836373	-0.333081
H	-1.527047	-0.873650	-0.752857
C	-4.591820	1.340652	0.158756
H	-3.207247	2.996059	0.103682
C	-4.736368	-0.044229	-0.000655
H	-3.753041	-1.908027	-0.451124
H	-5.454332	1.949033	0.410591
C	-6.080241	-0.679128	0.247826
F	-6.276723	-0.917450	1.564576
F	-6.210263	-1.859617	-0.393233
F	-7.092390	0.119421	-0.160355

distal-TS2h

Total SCF energy: -1341.70168211 a.u.
Enthalpy at 298K: -1341.379720 a.u.
Gibbs free energy at 298K: -1341.452982 a.u.
Free energy in solution: -1341.453970 a.u.
Imaginary frequency: -186.4407 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.715085	0.394876	-1.970905
C	-1.324570	0.393812	-2.055194
C	-2.387607	0.510320	-1.030408
C	-2.867672	-0.614998	-0.361065
C	-2.297970	-2.010990	-0.569747
C	-0.764423	-1.943976	-0.444622
C	1.407990	0.101070	-0.931122
Rh	-0.400263	0.070645	0.049829
Cl	-0.138887	2.476610	0.678363
C	0.030528	-0.376459	1.790337
O	0.305749	-0.659417	2.873737
H	-0.246751	-2.167646	-1.381723
H	-0.397861	-2.633495	0.318608
H	-2.640123	-2.394404	-1.543721
H	-2.709585	-2.691031	0.178876
O	-3.981354	-0.417372	0.374497
C	-4.380410	-1.355763	1.375203
H	-3.561009	-1.555394	2.075180
H	-5.201209	-0.873627	1.907833
H	-4.737616	-2.292785	0.935434
H	-1.334873	-0.518235	-2.648391
H	-1.285032	1.293494	-2.661916
C	-3.073579	1.848332	-0.860955
H	-2.379910	2.661858	-1.078555
H	-3.932594	1.914439	-1.543545
H	-3.438811	1.984418	0.157828
H	0.828671	0.779879	-2.969540
C	2.773805	-0.101646	-0.472010
C	3.239961	0.544072	0.687287
C	3.647822	-0.930308	-1.198747
C	4.558954	0.368906	1.099574
H	2.565472	1.196492	1.233684
C	4.962408	-1.109929	-0.770550
H	3.287077	-1.432961	-2.091554
C	5.421847	-0.460764	0.377559
H	4.913563	0.880696	1.989972
H	5.628234	-1.756766	-1.335604
H	6.447113	-0.601347	0.708963

distal-TS2j

Total SCF energy: -1149.96616624 a.u.
Enthalpy at 298K: -1149.700493 a.u.
Gibbs free energy at 298K: -1149.766075 a.u.
Free energy in solution: -1149.768864 a.u.
Imaginary frequency: -225.3035 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.734473	1.045024	-1.562011
C	-0.231835	1.552226	-1.405669
C	-1.289031	1.274896	-0.402891
C	-2.063991	0.119279	-0.477967
C	-1.838596	-0.958061	-1.529459
C	-0.350033	-1.353557	-1.521725
C	2.269008	0.051194	-0.957431
Rh	0.473936	-0.155989	0.003948
Cl	1.305491	1.292871	1.859700
C	0.749800	-1.613333	1.099861
O	0.938576	-2.528410	1.776740
H	0.160522	-1.116879	-2.459657
H	-0.226939	-2.420909	-1.325532

H	-2.179723	-0.577028	-2.504430
H	-2.466677	-1.824745	-1.313321
O	-3.136717	0.082900	0.340750
C	-3.779125	-1.154453	0.652568
H	-3.052705	-1.895273	1.005904
H	-4.477205	-0.920071	1.457403
H	-4.336430	-1.551188	-0.202564
H	-0.438835	1.205531	-2.416248
H	0.055904	2.598745	-1.367848
C	-1.639469	2.369121	0.581883
H	-0.749200	2.940686	0.848703
H	-2.381675	3.045642	0.134869
H	-2.063797	1.960591	1.499921
C	3.544620	-0.681443	-0.769213
H	4.330798	-0.289933	-1.425495
H	3.869516	-0.577843	0.271897
H	3.416674	-1.750133	-0.974596
H	1.969498	1.872245	-2.209167

distal-TS2k

Total SCF energy: -1267.90526625 a.u.
Enthalpy at 298K: -1267.550396 a.u.
Gibbs free energy at 298K: -1267.624227 a.u.
Free energy in solution: -1267.624785 a.u.
Imaginary frequency: -189.4284 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.240172	0.956925	-1.548858
C	-0.766049	1.197936	-1.731207
C	-1.910441	1.017856	-0.805161
C	-2.531259	-0.221084	-0.659910
C	-2.046178	-1.480242	-1.364235
C	-0.532532	-1.632165	-1.126975
C	1.817993	0.202868	-0.686673
Rh	-0.061332	-0.006304	0.126398
Cl	0.303008	1.957622	1.628882
C	0.168710	-1.106465	1.588293
O	0.307522	-1.796515	2.503243
H	0.055828	-1.540176	-2.044057
H	-0.298232	-2.594742	-0.667539
H	-2.315110	-1.416473	-2.430177
H	-2.580945	-2.348956	-0.974687
O	-3.695901	-0.209634	0.022368
C	-4.246529	-1.413024	0.560235
H	-3.509076	-1.941981	1.174836
H	-5.077130	-1.090950	1.189794
H	-4.626189	-2.074250	-0.225750
H	-0.792081	0.594011	-2.636262
H	-0.611559	2.253644	-1.933628
C	-2.515462	2.254730	-0.177690
H	-1.741146	2.997403	0.020206
H	-3.264377	2.685558	-0.857383
H	-3.008456	2.025256	0.767810
C	3.186133	-0.299877	-0.313523
H	1.460985	1.644554	-2.346605
C	3.216119	-1.840650	-0.408662
H	2.495011	-2.294184	0.278166
H	2.984233	-2.181801	-1.424025
H	4.214886	-2.207933	-0.144980
C	4.214237	0.295931	-1.303183
H	4.216075	1.390078	-1.253271
H	5.222265	-0.056860	-1.055755
H	3.992365	-0.004626	-2.333566
C	3.539261	0.143648	1.122294
H	3.496012	1.231680	1.222092
H	2.845033	-0.277797	1.853723
H	4.552396	-0.196461	1.368812

distal-TS2l

Total SCF energy: -1223.96246175 a.u.
Enthalpy at 298K: -1223.715090 a.u.
Gibbs free energy at 298K: -1223.782034 a.u.
Free energy in solution: -1223.787675 a.u.
Imaginary frequency: -214.0628 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.518785	1.247391	-1.546384
C	-0.526763	1.497468	-1.487881
C	-1.561613	1.135643	-0.494114
C	-2.175080	-0.118825	-0.516365
C	-1.785624	-1.212472	-1.500911
C	-0.260392	-1.412941	-1.434546
C	2.117892	0.309814	-0.902922
Rh	0.355895	-0.034030	0.034523
Cl	0.910705	1.631440	1.798322
C	0.787151	-1.383948	1.227150
O	1.035195	-2.218294	1.978532
H	1.689042	2.074864	-2.215057
H	0.242232	-1.174490	-2.376512
H	-0.004764	-2.438789	-1.163794
H	-0.374455	2.572642	-1.509280
H	-0.633830	1.059798	-2.478567
H	-2.143878	-0.929822	-2.502651
H	-2.304826	-2.139595	-1.250382
O	-3.247916	-0.249308	0.287556
C	-3.767557	-1.538391	0.623816
H	-2.979482	-2.185960	1.024133
H	-4.511720	-1.352003	1.399038
H	-4.251556	-2.016913	-0.233643
C	3.455247	-0.288223	-0.773937
O	3.691689	-1.306964	-0.160273
H	4.261389	0.263752	-1.297688
C	-2.080703	2.224080	0.420379
H	-1.285617	2.931972	0.658778
H	-2.906595	2.757268	-0.071160
H	-2.453017	1.813100	1.359527

distal-TS2m

Total SCF energy: -1202.88150152 a.u.
Enthalpy at 298K: -1202.645021 a.u.
Gibbs free energy at 298K: -1202.711311 a.u.
Free energy in solution: -1202.717669 a.u.
Imaginary frequency: -201.3159 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.635978	1.016764	-1.563118
C	-0.381985	1.368865	-1.592602
C	-1.456060	1.125320	-0.606290
C	-2.129704	-0.101817	-0.563829
C	-1.761352	-1.280905	-1.451994
C	-0.249194	-1.534733	-1.319135
C	2.203942	0.111661	-0.848317
Rh	0.379331	-0.070088	0.064082
Cl	0.951546	1.695042	1.713943
C	0.620480	-1.322412	1.408161
O	0.780269	-2.097283	2.242815
H	0.294119	-1.387631	-2.256739
H	-0.044955	-2.545857	-0.962628
H	-2.078043	-1.059642	-2.482441
H	-2.326991	-2.164216	-1.149502
O	-3.222421	-0.123222	0.215909
C	-3.859698	-1.352636	0.579321
H	-3.145860	-2.040230	1.045690
H	-4.621090	-1.071770	1.307505
H	-4.339102	-1.828545	-0.281683
H	-0.481370	0.863732	-2.551323
H	-0.178741	2.431386	-1.686840
C	-1.965000	2.296692	0.205858
H	-1.169140	3.024951	0.365992
H	-2.796873	2.779259	-0.325980
H	-2.326889	1.978822	1.184426

H	1.869125	1.785344	-2.280744
C	3.435526	-0.513628	-0.644769
N	4.439895	-1.077471	-0.462278

distal-TS2n

Total SCF energy: -1166.00019600 a.u.
Enthalpy at 298K: -1165.745699 a.u.
Gibbs free energy at 298K: -1165.810794 a.u.
Free energy in solution: -1165.815750 a.u.
Imaginary frequency: -215.4581 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.807806	1.074008	-1.503312
C	-0.187395	1.609960	-1.369596
C	-1.247411	1.321451	-0.379638
C	-2.026177	0.169040	-0.486687
C	-1.815770	-0.869664	-1.581849
C	-0.325189	-1.253598	-1.616648
C	2.288973	0.030349	-0.898228
Rh	0.482829	-0.152430	-0.015285
Cl	1.305062	1.158064	1.956986
C	0.626428	-1.670173	1.032837
O	0.749223	-2.616528	1.681527
H	2.138838	2.054612	-1.795292
H	0.184035	-0.943053	-2.532748
H	-0.185432	-2.329373	-1.492887
H	-2.182097	-0.460425	-2.536105
H	-2.430492	-1.748977	-1.378618
O	-3.095691	0.110633	0.335399
C	-3.741382	-1.133723	0.609079
H	-3.016839	-1.885969	0.941720
H	-4.440587	-0.922026	1.419209
H	-4.297494	-1.504206	-0.258520
H	-0.381297	1.287615	-2.388257
H	0.125974	2.646898	-1.303501
C	-1.579659	2.379419	0.649236
H	-0.683965	2.940667	0.920399
H	-2.327779	3.072474	0.239137
H	-1.987740	1.939622	1.560125
N	3.395043	-0.754493	-0.817744
H	4.255318	-0.358660	-1.184559
H	3.521283	-1.230717	0.066593

distal-TS3d-a

Total SCF energy: -1519.33833406 a.u.
Enthalpy at 298K: -1518.991497 a.u.
Gibbs free energy at 298K: -1519.070154 a.u.
Free energy in solution: -1519.064672 a.u.
Imaginary frequency: -205.9810 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.870010	-0.369814	-1.932733
C	1.099145	-0.496121	-2.150588
C	2.213436	-0.621369	-1.180852
C	2.825606	0.452538	-0.550808
C	2.349768	1.881250	-0.718926
C	0.824252	1.914069	-0.463681
C	-1.477371	-0.080535	-0.837772
Rh	0.399196	-0.115236	0.042801
Cl	0.258139	-2.579733	0.522316
C	0.059461	0.238879	1.816980
O	-0.149854	0.429318	2.936245
H	-1.097792	-0.642554	-2.950922
H	0.278350	2.062732	-1.401209
H	2.553675	-1.629144	-0.979333
O	3.903931	0.345179	0.237687
C	4.395309	-0.959202	0.577335
H	4.763573	-1.480241	-0.313506
H	5.218561	-0.787763	1.270850
H	3.608608	-1.548969	1.059887
H	1.147846	0.383457	-2.790757
H	0.991664	-1.423699	-2.705585
H	2.885809	2.489861	0.016264
H	2.631569	2.262765	-1.711514
C	0.421648	3.007975	0.518544
H	0.685063	4.002419	0.124177
H	-0.657700	3.002664	0.700829
H	0.928098	2.899949	1.485409
Si	-3.204847	0.053909	-0.113903
C	-3.459235	1.803435	0.556379
H	-2.771481	2.020564	1.381443
H	-3.309935	2.563329	-0.219475
H	-4.480968	1.915837	0.940492
C	-4.434718	-0.286393	-1.513270
H	-4.296973	-1.292290	-1.926488
H	-5.465881	-0.217503	-1.144524
H	-4.326321	0.434360	-2.332364
C	-3.375909	-1.226034	1.257041
H	-3.032229	-2.209204	0.919383
H	-2.776002	-0.958486	2.133363
H	-4.422785	-1.309793	1.575448

distal-TS3d-b

Total SCF energy: -1519.34018269 a.u.
Enthalpy at 298K: -1518.993512 a.u.
Gibbs free energy at 298K: -1519.072754 a.u.
Free energy in solution: -1519.067591 a.u.
Imaginary frequency: -207.7403 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.986401	0.102805	-1.937021
C	0.968451	-0.208759	-2.176723
C	2.059898	-0.573129	-1.244187
C	2.737597	0.352420	-0.458245
C	2.316473	1.819450	-0.432599
C	0.869348	1.809617	0.111580
C	-1.585765	0.202168	-0.806513
Rh	0.256796	-0.222234	0.046515
Cl	-0.109394	-2.693718	-0.058105
C	-0.087235	-0.222394	1.851778
O	-0.288790	-0.227271	2.988912
H	-1.206468	0.096218	-2.992525
H	0.182932	2.413876	-0.488277
H	0.856322	2.175193	1.141508
H	2.334635	-1.619859	-1.213712
H	2.310925	2.160152	-1.477634
O	3.791191	0.055877	0.307247
C	4.178964	-1.316162	0.465656
H	4.519296	-1.735898	-0.487206
H	5.001983	-1.305020	1.180172
H	3.341637	-1.903572	0.857333
H	1.097231	0.750106	-2.675018
C	3.265875	2.730730	0.351977
H	4.282907	2.711475	-0.054275
H	2.896519	3.760652	0.304025
H	3.316922	2.436219	1.404947
H	0.773324	-1.027535	-2.863626
Si	-3.277086	0.432721	-0.028925
C	-3.267840	2.065141	0.925180
H	-2.514759	2.059131	1.721495
H	-3.056316	2.916082	0.267242
H	-4.244634	2.239643	1.393520
C	-3.620368	-1.024721	1.114506
H	-2.994598	-0.987468	2.012335
H	-4.669990	-1.023310	1.434748
H	-3.411027	-1.974773	0.611680
C	-4.548607	0.500483	-1.430291
H	-4.550513	-0.431378	-2.007465
H	-5.559277	0.644114	-1.027913
H	-4.345534	1.326823	-2.121644

distal-TS3e-a

Total SCF energy: -1338.52072255 a.u.
Enthalpy at 298K: -1338.236726 a.u.
Gibbs free energy at 298K: -1338.309231 a.u.
Free energy in solution: -1338.311590 a.u.
Imaginary frequency: -189.4690 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.153679	-0.605188	-1.751659
C	0.883546	-0.732424	-2.075655
C	2.029942	-0.727308	-1.148729
C	2.624117	0.425161	-0.643155
C	2.109014	1.819871	-0.942351
C	0.588727	1.842935	-0.657816
C	-1.650216	-0.153320	-0.659689
Rh	0.241796	-0.129773	0.067141
Cl	0.157009	-2.530036	0.803626
C	0.020613	0.388248	1.834505
O	-0.108451	0.666236	2.942757
H	0.022291	1.886549	-1.594507
H	2.400706	-1.699540	-0.849674
O	3.723845	0.422992	0.119370
C	4.257599	-0.826278	0.583041
H	4.615978	-1.431517	-0.256919
H	5.093486	-0.561467	1.230305
H	3.498758	-1.377167	1.148808
H	0.849218	0.079352	-2.798957
H	0.739361	-1.716222	-2.511592
H	2.644011	2.509823	-0.282112
H	2.362869	2.106384	-1.973608
C	0.159116	3.005034	0.229979
H	0.349028	3.968058	-0.270003
H	-0.909449	2.951161	0.461736
H	0.708519	3.019574	1.179169
H	-1.412956	-1.018774	-2.711302
C	-2.952050	0.213218	-0.071874
O	-3.097905	0.986860	0.850952
O	-3.961972	-0.417785	-0.702026
C	-5.275844	-0.134684	-0.185848
H	-5.505410	0.929356	-0.287744
H	-5.957235	-0.736089	-0.787507
H	-5.338605	-0.417081	0.868007

distal-TS3e-b

Total SCF energy: -1338.52147060 a.u.
Enthalpy at 298K: -1338.237571 a.u.
Gibbs free energy at 298K: -1338.310407 a.u.
Free energy in solution: -1338.312829 a.u.
Imaginary frequency: -189.2303 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.293619	-0.013632	-1.807287
C	-0.736985	0.290348	-2.156647
C	-1.857746	0.613149	-1.258862
C	-2.552791	-0.342638	-0.519534
C	-2.141753	-1.813426	-0.544845
C	-0.691665	-1.835870	-0.006918
C	1.767189	-0.189107	-0.631000
Rh	-0.096113	0.198104	0.070014
Cl	0.257338	2.670424	0.109388
C	0.137570	0.117901	1.906199
O	0.268274	0.082919	3.048058
H	1.556525	0.073845	-2.847477
H	-0.006249	-2.392903	-0.652452
H	-0.664350	-2.273669	0.993456
H	-2.131639	1.658415	-1.191593
H	-2.147941	-2.120464	-1.600607
O	-3.623397	-0.069219	0.227597
C	-4.004466	1.298513	0.440150
H	-4.327245	1.761295	-0.498624
H	-4.838510	1.261581	1.140663
H	-3.168821	1.860906	0.870184
H	-0.797792	-0.662503	-2.676899
C	-3.094103	-2.739753	0.218517
H	-4.114103	-2.697997	-0.177890
H	-2.734669	-3.770744	0.134963
H	-3.132684	-2.478330	1.280751
H	-0.486609	1.129740	-2.798153
C	3.030502	-0.507417	0.060334
O	3.110784	-0.900190	1.204522
O	4.088038	-0.310266	-0.752353
C	5.371566	-0.574919	-0.156773
H	5.444446	-1.623281	0.144762
H	6.102107	-0.344661	-0.932268
H	5.522642	0.062058	0.718356

distal-TS3f-a

Total SCF energy: -1263.29508504 a.u.
Enthalpy at 298K: -1263.017672 a.u.
Gibbs free energy at 298K: -1263.087584 a.u.
Free energy in solution: -1263.088110 a.u.
Imaginary frequency: -197.8698 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.254777	-0.247062	-1.989177
C	0.739269	-0.427108	-2.153094
C	1.809897	-0.611985	-1.147161
C	2.421998	0.423789	-0.446720
C	1.990665	1.872646	-0.565091
C	0.454253	1.926406	-0.409538
C	-1.845000	0.038032	-0.888219
Rh	-0.019731	-0.106523	0.023202
Cl	-0.287249	-2.575477	0.425774
C	-0.350796	0.188860	1.818434
O	-0.555659	0.332408	2.942570
H	-0.028333	2.095680	-1.377184
H	2.122252	-1.634027	-0.973877
O	3.463125	0.251520	0.375136
C	3.911190	-1.078063	0.679801
H	4.300835	-1.571964	-0.217021
H	4.710950	-0.953489	1.409527
H	3.092609	-1.665161	1.109612
H	0.819962	0.474989	-2.755965
H	0.616573	-1.333259	-2.739081
H	2.487016	2.422489	0.240764
H	2.349417	2.303912	-1.511492
C	-0.025301	2.992441	0.566921
H	0.247295	3.996696	0.205685
H	-1.114522	2.963813	0.673691
H	0.422533	2.874115	1.561134
H	-1.465236	-0.476209	-3.020460
C	-3.155076	0.299097	-0.244374
O	-3.526226	1.438146	-0.026424
C	-3.939796	-0.936483	0.135457
H	-3.292918	-1.647355	0.662617
H	-4.796891	-0.652215	0.750245
H	-4.289505	-1.441375	-0.774122

distal-TS3f-b

Total SCF energy: -1263.29572355 a.u.
Enthalpy at 298K: -1263.018399 a.u.
Gibbs free energy at 298K: -1263.088602 a.u.
Free energy in solution: -1263.089112 a.u.
Imaginary frequency: -200.6506 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.396771	-0.323349	-1.939751
C	-0.537869	0.229085	-2.169413

C	-1.557168	0.721102	-1.220053
C	-2.345218	-0.118544	-0.432529
C	-2.135722	-1.630520	-0.438514
C	-0.679363	-1.828738	0.039680
C	1.938772	-0.515652	-0.797110
Rh	0.176797	0.113172	0.043598
Cl	0.891328	2.510491	0.022790
C	0.473509	0.033316	1.863864
O	0.654514	-0.005244	3.000844
H	1.615722	-0.327795	-2.994079
H	-0.089474	-2.469337	-0.620763
H	-0.663665	-2.251135	1.046747
H	-1.692332	1.794401	-1.175239
H	-2.229370	-1.954682	-1.484694
O	-3.334007	0.311381	0.350637
C	-3.525932	1.722193	0.538872
H	-3.826858	2.200307	-0.399324
H	-4.326525	1.810066	1.272940
H	-2.607112	2.181345	0.918804
H	-0.775090	-0.711142	-2.661665
C	-3.166025	-2.407733	0.387263
H	-4.188153	-2.239842	0.031898
H	-2.948144	-3.478300	0.314505
H	-3.123417	-2.123342	1.443441
H	-0.236316	1.018013	-2.852065
C	3.186697	-0.903166	-0.094184
O	3.367280	-2.051660	0.265151
C	4.164403	0.225452	0.147124
H	3.645559	1.097724	0.560703
H	4.958860	-0.115289	0.815057
H	4.598450	0.541414	-0.810153

distal-TS3j-a

Total SCF energy: -1149.97125831 a.u.
Enthalpy at 298K: -1149.705225 a.u.
Gibbs free energy at 298K: -1149.769490 a.u.
Free energy in solution: -1149.771195 a.u.
Imaginary frequency: -226.3461 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.645625	-0.262682	-1.910619
C	0.368667	-0.498243	-2.120619
C	1.463679	-0.671802	-1.143538
C	2.103622	0.373970	-0.492147
C	1.690725	1.823177	-0.656311
C	0.159292	1.919519	-0.455689
C	-2.218946	0.054927	-0.810748
Rh	-0.360319	-0.088234	0.038095
Cl	-0.653875	-2.536386	0.517933
C	-0.683076	0.265008	1.822555
O	-0.901522	0.454068	2.939147
H	-1.852327	-0.543012	-2.929070
H	-0.344508	2.091897	-1.412757
H	1.756828	-1.693366	-0.937209
O	3.162558	0.218357	0.314458
C	3.597561	-1.105930	0.652252
H	3.958548	-1.635843	-0.236331
H	4.416360	-0.971124	1.359014
H	2.781248	-1.667107	1.119630
H	0.444650	0.379839	-2.758502
H	0.198260	-1.420062	-2.667939
H	2.224584	2.398306	0.107048
H	2.024836	2.206825	-1.631838
C	-0.240130	3.026920	0.513421
H	0.060686	4.013894	0.127557
H	-1.325053	3.052736	0.665863
H	0.233096	2.905388	1.495288
C	-3.543173	0.316910	-0.194245
H	-4.344715	0.286095	-0.941535
H	-3.745427	-0.441496	0.570032
H	-3.560686	1.296068	0.296896

distal-TS3j-b

Total SCF energy: -1149.97263903 a.u.
Enthalpy at 298K: -1149.706686 a.u.
Gibbs free energy at 298K: -1149.771282 a.u.
Free energy in solution: -1149.772525 a.u.
Imaginary frequency: -225.0985 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.726384	-0.758925	-1.783762
C	-0.120948	0.052973	-2.142992
C	-1.107100	0.734370	-1.282085
C	-2.017572	0.055242	-0.479190
C	-1.993368	-1.468114	-0.377746
C	-0.598264	-1.814919	0.193520
C	2.217101	-0.932379	-0.615694
Rh	0.520307	-0.014919	0.082789
Cl	1.537731	2.260281	-0.089668
C	0.786021	-0.005857	1.907700
O	0.964044	-0.003874	3.047625
H	1.956129	-0.842706	-2.831792
H	-0.088809	-2.596602	-0.378163
H	-0.691968	-2.142036	1.232308
H	-1.099983	1.816838	-1.304882
H	-2.072257	-1.849496	-1.405757
O	-2.975909	0.651386	0.234760
C	-2.998244	2.083025	0.322410
H	-3.195176	2.529194	-0.658421
H	-3.812799	2.319751	1.006882
H	-2.046859	2.453288	0.719376
H	-0.458575	-0.876960	-2.594290
C	-3.153566	-2.058779	0.430256
H	-4.127303	-1.792422	0.005492
H	-3.068142	-3.150590	0.435508
H	-3.130881	-1.710778	1.467890
H	0.323629	0.746581	-2.850015
C	3.409621	-1.421876	0.118573
H	4.157205	-1.837349	-0.567263
H	3.863513	-0.593595	0.673519
H	3.131589	-2.195217	0.843436

distal-TS3l-a

Total SCF energy: -1223.96794413 a.u.
Enthalpy at 298K: -1223.720320 a.u.
Gibbs free energy at 298K: -1223.786524 a.u.
Free energy in solution: -1223.790365 a.u.
Imaginary frequency: -214.0053 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.380503	-0.636432	-1.968034
C	0.679567	-0.635218	-2.086679
C	1.724324	-0.604646	-1.047241
C	2.199963	0.556501	-0.446330
C	1.634450	1.930922	-0.743238
C	0.095559	1.860965	-0.597954
C	-2.014011	-0.247369	-0.919251
Rh	-0.210323	-0.161807	0.003894
Cl	-0.235988	-2.595395	0.610492
C	-0.661571	0.258115	1.753894
O	-0.920690	0.474443	2.852830
H	-1.519645	-1.026318	-2.962828
H	-0.385226	1.922731	-1.580717
H	2.122005	-1.566530	-0.749451
O	3.219732	0.582988	0.418664
C	3.786795	-0.652839	0.879601
H	4.255461	-1.197147	0.052394
H	4.543309	-0.369009	1.610861
H	3.016232	-1.271999	1.350930
H	0.668731	0.203279	-2.780142
H	0.640696	-1.606120	-2.570906

H	2.068563	2.623222	-0.015053
H	1.961688	2.269929	-1.737167
C	-0.471086	2.958339	0.295823
H	-0.281734	3.952104	-0.139931
H	-1.553167	2.849257	0.422034
H	-0.015131	2.950514	1.293264
C	-3.392453	0.015946	-0.477811
O	-3.683290	0.591529	0.549339
H	-4.177692	-0.348248	-1.170226

distal-TS3l-b

Total SCF energy: -1223.96906828 a.u.
Enthalpy at 298K: -1223.721474 a.u.
Gibbs free energy at 298K: -1223.787659 a.u.
Free energy in solution: -1223.791675 a.u.
Imaginary frequency: -209.7637 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.584901	-0.096542	-1.994236
C	-0.410482	0.478062	-2.132297
C	-1.402870	0.850970	-1.112105
C	-2.159984	-0.075467	-0.396442
C	-1.946610	-1.576741	-0.574382
C	-0.475035	-1.826453	-0.169714
C	2.122106	-0.459263	-0.886217
Rh	0.391988	0.099463	0.016743
Cl	1.077794	2.489488	0.209935
C	0.775576	-0.184448	1.807001
O	0.990959	-0.340583	2.925558
H	1.778632	0.067086	-3.041208
H	0.076894	-2.408543	-0.913907
H	-0.430635	-2.352262	0.786751
H	-1.531459	1.911450	-0.936286
H	-2.074572	-1.784553	-1.646483
O	-3.127937	0.257955	0.457020
C	-3.328654	1.638847	0.795969
H	-3.655754	2.208349	-0.080474
H	-4.112905	1.640202	1.552621
H	-2.406345	2.067388	1.201922
H	-0.633691	-0.410274	-2.718875
C	-2.948851	-2.443991	0.194636
H	-3.982649	-2.241457	-0.104313
H	-2.734104	-3.499459	-0.002549
H	-2.869054	-2.276818	1.273494
H	-0.108641	1.335749	-2.725607
C	3.388077	-1.002941	-0.370747
O	3.552308	-1.395646	0.764501
H	4.210619	-1.039990	-1.112856

proximal-TS1a

Total SCF energy: -1228.59087802 a.u.
Enthalpy at 298K: -1228.264558 a.u.
Gibbs free energy at 298K: -1228.335497 a.u.
Free energy in solution: -1228.336230 a.u.
Imaginary frequency: -246.9539 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.898391	0.109341	0.092748
C	-0.505154	-1.430743	0.587323
C	0.979131	-1.459371	0.526934
C	1.716681	-1.622040	-0.636081
C	1.066892	-1.558797	-1.999113
C	0.478570	-0.139616	-2.122319
C	-1.422753	1.243966	-0.270732
Rh	0.490401	0.637886	-0.139532
Cl	0.780504	1.357073	2.234385
C	1.360517	2.159563	-0.687770
O	1.899011	3.121384	-1.028493
H	-1.788271	2.214642	-0.568745
H	-0.544440	-0.133415	-2.505856
H	1.104870	0.476697	-2.770204
H	1.486513	-1.435408	1.484223
H	0.291621	-2.332529	-2.067726
H	1.817393	-1.783760	-2.762903
O	3.039163	-1.818038	-0.677261
C	3.794754	-1.749708	0.540004
H	3.492263	-2.544095	1.231028
H	4.834556	-1.891189	0.245575
H	3.663990	-0.770671	1.013589
C	-0.986029	-1.740742	2.001606
H	-2.065805	-1.871214	2.064904
H	-0.522738	-2.675839	2.342216
H	-0.681279	-0.938880	2.680888
H	-0.966692	-2.022917	-0.201601
C	-3.221142	-0.568556	0.252878
H	-3.528285	-0.551736	1.306695
H	-3.151047	-1.627484	-0.031537
C	-4.316329	0.108799	-0.595517
H	-4.391262	1.164214	-0.306762
H	-4.014743	0.092164	-1.650114
C	-5.677829	-0.573003	-0.425691
H	-6.013275	-0.539878	0.617881
H	-6.441303	-0.079046	-1.036572
H	-5.637594	-1.626104	-0.730179

proximal-TS1b

Total SCF energy: -1225.16708146 a.u.
Enthalpy at 298K: -1224.894951 a.u.
Gibbs free energy at 298K: -1224.961771 a.u.
Free energy in solution: -1224.965516 a.u.
Imaginary frequency: -250.1681 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.096513	0.057766	-0.667569
C	-0.827403	-1.512930	0.061776
C	0.607926	-1.486029	0.434953
C	1.664069	-1.500672	-0.465961
C	1.441863	-1.316814	-1.949832
C	0.794124	0.072279	-2.115654
C	-1.603670	1.238477	-0.785722
Rh	0.206601	0.652500	-0.151528
Cl	-0.254041	1.152732	2.248098
C	1.153299	2.223887	-0.276723
O	1.736455	3.215879	-0.354476
H	-1.924369	2.219785	-1.103431
H	-0.086780	0.055906	-2.761843
H	1.515753	0.784617	-2.519685
H	0.811366	-1.551439	1.497376
H	0.796182	-2.121613	-2.323637
H	2.402399	-1.407278	-2.465522
O	2.948100	-1.647549	-0.127581
C	3.308889	-1.679282	1.261134
H	2.873890	-2.554123	1.756150
H	4.396476	-1.746927	1.277170
H	2.977412	-0.761670	1.759033
C	-1.676681	-1.999119	1.230795
H	-2.743281	-2.020983	1.015952
H	-1.352614	-3.014007	1.498749
H	-1.516390	-1.346299	2.094045
H	-1.010846	-2.010566	-0.889677
C	-3.403673	-0.623194	-0.938116
H	-3.859686	-0.086560	-1.785469
H	-3.263212	-1.662893	-1.250518
O	-4.297131	-0.666042	0.165295
H	-4.267408	0.200590	0.601987

proximal-TS1c

Total SCF energy: -1303.79667346 a.u.
Enthalpy at 298K: -1303.465866 a.u.

Gibbs free energy at 298K: -1303.537837 a.u.
Free energy in solution: -1303.539176 a.u.
Imaginary frequency: -228.1855 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.845327	0.221629	-0.187080
C	-0.517034	-1.385558	0.473700
C	0.964742	-1.437851	0.553335
C	1.811291	-1.631980	-0.529027
C	1.306385	-1.547375	-1.950604
C	0.768098	-0.113986	-2.124838
C	-1.260180	1.326906	-0.484210
Rh	0.599149	0.667973	-0.149684
Cl	0.629838	1.407202	2.231093
C	1.558087	2.166514	-0.611019
O	2.151930	3.113158	-0.897616
H	-1.541069	2.314129	-0.819358
H	-0.211081	-0.083237	-2.608200
H	1.469614	0.486740	-2.706958
H	1.372937	-1.423165	1.557191
H	0.524828	-2.302348	-2.103427
H	2.125757	-1.787070	-2.634923
O	3.122764	-1.872064	-0.436682
C	3.752702	-1.849916	0.852024
H	3.346035	-2.636121	1.497133
H	4.809586	-2.036072	0.661857
H	3.619581	-0.870574	1.323970
C	-1.133674	-1.683951	1.834271
H	-2.220845	-1.668325	1.822376
H	-0.795133	-2.676411	2.163589
H	-0.784838	-0.944692	2.561861
H	-0.908347	-1.958283	-0.362119
C	-3.285303	-0.279345	-0.194209
C	-3.476937	-1.664213	-0.823408
C	-4.117121	0.758556	-0.984539
H	-3.083531	-1.685718	-1.844530
H	-2.995256	-2.447857	-0.235045
H	-4.547470	-1.889109	-0.856955
H	-5.168274	0.454793	-0.953267
H	-4.033531	1.750853	-0.529390
H	-3.794960	0.826146	-2.028161
O	-3.826557	-0.380452	1.128059
H	-3.592419	0.433375	1.605078

proximal-TS1d
Total SCF energy: -1519.32950811 a.u.
Enthalpy at 298K: -1518.982701 a.u.
Gibbs free energy at 298K: -1519.061299 a.u.
Free energy in solution: -1519.063817 a.u.
Imaginary frequency: -229.7117 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.585549	-0.324791	-0.077651
C	0.377956	1.326497	0.497528
C	-1.098435	1.460983	0.562982
C	-1.919913	1.690218	-0.531548
C	-1.397642	1.592232	-1.947284
C	-0.916985	0.137876	-2.123812
C	0.984468	-1.418615	-0.402237
Rh	-0.856901	-0.665315	-0.152963
Cl	-1.028143	-1.375592	2.231765
C	-1.894917	-2.097281	-0.648982
O	-2.539815	-3.003279	-0.957313
H	1.246164	-2.419955	-0.711320
H	0.079535	0.069715	-2.566538
H	-1.619875	-0.423791	-2.741834
H	-1.524063	1.455007	1.559531
H	-0.583771	2.315305	-2.085807
H	-2.197831	1.868860	-2.640208
O	-3.222416	1.984841	-0.456722
C	-3.873877	1.958082	0.820934
H	-3.457306	2.721863	1.486630
H	-4.922146	2.176495	0.617583
H	-3.773902	0.967224	1.277034
C	1.001432	1.581361	1.862516
H	2.089828	1.611755	1.826996
H	0.653900	2.549399	2.247424
H	0.694257	0.799860	2.563986
H	0.813542	1.885366	-0.326725
C	3.606281	1.975407	-0.688020
C	4.287348	-0.154799	1.491007
C	4.173219	-0.945603	-1.473982
H	3.117029	2.163302	-1.651298
H	3.212838	2.693540	0.039063
H	4.673465	2.195957	-0.817620
H	4.150579	-1.198072	1.797708
H	5.364673	0.021355	1.375468
H	3.931476	0.477183	2.310530
H	5.244161	-0.730927	-1.580384
H	4.073777	-2.005139	-1.211458
H	3.701276	-0.795764	-2.451461
Si	3.405879	0.170271	-0.150744

proximal-TS1e
Total SCF energy: -1338.52096958 a.u.
Enthalpy at 298K: -1338.236790 a.u.
Gibbs free energy at 298K: -1338.308409 a.u.
Free energy in solution: -1338.308202 a.u.
Imaginary frequency: -207.6276 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.744172	0.270127	-0.057638
C	-0.487187	-1.330344	0.689996
C	0.983336	-1.396132	0.690065
C	1.753226	-1.687352	-0.432413
C	1.146549	-1.740883	-1.816730
C	0.613062	-0.323460	-2.103510
C	-1.259201	1.405340	-0.419989
Rh	0.583402	0.637289	-0.201345
Cl	0.796375	1.590050	2.098410
C	1.665843	2.002296	-0.813143
O	2.327854	2.864749	-1.195762
H	-1.589670	2.381120	-0.741805
H	-0.395142	-0.324847	-2.523200
H	1.281149	0.207020	-2.784207
H	1.462422	-1.284381	1.656010
H	0.345899	-2.490193	-1.831028
H	1.911708	-2.066132	-2.527899
O	3.067100	-1.914378	-0.409792
C	3.789833	-1.755330	0.820939
H	3.445480	-2.476961	1.569109
H	4.832836	-1.948417	0.571392
H	3.672157	-0.734197	1.198962
C	-1.088160	-1.405573	2.083491
H	-2.176899	-1.446427	2.054260
H	-0.736724	-2.327804	2.565495
H	-0.763985	-0.554228	2.688464
H	-0.978854	-1.950780	-0.053206
C	-3.038678	-0.418618	-0.163569
O	-3.212560	-1.617435	-0.281072
O	-4.041786	0.484351	-0.152348
C	-5.361249	-0.065350	-0.320888
H	-6.035220	0.790252	-0.279894
H	-5.444008	-0.576560	-1.283795
H	-5.586689	-0.772961	0.481035

proximal-TS1f
Total SCF energy: -1263.29575183 a.u.
Enthalpy at 298K: -1263.018307 a.u.
Gibbs free energy at 298K: -1263.087897 a.u.
Free energy in solution: -1263.087626 a.u.

Imaginary frequency: -211.2704 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.998402	0.166202	-0.138354
C	-0.709953	-1.362908	0.640670
C	0.762926	-1.384178	0.694059
C	1.582872	-1.649536	-0.398170
C	1.029140	-1.713855	-1.803747
C	0.472118	-0.308989	-2.105585
C	-1.532330	1.322436	-0.472096
Rh	0.331836	0.640387	-0.202208
Cl	0.408180	1.598457	2.103753
C	1.370728	2.056579	-0.774775
O	2.002504	2.951888	-1.132549
H	-1.882047	2.290946	-0.797228
H	-0.515320	-0.334076	-2.571496
H	1.156592	0.243990	-2.751237
H	1.201322	-1.263175	1.678162
H	0.247033	-2.481255	-1.848608
H	1.826710	-2.018112	-2.488095
O	2.901413	-1.839534	-0.328173
C	3.573313	-1.663500	0.928240
H	3.221078	-2.394958	1.663107
H	4.629730	-1.828247	0.717713
H	3.414428	-0.646298	1.301952
C	-1.351668	-1.466306	2.015485
H	-2.436757	-1.548113	1.951574
H	-0.981251	-2.375844	2.507087
H	-1.080283	-0.605323	2.632690
H	-1.154038	-2.004716	-0.114926
C	-3.273913	-0.559844	-0.312447
O	-3.352296	-1.770072	-0.449341
C	-4.508600	0.328689	-0.324340
H	-4.397400	1.149037	-1.041011
H	-5.379185	-0.277443	-0.583768
H	-4.652632	0.775422	0.666519

proximal-TS1g

Total SCF energy: -1792.06433109 a.u.
Enthalpy at 298K: -1791.721901 a.u.
Gibbs free energy at 298K: -1791.808652 a.u.
Free energy in solution: -1791.805210 a.u.
Imaginary frequency: -213.3446 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	0.072202	-0.335431	-0.230592
C	1.589758	-1.381151	0.851491
C	3.022949	-1.056842	0.962191
C	3.964002	-1.336772	-0.023994
C	3.547934	-1.779419	-1.407764
C	2.755505	-0.601840	-2.006761
C	0.306851	0.796764	-0.802522
Rh	2.246970	0.624249	-0.335878
Cl	1.904973	1.972654	1.739092
C	2.989960	2.106403	-1.144267
O	3.438253	3.039349	-1.651459
H	-0.218692	1.565899	-1.348464
H	1.842536	-0.917713	-2.515562
H	3.377847	-0.039242	-2.704726
H	2.934765	-2.684727	-1.328979
H	4.441009	-2.037190	-1.984941
O	5.282321	-1.213485	0.129942
C	5.802855	-0.667432	1.351974
H	5.551569	-1.310521	2.201788
H	6.883650	-0.634719	1.217419
H	5.408879	0.341766	1.512195
H	1.354907	-2.223058	0.205755
C	-0.998921	-1.351226	-0.270909
O	-0.759737	-2.545042	-0.416744
C	-2.409981	-0.852645	-0.169995
C	-3.436381	-1.711393	-0.595049
C	-2.735313	0.401950	0.365961
C	-4.765021	-1.313142	-0.509649
H	-3.170462	-2.686903	-0.987683
C	-4.068277	0.797231	0.461685
H	-1.952213	1.057550	0.731760
C	-5.081430	-0.055923	0.018267
H	-5.557861	-1.975623	-0.840661
H	-4.320702	1.760823	0.891016
C	-6.518573	0.396958	0.060253
F	-7.365217	-0.640565	0.235160
F	-6.739435	1.278382	1.058353
F	-6.874284	1.006636	-1.093545
C	0.884372	-1.391128	2.198576
H	0.916315	-0.398220	2.656160
H	-0.151806	-1.722729	2.117632
H	1.403969	-2.095426	2.861605
H	3.346873	-0.662712	1.918638

proximal-TS1h

Total SCF energy: -1341.69980294 a.u.
Enthalpy at 298K: -1341.377645 a.u.
Gibbs free energy at 298K: -1341.450217 a.u.
Free energy in solution: -1341.449038 a.u.
Imaginary frequency: -262.8189 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.422199	-0.492623	-0.350758
C	0.410286	1.085522	0.675217
C	-1.041545	1.348277	0.850845
C	-1.865494	1.892670	-0.122463
C	-1.410589	2.019315	-1.557578
C	-1.160418	0.580122	-2.049716
C	0.685720	-1.427888	-0.837629
Rh	-1.057863	-0.612082	-0.286665
Cl	-1.159654	-1.785788	1.906245
C	-2.214397	-1.845775	-0.995555
O	-2.937027	-2.628376	-1.438645
H	0.843130	-2.342367	-1.390684
H	-0.228536	0.476758	-2.610165
H	-1.990669	0.245462	-2.674920
H	-1.425558	1.187369	1.851328
H	-0.499726	2.629847	-1.596996
H	-2.178654	2.545539	-2.132503
O	-3.119749	2.307542	0.084239
C	-3.722579	2.102612	1.369533
H	-3.186737	2.661502	2.144404
H	-4.740601	2.480675	1.276999
H	-3.735381	1.035740	1.617578
C	1.109304	0.982631	2.023435
H	2.187327	0.857709	1.925727
H	0.928256	1.905593	2.590242
H	0.701247	0.141950	2.592799
H	0.877161	1.765415	-0.034653
C	2.833020	-0.134545	-0.238843
C	3.701690	-0.952058	0.509073
C	3.359014	0.990731	-0.898744
C	5.061189	-0.652782	0.583701
H	3.296712	-1.815807	1.027292
C	4.718538	1.287763	-0.815282
H	2.703329	1.618147	-1.496272
C	5.573246	0.468317	-0.074093
H	5.720713	-1.295006	1.160935
H	5.112427	2.155483	-1.337436
H	6.632625	0.701035	-0.011494

proximal-TS1j

Total SCF energy: -1149.96410229 a.u.
Enthalpy at 298K: -1149.697921 a.u.
Gibbs free energy at 298K: -1149.761869 a.u.
Free energy in solution: -1149.763925 a.u.

Imaginary frequency: -258.6994 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.317606	-0.389907	-0.557326
C	-0.759014	-1.685364	0.137111
C	0.666431	-1.410869	0.450819
C	1.667841	-1.261288	-0.497334
C	1.352710	-1.149931	-1.971518
C	0.481793	0.112115	-2.127002
C	-2.036959	0.851763	-0.707046
Rh	-0.120119	0.614742	-0.146813
Cl	-0.546548	1.055732	2.273105
C	0.503298	2.332263	-0.338112
O	0.885471	3.414296	-0.456637
H	-2.534387	1.759517	-1.013456
H	-0.406760	-0.055428	-2.740451
H	1.064407	0.926312	-2.562172
H	0.921792	-1.415782	1.503897
H	0.828902	-2.056353	-2.301001
H	2.291250	-1.097952	-2.531471
O	2.973117	-1.178808	-0.217484
C	3.393716	-1.124857	1.152784
H	3.133969	-2.051256	1.676610
H	4.477015	-1.009580	1.120173
H	2.935697	-0.267187	1.657280
C	-1.466275	-2.277082	1.352384
H	-2.473893	-2.626805	1.130526
H	-0.894096	-3.140539	1.715538
H	-1.512560	-1.533473	2.153960
H	-0.886347	-2.239806	-0.791675
C	-3.455873	-1.329717	-0.759008
H	-4.005946	-1.520894	0.168330
H	-4.152458	-0.874013	-1.471735
H	-3.138974	-2.294256	-1.172089

proximal-TS1k

Total SCF energy: -1267.89252500 a.u.
Enthalpy at 298K: -1267.537321 a.u.
Gibbs free energy at 298K: -1267.609660 a.u.
Free energy in solution: -1267.609469 a.u.
Imaginary frequency: -236.0856 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.862645	0.218827	-0.141013
C	-0.509792	-1.349796	0.581952
C	0.973668	-1.429938	0.601332
C	1.766365	-1.679335	-0.509159
C	1.197149	-1.628727	-1.907289
C	0.728157	-0.175565	-2.111778
C	-1.257783	1.307579	-0.453870
Rh	0.616111	0.661099	-0.155136
Cl	0.762722	1.470446	2.199477
C	1.535975	2.157485	-0.693207
O	2.107401	3.102542	-1.027272
H	-1.527152	2.291207	-0.808438
H	-0.250169	-0.107073	-2.592384
H	1.458670	0.375351	-2.707806
H	1.428493	-1.380172	1.583928
H	0.366508	-2.341358	-1.985935
H	1.964369	-1.943352	-2.621418
O	3.078257	-1.934338	-0.468391
C	3.768110	-1.860267	0.786877
H	3.386753	-2.612451	1.485952
H	4.813646	-2.064758	0.556791
H	3.664158	-0.859292	1.219412
C	-1.064679	-1.540976	1.986732
H	-2.149027	-1.614813	2.007350
H	-0.661627	-2.470795	2.411192
H	-0.754955	-0.709557	2.626782
H	-0.945777	-1.975362	-0.190543
C	-3.305199	-0.282023	-0.195546
C	-3.460953	-1.789330	-0.484041
C	-4.072291	0.106828	1.092507
C	-3.964151	0.479647	-1.378702
H	-2.941020	-2.075840	-1.405661
H	-3.101240	-2.424295	0.329026
H	-4.524179	-2.014340	-0.623666
H	-4.015124	1.186749	1.259992
H	-5.128706	-0.170091	0.988085
H	-3.682193	-0.387121	1.984649
H	-5.016775	0.183906	-1.464525
H	-3.929961	1.561963	-1.221315
H	-3.462797	0.252397	-2.324914

proximal-TS1l

Total SCF energy: -1223.97149447 a.u.
Enthalpy at 298K: -1223.723710 a.u.
Gibbs free energy at 298K: -1223.789075 a.u.
Free energy in solution: -1223.789856 a.u.
Imaginary frequency: -216.8161 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.172335	0.400948	-0.277195
C	-1.082366	-1.247412	0.592399
C	0.376838	-1.402130	0.713006
C	1.218087	-1.754723	-0.338296
C	0.727325	-1.783683	-1.768015
C	0.315868	-0.338207	-2.108525
C	-1.588068	1.509759	-0.596429
Rh	0.173140	0.643546	-0.219298
Cl	0.240499	1.616731	2.078132
C	1.393605	1.932000	-0.741462
O	2.136594	2.749277	-1.069066
H	-1.837614	2.501631	-0.944367
H	-0.645170	-0.279488	-2.623944
H	1.078903	0.142955	-2.722624
H	0.779624	-1.308606	1.715042
H	-0.117882	-2.478030	-1.845824
H	1.525288	-2.167105	-2.410880
O	2.507723	-2.064703	-0.204729
C	3.131887	-1.952356	1.083857
H	2.671684	-2.642387	1.798717
H	4.175266	-2.223160	0.924757
H	3.058356	-0.923165	1.451067
C	-1.798773	-1.262386	1.932500
H	-2.880998	-1.221911	1.814641
H	-1.556603	-2.203513	2.444682
H	-1.461364	-0.431663	2.558416
H	-1.549745	-1.853572	-0.178214
C	-3.486985	-0.184398	-0.524508
O	-3.779618	-1.366182	-0.538638
H	-4.247615	0.592397	-0.745832

proximal-TS1m

Total SCF energy: -1202.88724595 a.u.
Enthalpy at 298K: -1202.650381 a.u.
Gibbs free energy at 298K: -1202.715624 a.u.
Free energy in solution: -1202.717377 a.u.
Imaginary frequency: -243.9986 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.227000	0.170983	-0.376747
C	-0.999293	-1.464646	0.342200
C	0.461665	-1.469376	0.539670
C	1.388331	-1.636857	-0.485433
C	0.989347	-1.518802	-1.937722
C	0.487212	-0.073243	-2.127598
C	-1.693424	1.323913	-0.610315
Rh	0.134869	0.672763	-0.158238
Cl	-0.011392	1.326246	2.227497

C	1.122402	2.181169	-0.502963
O	1.735110	3.133004	-0.715943
H	-2.023461	2.303402	-0.925421
H	-0.437791	-0.019612	-2.705782
H	1.250799	0.531344	-2.620059
H	0.794707	-1.458021	1.570872
H	0.207809	-2.255218	-2.160656
H	1.851692	-1.761383	-2.565615
O	2.687202	-1.857461	-0.298985
C	3.223995	-1.867052	1.034910
H	2.776895	-2.673891	1.624462
H	4.292588	-2.041557	0.914320
H	3.049499	-0.901388	1.520517
C	-1.766036	-1.760295	1.619202
H	-2.843539	-1.801191	1.457168
H	-1.447200	-2.741158	1.996038
H	-1.538835	-1.006636	2.379079
H	-1.327378	-2.005623	-0.542017
C	-3.448918	-0.483366	-0.512530
N	-4.441344	-1.086926	-0.638038

proximal-TS1n

Total SCF energy: -1165.99501441 a.u.
Enthalpy at 298K: -1165.740426 a.u.
Gibbs free energy at 298K: -1165.804272 a.u.
Free energy in solution: -1165.809372 a.u.
Imaginary frequency: -319.7979 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.251665	-0.696321	-0.680684
C	-0.587225	-1.760711	0.051273
C	0.813377	-1.361882	0.397887
C	1.807033	-1.092135	-0.524479
C	1.488848	-0.930885	-1.992019
C	0.545180	0.282605	-2.092867
C	-2.039721	0.573629	-0.795382
Rh	-0.172797	0.622758	-0.115600
Cl	-0.642255	0.916614	2.310486
C	0.102958	2.428934	-0.276224
O	0.263990	3.566813	-0.373499
H	-2.629703	1.383868	-1.200410
H	-0.296814	0.112147	-2.768259
H	1.097959	1.163098	-2.427307
H	1.055031	-1.390144	1.453866
H	1.013526	-1.847217	-2.364553
H	2.420592	-0.798407	-2.550439
O	3.100593	-0.900302	-0.227509
C	3.500989	-0.875013	1.147501
H	3.313402	-1.842287	1.627161
H	4.571443	-0.669308	1.136814
H	2.969053	-0.082555	1.685629
C	-1.225651	-2.465131	1.244951
H	-2.232108	-2.829099	1.031364
H	-0.619497	-3.335543	1.527921
H	-1.272218	-1.782495	2.099264
H	-0.615544	-2.332297	-0.878833
N	-3.287014	-1.589833	-0.776227
H	-3.046711	-2.506670	-1.141391
H	-3.866508	-1.671460	0.054834

proximal-TS2a

Total SCF energy: -1228.59071033 a.u.
Enthalpy at 298K: -1228.264888 a.u.
Gibbs free energy at 298K: -1228.337469 a.u.
Free energy in solution: -1228.339923 a.u.
Imaginary frequency: -248.0959 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.002389	-0.139553	-0.269621
C	-0.562425	-1.502974	0.236002
C	0.845041	-1.435835	0.712511
C	1.911287	-1.408949	-0.183150
C	1.723793	-1.359450	-1.692338
C	0.737797	-0.225855	-2.029106
C	-1.608720	1.014258	-0.669704
Rh	0.303500	0.627727	-0.151899
Cl	-0.062123	1.531205	2.143691
C	1.132398	2.209785	-0.595389
O	1.639719	3.205501	-0.881184
H	-0.196831	-0.585936	-2.468758
H	1.183078	0.494007	-2.719150
H	1.387623	-2.347953	-2.042456
H	2.685691	-1.183183	-2.178364
O	3.132949	-1.595989	0.362453
C	4.316451	-1.221936	-0.344038
H	4.256156	-0.183569	-0.690164
H	5.125105	-1.313916	0.382434
H	4.515015	-1.889476	-1.189212
H	-0.712224	-2.058856	-0.688079
H	-1.197819	-1.850389	1.044763
C	1.101077	-1.620043	2.192617
H	0.276678	-1.209291	2.777130
H	1.206277	-2.690719	2.418676
H	2.016419	-1.116478	2.506158
H	-2.038456	1.927102	-1.051005
C	-3.239331	-0.919840	0.021954
H	-3.336348	-1.042809	1.110303
H	-3.162293	-1.932836	-0.398703
C	-4.500812	-0.228123	-0.526208
H	-4.572096	0.776348	-0.092086
H	-4.396738	-0.097393	-1.610675
C	-5.773056	-1.022914	-0.214378
H	-5.912851	-1.141763	0.866775
H	-6.658308	-0.513714	-0.610514
H	-5.737492	-2.024898	-0.659411

proximal-TS2b

Total SCF energy: -1225.16647051 a.u.
Enthalpy at 298K: -1224.894669 a.u.
Gibbs free energy at 298K: -1224.963151 a.u.
Free energy in solution: -1224.969541 a.u.
Imaginary frequency: -243.9262 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.345224	-0.123818	-0.218515
C	-0.900783	-1.381788	0.575321
C	0.517243	-1.233547	0.982372
C	1.551322	-1.385903	0.058956
C	1.296964	-1.633865	-1.420188
C	0.354269	-0.533906	-1.940276
C	-1.964569	0.961443	-0.785547
Rh	-0.051658	0.631906	-0.230211
Cl	-0.413839	1.935891	1.863765
C	0.811419	2.102986	-0.932429
O	1.335455	3.027327	-1.380391
H	-2.397048	1.803197	-1.304176
H	-0.590047	-0.929189	-2.324387
H	0.828382	0.050615	-2.731540
H	0.882612	-2.646182	-1.539441
H	2.240302	-1.630427	-1.969942
O	2.793924	-1.459229	0.579170
C	3.944740	-1.231246	-0.236446
H	3.854953	-0.287238	-0.786216
H	4.781486	-1.165894	0.460361
H	4.120550	-2.057768	-0.932889
H	-1.107426	-2.121812	-0.193520
C	-3.573665	-0.924958	0.070555
H	-3.666827	-1.138248	1.139035
H	-4.433357	-0.300743	-0.217700
O	-3.606862	-2.189474	-0.578605
H	-3.614750	-2.023547	-1.535216

H	-1.525402	-1.504444	1.454587
C	0.824784	-1.130575	2.460880
H	0.038247	-0.577506	2.976124
H	0.899285	-2.138924	2.891907
H	1.769789	-0.615763	2.639015

proximal-TS2c

Total SCF energy: -1303.80582554 a.u.
Enthalpy at 298K: -1303.475060 a.u.
Gibbs free energy at 298K: -1303.547467 a.u.
Free energy in solution: -1303.547738 a.u.
Imaginary frequency: -245.9146 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.852870	0.011555	-0.724584
C	-0.510751	-1.443396	-0.378731
C	0.761891	-1.499964	0.394560
C	1.997718	-1.310575	-0.219179
C	2.153975	-0.956924	-1.691315
C	1.198219	0.201191	-2.024807
C	-1.400502	1.192546	-0.973063
Rh	0.374614	0.698060	-0.158371
Cl	-0.576154	1.127282	2.145364
C	1.262339	2.313398	-0.139188
O	1.804595	3.331561	-0.136970
H	-1.781517	2.155951	-1.273314
H	0.380448	-0.086764	-2.691600
H	1.729076	1.039001	-2.481002
H	1.981574	-1.857631	-2.301091
H	3.185155	-0.655837	-1.887073
O	3.071778	-1.632222	0.535050
C	4.376929	-1.163845	0.193591
H	4.382474	-0.075416	0.062503
H	5.007544	-1.428030	1.043629
H	4.763912	-1.653024	-0.706639
H	-0.439156	-1.754459	-1.418526
C	-3.185500	-0.584601	-0.275671
O	-3.043820	-1.042732	1.067580
H	-2.575705	-0.345030	1.575459
H	-1.277102	-1.964446	0.184933
C	0.698210	-1.990452	1.825479
H	-0.279677	-1.778908	2.258727
H	0.869586	-3.075764	1.850013
H	1.456185	-1.515650	2.450292
C	-3.635636	-1.790787	-1.107257
H	-4.561602	-2.190240	-0.681424
H	-3.823591	-1.494142	-2.143929
H	-2.892766	-2.592517	-1.102807
C	-4.247955	0.530007	-0.340155
H	-4.368815	0.910865	-1.360235
H	-5.206382	0.123789	-0.001418
H	-3.969491	1.359998	0.315676

proximal-TS2d

Total SCF energy: -1519.32947967 a.u.
Enthalpy at 298K: -1518.983159 a.u.
Gibbs free energy at 298K: -1519.063544 a.u.
Free energy in solution: -1519.059289 a.u.
Imaginary frequency: -240.7609 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.708368	0.200514	-0.424934
C	-0.486780	-1.339850	0.115656
C	0.885649	-1.428791	0.682998
C	2.005618	-1.513375	-0.140436
C	1.927942	-1.433429	-1.658476
C	1.097470	-0.195296	-2.041928
C	-1.146339	1.309133	-0.772016
Rh	0.673972	0.700154	-0.181474
Cl	0.313904	1.638227	2.098393
C	1.718342	2.162758	-0.568640
O	2.363582	3.085617	-0.820115
H	0.150063	-0.446254	-2.527438
H	1.655631	0.467091	-2.706860
H	1.512403	-2.376470	-2.046867
H	2.934510	-1.357922	-2.074921
O	3.160259	-1.843816	0.480695
C	4.422563	-1.575613	-0.130866
H	4.489318	-0.529031	-0.450201
H	5.163973	-1.763791	0.647045
H	4.615548	-2.241047	-0.979096
H	-0.629702	-1.851221	-0.833027
H	-1.200473	-1.651642	0.871229
C	1.019208	-1.644270	2.174963
H	0.220080	-1.127169	2.708253
H	0.967130	-2.719157	2.400069
H	1.970194	-1.264820	2.550486
H	-1.450419	2.273886	-1.149878
Si	-3.467093	-0.413403	-0.163073
C	-3.735230	-2.028221	-1.113317
H	-3.077031	-2.833104	-0.766332
H	-4.768246	-2.374501	-0.982878
H	-3.564229	-1.892604	-2.187648
C	-3.776895	-0.670487	1.682379
H	-4.837452	-0.887965	1.862150
H	-3.198546	-1.504527	2.096291
H	-3.511261	0.229005	2.248208
C	-4.597188	0.939112	-0.844488
H	-5.649589	0.646744	-0.740944
H	-4.458006	1.881847	-0.303634
H	-4.406381	1.125967	-1.907369

proximal-TS2e

Total SCF energy: -1338.51696365 a.u.
Enthalpy at 298K: -1338.233208 a.u.
Gibbs free energy at 298K: -1338.306257 a.u.
Free energy in solution: -1338.308568 a.u.
Imaginary frequency: -190.1239 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.901217	0.070095	-0.350573
C	-0.486361	-1.512961	0.075734
C	0.876466	-1.478179	0.606581
C	1.978024	-1.365532	-0.253220
C	1.840200	-1.234509	-1.764372
C	0.849194	-0.095679	-2.064781
C	-1.471305	1.232473	-0.677428
Rh	0.383892	0.635381	-0.141342
Cl	0.014238	1.416028	2.198108
C	1.385457	2.171776	-0.401990
O	1.989591	3.138263	-0.570842
H	-1.836823	2.192715	-1.006160
H	-0.070414	-0.438738	-2.546675
H	1.302012	0.669527	-2.698257
H	1.532330	-2.205822	-2.180500
H	2.814550	-1.015045	-2.205422
O	3.176147	-1.559442	0.327266
C	4.391362	-1.209762	-0.339538
H	4.373767	-0.162959	-0.662990
H	5.174476	-1.344440	0.407421
H	4.588908	-1.866315	-1.192956
H	-0.626825	-1.923727	-0.920370
C	-3.171958	-0.634955	-0.118160
O	-3.329355	-1.715715	0.414063
O	-4.184395	0.117772	-0.599185
C	-5.499348	-0.432455	-0.400044
H	-6.183542	0.299310	-0.829614
H	-5.593391	-1.395201	-0.909356
H	-5.698748	-0.568657	0.665896
H	-1.222446	-1.862820	0.790173
C	1.090182	-1.747288	2.080299

H	0.207550	-1.456659	2.651140
H	1.278816	-2.819154	2.231424
H	1.942518	-1.191801	2.473315

proximal-TS2f

Total SCF energy: -1263.29247894 a.u.
Enthalpy at 298K: -1263.015413 a.u.
Gibbs free energy at 298K: -1263.086714 a.u.
Free energy in solution: -1263.088881 a.u.
Imaginary frequency: -188.5065 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.142241	-0.093406	-0.449156
C	-0.645848	-1.589795	-0.074676
C	0.683980	-1.505963	0.531027
C	1.817100	-1.272723	-0.260957
C	1.746707	-1.083026	-1.771315
C	0.707185	0.011571	-2.071205
C	-1.757836	1.107053	-0.705670
Rh	0.113422	0.612553	-0.139220
Cl	-0.405628	1.256083	2.215682
C	1.021705	2.221525	-0.284267
O	1.566471	3.232199	-0.382144
H	-2.166993	2.062040	-0.998559
H	-0.165312	-0.357980	-2.617165
H	1.144567	0.833024	-2.642133
H	1.514156	-2.049920	-2.242512
H	2.727399	-0.790981	-2.152038
O	2.997625	-1.418221	0.371376
C	4.206471	-0.909227	-0.196348
H	4.101584	0.151580	-0.451262
H	4.958482	-1.021050	0.585620
H	4.513975	-1.481544	-1.077535
H	-0.706754	-1.945018	-1.099724
C	-3.394145	-0.859496	-0.271779
O	-3.460013	-1.995328	0.163472
C	-4.641949	-0.081291	-0.666930
H	-4.546618	0.335345	-1.675009
H	-5.502987	-0.750856	-0.617921
H	-4.788787	0.753619	0.027928
H	-1.392314	-2.038205	0.572352
C	0.838550	-1.840234	1.998212
H	-0.084261	-1.622143	2.537001
H	1.072128	-2.908556	2.105340
H	1.642694	-1.266783	2.460651

proximal-TS2g

Total SCF energy: -1792.05925965 a.u.
Enthalpy at 298K: -1791.717265 a.u.
Gibbs free energy at 298K: -1791.806321 a.u.
Free energy in solution: -1791.804998 a.u.
Imaginary frequency: -202.6877 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-0.022650	-0.521482	-0.351471
C	1.602539	-1.534447	0.556831
C	2.924477	-1.090217	1.027555
C	4.026143	-1.075682	0.164282
C	3.914760	-1.416911	-1.313859
C	2.811605	-0.539659	-1.932368
C	0.181777	0.607646	-0.932744
Rh	2.091505	0.584993	-0.298698
Cl	1.328172	1.865858	1.705436
C	2.771330	2.158519	-0.991918
O	3.180387	3.141329	-1.433259
H	-0.360884	1.350554	-1.496772
H	1.983369	-1.122540	-2.343238
H	3.209927	0.098334	-2.723487
H	3.711915	-2.493688	-1.410311
H	4.870795	-1.245119	-1.812423
O	5.218310	-0.883325	0.755054
C	6.382256	-0.553162	-0.008025
H	6.199611	0.322482	-0.640767
H	7.147666	-0.313186	0.730783
H	6.719641	-1.397577	-0.617228
H	1.569999	-2.290899	-0.220787
C	-1.092497	-1.523567	-0.168574
O	-0.875434	-2.726209	-0.102358
H	0.939294	-1.756065	1.385177
C	3.121696	-0.866101	2.511879
H	2.196404	-0.513572	2.969199
H	3.422909	-1.808974	2.988898
H	3.897369	-0.124399	2.707702
C	-2.490956	-0.982187	-0.107161
C	-3.538586	-1.849359	-0.455382
C	-2.782296	0.318409	0.330515
C	-4.857215	-1.413468	-0.400259
H	-3.298650	-2.860612	-0.766108
C	-4.105892	0.749070	0.401447
H	-1.982476	0.979471	0.648494
C	-5.140858	-0.111279	0.027014
H	-5.667002	-2.080518	-0.676144
H	-4.333973	1.747566	0.758830
C	-6.565070	0.382025	0.035988
F	-7.443550	-0.622841	0.242001
F	-6.769815	1.308066	0.996485
F	-6.892421	0.957135	-1.144135

proximal-TS2h

Total SCF energy: -1341.69762875 a.u.
Enthalpy at 298K: -1341.375747 a.u.
Gibbs free energy at 298K: -1341.450184 a.u.
Free energy in solution: -1341.450487 a.u.
Imaginary frequency: -282.3531 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.542747	0.366776	-0.573365
C	-0.511664	-1.147193	0.306620
C	0.835421	-1.309493	0.925671
C	1.938624	-1.684155	0.165184
C	1.875821	-1.839306	-1.346368
C	1.276089	-0.555477	-1.948624
C	-0.839254	1.332339	-1.052606
Rh	0.886540	0.668582	-0.275690
Cl	0.541947	1.993354	1.803130
C	2.039677	1.968729	-0.867704
O	2.755502	2.789212	-1.248043
H	0.333933	-0.730084	-2.475423
H	1.973996	-0.084664	-2.644207
H	1.288774	-2.739725	-1.583854
H	2.875196	-2.022620	-1.746377
O	3.037190	-2.050400	0.860880
C	4.325577	-2.052701	0.244068
H	4.527033	-1.093349	-0.246813
H	5.034535	-2.196785	1.060646
H	4.433168	-2.872810	-0.473675
H	-0.715412	-1.817455	-0.526836
H	-1.270950	-1.198738	1.080198
C	0.912958	-1.296137	2.436946
H	0.227168	-0.552633	2.846020
H	0.644904	-2.287572	2.828924
H	1.918316	-1.055289	2.784715
H	-1.032037	2.237269	-1.609241
C	-2.932329	-0.024585	-0.343541
C	-3.528358	-1.066517	-1.074322
C	-3.689009	0.654614	0.628904
C	-4.859923	-1.412309	-0.847117
H	-2.950389	-1.588643	-1.831923
C	-5.019756	0.302758	0.850877
H	-3.221203	1.451173	1.199442
C	-5.607441	-0.729829	0.115725

H	-5.315117	-2.211965	-1.425075
H	-5.598193	0.836372	1.599988
H	-6.644762	-1.001253	0.291542

proximal-TS2j

Total SCF energy: -1149.96363525 a.u.
Enthalpy at 298K: -1149.698000 a.u.
Gibbs free energy at 298K: -1149.763680 a.u.
Free energy in solution: -1149.767361 a.u.
Imaginary frequency: -264.1926 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.257150	-0.949083	-0.739442
C	-0.508052	-1.841539	-0.144875
C	0.732410	-1.402866	0.548195
C	1.816987	-0.899695	-0.166360
C	1.782322	-0.687302	-1.672343
C	0.530691	0.138525	-2.021965
C	-2.236906	0.318076	-0.933640
Rh	-0.382786	0.485275	-0.153753
Cl	-1.303009	0.836675	2.136161
C	-0.096462	2.300018	-0.268157
O	0.071686	3.438213	-0.348284
H	-0.175548	-0.402488	-2.658017
H	0.799831	1.069028	-2.526197
H	1.803908	-1.669931	-2.168419
H	2.687574	-0.170413	-1.997271
O	2.962471	-0.759950	0.534869
C	4.019021	0.073047	0.054995
H	3.648300	1.074195	-0.193553
H	4.725804	0.144776	0.882867
H	4.523742	-0.367431	-0.811335
H	-0.358310	-2.272865	-1.133649
H	-1.080778	-2.485641	0.515344
C	0.872891	-1.723179	2.020586
H	-0.099145	-1.684560	2.514307
H	1.299305	-2.729303	2.140610
H	1.532023	-1.014444	2.523619
H	-2.905218	1.092002	-1.277828
C	-3.165068	-2.125597	-0.749945
H	-3.419393	-2.436439	0.270627
H	-4.093674	-1.849420	-1.261162
H	-2.729236	-2.986457	-1.270762

proximal-TS2k

Total SCF energy: -1267.89904987 a.u.
Enthalpy at 298K: -1267.544173 a.u.
Gibbs free energy at 298K: -1267.617777 a.u.
Free energy in solution: -1267.618685 a.u.
Imaginary frequency: -236.1952 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.963590	0.039774	-0.449985
C	-0.569684	-1.425320	0.073194
C	0.796498	-1.430069	0.655730
C	1.928769	-1.404962	-0.156767
C	1.859949	-1.301437	-1.673373
C	0.920529	-0.139379	-2.041884
C	-1.447593	1.161954	-0.800333
Rh	0.401102	0.672863	-0.169218
Cl	-0.062192	1.532381	2.128615
C	1.313471	2.236544	-0.512635
O	1.871701	3.220948	-0.735789
H	0.006440	-0.466393	-2.545523
H	1.421504	0.587156	-2.685103
H	1.541094	-2.271501	-2.086135
H	2.859257	-1.121242	-2.075118
O	3.098750	-1.656858	0.471795
C	4.343350	-1.292452	-0.125908
H	4.339519	-0.239295	-0.430432
H	5.090779	-1.439821	0.655013
H	4.587651	-1.930470	-0.981976
H	-0.666209	-1.916583	-0.891335
H	-1.273196	-1.791607	0.810633
C	0.935975	-1.675293	2.142646
H	0.076596	-1.271719	2.679985
H	1.006336	-2.755619	2.333440
H	1.832380	-1.201445	2.544524
H	-1.784899	2.107601	-1.194833
C	-3.328706	-0.574050	-0.217796
C	-3.628414	-0.699333	1.294155
H	-4.669291	-1.014950	1.433882
H	-2.993334	-1.441751	1.787905
H	-3.477454	0.257211	1.802405
C	-3.509854	-1.937991	-0.918700
H	-4.547532	-2.270599	-0.802029
H	-3.297503	-1.862762	-1.991157
H	-2.870232	-2.717411	-0.495150
C	-4.340714	0.426941	-0.832300
H	-5.359309	0.044772	-0.698017
H	-4.274249	1.403174	-0.342377
H	-4.164200	0.561690	-1.904588

proximal-TS2l

Total SCF energy: -1223.96827709 a.u.
Enthalpy at 298K: -1223.720852 a.u.
Gibbs free energy at 298K: -1223.787596 a.u.
Free energy in solution: -1223.790544 a.u.
Imaginary frequency: -190.6259 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.318532	-0.106115	-0.648912
C	-0.861212	-1.596488	-0.127728
C	0.424308	-1.491199	0.563120
C	1.607028	-1.271554	-0.158046
C	1.634946	-1.106789	-1.672673
C	0.613509	-0.022694	-2.061311
C	-1.934971	1.099837	-0.892264
Rh	-0.114608	0.611100	-0.185727
Cl	-0.795241	1.292150	2.113193
C	0.817200	2.211920	-0.284744
O	1.375751	3.216724	-0.355580
H	-2.338950	2.043325	-1.227696
H	-0.217573	-0.407214	-2.659050
H	1.085734	0.790465	-2.615939
H	-1.648701	-2.031008	0.479086
H	-0.852934	-1.976138	-1.145766
H	1.438139	-2.082774	-2.141290
H	2.637367	-0.816178	-1.993029
O	2.742079	-1.398840	0.553608
C	3.989369	-0.911065	0.052897
H	3.908586	0.142858	-0.236502
H	4.687128	-1.005504	0.885683
H	4.349794	-1.509038	-0.790217
C	-3.558305	-0.875875	-0.590357
O	-3.721070	-2.001298	-0.161502
H	-4.407968	-0.295382	-1.003971
C	0.482160	-1.797343	2.043476
H	-0.471964	-1.564669	2.517864
H	0.702473	-2.864369	2.185394
H	1.258228	-1.218931	2.545936

proximal-TS2m

Total SCF energy: -1202.88145863 a.u.
Enthalpy at 298K: -1202.644901 a.u.
Gibbs free energy at 298K: -1202.711670 a.u.
Free energy in solution: -1202.715925 a.u.
Imaginary frequency: -253.4095 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.317893	-0.487123	-0.523321
C	-0.738607	-1.678765	0.159082
C	0.583119	-1.364469	0.737592
C	1.701445	-1.207988	-0.087622
C	1.601828	-1.186741	-1.604165
C	0.540116	-0.147535	-2.013671
C	-2.075582	0.738851	-0.846143
Rh	-0.193882	0.612309	-0.179865
Cl	-0.868235	1.425628	2.056154
C	0.432153	2.302102	-0.545859
O	0.817082	3.361654	-0.781237
H	-0.293283	-0.588369	-2.567057
H	0.980799	0.639242	-2.628756
H	1.364029	-2.202460	-1.953453
H	2.571289	-0.940995	-2.041544
O	2.883300	-1.191426	0.546723
C	4.092883	-0.824025	-0.124999
H	4.002554	0.167757	-0.581021
H	4.852414	-0.795757	0.656740
H	4.375865	-1.564789	-0.879141
H	-0.738148	-2.233580	-0.775674
H	-1.405536	-2.091411	0.908990
C	0.758115	-1.484311	2.237009
H	-0.180536	-1.270284	2.749178
H	1.082703	-2.503132	2.489290
H	1.508008	-0.785603	2.610621
H	-2.624978	1.577667	-1.247328
C	-3.339924	-1.433047	-0.486108
N	-4.148499	-2.274482	-0.448028

proximal-TS2n

Total SCF energy: -1165.99122161 a.u.
Enthalpy at 298K: -1165.737192 a.u.
Gibbs free energy at 298K: -1165.802966 a.u.
Free energy in solution: -1165.810328 a.u.
Imaginary frequency: -340.9423 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.231224	-1.026411	-0.797304
C	-0.458106	-1.868957	-0.251168
C	0.772938	-1.431865	0.469892
C	1.841556	-0.857177	-0.208861
C	1.803336	-0.569215	-1.702051
C	0.515853	0.214411	-2.017462
C	-2.209836	0.256051	-0.952617
Rh	-0.392404	0.472378	-0.131350
Cl	-1.250064	0.741580	2.187015
C	-0.225776	2.301231	-0.217904
O	-0.135536	3.449194	-0.282923
H	-0.174345	-0.334215	-2.665215
H	0.741527	1.171010	-2.493815
H	1.874298	-1.521234	-2.251052
H	2.683688	0.008403	-1.991921
O	2.985520	-0.717973	0.500845
C	3.982663	0.218710	0.093401
H	3.545416	1.210545	-0.072107
H	4.687836	0.268982	0.924443
H	4.512307	-0.113008	-0.806249
H	-0.274971	-2.253231	-1.255148
H	-1.023638	-2.551321	0.375062
C	0.910260	-1.825240	1.924480
H	-0.063573	-1.816816	2.416332
H	1.339284	-2.835033	1.994070
H	1.566199	-1.140870	2.464080
H	-2.874011	1.003903	-1.358447
N	-3.088575	-2.083604	-0.646807
H	-4.062076	-1.827613	-0.528404
H	-2.958509	-2.867154	-1.278294

proximal-TS3d-a

Total SCF energy: -1519.33523408 a.u.
Enthalpy at 298K: -1518.988520 a.u.
Gibbs free energy at 298K: -1519.067992 a.u.
Free energy in solution: -1519.062845 a.u.
Imaginary frequency: -235.8049 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.692485	-0.314647	0.162147
C	-0.571389	1.381271	0.305515
C	0.822929	1.720221	-0.068949
C	1.931633	1.517422	0.739979
C	1.860038	0.819901	2.084161
C	1.055555	-0.488489	1.907270
C	-1.062741	-1.432435	0.020907
Rh	0.716440	-0.524832	-0.196710
Cl	0.451448	-0.213211	-2.670832
C	1.842694	-1.946304	-0.518961
O	2.535569	-2.838020	-0.753699
H	0.049872	-0.382750	2.327621
H	0.951938	2.165521	-1.047269
O	3.167439	1.943882	0.437570
C	3.413816	2.516916	-0.853581
H	2.860044	3.454711	-0.975820
H	4.485261	2.715428	-0.883613
H	3.136402	1.810953	-1.643743
H	-0.803863	1.503312	1.360287
H	-1.255107	1.910181	-0.350058
H	2.889670	0.607549	2.389677
H	1.436678	1.492595	2.845257
C	1.732273	-1.691127	2.555023
H	1.831072	-1.545124	3.642479
H	1.153121	-2.608399	2.398933
H	2.741011	-1.859540	2.158913
H	-1.306825	-2.482372	-0.044612
Si	-3.484591	0.258756	0.159352
C	-3.853145	1.169826	-1.453132
H	-4.925164	1.393439	-1.525481
H	-3.314370	2.120934	-1.534239
H	-3.571372	0.558083	-2.316881
C	-3.808685	1.382633	1.647740
H	-4.868119	1.666821	1.678083
H	-3.575340	0.875017	2.591054
H	-3.226147	2.310196	1.610279
C	-4.532549	-1.308408	0.291743
H	-5.599816	-1.054201	0.303453
H	-4.358527	-1.976196	-0.559415
H	-4.312291	-1.864310	1.210122

proximal-TS3d-b

Total SCF energy: -1519.33638142 a.u.
Enthalpy at 298K: -1518.989733 a.u.
Gibbs free energy at 298K: -1519.069690 a.u.
Free energy in solution: -1519.064001 a.u.
Imaginary frequency: -234.2285 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.761463	-0.044794	-0.376260
C	0.525395	1.024767	0.866867
C	-0.879177	0.862555	1.306094
C	-1.973030	1.341760	0.594353
C	-1.798632	1.995472	-0.774405
C	-1.141662	0.909550	-1.658262
C	1.206000	-0.917111	-1.145827
Rh	-0.613276	-0.657840	-0.327891
Cl	-0.222342	-2.324081	1.487501
C	-1.616851	-1.876128	-1.272071
O	-2.239586	-2.644514	-1.866166
H	1.505154	-1.614591	-1.913781
H	-0.242299	1.263447	-2.170426

H	-1.854298	0.550574	-2.404955
H	-1.027392	0.358915	2.253038
H	-1.098811	2.832143	-0.636483
O	-3.232328	1.300878	1.041599
C	-3.526022	0.573814	2.242494
H	-3.051988	1.047028	3.109482
H	-4.610283	0.612114	2.347993
H	-3.187763	-0.463906	2.149839
H	0.731100	1.945389	0.328252
C	-3.094625	2.562043	-1.363944
H	-3.544557	3.320340	-0.714512
H	-2.876411	3.024453	-2.332491
H	-3.834938	1.771453	-1.523637
H	1.193336	0.851192	1.703798
Si	3.506552	0.512466	0.050132
C	4.638426	-0.315150	-1.216886
H	5.683437	-0.031619	-1.039955
H	4.573886	-1.407091	-1.151678
H	4.381281	-0.020532	-2.240586
C	3.636387	2.395858	-0.089131
H	3.351623	2.745012	-1.088575
H	3.006424	2.914762	0.642514
H	4.670822	2.714555	0.090950
C	3.951306	-0.049431	1.797952
H	3.812207	-1.130433	1.907095
H	5.002074	0.183533	2.012801
H	3.344327	0.440781	2.567737

proximal-TS3e-a

Total SCF energy: -1338.52233728 a.u.
Enthalpy at 298K: -1338.238294 a.u.
Gibbs free energy at 298K: -1338.310448 a.u.
Free energy in solution: -1338.311468 a.u.
Imaginary frequency: -190.4280 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.881490	0.149459	-0.054936
C	-0.565112	-1.483486	-0.597002
C	0.841920	-1.711998	-0.282443
C	1.903166	-1.187893	-1.022311
C	1.704832	-0.273081	-2.215498
C	0.746342	0.863452	-1.791816
C	-1.387184	1.277133	0.302735
Rh	0.441206	0.417299	0.273028
Cl	0.266851	-0.397927	2.640711
C	1.542928	1.775901	0.892157
O	2.213493	2.613376	1.310880
H	-0.240991	0.727386	-2.245028
H	1.046893	-2.312785	0.594991
O	3.186687	-1.482329	-0.793184
C	3.537321	-2.266488	0.358446
H	3.124506	-3.277825	0.277775
H	4.626225	-2.310156	0.357103
H	3.177132	-1.782636	1.272286
H	-0.828430	-1.358701	-1.643191
H	-1.243623	-2.128659	-0.053241
H	2.689481	0.121525	-2.485536
H	1.344349	-0.848608	-3.080554
C	1.264356	2.250033	-2.154833
H	1.358084	2.357854	-3.246933
H	0.583335	3.034306	-1.805353
H	2.253196	2.448387	-1.724278
H	-1.704151	2.268689	0.586430
C	-3.184736	-0.509300	-0.238470
O	-3.390911	-1.687202	-0.450843
O	-4.161021	0.418616	-0.140823
C	-5.500336	-0.091290	-0.275025
H	-6.149192	0.778058	-0.168757
H	-5.636315	-0.557992	-1.254200
H	-5.709263	-0.826885	0.505891

proximal-TS3e-b

Total SCF energy: -1338.52328330 a.u.
Enthalpy at 298K: -1338.239354 a.u.
Gibbs free energy at 298K: -1338.312519 a.u.
Free energy in solution: -1338.311802 a.u.
Imaginary frequency: -184.2276 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.959206	-0.052814	-0.238686
C	-0.549896	-1.111569	1.046588
C	0.842922	-0.826207	1.369459
C	1.921217	-1.234025	0.577705
C	1.702839	-1.993735	-0.729867
C	0.834308	-1.054050	-1.598691
C	-1.523249	0.799068	-1.089280
Rh	0.328900	0.555416	-0.310848
Cl	-0.004840	2.313488	1.432145
C	1.326821	1.753919	-1.310471
O	1.935422	2.505843	-1.936107
H	-1.876524	1.456328	-1.868208
H	-0.083247	-1.528993	-1.958089
H	1.404483	-0.695350	-2.458734
H	1.022302	-0.258117	2.273855
H	1.133637	-2.898964	-0.474620
O	3.196873	-1.050330	0.915895
C	3.517115	-0.240464	2.059027
H	3.169960	-0.719775	2.980364
H	4.604435	-0.167824	2.065958
H	3.067353	0.752650	1.956607
H	-0.765011	-2.028786	0.507555
C	3.001048	-2.431692	-1.415718
H	3.605176	-3.082391	-0.775302
H	2.754611	-2.981681	-2.329994
H	3.613232	-1.567391	-1.693280
H	-1.236661	-0.913751	1.859520
C	-3.217560	-0.638736	0.247979
O	-3.360374	-1.408176	1.176737
O	-4.234365	-0.190289	-0.519682
C	-5.537837	-0.670651	-0.143407
H	-6.226931	-0.214075	-0.853885
H	-5.579134	-1.761019	-0.210726
H	-5.777489	-0.364500	0.878093

proximal-TS3f-a

Total SCF energy: -1263.29758259 a.u.
Enthalpy at 298K: -1263.020250 a.u.
Gibbs free energy at 298K: -1263.090349 a.u.
Free energy in solution: -1263.091417 a.u.
Imaginary frequency: -189.7940 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.139829	0.055948	-0.187064
C	-0.742819	-1.512091	-0.660093
C	0.649071	-1.708849	-0.262405
C	1.739293	-1.164844	-0.943108
C	1.588155	-0.262692	-2.153190
C	0.579157	0.851836	-1.794365
C	-1.682465	1.199922	0.183322
Rh	0.172247	0.414347	0.253544
Cl	-0.115884	-0.382503	2.616580
C	1.192282	1.816385	0.917533
O	1.808154	2.681670	1.363174
H	-0.377336	0.686094	-2.300760
H	0.816279	-2.303108	0.627497
O	3.014673	-1.429720	-0.640366
C	3.315269	-2.193469	0.538344
H	2.932286	-3.215480	0.445316
H	4.403081	-2.210684	0.601977
H	2.889832	-1.709193	1.423568
H	-0.943013	-1.393408	-1.721001

H	-1.435113	-2.183452	-0.166866
H	2.576637	0.155375	-2.368552
H	1.293206	-0.852202	-3.033558
C	1.081933	2.247878	-2.143040
H	1.234358	2.347105	-3.229321
H	0.363748	3.018882	-1.841308
H	2.039906	2.475256	-1.660279
H	-2.037380	2.184834	0.446971
C	-3.429757	-0.633416	-0.403775
O	-3.549203	-1.815507	-0.670816
C	-4.638400	0.279904	-0.246918
H	-4.543513	1.171809	-0.875170
H	-5.536265	-0.277151	-0.521973
H	-4.718163	0.611639	0.794715

proximal-TS3f-b

Total SCF energy: -1263.29857103 a.u.
Enthalpy at 298K: -1263.021260 a.u.
Gibbs free energy at 298K: -1263.091636 a.u.
Free energy in solution: -1263.090903 a.u.
Imaginary frequency: -186.1792 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.201974	-0.312281	-0.257114
C	-0.699853	-1.296756	0.946241
C	0.645556	-0.881506	1.328609
C	1.782329	-1.125857	0.551584
C	1.685294	-1.843059	-0.794957
C	0.710705	-0.986785	-1.637193
C	-1.825558	0.605765	-1.073726
Rh	0.037661	0.517991	-0.301357
Cl	-0.489331	2.168651	1.498130
C	0.918474	1.846098	-1.247308
O	1.452298	2.677261	-1.840310
H	-2.230600	1.261192	-1.829573
H	-0.153409	-1.550825	-2.000076
H	1.227339	-0.546357	-2.492866
H	0.740438	-0.352279	2.268539
H	1.244100	-2.830094	-0.595257
O	3.021889	-0.827013	0.942021
C	3.219419	-0.040511	2.128108
H	2.898363	-0.594365	3.016636
H	4.292113	0.145913	2.175853
H	2.669479	0.903472	2.051716
H	-0.791765	-2.191658	0.337569
C	3.040687	-2.062650	-1.475176
H	3.722259	-2.650762	-0.852614
H	2.885484	-2.598935	-2.417204
H	3.528093	-1.108754	-1.702770
H	-1.419181	-1.250500	1.754503
C	-3.430702	-0.987552	0.210569
O	-3.473702	-1.803156	1.113883
C	-4.682445	-0.557113	-0.542860
H	-5.520590	-1.172778	-0.210214
H	-4.896328	0.497073	-0.332140
H	-4.547375	-0.660518	-1.624663

proximal-TS3j-a

Total SCF energy: -1149.96940262 a.u.
Enthalpy at 298K: -1149.703306 a.u.
Gibbs free energy at 298K: -1149.767257 a.u.
Free energy in solution: -1149.769727 a.u.
Imaginary frequency: -266.4137 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.344362	-0.241275	-0.913583
C	-0.631814	-1.224160	-1.472567
C	0.710983	-1.399967	-0.870906
C	1.763865	-0.508593	-1.019418
C	1.630661	0.811005	-1.751958
C	0.371869	1.534780	-1.219789
C	-2.234498	0.679365	-0.027504
Rh	-0.299619	0.216147	0.316526
Cl	-0.834715	-1.578792	1.986993
C	0.112703	1.356237	1.706252
O	0.352388	2.046938	2.597735
H	-0.432793	1.505300	-1.962211
H	0.848546	-2.298440	-0.283004
O	3.005276	-0.732353	-0.564769
C	3.260049	-1.893291	0.237583
H	3.097888	-2.809598	-0.341151
H	4.308257	-1.821271	0.527835
H	2.619813	-1.891950	1.126220
H	-0.638476	-0.750190	-2.452631
H	-1.170628	-2.165866	-1.442684
H	2.536037	1.389415	-1.541427
H	1.608188	0.644030	-2.839305
C	0.640818	2.988080	-0.846420
H	0.966389	3.564912	-1.726640
H	-0.259295	3.472321	-0.451126
H	1.430261	3.078183	-0.090495
C	-3.344647	-0.975399	-1.731819
H	-3.517471	-1.981954	-1.332107
H	-4.294532	-0.430836	-1.700619
H	-3.038706	-1.072220	-2.780162
H	-2.865548	1.403616	0.463969

proximal-TS3j-b

Total SCF energy: -1149.97068700 a.u.
Enthalpy at 298K: -1149.704643 a.u.
Gibbs free energy at 298K: -1149.768983 a.u.
Free energy in solution: -1149.771087 a.u.
Imaginary frequency: -264.8993 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.189936	1.406494	0.041289
C	-0.518064	1.483598	-1.172197
C	0.633505	0.590001	-1.423457
C	1.782128	0.575256	-0.639946
C	1.892290	1.442433	0.611055
C	0.737759	0.975548	1.527642
C	-2.193332	0.531390	0.976523
Rh	-0.466093	-0.292687	0.324802
Cl	-1.586191	-1.790651	-1.329445
C	-0.278494	-1.690626	1.508482
O	-0.170703	-2.565592	2.252093
H	-2.827653	0.218070	1.790905
H	0.128390	1.803928	1.900733
H	1.137623	0.420715	2.380109
H	0.553710	-0.061668	-2.284380
H	1.711316	2.478444	0.290122
O	2.865923	-0.155956	-0.916008
C	2.814142	-1.110440	-1.985478
H	2.691014	-0.606254	-2.950212
H	3.772535	-1.628979	-1.959185
H	1.993136	-1.817356	-1.823908
H	-0.261044	2.463890	-0.776367
C	3.267791	1.393798	1.284528
H	4.066935	1.720486	0.610768
H	3.263835	2.053583	2.158663
H	3.505261	0.380523	1.624145
H	-1.162141	1.518976	-2.045084
C	-3.021469	2.449947	-0.611202
H	-3.406790	2.101061	-1.576873
H	-3.877882	2.673302	0.034283
H	-2.468493	3.381214	-0.781342

proximal-TS3l-a

Total SCF energy: -1223.97329986 a.u.

Enthalpy at 298K: -1223.725657 a.u.
Gibbs free energy at 298K: -1223.791287 a.u.
Free energy in solution: -1223.793454 a.u.
Imaginary frequency: -187.8740 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.341172	0.223753	-0.275309
C	-1.046300	-1.460004	-0.648507
C	0.317687	-1.724188	-0.201229
C	1.460141	-1.274164	-0.865435
C	1.403526	-0.407108	-2.107886
C	0.455390	0.780089	-1.820427
C	-1.833486	1.352787	0.082223
Rh	-0.044033	0.443021	0.227270
Cl	-0.441943	-0.260175	2.602075
C	1.060713	1.787733	0.879478
O	1.725003	2.620008	1.316988
H	-0.492348	0.655886	-2.354405
H	0.422450	-2.293487	0.714088
O	2.705282	-1.605260	-0.510856
C	2.922002	-2.340089	0.704858
H	2.479898	-3.339837	0.636677
H	4.004209	-2.420142	0.804506
H	2.499989	-1.796251	1.556459
H	-1.211622	-1.369430	-1.718119
H	-1.793732	-2.064040	-0.147907
H	2.422376	-0.058499	-2.304095
H	1.099244	-1.007230	-2.977808
C	1.054913	2.129491	-2.198332
H	1.245719	2.180742	-3.281776
H	0.377061	2.952831	-1.946049
H	2.010165	2.315090	-1.692912
H	-2.143309	2.362937	0.305285
C	-3.649093	-0.374022	-0.531087
O	-3.905300	-1.538298	-0.765448
H	-4.451396	0.391174	-0.491910
H	-1.648976	-1.442545	1.584811
C	-3.535183	-1.312981	-0.133606
O	-3.639039	-2.164077	0.727253
H	-4.392362	-1.055440	-0.789319

S-CPX1
Total SCF energy: -1033.31547099 a.u.
Enthalpy at 298K: -1033.112883 a.u.
Gibbs free energy at 298K: -1033.170686 a.u.
Free energy in solution: -1033.172391 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	0.561165	-0.136273	-0.195003
C	-1.694555	-0.600282	-1.220161
C	-1.955117	0.351107	0.081653
C	-0.862411	1.295847	0.437102
C	-0.067464	1.932711	-0.534083
H	-0.380334	1.899484	-1.578836
H	-0.820401	1.610635	1.477358
C	-2.773321	0.454426	-1.156056
H	-3.794420	0.099824	-1.054691
H	-2.653041	1.337750	-1.776457
H	-0.904313	-0.442771	-1.960400
H	-1.971648	-1.638162	-1.076343
C	2.142492	0.286467	0.601120
O	3.134332	0.557165	1.125728
Cl	1.210974	-2.358589	-0.578774
O	-2.630072	-0.263886	1.118143
C	-1.862159	-1.059367	2.027499
H	-1.157045	-0.451544	2.606439
H	-2.587889	-1.511763	2.706247
H	-1.307361	-1.841004	1.495551
C	0.828444	3.102059	-0.203919
H	1.728901	3.100247	-0.826900
H	0.301022	4.046997	-0.393770
H	1.138001	3.094584	0.846215

proximal-TS3l-b
Total SCF energy: -1223.97435098 a.u.
Enthalpy at 298K: -1223.726728 a.u.
Gibbs free energy at 298K: -1223.792547 a.u.
Free energy in solution: -1223.792850 a.u.
Imaginary frequency: -186.0350 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-2.359826	-0.514139	-0.468461
C	-0.877050	-1.417432	0.825076
C	0.404119	-0.909096	1.300720
C	1.602385	-1.042276	0.591439
C	1.643252	-1.716153	-0.779889
C	0.666759	-0.901084	-1.660155
C	-2.021043	0.465604	-1.231376
Rh	-0.221170	0.490985	-0.325111
Cl	-0.996445	2.025969	1.482679
C	0.624966	1.920392	-1.151777
O	1.134944	2.812461	-1.671643
H	-2.438866	1.107090	-1.992626
H	-0.116320	-1.515610	-2.113645
H	1.208128	-0.381487	-2.453867
H	0.398550	-0.403262	2.258242
H	1.259492	-2.736843	-0.640164
O	2.787778	-0.663146	1.066775
C	2.855120	0.088990	2.289572
H	2.523515	-0.520749	3.136542
H	3.906215	0.350125	2.410099
H	2.242455	0.993166	2.211060
H	-0.862771	-2.300688	0.193492
C	3.051819	-1.821932	-1.373977
H	3.729425	-2.386269	-0.725573
H	2.994852	-2.333563	-2.340436
H	3.487518	-0.830964	-1.538638

S-CPX2
Total SCF energy: -1033.31225728 a.u.
Enthalpy at 298K: -1033.109650 a.u.
Gibbs free energy at 298K: -1033.167365 a.u.
Free energy in solution: -1033.170632 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	-0.842550	-0.065271	0.185732
C	1.152393	-1.506115	0.840166
C	1.758764	-0.182870	0.202311
C	0.945626	1.079972	0.334994
C	0.189783	1.286481	1.509836
H	-0.266040	2.259448	1.671194
H	0.367158	0.726494	2.426074
C	2.419739	-0.876508	1.358315
H	3.343326	-1.403128	1.139653
H	2.392938	-0.399950	2.333566
H	0.297520	-1.511475	1.524583
H	1.221524	-2.376922	0.198984
C	-2.171305	1.104250	-0.207114
O	-3.004208	1.864663	-0.453037
Cl	-1.996283	-1.912980	-0.664536
O	2.295179	-0.424145	-1.062753
C	3.628564	0.036765	-1.271933
H	4.336016	-0.435332	-0.578500
H	3.884959	-0.249806	-2.293511
H	3.707922	1.126072	-1.173633
C	1.168516	2.186031	-0.670158
H	2.121133	2.698162	-0.474191
H	1.191884	1.799267	-1.691533
H	0.372988	2.932849	-0.595701

S-CPX2'

Total SCF energy: -1402.72173105 a.u.
Enthalpy at 298K: -1402.439407 a.u.
Gibbs free energy at 298K: -1402.512215 a.u.
Free energy in solution: -1402.507163 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	1.743621	0.083567	0.143917
C	-0.108309	1.147016	1.477315
C	-0.756861	-0.146058	0.766084
C	0.173228	-1.300768	0.507804
C	1.214929	-1.564265	1.425081
H	1.783236	-2.483424	1.313470
H	1.220866	-1.163499	2.436915
C	-1.158297	0.288208	2.141979
H	-2.147073	0.723209	2.244456
H	-0.850670	-0.323000	2.985542
H	0.873573	1.169078	1.959833
H	-0.408796	2.084705	1.024948
C	3.040503	-0.824662	-0.746313
O	3.852698	-1.421028	-1.309921
Cl	2.442890	2.178371	-0.641953
O	-1.583282	0.156553	-0.295129
C	-0.209490	-2.281870	-0.573848
H	-1.095968	-2.855135	-0.266789
H	-0.447323	-1.774087	-1.510904
H	0.603835	-2.991664	-0.751008
Si	-3.272215	0.124618	-0.468623
C	-3.525260	-0.039856	-2.321593
H	-3.104895	-0.978039	-2.701090
H	-4.591466	-0.021570	-2.578451
H	-3.037011	0.783108	-2.855768
C	-4.005554	-1.342762	0.466152
H	-3.627803	-2.296562	0.079463
H	-3.787443	-1.307540	1.539777
H	-5.097231	-1.353677	0.355386
C	-4.012976	1.746738	0.149742
H	-3.519982	2.604374	-0.322926
H	-5.079239	1.798322	-0.105240
H	-3.934485	1.873409	1.236033

S-CPX3

Total SCF energy: -1033.31509477 a.u.
Enthalpy at 298K: -1033.112519 a.u.
Gibbs free energy at 298K: -1033.170679 a.u.
Free energy in solution: -1033.171332 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	-0.854193	-0.101389	-0.237348
C	1.465206	0.626923	-0.954687
C	1.680469	-0.410346	0.280354
C	0.631121	-1.452473	0.441746
C	-0.016111	-2.052431	-0.653691
H	0.377530	-1.993326	-1.666666
H	0.496530	-1.841719	1.447492
C	2.615311	-0.353160	-0.887281
H	2.524126	-1.197124	-1.569226
H	0.748953	0.490652	-1.771822
H	1.655223	1.663505	-0.697047
C	-2.455097	-0.767662	0.310477
O	-3.457610	-1.210393	0.671214
Cl	-1.664593	2.086778	-0.453576
O	2.188527	0.150258	1.435439
C	1.274097	0.838716	2.294965
H	0.552508	0.153609	2.755036
H	1.887938	1.290655	3.076825
H	0.729115	1.617063	1.748060
H	-0.659261	-2.908996	-0.475324
C	4.035371	0.149554	-0.713325
H	4.683412	-0.648806	-0.335357
H	4.432555	0.486276	-1.677210
H	4.078616	0.981837	-0.007888

S-distal-TS2l'

Total SCF energy: -1593.37426292 a.u.
Enthalpy at 298K: -1593.047226 a.u.
Gibbs free energy at 298K: -1593.129215 a.u.
Free energy in solution: -1593.126904 a.u.
Imaginary frequency: -205.1010 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	2.790422	1.171433	-1.177026
C	0.870814	1.941605	-1.259226
C	-0.353513	1.708780	-0.462519
C	-1.253067	0.693294	-0.796858
C	-0.995454	-0.301417	-1.922190
C	0.414177	-0.895706	-1.761245
C	3.045378	0.013100	-0.683484
Rh	1.137809	0.005314	0.002086
Cl	1.823405	1.150343	2.105714
C	1.049465	-1.588364	0.940393
O	0.975217	-2.570559	1.534531
H	3.244124	2.026522	-1.649799
H	1.085336	-0.638744	-2.586379
H	0.383173	-1.983597	-1.677804
H	1.282715	2.925177	-1.053170
H	0.805653	1.718132	-2.322416
H	-1.148937	0.203291	-2.888701
H	-1.754921	-1.085883	-1.871400
O	-2.437624	0.702699	-0.181888
C	4.161809	-0.935591	-0.560501
O	4.053828	-2.070493	-0.147072
H	5.143285	-0.538813	-0.889761
C	-0.719836	2.733146	0.589172
H	0.178727	3.141813	1.053985
H	-1.292889	3.549495	0.127125
H	-1.332620	2.293774	1.377312
Si	-3.687817	-0.428647	0.135120
C	-4.718235	-0.666868	-1.423659
H	-5.072835	0.295920	-1.810037
H	-4.167466	-1.168741	-2.227002
H	-5.602442	-1.277468	-1.200560
C	-4.686569	0.427476	1.471889
H	-5.048916	1.404040	1.131280
H	-5.559409	-0.173093	1.755677
H	-4.084079	0.589569	2.372688
C	-2.937463	-2.038458	0.753244
H	-2.388375	-2.583056	-0.022623
H	-2.248465	-1.857543	1.586302
H	-3.730461	-2.702435	1.120102

S-proximal-TS2l'

Total SCF energy: -1593.37986822 a.u.
Enthalpy at 298K: -1593.052751 a.u.
Gibbs free energy at 298K: -1593.134572 a.u.
Free energy in solution: -1593.129488 a.u.
Imaginary frequency: -183.9061 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-3.129139	-0.452679	-0.571437
C	-1.408470	-1.683218	-0.132307
C	-0.130213	-1.373238	0.506816
C	0.975141	-0.964869	-0.254768
C	0.910570	-0.754118	-1.763727
C	-0.307387	0.124335	-2.095661
C	-2.961104	0.801149	-0.813212
Rh	-1.057255	0.615908	-0.184440
Cl	-1.734354	1.143976	2.156479

C	-0.408570	2.349149	-0.299770
O	-0.024949	3.432714	-0.379727
H	-3.524745	1.669291	-1.120495
H	-1.083470	-0.404182	-2.656535
H	-0.018642	1.009705	-2.665723
H	-2.086613	-2.249957	0.496802
H	-1.383118	-2.041214	-1.157686
H	0.899187	-1.733079	-2.267112
H	1.833066	-0.261891	-2.082197
O	2.150827	-0.917376	0.372260
C	-4.214995	-1.423296	-0.475018
O	-4.165523	-2.563744	-0.057125
H	-5.168469	-0.994037	-0.845247
C	0.047127	-1.681527	1.977511
H	-0.918051	-1.695970	2.485351
H	0.524791	-2.664727	2.088493
H	0.674915	-0.939564	2.472670
Si	3.714878	-0.283525	0.060521
C	4.573726	-0.490212	1.714129
H	4.588427	-1.541521	2.022969
H	5.612281	-0.140867	1.664676
H	4.064133	0.081657	2.497580
C	4.553638	-1.319113	-1.270973
H	4.544110	-2.382631	-1.005015
H	4.082306	-1.214396	-2.254447
H	5.603202	-1.016075	-1.375993
C	3.575043	1.528569	-0.426008
H	3.111640	1.676653	-1.407557
H	2.988024	2.089535	0.310247
H	4.574207	1.980843	-0.465109

TS1i

Total SCF energy: -1110.64861984 a.u.
Enthalpy at 298K: -1110.412929 a.u.
Gibbs free energy at 298K: -1110.473436 a.u.
Free energy in solution: -1110.476129 a.u.
Imaginary frequency: -260.8434 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.826740	1.451035	-1.017906
C	-0.122449	1.936555	-0.491106
C	-1.138487	1.110467	0.201708
C	-1.965531	0.184976	-0.422699
C	-1.804416	-0.185650	-1.883546
C	-0.342753	-0.642720	-2.069227
C	2.307620	0.268065	-0.970915
Rh	0.543034	-0.331017	-0.166567
Cl	1.258267	0.124104	2.185302
C	0.806136	-2.135633	0.086255
O	0.983237	-3.264071	0.244453
H	3.212539	-0.282146	-1.172874
H	2.090199	2.472155	-1.232947
H	0.204847	-0.041418	-2.799667
H	-0.292295	-1.690584	-2.369235
H	-1.256871	1.304781	1.260926
H	-2.065281	0.674548	-2.514958
H	-2.522827	-0.978063	-2.111147
O	-2.976300	-0.449881	0.181101
C	-3.153576	-0.299444	1.597277
H	-3.406656	0.736099	1.849791
H	-3.983407	-0.956468	1.857162
H	-2.245100	-0.605550	2.126933
C	0.225873	3.185518	0.309712
H	0.904723	3.850269	-0.232586
H	-0.690347	3.750464	0.521117
H	0.690305	2.906183	1.260577
H	-0.357330	2.118324	-1.539475

TS2i

Total SCF energy: -1110.64190644 a.u.
Enthalpy at 298K: -1110.406504 a.u.
Gibbs free energy at 298K: -1110.468187 a.u.
Free energy in solution: -1110.473143 a.u.
Imaginary frequency: -258.8826 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.887529	-1.082695	1.637095
C	0.003638	-1.742648	1.166981
C	-0.970973	-1.396931	0.106112
C	-1.879077	-0.350751	0.275344
C	-1.893290	0.540486	1.509076
C	-0.469738	1.078512	1.740382
C	2.316116	0.061340	1.266370
Rh	0.631880	0.255498	0.143376
Cl	1.774364	-0.758320	-1.826633
C	0.864406	1.903611	-0.652312
O	1.025380	2.935768	-1.139931
H	2.155126	-1.984381	2.159576
H	-0.027982	0.734690	2.679821
H	-0.452950	2.170308	1.734926
H	-2.282903	-0.038846	2.360225
H	-2.595618	1.363647	1.363343
O	-2.857554	-0.277850	-0.650033
C	-3.615604	0.920767	-0.826194
H	-2.955691	1.784968	-0.963936
H	-4.196296	0.760579	-1.735577
H	-4.299233	1.096974	0.010734
H	-0.335808	-1.593979	2.190204
H	0.413325	-2.733565	0.994151
C	-1.098594	-2.333709	-1.075448
H	-0.132411	-2.779952	-1.315068
H	-1.815461	-3.131835	-0.835907
H	-1.456733	-1.812426	-1.963911
H	3.174765	0.706592	1.357525

TS3i-a

Total SCF energy: -1110.64733227 a.u.
Enthalpy at 298K: -1110.411642 a.u.
Gibbs free energy at 298K: -1110.472199 a.u.
Free energy in solution: -1110.476183 a.u.
Imaginary frequency: -259.8158 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	-1.821527	-0.001811	-1.978785
C	0.154574	-0.519008	-2.125186
C	1.185633	-0.830921	-1.114129
C	1.949072	0.121527	-0.448948
C	1.751279	1.613561	-0.633031
C	0.245202	1.922715	-0.468093
C	-2.331682	0.419896	-0.886129
Rh	-0.557923	0.008759	0.019672
Cl	-1.176249	-2.375642	0.501421
C	-0.892656	0.413370	1.791280
O	-1.120266	0.634235	2.899242
H	-3.263599	0.781909	-0.482533
H	-2.043397	-0.262519	-2.999053
H	-0.208231	2.156574	-1.437045
H	1.327192	-1.881233	-0.892903
O	2.950762	-0.175820	0.388454
C	3.183753	-1.545501	0.748064
H	3.489689	-2.130319	-0.126449
H	3.993857	-1.519941	1.476768
H	2.283648	-1.979843	1.195906
H	0.366453	0.335148	-2.764959
H	-0.125854	-1.414577	-2.671198
H	2.344579	2.114795	0.138425
H	2.157233	1.934943	-1.603694
C	-0.022414	3.077690	0.489762
H	0.427160	4.010215	0.113421
H	-1.097094	3.256291	0.608434
H	0.399780	2.893895	1.485098

TS3i-b

Total SCF energy: -1110.64860179 a.u.
Enthalpy at 298K: -1110.412982 a.u.
Gibbs free energy at 298K: -1110.474051 a.u.
Free energy in solution: -1110.477398 a.u.
Imaginary frequency: -257.9509 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.762245	-1.397116	-1.614798
C	0.113735	-0.264674	-2.126032
C	-0.717261	0.693701	-1.374819
C	-1.770820	0.314998	-0.546030
C	-2.090406	-1.157942	-0.301449
C	-0.811718	-1.743229	0.342053
C	2.129065	-1.544014	-0.402053
Rh	0.663999	-0.232574	0.132403
Cl	2.115436	1.774576	-0.188703
C	0.887856	-0.112366	1.959213
O	1.037689	-0.040302	3.100009
H	2.872441	-2.039798	0.200660
H	2.005476	-1.621457	-2.638518
H	-0.465715	-2.656612	-0.150243
H	-0.987706	-1.956770	1.399188
H	-0.474541	1.741165	-1.501421
H	-2.246103	-1.612095	-1.290378
O	-2.583606	1.177650	0.067045
C	-2.278676	2.579825	0.028894
H	-2.359000	2.966808	-0.992605
H	-3.024606	3.056454	0.664700
H	-1.271577	2.757547	0.421024
H	-0.400148	-1.152224	-2.487824
C	-3.357737	-1.392327	0.527151
H	-4.245000	-0.960511	0.052176
H	-3.518347	-2.469717	0.640010
H	-3.263079	-0.956094	1.526711
H	0.705178	0.241408	-2.882891

TS4-a

Total SCF energy: -1033.31147174 a.u.
Enthalpy at 298K: -1033.109995 a.u.
Gibbs free energy at 298K: -1033.166033 a.u.
Free energy in solution: -1033.168041 a.u.
Imaginary frequency: -122.1370 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.402643	0.885299	-0.975322
C	1.784738	-0.792693	-0.037156
Rh	-0.653522	-0.056438	-0.247306
C	-0.087582	-1.799696	-1.356256
H	0.735392	1.010446	-1.836254
C	0.660805	-1.704098	-0.157275
H	0.479761	-2.387893	0.666279
H	0.310212	-1.468522	-2.312708
Cl	-1.455423	2.081809	0.400765
C	2.471834	-0.170864	-1.189028
H	2.422010	-0.734557	-2.119607
H	3.489878	0.147044	-0.963064
C	-2.320067	-0.761766	0.205940
O	-3.334543	-1.218129	0.505609
O	2.403809	-0.588650	1.137960
C	1.662684	-0.723670	2.363781
H	1.486608	-1.778055	2.600982
H	2.294066	-0.280604	3.134333
H	0.710583	-0.186785	2.289855
H	-0.824786	-2.592944	-1.436110
C	1.850522	2.146610	-0.279160
H	2.582356	2.677664	-0.906682
H	1.009081	2.808830	-0.072728
H	2.347952	1.913855	0.669768

TS4-b

Total SCF energy: -1033.31349496 a.u.
Enthalpy at 298K: -1033.112123 a.u.
Gibbs free energy at 298K: -1033.168290 a.u.
Free energy in solution: -1033.170728 a.u.
Imaginary frequency: -147.7988 cm-1

Cartesian coordinates

ATOM	X	Y	Z
C	1.277638	0.850780	-0.925281
C	1.655237	-0.557754	0.225646
Rh	-0.774126	-0.042121	-0.280047
C	-0.027445	-1.891257	-1.089089
H	1.401851	1.797515	-0.409400
H	0.707605	0.898382	-1.858313
C	0.608539	-1.577629	0.134149
H	0.408739	-2.160286	1.028299
H	0.417995	-1.655953	-2.052969
Cl	-1.546093	2.171216	0.032993
C	2.473054	-0.081757	-0.919299
H	2.462178	-0.783852	-1.753717
C	-2.446757	-0.738896	0.143170
O	-3.468786	-1.192117	0.422603
O	2.109344	-0.150421	1.428521
C	1.209919	-0.065046	2.546167
H	0.949220	-1.059752	2.922999
H	1.757764	0.479774	3.315985
H	0.304027	0.479754	2.259792
H	-0.705452	-2.739135	-1.109130
C	3.859260	0.489186	-0.663746
H	4.576927	-0.307588	-0.438951
H	4.204809	1.020693	-1.556758
H	3.852476	1.189767	0.174118