Supporting Information

Theoretical Studies on the Mechanism and Stereoselectivity of Rh(Phebox)-catalyzed Asymmetric Reductive Aldol Reaction

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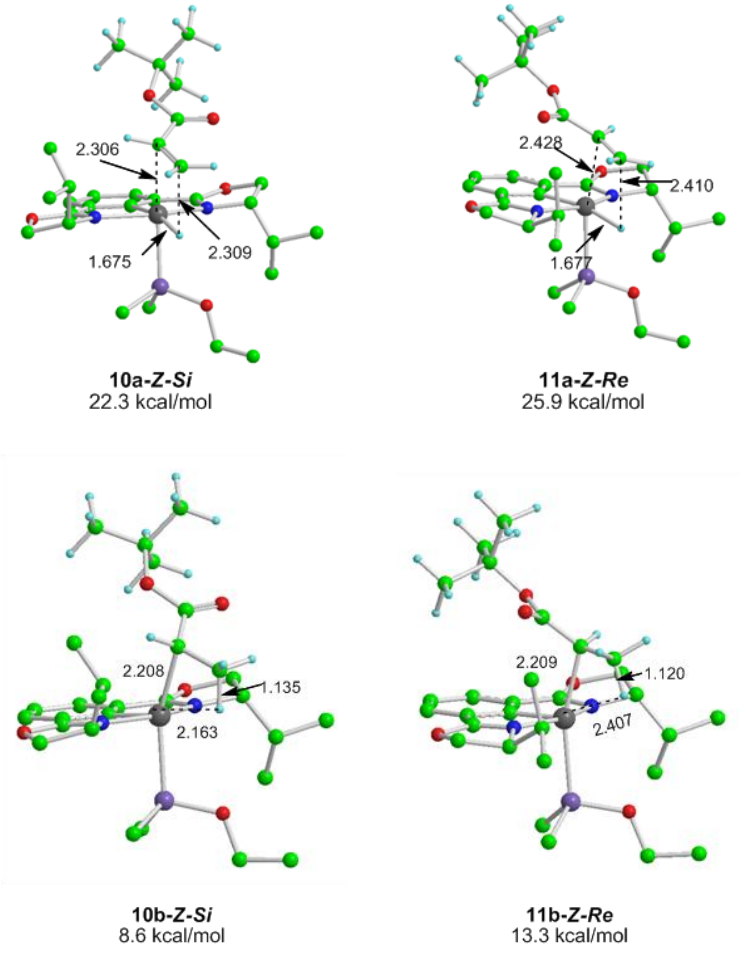


Figure S1. Optimized structures of **10a**, **11a**, **10b** and **11b**, and hydrogen atoms of Rh(Phebox-ip)

are omitted for clarity; Distances are in angstrom(Å).

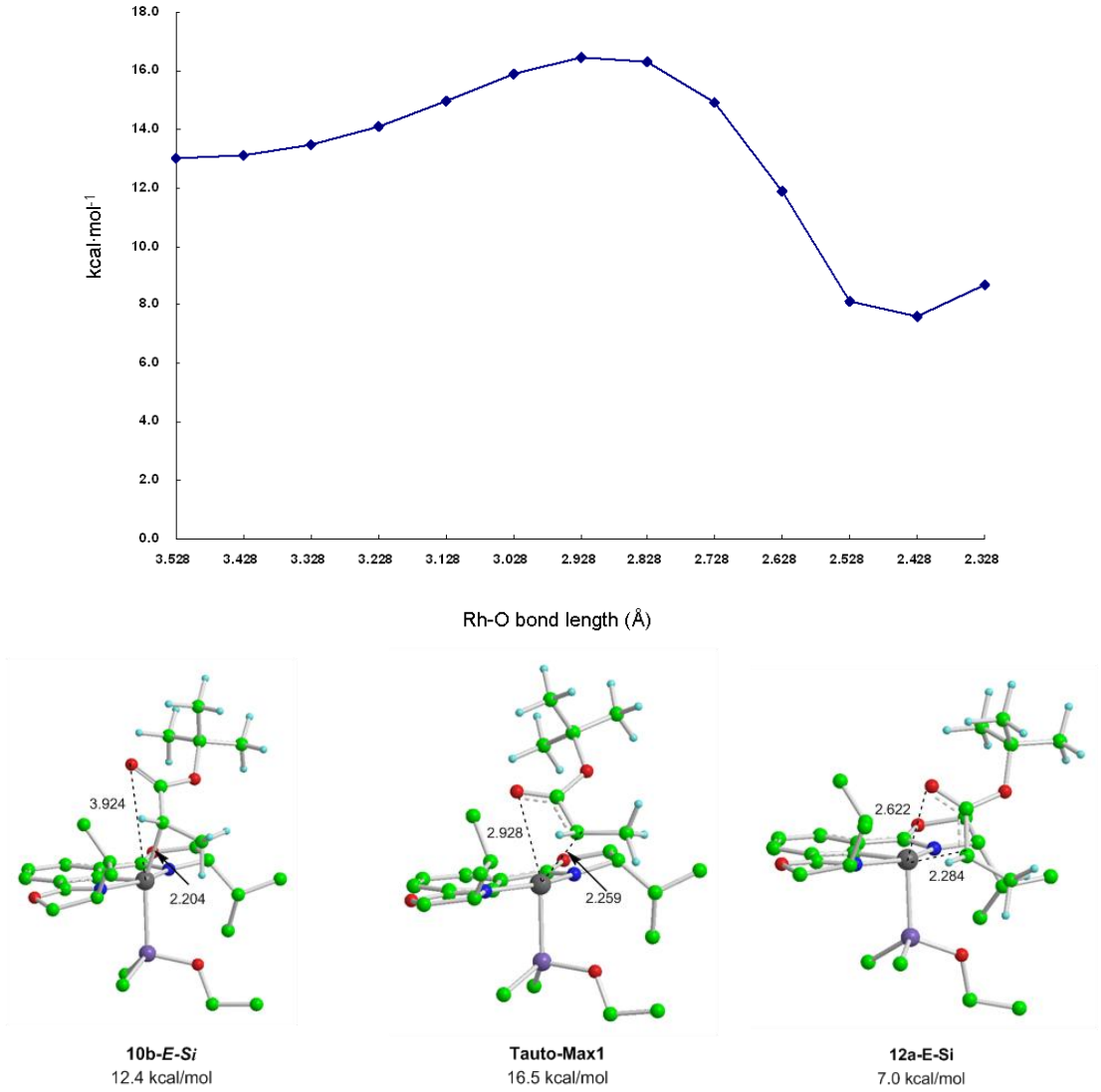
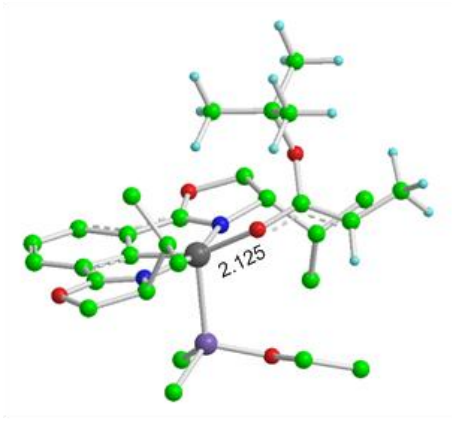
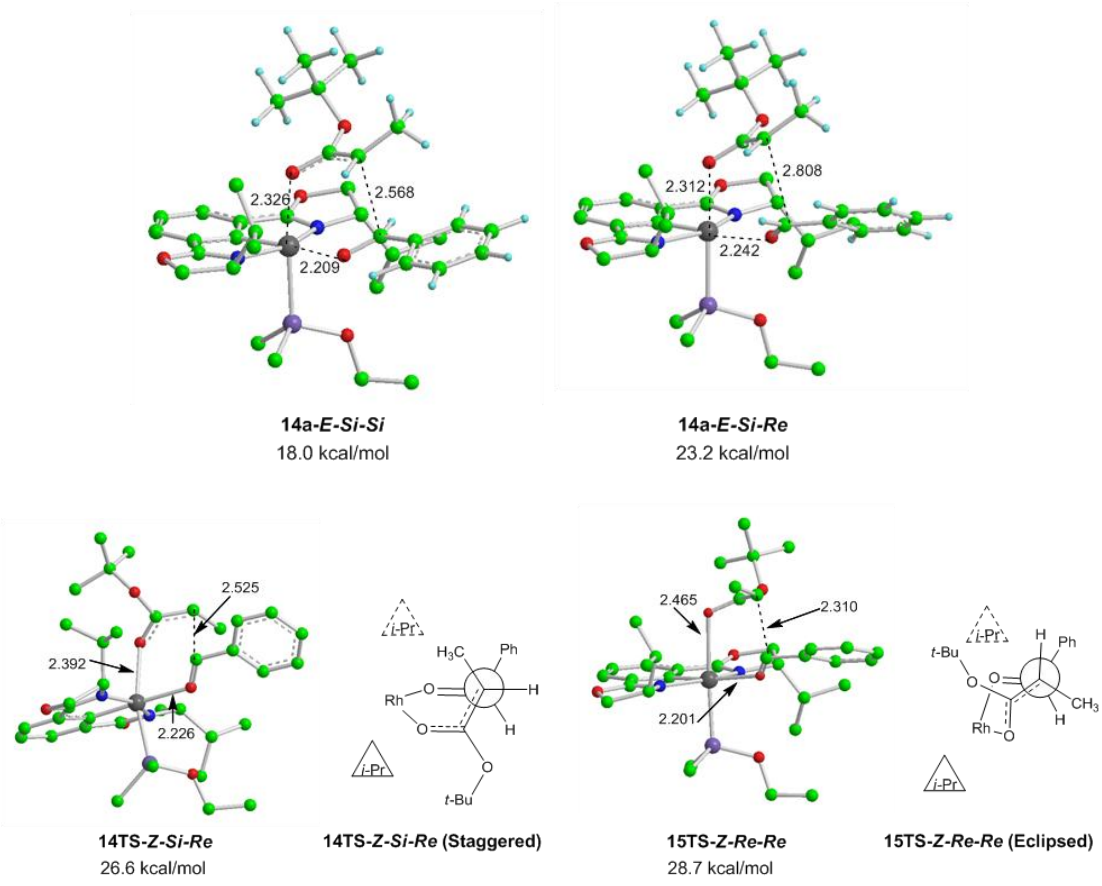


Figure S2. Relative electron energy changes along the Rh-O bond length and structure of **10b-*E*-*Si***, **Tauto-Max1** and **12a-*E*-*Si*** on the surface.



13b-*E*-*Si*
9.7 kcal/mol

Figure S3. Optimized structure of **13b-*E*-*Si*.**



14a-*E*-*Si*-*Si*
18.0 kcal/mol

14a-*E*-*Si*-*Re*
23.2 kcal/mol

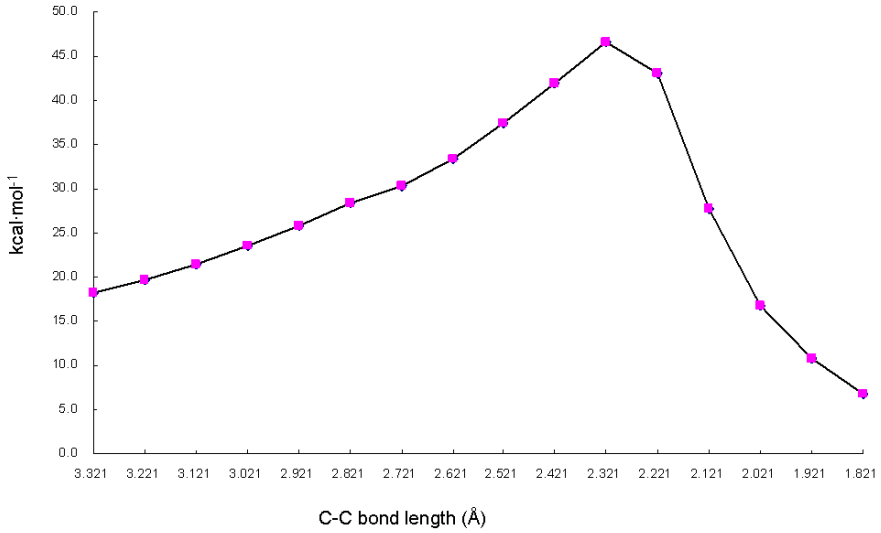
14TS-*Z*-*Si*-*Re*
26.6 kcal/mol

14TS-*Z*-*Si*-*Re* (Staggered)

15TS-*Z*-*Re*-*Re*
28.7 kcal/mol

15TS-*Z*-*Re*-*Re* (Eclipsed)

Figure S4. Optimized structures of **14a**, **14TS-*Z*-*Si*-*Re*** and **15TS-*Z*-*Re*-*Re*** and their corresponding Newman projections. All hydrogen atoms are omitted for clarity and distances are in angstrom (Å).



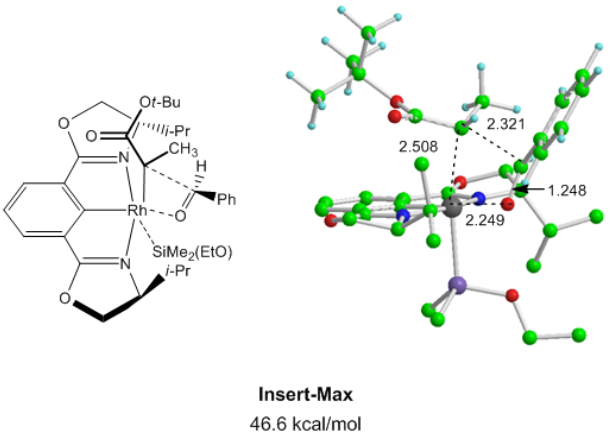


Figure S5. Relative electron energy changes along the $C^{\delta+}$-$C^{\delta-}$ bond length in reaction between Rh bound C-enolate and aldehyde. Structures of **Insert-Max**. and hydrogen atoms of Rh(Phebox-ip) are ignored for clarity; Distances are in angstrom (Å).

P. S. Scanned energy is electronic energy. But all the energies we discussed in our manuscript is Gibbs free energy. In order to facilitate our analysis, we take the electronic energy difference as Gibbs free energy difference as an approximation.

An alternative pathway is the C-enolate species reacting directly with the rhodium-bound aldehyde. Such pathway is relevant in rhodium(I) mediated arylation of aldehydes with arylboronic acids under base and water free conditions.[30] Since this four-membered ring transition state structure has large steric congestion, every time we try to locate it failed. It goes easily to

transform to the six-membered ring transition state (**14TS-*E*-*Si*-*Si***). We failed to locate the expected exact transition states for the aldehyde migration into the Rh-C bond, so we scanned the potential surface along the reaction coordinates (distances between $C^{\delta+}$-$C^{\delta-}$ bond length) and found a maximum point at 2.321 Å. The structure **Insert-Max** is energetically disfavorable relative to the aldol reaction structure.

The Cartesian coordinates and energies for all of the optimized structures and transition states structures

2

Cartesian coordinates

ATOM	X	Y	Z
C	1.769163	0.148426	-0.096657
C	2.065027	1.520577	0.027376
C	3.397699	1.946078	-0.075186
C	4.407747	0.997085	-0.299861
C	4.118489	-0.369018	-0.420769
C	2.784986	-0.798351	-0.316457
H	3.661494	2.997884	0.017389
H	5.438628	1.330133	-0.380215
H	4.927066	-1.076946	-0.592912
C	0.850299	2.288272	0.282059
N	-0.254336	1.603129	0.349414
C	2.235357	-2.143460	-0.388857
N	0.945020	-2.266198	-0.231392
Rh	-0.091390	-0.437916	0.062519
H	-1.524894	-0.139049	2.324921
C	-1.475180	-0.997220	1.659897
C	-2.310865	-1.052125	0.544127
H	-1.102965	-1.917180	2.103220
H	-2.526284	-1.991187	0.044964
C	-3.140041	0.093052	0.160333
O	-3.111734	1.219475	0.646816
O	-3.993828	-0.233308	-0.847552
H	0.857528	3.371501	0.426488
H	2.869006	-3.017931	-0.559092
H	0.608104	-3.226234	-0.291551

SiH4

Cartesian coordinates

ATOM	X	Y	Z
Si	0.000000	0.000000	0.000000
H	0.856235	0.856235	0.856235
H	-0.856235	-0.856235	0.856235
H	-0.856235	0.856235	-0.856235
H	0.856235	-0.856235	-0.856235

Total SCF energy -6.26359563

Gibbs free energy at 298K -6.25186400

PhCHO

Cartesian coordinates

ATOM	X	Y	Z
C	-0.045314	-1.100899	0.000053
C	-0.533981	0.214832	0.000029
C	0.361362	1.292267	0.000002
C	1.735989	1.060440	-0.000028
C	2.216766	-0.251094	-0.000037
C	1.326171	-1.331321	0.000021
H	-0.759126	-1.919168	0.000080
H	-0.024469	2.309833	0.000037
H	2.430388	1.895980	-0.000075
H	3.288177	-0.433654	-0.000076
H	1.707339	-2.348842	0.000042
C	-1.992237	0.468805	0.000055
H	-2.274062	1.545928	0.000245

H	-1.125602	2.099268	0.542768
C	-4.836355	0.828510	-1.305906
H	-5.451959	0.395409	-2.095851
H	-5.465995	1.204887	-0.494351
H	-4.239831	1.656841	-1.700018
Total SCF energy		-834.56859968	
Gibbs free energy at 298K		-834.38008400	

3a

Cartesian coordinates

ATOM	X	Y	Z
C	-1.290957	0.566795	0.155687
C	-1.905339	1.250444	-0.908839
C	-2.752128	2.336481	-0.636321
C	-2.972546	2.714554	0.697521
C	-2.372064	2.029734	1.764610
C	-1.524528	0.943829	1.489893
H	-3.243282	2.887936	-1.436325
H	-3.630036	3.553065	0.908774
H	-2.575028	2.347159	2.786038
C	-1.541644	0.646455	-2.181703
N	-0.754200	-0.392736	-2.138362
C	-0.817122	0.058692	2.400797
N	-0.115742	-0.904551	1.866338
Rh	-0.115792	-0.989698	-0.233979
Si	-1.635417	-2.787187	-0.216865
H	0.726347	-2.433753	-0.576082
H	2.575939	-1.979554	0.343283
C	3.540748	-1.618775	0.700045
C	3.891148	-0.333979	0.579253
H	4.222028	-2.337896	1.147466
H	4.855247	0.040086	0.911710
C	2.997481	0.663189	-0.047882
O	1.856523	0.488326	-0.450793
O	3.613161	1.859807	-0.146386
C	2.843626	2.914584	-0.744360
H	1.918644	3.079763	-0.185762
H	3.481529	3.797966	-0.705330
H	2.594417	2.666752	-1.779839
H	-1.325174	-3.824220	0.812666
H	-3.033455	-2.335107	0.095747
H	-1.737921	-3.493564	-1.528540
H	-0.874599	0.169119	3.486852
H	-1.915484	1.024011	-3.137085

O	-2.847598	-0.396032	-0.000103
Total SCF energy		-345.56649002	
Gibbs free energy at 298K		-345.48672200	
Free energy in solution		-345.56772700	

4a

Cartesian coordinates

ATOM	X	Y	Z
C	0.445922	1.019821	0.006291
C	-0.119841	1.608153	1.152580
C	-0.270205	3.002435	1.201040
C	0.154996	3.778453	0.111162
C	0.737331	3.195716	-1.022816
C	0.889745	1.799936	-1.076203
H	-0.705557	3.492976	2.069548
H	0.039000	4.857506	0.152247
H	1.068061	3.831116	-1.842134
C	-0.449845	0.597516	2.143218
N	-0.144247	-0.633204	1.843241
C	1.495341	0.970989	-2.100116
N	1.542425	-0.313923	-1.868140
Rh	0.709084	-0.945037	-0.035775
Si	2.907366	-0.836133	0.966766
H	1.352019	-2.486047	0.146200
H	-0.995839	-3.218641	0.089481
C	-0.667747	-2.650031	-0.773654
C	-1.312937	-1.455316	-1.088675
H	-0.134879	-3.200707	-1.539100
H	-1.218773	-1.018531	-2.076547
C	-2.439988	-0.959274	-0.273616
O	-2.819177	-1.407210	0.794841
O	-3.052444	0.086566	-0.890126
H	-0.929470	0.836435	3.094251
H	1.916351	1.387273	-3.018152
H	3.979715	-1.379403	0.080782
H	3.013178	-1.567599	2.263025
H	3.315616	0.573733	1.267742
H	2.002548	-0.874274	-2.582234
H	-0.411546	-1.340730	2.522847
C	-4.182540	0.627859	-0.197826
H	-4.566438	1.423403	-0.838005

H	-0.526267	-0.814470	-3.035887
H	0.345632	-1.526338	2.526871

Total SCF energy -840.80762382

Gibbs free energy at 298K -840.59388300

H	-4.946125	-0.139419	-0.040365
H	-3.885422	1.032948	0.773840

Total SCF energy -840.82197468

Gibbs free energy at 298K -840.60467900

5a

Cartesian coordinates

ATOM	X	Y	Z
C	1.660730	0.261044	-0.158192
C	1.967273	1.532837	0.362459
C	3.273829	2.026348	0.229873
C	4.245221	1.240190	-0.410266
C	3.945460	-0.032894	-0.913806
C	2.638777	-0.533819	-0.783281
H	3.548398	3.005799	0.616658
H	5.255684	1.625360	-0.510596
H	4.727905	-0.617595	-1.393744
C	0.793642	2.136174	0.971794
N	-0.286765	1.409137	0.991652
C	2.095083	-1.820807	-1.170642
N	0.838528	-2.040857	-0.887307
Rh	-0.166283	-0.466365	0.095155
Si	0.396986	-1.483976	2.228136
H	-1.446578	-1.294848	0.807404
H	-0.757044	1.564275	-1.735293
C	-0.839629	0.491481	-1.870759
C	-1.941087	-0.189514	-1.360646
H	-0.239650	0.046473	-2.656763
H	-2.206073	-1.174295	-1.727537
C	-3.009513	0.524299	-0.620161
O	-2.937541	1.651554	-0.154686
O	-4.130131	-0.228948	-0.546754
H	0.792061	3.149512	1.378761
H	2.700034	-2.589429	-1.657215
H	0.263721	-2.970996	2.232810
H	-0.411386	-0.978522	3.375195
H	1.824577	-1.214255	2.596832
H	0.484761	-2.962603	-1.133870
H	-1.144310	1.842065	1.328722
C	-5.215407	0.351605	0.187041
H	-6.033429	-0.366399	0.117330
H	-4.932766	0.505375	1.232744
H	-5.508222	1.311711	-0.246694

6a

Cartesian coordinates

ATOM	X	Y	Z
C	0.839163	-0.992632	0.176713
C	1.629916	-0.640795	1.282762
C	2.930618	-1.159046	1.379370
C	3.400776	-2.026920	0.381106
C	2.597086	-2.403529	-0.703931
C	1.294575	-1.886229	-0.805129
H	3.577634	-0.906368	2.217147
H	4.407357	-2.427056	0.458846
H	2.988514	-3.095500	-1.447040
C	0.898865	0.232879	2.189096
N	-0.333098	0.502690	1.871918
C	0.256806	-2.161446	-1.783560
N	-0.893102	-1.573644	-1.606709
Rh	-1.038042	-0.343021	0.098398
Si	-3.517774	-0.459172	0.521998
H	-1.327759	-1.652380	0.927296
H	-2.173528	2.268151	-0.044058
C	-1.880682	1.595026	-0.842670
C	-0.535197	1.514933	-1.204210
H	-2.648657	1.340080	-1.564194
H	-0.246110	1.106687	-2.166405
C	0.491581	2.339177	-0.536031
O	0.348146	3.009604	0.471936
O	1.667074	2.284681	-1.218761
H	1.346428	0.649860	3.093153
H	0.411374	-2.843596	-2.622775
H	-4.291017	-0.680012	-0.749019
H	-4.137883	0.765341	1.129794
H	-3.967129	-1.571371	1.417347
H	-1.618032	-1.798538	-2.284948
H	-0.825500	1.146905	2.485466
C	2.729376	3.073257	-0.672151
H	3.569541	2.950523	-1.357166
H	2.438915	4.125690	-0.606533
H	3.000910	2.720276	0.327127

Total SCF energy	-840.82376602
Gibbs free energy at 298K	-840.60501900

3TS

Cartesian coordinates

ATOM	X	Y	Z
C	1.445500	0.439121	0.060967
C	2.112116	0.548671	1.292548
C	3.193282	1.437321	1.409823
C	3.581918	2.194272	0.294891
C	2.915575	2.086944	-0.935364
C	1.834841	1.199157	-1.055252
H	3.732840	1.549363	2.348388
H	4.419373	2.879769	0.385624
H	3.244871	2.692609	-1.777590
C	1.524479	-0.340785	2.279662
N	0.520441	-1.076813	1.888653
C	0.995260	0.899521	-2.203861
N	0.062958	0.004713	-2.031455
Rh	-0.087405	-0.786740	-0.103621
Si	1.160576	-2.685446	-0.762968
H	-1.375841	-1.980267	-0.324973
H	-2.230554	-1.597172	1.447686
C	-2.868174	-1.693250	0.577857
C	-3.561979	-0.595106	0.115904
H	-3.265473	-2.692036	0.417297
H	-4.461274	-0.689427	-0.482772
C	-2.953498	0.696570	0.237951
O	-1.733923	0.900144	0.405296
O	-3.806243	1.740030	0.092930
C	-3.214247	3.042530	0.087180
H	-2.459043	3.127431	-0.700178
H	-4.036356	3.736262	-0.097129
H	-2.742738	3.262350	1.049527
H	0.790681	-3.168638	-2.126759
H	2.639578	-2.448979	-0.804658
H	0.963679	-3.831738	0.174855
H	1.135031	1.382258	-3.173904
H	1.903079	-0.410900	3.301946
H	0.142367	-1.707685	2.592885
H	-0.507959	-0.210126	-2.845774

Total SCF energy	-840.79106825
Gibbs free energy at 298K	-840.57566900
Imaginary frequency	-584.488

Total SCF energy	-840.82094354
Gibbs free energy at 298K	-840.60274000

4TS

Cartesian coordinates

ATOM	X	Y	Z
C	0.856616	0.852810	-0.013634
C	0.530624	1.654188	1.098228
C	0.944136	2.994280	1.119043
C	1.680330	3.505604	0.038542
C	2.019662	2.706290	-1.061205
C	1.607332	1.363453	-1.089757
H	0.706094	3.643530	1.959376
H	2.000265	4.543206	0.059164
H	2.600982	3.133513	-1.875964
C	-0.220453	0.893920	2.080264
N	-0.422288	-0.364653	1.807701
C	1.860836	0.337504	-2.079129
N	1.380090	-0.851829	-1.827216
Rh	0.317550	-1.041535	-0.021591
Si	2.350205	-1.785313	1.073081
H	0.219650	-2.714536	0.182122
H	-2.000243	-2.772473	0.091216
C	-1.466988	-2.332385	-0.744344
C	-1.735512	-0.993800	-1.079557
H	-1.142156	-3.022193	-1.514885
H	-1.527725	-0.621616	-2.076276
C	-2.696849	-0.210903	-0.283340
O	-3.194316	-0.536186	0.782935
O	-3.004439	0.958204	-0.907383
H	-0.610003	1.335213	2.999555
H	2.440941	0.524323	-2.985356
H	3.146191	-2.740368	0.244388
H	2.111652	-2.461870	2.382182
H	3.276369	-0.647337	1.371161
H	1.596668	-1.569264	-2.515702
H	-0.996254	-0.883716	2.467352
C	-3.965453	1.776568	-0.232716
H	-4.096884	2.656917	-0.863590
H	-4.914795	1.245389	-0.115749
H	-3.603624	2.068777	0.757283

Total SCF energy	-840.82162374
Gibbs free energy at 298K	-840.60443500
Imaginary frequency	-220.857

5TS

Cartesian coordinates

ATOM	X	Y	Z
C	1.765252	0.230276	-0.167179
C	2.075565	1.569730	0.160041
C	3.404532	2.004162	0.055976
C	4.397489	1.104475	-0.362926
C	4.093744	-0.226508	-0.677591
C	2.766482	-0.675551	-0.578954
H	3.678006	3.029870	0.295525
H	5.425079	1.447241	-0.440212
H	4.889523	-0.898767	-0.992475
C	0.884327	2.293901	0.552589
N	-0.219668	1.600463	0.581874
C	2.215518	-1.989046	-0.815572
N	0.928293	-2.123456	-0.619506
Rh	-0.068722	-0.389867	0.019944
Si	0.189447	-1.122086	2.342367
H	-1.609114	-1.033375	0.447859
H	-1.069940	1.116416	-2.066691
C	-1.086822	0.041961	-1.921613
C	-2.111185	-0.525110	-1.115699
H	-0.639840	-0.563500	-2.702604
H	-2.457352	-1.530816	-1.331978
C	-3.167484	0.370662	-0.545483
O	-3.042349	1.555850	-0.295063
O	-4.312922	-0.310542	-0.341959
H	0.886863	3.356852	0.800653
H	2.827798	-2.840240	-1.119583
H	-0.153319	-2.560298	2.572634
H	-0.635357	-0.349221	3.321024
H	1.603809	-0.981498	2.814436
H	0.559736	-3.062419	-0.753106
H	-1.089846	2.088872	0.784739
C	-5.389246	0.446041	0.234582
H	-6.223103	-0.251242	0.319181
H	-5.104759	0.825327	1.219844
H	-5.655215	1.288548	-0.409306

Total SCF energy -840.81603866

Gibbs free energy at 298K -840.59876900

Imaginary frequency -674.480

6TS

Cartesian coordinates

ATOM	X	Y	Z
C	1.544995	-0.220100	0.137432
C	1.980474	0.685234	1.129296
C	3.325382	1.078630	1.138730
C	4.207458	0.564920	0.175339
C	3.773264	-0.335452	-0.805478
C	2.428220	-0.738373	-0.833177
H	3.693610	1.780624	1.884002
H	5.248412	0.873448	0.190647
H	4.481978	-0.716509	-1.537818
C	0.883635	1.092651	1.982498
N	-0.266199	0.537093	1.731641
C	1.754756	-1.653123	-1.724586
N	0.482022	-1.841055	-1.501013
Rh	-0.290492	-0.793778	0.137347
Si	-2.405423	-2.349753	0.747629
H	0.291187	-1.956170	1.098752
H	-3.373991	-0.119308	0.070086
C	-2.612200	-0.559587	-0.573875
C	-1.649059	0.437803	-1.064592
H	-3.054534	-1.166452	-1.365182
H	-1.342080	0.378666	-2.104137
C	-1.762739	1.794088	-0.531554
O	-2.353713	2.131800	0.489788
O	-1.110628	2.700390	-1.317179
H	0.990816	1.837037	2.772912
H	2.269996	-2.177076	-2.531386
H	-1.833776	-3.619416	0.217630
H	-3.877339	-2.516888	0.562789
H	-2.233493	-2.286347	2.223821
H	0.018077	-2.508761	-2.113084
H	-1.071008	0.883069	2.249479
C	-1.164840	4.053756	-0.861416
H	-0.602650	4.634676	-1.594836
H	-2.198483	4.409032	-0.807302
H	-0.710742	4.154477	0.129224

Total SCF energy -840.80580866

Gibbs free energy at 298K -840.58557200

Imaginary frequency -161.452

3b

4b

Cartesian coordinates

ATOM	X	Y	Z
C	1.636695	-0.159808	0.147844
C	2.578004	-0.476836	-0.856422
C	3.840633	-0.953336	-0.468524
C	4.127304	-1.130836	0.891427
C	3.166481	-0.878017	1.883069
C	1.901127	-0.398893	1.516670
H	4.593817	-1.200646	-1.213609
H	5.106495	-1.497451	1.183779
H	3.406915	-1.072053	2.926079
C	2.016491	-0.313089	-2.181760
N	0.759748	0.038792	-2.242693
C	0.711390	-0.199773	2.326032
N	-0.366402	0.139344	1.678142
Rh	-0.157430	0.280285	-0.369481
Si	0.770876	2.477469	-0.199466
H	-2.722206	2.117630	-0.140901
H	-3.112383	2.396156	1.563987
C	-3.447596	1.887703	0.645864
C	-3.609276	0.404336	0.820273
H	-4.398493	2.365184	0.364847
H	-4.384895	0.044655	1.490813
C	-2.957566	-0.539383	0.088864
O	-2.066364	-0.343733	-0.858381
O	-3.251537	-1.859805	0.387779
C	-3.057208	-2.801137	-0.658894
H	-2.015011	-2.840325	-0.991347
H	-3.346258	-3.770156	-0.243371
H	-3.693487	-2.576494	-1.526012
H	-0.317366	3.402553	-0.628489
H	1.171151	2.845547	1.186877
H	1.943542	2.709794	-1.088708
H	0.696111	-0.368000	3.403801
H	2.598472	-0.490625	-3.087672
H	0.366490	0.147067	-3.175265
H	-1.249881	0.225519	2.184375

Total SCF energy -840.83349967

Gibbs free energy at 298K -840.61398400

Cartesian coordinates

ATOM	X	Y	Z
C	-1.245272	0.519389	0.035761
C	-1.211705	1.505877	-0.980772
C	-2.120470	2.569466	-0.907959
C	-3.025980	2.644136	0.161820
C	-3.033325	1.683950	1.180942
C	-2.131454	0.608688	1.136632
H	-2.123649	3.345599	-1.670166
H	-3.727394	3.471632	0.206334
H	-3.735258	1.780139	2.006435
C	-0.142954	1.257848	-1.919556
N	0.564633	0.184999	-1.695689
C	-1.928238	-0.466105	2.072512
N	-0.973469	-1.310939	1.773147
Rh	0.017878	-0.894747	-0.017386
Si	-1.733697	-2.099979	-1.266047
H	3.056562	-2.149728	-0.309790
C	2.234267	-2.115148	0.410342
C	1.985196	-0.697894	0.895494
H	2.421116	-2.811635	1.233935
H	1.891127	-0.566884	1.970483
C	2.790385	0.343507	0.254444
O	3.347750	0.268746	-0.837744
O	2.850565	1.477994	1.011720
H	0.095119	1.932144	-2.742567
H	-2.527888	-0.585713	2.975325
H	-3.013938	-2.271788	-0.511989
H	-1.264137	-3.485726	-1.590078
H	-2.097535	-1.475115	-2.574133
H	-0.843172	-2.079861	2.426534
H	1.397347	0.044092	-2.264395
H	1.360871	-2.573228	-0.145519
C	3.586847	2.559073	0.436228
H	3.528498	3.374089	1.159942
H	4.630399	2.276941	0.265727
H	3.150731	2.869299	-0.518401

Total SCF energy -840.85361734

Gibbs free energy at 298K -840.63242300

5b

Cartesian coordinates

ATOM	X	Y	Z
C	1.758728	0.286907	-0.219277

6b

Cartesian coordinates

ATOM	X	Y	Z
C	1.183941	-0.727000	0.279026

C	1.942677	1.668919	0.046205
C	3.192637	2.235066	-0.234903
C	4.216703	1.442852	-0.777555
C	4.018196	0.086325	-1.063349
C	2.776880	-0.512168	-0.795615
H	3.374463	3.290486	-0.043337
H	5.181028	1.894772	-0.989220
H	4.827623	-0.496581	-1.497821
C	0.732641	2.279103	0.543668
N	-0.286616	1.473770	0.664778
C	2.329527	-1.859356	-1.028537
N	1.085713	-2.111058	-0.702171
Rh	0.063764	-0.477478	0.111706
Si	0.915020	-1.060325	2.382449
H	-2.039206	-1.277726	0.405098
H	-1.523304	0.715298	-1.782891
C	-1.333560	-0.311184	-1.468194
C	-2.446537	-0.890617	-0.571752
H	-1.120966	-0.944883	-2.330408
H	-2.941493	-1.754789	-1.023492
C	-3.470551	0.154594	-0.184605
O	-3.237648	1.167309	0.450579
O	-4.697352	-0.152080	-0.648417
H	0.655703	3.337988	0.792089
H	2.976493	-2.634479	-1.440432
H	-0.120472	-1.820904	3.161238
H	1.264687	0.111807	3.246820
H	2.126352	-1.943479	2.392979
H	0.781044	-3.071034	-0.846193
H	-1.187863	1.849067	0.956059
C	-5.729673	0.805551	-0.356578
H	-6.638429	0.398243	-0.800300
H	-5.847659	0.924359	0.723656
H	-5.487349	1.776122	-0.797511

Total SCF energy -840.83849839

Gibbs free energy at 298K -840.61842000

C	1.787249	-0.042069	1.353342
C	3.181099	0.114346	1.348647
C	3.936300	-0.403731	0.286343
C	3.327391	-1.070409	-0.785242
C	1.934025	-1.235127	-0.800456
H	3.681760	0.636650	2.161021
H	5.015106	-0.280566	0.291968
H	3.939173	-1.452332	-1.599712
C	0.804693	0.415750	2.312372
N	-0.431674	0.102463	2.051788
C	1.083761	-1.854674	-1.791561
N	-0.194530	-1.840971	-1.535309
Rh	-0.713368	-0.908686	0.256824
Si	-3.687057	-0.362929	-0.054237
H	-0.491997	-2.328301	1.026303
H	-2.634672	1.710897	0.830540
C	-2.761000	1.291574	-0.173780
C	-1.384102	0.993955	-0.775616
H	-3.334472	2.035560	-0.748328
H	-1.428865	0.744428	-1.837194
C	-0.367625	2.018896	-0.519194
O	-0.296742	2.757325	0.456605
O	0.583921	2.054956	-1.509975
H	1.069786	0.988789	3.200738
H	1.475072	-2.312681	-2.701139
H	-4.199151	-0.839052	-1.364983
H	-4.786612	-0.429189	0.944397
H	-2.682839	-1.420421	0.394575
H	-0.792097	-2.284830	-2.228695
H	-1.122912	0.445476	2.713857
C	1.656567	2.970780	-1.288940
H	2.277627	2.921984	-2.185987
H	1.282493	3.988514	-1.141809
H	2.245149	2.684509	-0.411355

Total SCF energy -840.82368771

Gibbs free energy at 298K -840.60289500

7a

Cartesian coordinates

ATOM	X	Y	Z
C	2.534465	-0.470222	-0.899909
C	1.621210	0.216283	-0.077090
C	2.032501	1.293873	0.731762
C	3.381083	1.685184	0.717712

7TS

Cartesian coordinates

ATOM	X	Y	Z
C	3.477751	-0.626237	-1.123914
C	2.732309	-0.202041	-0.005801
C	3.319879	0.544946	1.034326
C	4.690943	0.840839	0.965744

C	4.288051	0.998560	-0.101486
C	3.879726	-0.072205	-0.911063
H	3.732258	2.512120	1.331787
H	5.330488	1.302532	-0.110217
H	4.610431	-0.579565	-1.537900
C	1.870480	-1.528709	-1.639547
N	0.596805	-1.686748	-1.411758
Rh	-0.251443	-0.327031	-0.060681
C	0.915714	1.832903	1.483187
N	-0.239845	1.251664	1.305850
C	-2.501230	-0.940720	-0.284812
H	-2.330172	-1.717960	-1.028078
C	-2.453654	0.373491	-0.843561
C	-3.491173	-1.291407	0.804126
H	-4.521496	-1.365565	0.423862
H	-3.241480	-2.256347	1.259249
H	-3.496130	-0.541124	1.601396
O	-1.619792	0.723378	-1.726475
O	-3.254650	1.310750	-0.252774
C	-3.078561	2.654973	-0.710724
Si	0.010819	-1.879769	1.717871
H	1.399593	-1.942676	2.267972
H	-0.877988	-1.547975	2.871123
H	-0.329727	-3.271098	1.293157
H	-3.289425	2.737238	-1.780822
H	-3.793035	3.252644	-0.140769
H	-2.058207	3.006903	-0.529764
H	2.397461	-2.167326	-2.351601
H	0.136380	-2.425180	-1.940403
H	1.020298	2.673238	2.172540
H	-1.020632	1.623860	1.842674
Total SCF energy		-840.84822414	
Gibbs free energy at 298K		-840.62739600	

C	5.437859	0.400987	-0.135418
C	4.845019	-0.320810	-1.182495
H	5.178844	1.411199	1.753387
H	6.497708	0.631825	-0.184094
H	5.450419	-0.630633	-2.031672
C	2.633378	-1.312103	-2.086091
N	1.380361	-1.444157	-1.760031
Rh	0.844969	-0.541580	0.031627
C	2.335895	0.913765	2.033773
N	1.111582	0.522109	1.814822
C	-2.124209	1.727170	-1.152262
H	-2.264680	0.971359	-1.917623
C	-0.796098	1.948892	-0.798373
C	-3.229350	2.719993	-0.929160
H	-3.479358	3.260190	-1.855744
H	-4.157104	2.233466	-0.597527
H	-2.945927	3.464477	-0.180545
O	0.202762	1.269525	-1.194921
O	-0.592626	2.959189	0.134063
C	0.678962	3.598882	0.091541
Si	1.309836	-2.611252	1.158217
H	-5.762222	-2.551066	-1.365379
C	-5.427973	-1.768823	-0.688722
C	-6.361543	-1.070886	0.086741
C	-4.072766	-1.469532	-0.592009
C	-5.930683	-0.070681	0.960951
H	-7.419142	-1.309390	0.011305
C	-3.631278	-0.459625	0.279748
H	-3.335449	-2.009428	-1.177436
C	-4.572616	0.233893	1.056597
H	-6.651079	0.469987	1.569034
H	-4.233937	1.007977	1.741401
C	-2.191692	-0.164767	0.420079
H	-1.930753	0.563454	1.201316
O	-1.316752	-0.935387	-0.049436
H	0.693514	4.296198	0.933519
H	1.502734	2.887785	0.177796
H	0.799010	4.162830	-0.843338
H	2.407853	-3.391790	0.512916
H	1.710098	-2.429778	2.586354
H	0.099198	-3.481947	1.147267
H	3.013471	-1.690990	-3.036292
H	2.592309	1.492002	2.923191
H	0.770988	-1.895168	-2.438719

H	0.428789	0.790640	2.519912
Total SCF energy		-1186.41612278	
Gibbs free energy at 298K		-1186.09461300	
Imaginary frequency		-74.110	

7b

Cartesian coordinates

ATOM	X	Y	Z
C	3.559759	-0.707271	-1.026037
C	2.760355	-0.297041	0.060522
C	3.324184	0.338614	1.184265
C	4.712787	0.543588	1.230538
C	5.506376	0.121389	0.154861
C	4.945055	-0.495804	-0.974240
H	5.181439	1.025557	2.086482
H	6.579953	0.280233	0.193094
H	5.591015	-0.798567	-1.796118
C	2.742538	-1.287713	-2.079267
N	1.459696	-1.336935	-1.854614
Rh	0.840097	-0.500480	-0.060011
C	2.301187	0.677846	2.155346
N	1.067775	0.388835	1.836517
C	-2.076593	1.502878	-0.897000
H	-2.062235	1.053218	-1.895687
C	-0.745854	2.188273	-0.720777
C	-3.272028	2.454496	-0.762294
H	-3.158896	3.327539	-1.413696
H	-4.193485	1.936580	-1.037748
H	-3.384797	2.822072	0.262870
O	0.351833	1.710731	-1.001052
O	-0.840280	3.411714	-0.160203
C	0.397601	4.102501	0.067986
Si	0.838863	-2.640520	0.949552
H	-5.601925	-2.438448	-1.546580
C	-5.265101	-1.753941	-0.771430
C	-6.122521	-1.414085	0.279579
C	-3.974810	-1.227510	-0.824278
C	-5.675959	-0.547712	1.278300
H	-7.126312	-1.829274	0.323654
C	-3.521591	-0.345582	0.165686
H	-3.289718	-1.510694	-1.617162
C	-4.383748	-0.019212	1.218286
H	-6.329643	-0.287340	2.107461
H	-4.038546	0.650682	2.003844

8TS

Cartesian coordinates

ATOM	X	Y	Z
C	3.675494	-1.145429	-0.786912
C	2.891137	-0.361047	0.086471
C	3.470537	0.286600	1.197560
C	4.848119	0.151282	1.432546
C	5.622389	-0.624715	0.559167
C	5.050941	-1.273920	-0.546142
H	5.322317	0.637939	2.282617
H	6.687675	-0.728022	0.742716
H	5.681379	-1.870666	-1.202439
C	2.856922	-1.720447	-1.839550
N	1.581509	-1.450186	-1.793680
Rh	0.996421	-0.211867	-0.230932
C	2.465938	1.009474	1.951380
N	1.239288	0.945724	1.504848
C	-2.269554	1.504773	-0.866209
H	-2.439580	1.088026	-1.863657
C	-0.959830	2.263989	-0.968353
C	-3.430098	2.439360	-0.483593
H	-3.468390	3.308154	-1.150493
H	-4.383703	1.911222	-0.559864
H	-3.322691	2.810416	0.540482
O	-0.158048	2.180081	-1.878583
O	-0.764876	3.094619	0.092033
C	0.397532	3.934092	0.007542
Si	-0.082142	-1.997301	0.940912
H	-5.382262	-2.703180	-1.459744
C	-5.071910	-2.023968	-0.669385
C	-5.889471	-1.833442	0.448319
C	-3.854446	-1.351347	-0.772491
C	-5.476910	-0.969233	1.463468
H	-6.836415	-2.360910	0.529964
C	-3.435033	-0.474494	0.237270
H	-3.203946	-1.514892	-1.626278
C	-4.256889	-0.297048	1.356105
H	-6.099593	-0.822510	2.342561
H	-3.936384	0.368746	2.154858

C	-2.102119	0.219749	0.084201
H	-1.856156	0.620000	1.094980
O	-1.224172	-0.724800	-0.360999
H	0.117869	5.061531	0.505608
H	1.034556	3.537207	0.753052
H	0.934334	4.251272	-0.872731
H	0.249403	-3.640001	0.017143
H	2.192506	-3.142466	1.333347
H	0.019195	-2.616898	2.193708
H	3.165432	-1.662969	-3.013354
H	2.538706	1.135919	3.118180
H	0.873234	-1.741015	-2.582087
H	0.367177	0.589492	2.547765

Total SCF energy -1186.43756544

Gibbs free energy at 298K -1186.11150200

C	-2.109480	0.269961	0.098698
H	-1.845793	0.671682	1.094959
O	-1.121571	-0.578820	-0.408112
H	0.346787	4.592187	0.876723
H	1.311116	3.335214	0.030777
H	0.379993	4.519335	-0.915584
H	-0.590300	-3.101262	0.088446
H	1.066278	-2.609840	1.710186
H	-1.047627	-1.610474	2.006211
H	3.271715	-2.349506	-2.629877
H	2.706664	1.578851	2.851939
H	1.004883	-1.855620	-2.528344
H	0.546983	1.458918	2.046796

Total SCF energy -1186.43017693

Gibbs free energy at 298K -1186.10297700

Imaginary frequency -88.810

8

Cartesian coordinates

ATOM	X	Y	Z
C	-3.907127	0.418509	0.355665
C	-2.990404	-0.594649	-0.032532
C	-3.463112	-1.810541	-0.589902
C	-4.842108	-2.002059	-0.766591
C	-5.736511	-0.991605	-0.386506
C	-5.282705	0.211811	0.173400
H	-5.225797	-2.927879	-1.192170
H	-6.803212	-1.145065	-0.524951
H	-6.003268	0.974848	0.463284
C	-3.205308	1.557052	0.903101
N	-1.897957	1.458123	0.946428
Rh	-1.131037	-0.326635	0.227453
C	-2.362096	-2.699240	-0.876349
N	-1.162807	-2.248677	-0.591689
C	2.537993	1.813660	-0.326425
H	3.050388	2.035638	0.615058
C	1.280850	2.679621	-0.308512
C	3.462261	2.141848	-1.511137
H	3.706435	3.209120	-1.526269
H	4.397395	1.580025	-1.437018
H	2.984065	1.894194	-2.463135
O	0.805594	3.185194	0.690048
O	0.755583	2.810406	-1.539057
C	-0.468019	3.562042	-1.638061

9TS

Cartesian coordinates

ATOM	X	Y	Z
C	2.981151	0.774349	-0.855379
C	2.451960	-0.152134	0.061966
C	3.196536	-0.612186	1.162587
C	4.507231	-0.139593	1.343146
C	5.038451	0.776076	0.425445
C	4.289848	1.240958	-0.667934
H	5.112942	-0.472900	2.183101
H	6.052414	1.138467	0.564792
H	4.732113	1.960827	-1.353318
C	1.988548	1.137866	-1.858082
N	0.838438	0.537603	-1.777862
Rh	0.638256	-0.771600	-0.185193
C	2.419967	-1.541957	1.964043
N	1.211224	-1.805408	1.550070
C	-1.349065	1.129631	1.171983
H	-2.424075	1.254585	1.252337
C	-0.877721	2.096978	0.187079
O	-1.431926	2.391746	-0.868189
O	0.307628	2.716927	0.551511
C	0.667783	3.842211	-0.244997
Si	1.512431	-2.544969	-1.506391
C	-0.678226	1.054134	2.533112
H	-0.911226	1.927770	3.161657
H	0.411333	0.993203	2.462896

Si	1.460736	-0.019108	2.401139	H	-1.026562	0.169633	3.085926
H	6.264416	-1.348715	1.144655	C	-5.780930	-0.308566	1.038702
C	5.377539	-1.501034	0.535554	C	-4.429727	-0.581528	1.251043
C	5.229254	-2.675465	-0.204183	C	-3.521105	-0.550438	0.183855
C	4.390847	-0.513970	0.493268	C	-3.984248	-0.242887	-1.102636
C	4.089474	-2.856970	-0.990256	C	-5.333280	0.032139	-1.313994
H	5.998906	-3.441742	-0.172150	C	-6.235310	0.000297	-0.245753
C	3.238164	-0.686890	-0.287412	H	-6.478602	-0.341154	1.871623
H	4.529809	0.396209	1.069410	H	-4.074480	-0.827024	2.250206
C	3.105667	-1.869094	-1.030112	H	-3.272017	-0.222708	-1.919897
H	3.968809	-3.764779	-1.575275	H	-5.684889	0.274601	-2.313552
H	2.220719	-2.008968	-1.646887	H	-7.287620	0.214228	-0.414227
C	2.103419	0.324500	-0.330252	C	-2.084365	-0.884046	0.407271
H	1.530137	0.154219	-1.246392	H	-1.859698	-1.237501	1.427296
O	1.139056	0.082095	0.719705	O	-1.410491	-1.345564	-0.576909
H	-0.654835	3.671360	-2.706615	H	0.095537	0.853447	-2.399425
H	-1.280773	3.008463	-1.163294	H	2.174801	1.897249	-2.619117
H	-0.353231	4.539715	-1.163123	H	0.679615	-2.460005	2.120332
H	0.268258	0.503989	3.092283	H	2.816921	-2.005913	2.868923
H	1.728179	-1.420570	2.803840	H	0.376389	-3.421535	-1.893423
H	2.644970	0.807282	2.747552	H	2.181761	-2.048648	-2.741145
H	-3.719811	2.452939	1.258894	H	2.511628	-3.362299	-0.760424
H	-2.508036	-3.697272	-1.296626	H	1.630993	4.186061	0.138628
H	-1.406057	2.273507	1.311974	H	0.750794	3.583525	-1.304453
H	-0.416123	-2.913247	-0.789675	H	-0.077915	4.639600	-0.151059
Total SCF energy		-1186.44655234		Total SCF energy		-1186.38149498	
Gibbs free energy at 298K		-1186.12077100		Gibbs free energy at 298K		-1186.06005300	
				Imaginary frequency		-241.230	

Rh-acrylate

Cartesian coordinates

ATOM	X	Y	Z
C	-3.083111	-1.308593	-0.275870
C	-1.707967	-1.584819	-0.298185
C	-1.261982	-2.817725	-0.789276
C	-2.171339	-3.777730	-1.249904
C	-3.543319	-3.489066	-1.200893
C	-4.012441	-2.259748	-0.717888
H	-1.826083	-4.731172	-1.641232
H	-4.255945	-4.230724	-1.549901
H	-5.079015	-2.051508	-0.694093
C	-3.306035	0.034816	0.235666
O	-4.527820	0.582923	0.362573

C	-2.794692	2.114142	0.930395
C	-4.325344	1.871778	1.006080
H	-4.925943	2.607593	0.468466
N	-2.287398	0.774934	0.579038
H	-2.405061	2.396715	1.915455
H	-4.691433	1.788454	2.034163
Rh	-0.413399	-0.225977	0.342536
C	0.193300	-2.864393	-0.745859
O	0.894697	-3.890628	-1.256240
C	2.305103	-2.232650	-0.286721
C	2.291373	-3.485800	-1.200643
H	2.862799	-4.331523	-0.814538
N	0.867408	-1.879848	-0.219723
H	2.839928	-1.404383	-0.757669
H	2.611466	-3.271927	-2.225478
C	-2.344070	3.192173	-0.088027
H	-1.247756	3.146174	-0.100753
C	-2.754096	4.592851	0.392162
H	-3.845126	4.714718	0.412304
H	-2.374924	4.800610	1.400356
H	-2.355294	5.361587	-0.278727
C	-2.829471	2.915767	-1.518031
H	-2.489141	1.936756	-1.870166
H	-3.923691	2.948955	-1.598251
H	-2.431738	3.672809	-2.203227
C	2.937445	-2.460182	1.107943
H	2.836276	-1.503346	1.626649
C	4.443708	-2.732804	0.971154
H	4.910026	-2.802537	1.960406
H	4.650554	-3.677170	0.449736
H	4.941826	-1.923820	0.424604
C	2.230334	-3.547146	1.928486
H	1.170343	-3.311436	2.070713
H	2.298232	-4.535043	1.453842
H	2.690435	-3.633784	2.919713
C	0.883237	1.456504	1.299374
H	0.272173	2.352097	1.295165
C	2.158670	1.568569	0.583307
O	3.076210	0.755694	0.601139
O	2.191556	2.737427	-0.115274
C	3.351505	3.130779	-0.918130
C	2.915906	4.479455	-1.501346
H	3.712891	4.899383	-2.124631
H	2.018872	4.360845	-2.118301

H	2.690298	5.190850	-0.700029
C	3.596178	2.116139	-2.042157
H	4.369992	2.494787	-2.720344
H	3.920414	1.156168	-1.638332
H	2.678918	1.965007	-2.622185
C	4.583147	3.305960	-0.020181
H	5.415497	3.711009	-0.607616
H	4.364797	4.010394	0.790354
H	4.889188	2.353490	0.415120
C	0.582641	0.407247	2.170301
H	-0.201121	0.535069	2.913165
H	1.341004	-0.328209	2.417842

Total SCF energy	-1493.68656682
Gibbs free energy at 298K	-1493.18355300
Free energy in solution	-1493.67166100

10a-*Z*-*Si*

Cartesian coordinates

ATOM	X	Y	Z
C	-1.136598	1.197099	2.029986
C	-0.506681	0.139278	1.360880
C	-0.442740	-1.126930	1.957684
C	-1.023881	-1.348932	3.212169
C	-1.650218	-0.278182	3.869814
C	-1.709963	0.998323	3.294129
H	-0.991168	-2.330689	3.677888
H	-2.094983	-0.442098	4.846946
H	-2.193303	1.814894	3.824492
C	-1.043799	2.407453	1.231470
O	-1.500273	3.601975	1.648934
C	-0.558596	3.730035	-0.531874
C	-1.013791	4.576817	0.683155
H	-1.828750	5.270955	0.473416
N	-0.466823	2.378942	0.058479
H	0.440411	4.031853	-0.856996
H	-0.187188	5.119040	1.153072
Rh	0.380525	0.441618	-0.416844
C	0.244832	-2.051410	1.066107
O	0.287179	-3.376287	1.265478
C	1.354979	-2.747051	-0.778406
C	0.793078	-3.951527	0.021010
H	1.535976	-4.704411	0.287563
N	0.805847	-1.601252	-0.022794

11a-*Z*-*Re*

Cartesian coordinates

ATOM	X	Y	Z
C	-1.401399	0.178255	1.978045
C	-0.447837	-0.530005	1.236824
C	-0.099126	-1.834998	1.606231
C	-0.691914	-2.438953	2.723123
C	-1.629355	-1.708456	3.468691
C	-1.996821	-0.403522	3.105271
H	-0.435290	-3.454511	3.013844
H	-2.085150	-2.164849	4.342477
H	-2.733267	0.139576	3.692098
C	0.842973	-2.378466	0.639501
C	1.885122	-3.877017	-0.658223
C	2.166149	-2.446108	-1.193481
H	1.212677	-4.450933	-1.303534
C	-1.602171	1.496491	1.394759
C	-1.172945	3.316948	0.140875
C	-2.453533	3.518422	0.976458
H	-0.343497	3.840811	0.630175
H	-3.367741	3.429861	0.382932
N	-0.914788	1.866654	0.346401
N	1.321802	-1.617108	-0.307708
H	-2.471696	4.442199	1.556046
H	1.783637	-2.342264	-2.215966
H	2.781881	-4.465024	-0.459103
O	1.198515	-3.674276	0.610110

H	0.901435	-2.730271	-1.772427	O	-2.440483	2.405457	1.919277
H	-0.054973	-4.419456	-0.482700	Rh	0.407275	0.336921	-0.365475
C	-1.498248	3.788438	-1.761515	Si	2.282326	1.341065	0.771745
H	-1.156816	2.986774	-2.428373	C	-1.197557	3.807486	-1.322914
C	-1.322738	5.122217	-2.505199	H	-0.357562	3.290078	-1.804678
H	-1.628489	5.974717	-1.884145	C	3.651566	-2.019905	-1.200421
H	-0.280108	5.282104	-2.804592	H	3.649517	-0.938317	-1.373425
H	-1.938878	5.144217	-3.410947	H	-0.775819	-1.799907	-1.854224
C	-2.975822	3.533462	-1.425843	C	-1.161311	-0.787340	-1.838602
H	-3.112905	2.622152	-0.835292	C	-0.499134	0.205128	-2.536124
H	-3.415655	4.366319	-0.863221	C	-2.551963	-0.668906	-1.352866
H	-3.559688	3.423947	-2.346476	O	-3.226908	0.349492	-1.329966
C	2.891135	-2.699013	-0.930488	O	-2.996248	-1.890394	-0.967701
H	3.123445	-1.696923	-1.307015	C	-4.399406	-2.134120	-0.602468
C	3.348677	-3.735922	-1.968653	C	-2.482439	3.479622	-2.098306
H	4.429382	-3.663588	-2.136062	H	-2.331331	3.681649	-3.165698
H	3.139234	-4.763659	-1.640891	H	-2.781620	2.435108	-1.981173
H	2.850243	-3.585548	-2.934114	H	-3.318709	4.113248	-1.774012
C	3.645073	-2.869852	0.395309	C	-0.907156	5.318264	-1.372482
H	3.315542	-2.139531	1.140070	H	-0.866726	5.666476	-2.410528
H	3.521503	-3.875149	0.819434	H	-1.692850	5.895315	-0.866269
H	4.718433	-2.715917	0.238971	H	0.050288	5.565059	-0.898692
C	-1.570995	-0.091417	-1.719660	C	4.395200	-2.709889	-2.354695
H	-2.225164	0.750072	-1.532810	H	5.433830	-2.364157	-2.403668
C	-2.134080	-1.409220	-1.368459	H	4.423090	-3.801687	-2.231852
O	-1.626477	-2.495835	-1.612723	H	3.927236	-2.493830	-3.323113
O	-3.337767	-1.242220	-0.767443	C	4.357333	-2.260656	0.140785
C	-4.198160	-2.375133	-0.402694	H	4.471916	-3.328527	0.368705
C	-5.438397	-1.681548	0.170330	H	5.363130	-1.827908	0.115768
H	-6.175726	-2.427352	0.486596	H	3.817811	-1.787347	0.966009
H	-5.170547	-1.067695	1.036461	C	2.510870	0.666419	2.549023
H	-5.900631	-1.033598	-0.581751	H	3.407246	1.084258	3.025458
C	-3.522884	-3.237377	0.669448	H	1.647452	0.938722	3.166955
H	-4.219851	-4.012370	1.009671	H	2.596199	-0.424904	2.572606
H	-2.625085	-3.720784	0.281880	C	2.209663	3.238700	0.980908
H	-3.245483	-2.623702	1.532635	H	3.171537	3.619160	1.347606
C	-4.564906	-3.185324	-1.652644	H	1.992914	3.741466	0.033295
H	-5.310714	-3.944884	-1.391302	H	1.452049	3.531391	1.716735
H	-5.000758	-2.530792	-2.415834	O	3.756341	1.026099	-0.075303
H	-3.689321	-3.682068	-2.073094	C	5.019288	1.332154	0.495515
Si	2.515983	1.166380	0.456064	C	6.060588	1.426547	-0.613363
C	2.810968	3.047721	0.282345	H	5.309700	0.554521	1.219804
H	2.714509	3.370976	-0.759343	H	4.991089	2.285601	1.047180
H	2.104341	3.619968	0.894175	H	7.051589	1.648525	-0.198431

H	3.819760	3.315867	0.621440
C	2.728590	0.802395	2.323241
H	3.713527	1.125714	2.684119
H	1.968749	1.338844	2.902647
H	2.620189	-0.263030	2.551388
O	3.838678	0.408905	-0.354631
C	5.168685	0.517853	0.128911
H	5.390447	1.544051	0.465119
H	5.315079	-0.141965	0.998840
C	6.136074	0.133391	-0.983960
H	7.174427	0.195033	-0.635430
H	5.944161	-0.890656	-1.322425
H	6.014042	0.801847	-1.842800
C	-0.470710	0.050869	-2.552900
H	-0.319896	0.966329	-3.110433
H	0.030851	-0.827998	-2.942903
H	1.495817	0.811132	-1.611218

Total SCF energy -1732.46424108
Gibbs free energy at 298K -1731.81560500
Free energy in solution -1732.437

H	6.121018	0.483057	-1.167132
H	5.791769	2.217251	-1.321683
C	-4.794251	-1.319522	0.634011
H	-4.799202	-0.250631	0.417218
H	-5.797069	-1.619208	0.960996
H	-4.095275	-1.510594	1.454182
C	-5.304134	-1.834548	-1.804043
H	-4.975312	-2.403664	-2.680807
H	-6.333775	-2.130493	-1.572823
H	-5.293548	-0.770857	-2.048948
C	-4.402605	-3.631897	-0.280408
H	-5.409628	-3.955251	0.004568
H	-4.083580	-4.215622	-1.150256
H	-3.720317	-3.846953	0.548476
H	1.379215	1.213794	-1.413368
H	0.339195	-0.043905	-3.174196
H	-0.977973	1.159232	-2.719556

Total SCF energy -1732.45824132
Gibbs free energy at 298K -1731.80976900
Free energy in solution -1732.430

10TS-*Z*-*Si*

Cartesian coordinates

ATOM	X	Y	Z
C	-1.128086	1.206364	2.119924
C	-0.444498	0.171202	1.466180
C	-0.277079	-1.068295	2.102464
C	-0.795988	-1.279599	3.385278
C	-1.465897	-0.228626	4.031490
C	-1.636658	1.016818	3.412700
H	-0.683688	-2.240855	3.880228
H	-1.861530	-0.385278	5.030599
H	-2.159505	1.817438	3.929575
C	0.429060	-1.981586	1.217168
C	1.082658	-3.877411	0.229198
C	1.519232	-2.672097	-0.642431
H	0.249340	-4.425234	-0.216643
C	-1.178603	2.377875	1.265707
C	-0.916488	3.637687	-0.587744
C	-1.369529	4.508325	0.611207
H	0.028575	4.007886	-0.994506
H	-2.252789	5.119274	0.419784
N	-0.668392	2.334256	0.062525
N	0.894003	-1.542013	0.079904

11TS-*Z*-*Re*

Cartesian coordinates

ATOM	X	Y	Z
C	-1.123096	0.391518	2.229969
C	-0.204846	-0.358442	1.478436
C	0.345722	-1.529732	2.020177
C	-0.033103	-1.970591	3.294914
C	-0.949185	-1.207833	4.032522
C	-1.493764	-0.022957	3.515569
H	0.375511	-2.887304	3.712281
H	-1.240226	-1.538546	5.025063
H	-2.193174	0.560879	4.108469
C	1.251726	-2.133635	1.060424
C	2.385537	-3.702534	-0.063988
C	2.406971	-2.373895	-0.869174
H	1.753191	-4.469233	-0.522171
C	-1.508026	1.582167	1.492335
C	-1.603778	3.056709	-0.216308
C	-2.086781	3.703715	1.104489
H	-0.764499	3.618076	-0.632800
H	-3.053830	4.201690	1.039480
N	-1.084161	1.755194	0.268744
N	1.533379	-1.507178	-0.050451

H	-0.566822	5.143586	0.999024	H	-1.350369	4.390931	1.534281
H	1.037790	-2.739399	-1.620305	H	1.924592	-2.517631	-1.843624
H	1.887943	-4.565706	0.489459	H	3.373042	-4.121093	0.134774
O	0.594147	-3.287007	1.473752	O	1.786440	-3.356051	1.217010
O	-1.711170	3.550773	1.652644	O	-2.224405	2.585205	2.030164
Rh	0.286600	0.438383	-0.363720	Rh	0.337527	0.257030	-0.333818
Si	2.404364	1.374982	0.355501	Si	2.144112	1.703968	0.395791
C	-1.936096	3.550451	-1.751160	C	-2.690485	2.926307	-1.313220
H	-1.558175	2.764450	-2.417154	H	-2.339530	2.149568	-1.999461
C	3.042253	-2.507540	-0.839607	C	3.808901	-1.773405	-1.121282
H	3.185394	-1.513658	-1.277394	H	3.636325	-0.756517	-1.490417
H	-2.228920	0.553987	-1.603967	H	-0.435283	-2.098069	-1.601806
C	-1.487737	-0.221639	-1.743139	C	-0.894515	-1.133126	-1.778214
C	-0.365800	0.027309	-2.562954	C	-0.221911	-0.183345	-2.572018
C	-1.949625	-1.579400	-1.435644	C	-2.343672	-1.100137	-1.552633
O	-1.361640	-2.624191	-1.694256	O	-3.112072	-0.215861	-1.905145
O	-3.171333	-1.521505	-0.839191	O	-2.726846	-2.246711	-0.924330
C	-3.925604	-2.725020	-0.479913	C	-4.129462	-2.552074	-0.637198
C	-3.351822	3.155442	-1.304888	C	-4.057569	2.470439	-0.783026
H	-3.987876	2.979675	-2.179649	H	-4.705266	2.193527	-1.620234
H	-3.352587	2.240506	-0.704239	H	-3.967260	1.589097	-0.144329
H	-3.828977	3.946894	-0.713758	H	-4.566194	3.263575	-0.219529
C	-1.950809	4.865992	-2.546327	C	-2.814142	4.249219	-2.086493
H	-2.618227	4.785927	-3.411371	H	-3.560359	4.160511	-2.883875
H	-2.310309	5.705073	-1.936105	H	-3.133341	5.073024	-1.432852
H	-0.951321	5.124218	-2.916104	H	-1.862289	4.539624	-2.547994
C	3.557457	-3.562374	-1.831874	C	4.541551	-2.580011	-2.205015
H	4.625038	-3.415388	-2.031659	H	5.511139	-2.123995	-2.434427
H	3.437806	-4.583264	-1.443470	H	4.737123	-3.613264	-1.886114
H	3.026887	-3.506225	-2.790197	H	3.965203	-2.621702	-3.137632
C	3.839303	-2.540277	0.471552	C	4.656154	-1.651152	0.152164
H	3.813181	-3.527189	0.951558	H	4.945733	-2.629098	0.558301
H	4.891398	-2.303695	0.277961	H	5.581366	-1.107207	-0.066366
H	3.464264	-1.800682	1.184766	H	4.127067	-1.096120	0.931819
C	2.774950	1.139589	2.219178	C	2.677013	1.396117	2.208148
H	3.746716	1.567872	2.496859	H	3.550832	2.000477	2.483579
H	2.007128	1.639807	2.820866	H	1.859321	1.666795	2.886583
H	2.779264	0.083952	2.511127	H	2.920193	0.345514	2.397727
C	2.532877	3.262404	0.062568	C	1.801008	3.583906	0.307654
H	3.527723	3.637963	0.334022	H	2.691215	4.155834	0.598470
H	2.359930	3.511449	-0.989862	H	1.524605	3.894157	-0.705454
H	1.804630	3.807423	0.674036	H	0.997734	3.874526	0.993828
O	3.723732	0.681860	-0.521100	O	3.531824	1.446900	-0.606320
C	5.073019	0.953604	-0.174217	C	4.788338	2.036086	-0.306573

C	5.978369	0.545795	-1.330238
H	5.353608	0.399269	0.735684
H	5.221784	2.023661	0.044166
H	7.030916	0.733736	-1.084779
H	5.859995	-0.520135	-1.553561
H	5.722937	1.111171	-2.232795
C	-4.230940	-3.555890	-1.733090
H	-3.316617	-3.962014	-2.168040
H	-4.898868	-4.385335	-1.472908
H	-4.734855	-2.937460	-2.484465
C	-3.171655	-3.535166	0.581368
H	-2.923770	-2.901206	1.439343
H	-3.803740	-4.358261	0.935106
H	-2.249175	-3.952605	0.175773
C	-5.217682	-2.147986	0.108437
H	-5.886897	-2.957124	0.420861
H	-4.998100	-1.522238	0.979785
H	-5.738169	-1.533949	-0.633980
H	1.142548	0.704696	-1.798185
H	0.169526	-0.823022	-2.973894
H	-0.362176	0.912184	-3.190129
Total SCF energy		-1732.46203321	
Gibbs free energy at 298K		-1731.81400100	
Imaginary frequency		-516.390	
Free energy in solution		-1732.43422400	

C	5.676513	1.979266	-1.543771
H	5.272450	1.503237	0.527621
H	4.673462	3.085666	0.008565
H	6.659319	2.420578	-1.337137
H	5.824271	0.942428	-1.865671
H	5.213416	2.527729	-2.370906
C	-4.716920	-1.518554	0.331053
H	-4.812324	-0.544286	-0.149319
H	-5.708768	-1.845529	0.664925
H	-4.074936	-1.417841	1.213290
C	-4.931584	-2.640813	-1.942036
H	-4.467502	-3.361448	-2.624866
H	-5.950513	-2.983521	-1.727372
H	-4.983089	-1.669740	-2.436814
C	-4.043389	-3.926910	0.034778
H	-5.045094	-4.284260	0.297299
H	-3.580295	-4.655948	-0.638542
H	-3.442705	-3.872345	0.948688
H	0.929406	0.970280	-1.750482
H	0.641254	-0.497948	-3.148705
H	-0.800524	0.621246	-3.014621
Total SCF energy		-1732.45396191	
Gibbs free energy at 298K		-1731.80752200	
Imaginary frequency		-537.938	
Free energy in solution		-1732.42746200	

10TS-*E*-*Si*

Cartesian coordinates

ATOM	X	Y	Z
C	-1.756148	-0.931439	2.164176
C	-0.568886	-0.412869	1.628082
C	0.559157	-0.261601	2.447959
C	0.510804	-0.636766	3.796124
C	-0.686487	-1.148373	4.317529
C	-1.825913	-1.297361	3.515243
H	1.384324	-0.534771	4.434819
H	-0.730929	-1.436562	5.363497
H	-2.744697	-1.694477	3.939013
C	-2.778989	-0.981966	1.136867
O	-4.045774	-1.364974	1.374894
C	-3.703122	-0.828836	-0.916306
C	-4.790849	-1.06048	0.162108
H	-5.455774	-1.901566	-0.038415

11TS-*E*-*Re*

Cartesian coordinates

ATOM	X	Y	Z
C	-1.203153	-0.431254	2.20967
C	-0.100605	-0.816402	1.431342
C	0.621849	-1.969539	1.766313
C	0.271369	-2.723594	2.892834
C	-0.810647	-2.305893	3.681207
C	-1.561295	-1.171356	3.344958
H	0.81821	-3.626706	3.150682
H	-1.08321	-2.883293	4.559488
H	-2.409999	-0.876448	3.956608
C	1.610347	-2.244328	0.738732
C	2.909588	-3.430674	-0.642003
C	2.747904	-1.989354	-1.197902
H	2.359071	-4.176595	-1.223253
C	-1.809118	0.763382	1.653814

N	-2.498352	-0.615934	-0.086627	C	-1.921119	2.659492	0.455616
H	-3.906115	0.088719	-1.47463	C	-3.179243	2.499607	1.328469
H	-5.387831	-0.164414	0.359394	H	-1.230864	3.33887	0.969076
Rh	-0.473153	0.128571	-0.288991	H	-4.060123	2.183085	0.760587
C	1.658263	0.289062	1.674565	N	-1.317478	1.305096	0.56981
O	2.902095	0.437957	2.158521	N	1.785054	-1.399953	-0.242122
C	2.741657	1.119957	-0.133059	H	-3.422077	3.374484	1.93232
C	3.729278	0.883648	1.044837	H	2.268246	-2.017798	-2.183799
H	4.255641	1.782842	1.368272	H	3.945156	-3.75323	-0.527346
N	1.464222	0.639259	0.432314	O	2.310073	-3.388822	0.683935
H	2.991073	0.460445	-0.970019	O	-2.831041	1.416155	2.240912
H	4.457189	0.094574	0.844705	Rh	0.313502	0.180046	-0.234667
C	-3.543604	-1.985499	-1.935225	Si	1.932706	1.736035	0.688448
H	-2.617502	-1.772338	-2.483727	C	-2.09306	3.217054	-0.968909
C	-4.699384	-1.962913	-2.948734	H	-1.130743	3.025038	-1.461297
H	-5.666825	-2.147384	-2.463277	C	4.057582	-1.181386	-1.336378
H	-4.762923	-0.998199	-3.466238	H	3.749101	-0.146187	-1.517455
H	-4.563961	-2.742115	-3.706936	H	-0.053579	-2.017336	-1.867133
C	-3.403641	-3.370921	-1.285441	C	-0.767393	-1.206998	-1.770757
H	-2.621568	-3.391949	-0.520104	C	-0.472731	-0.006845	-2.456808
H	-4.340501	-3.69814	-0.817761	C	-2.043215	-1.749104	-1.28227
H	-3.144251	-4.11849	-2.043198	O	-2.11275	-2.888939	-0.841826
C	2.686248	2.571328	-0.661993	O	-3.123321	-0.925104	-1.401602
H	1.787003	2.631503	-1.284499	C	-4.472135	-1.446835	-1.105287
C	3.916599	2.855478	-1.538938	C	-3.19594	2.548044	-1.797097
H	3.862655	3.864022	-1.964174	H	-3.121106	2.864649	-2.844312
H	4.851131	2.796056	-0.963279	H	-3.130631	1.458617	-1.761112
H	3.992002	2.145913	-2.372094	H	-4.195414	2.839253	-1.449095
C	2.54038	3.627903	0.441498	C	-2.298963	4.741332	-0.916576
H	1.713095	3.392696	1.116652	H	-2.347367	5.156134	-1.929446
H	3.454813	3.737791	1.038768	H	-3.239122	5.003354	-0.412829
H	2.329438	4.605033	-0.004903	H	-1.481128	5.243916	-0.387102
C	0.148392	-1.860235	-1.262814	C	4.861846	-1.681916	-2.546636
H	-0.752509	-2.448446	-1.145553	H	5.760311	-1.07118	-2.689993
C	1.300022	-2.573531	-0.688504	H	5.19458	-2.721359	-2.418407
O	1.167551	-3.552407	0.03049	H	4.274234	-1.630895	-3.471696
O	2.514283	-2.088623	-1.083974	C	4.911807	-1.182573	-0.06142
C	3.731761	-2.889281	-0.878484	H	5.325667	-2.173876	0.164805
C	4.819643	-2.049169	-1.556025	H	5.760439	-0.500123	-0.180353
H	5.781753	-2.57037	-1.508785	H	4.337452	-0.844008	0.805533
H	4.572011	-1.873926	-2.60812	C	2.567104	1.214128	2.418257
H	4.935508	-1.077116	-1.065647	H	3.368462	1.872384	2.778068
C	3.595323	-4.239089	-1.596644	H	1.744409	1.266663	3.141523
H	4.542199	-4.787265	-1.531949	H	2.94358	0.185982	2.432552

H	2.809164	-4.846079	-1.14554
H	3.363284	-4.084956	-2.656493
C	4.0298	-3.070314	0.615936
H	5.027837	-3.506813	0.741809
H	4.012431	-2.106414	1.1353
H	3.292543	-3.722806	1.083764
Si	-1.317816	2.387366	0.034612
C	-3.147737	2.601781	-0.486188
H	-3.300607	2.325977	-1.535209
H	-3.808312	1.988178	0.136443
H	-3.471903	3.643605	-0.368636
C	-1.262742	2.990417	1.851432
H	-1.614875	4.025783	1.946204
H	-1.91188	2.359841	2.470286
H	-0.256295	2.93691	2.279413
O	-0.437496	3.529155	-0.921275
C	-0.663739	4.926227	-0.821067
H	-1.739808	5.155087	-0.757076
H	-0.197238	5.325872	0.093759
C	-0.075658	5.615703	-2.046552
H	-0.22302	6.701354	-1.991252
H	0.998907	5.415449	-2.121791
H	-0.553283	5.243145	-2.958995
C	0.181704	-0.868732	-2.263455
H	-0.6088	-0.843446	-3.005328
H	1.138005	-0.489599	-2.607721
H	-0.448443	0.863135	-1.801338

Total SCF energy	-1732.45336602
Gibbs free energy at 298K	-1731.80494900
Imaginary frequency	-384.154
Free energy in solution	-1732.42658800

C	1.382734	3.556746	0.925209
H	2.249687	4.189756	1.154416
H	0.908042	3.962689	0.02613
H	0.687643	3.659076	1.766623
O	3.305291	1.82833	-0.366675
C	4.493931	2.503364	0.014872
C	5.326962	2.794593	-1.227869
H	5.073943	1.887103	0.720335
H	4.269187	3.450854	0.530417
H	6.259586	3.30653	-0.960189
H	5.580575	1.864722	-1.748847
H	4.766288	3.429116	-1.922496
C	-4.790753	-2.644471	-2.011792
H	-4.157652	-3.49977	-1.776782
H	-5.840174	-2.932161	-1.879166
H	-4.645238	-2.372212	-3.06348
C	-4.596497	-1.796948	0.382948
H	-4.338271	-0.930802	1.002568
H	-5.63269	-2.07697	0.607852
H	-3.939424	-2.625932	0.646281
C	-5.400872	-0.280238	-1.454174
H	-6.443911	-0.585611	-1.317782
H	-5.21262	0.583149	-0.809287
H	-5.26538	0.030055	-2.49537
H	0.607514	1.108936	-1.643319
H	0.287908	-0.041549	-3.230675
H	-1.260804	0.715902	-2.634048

Total SCF energy	-1732.44443541
Gibbs free energy at 298K	-1731.79615500
Imaginary frequency	-699.369
Free energy in solution	-1732.41821900

10b-*Z*-*Si*

Cartesian coordinates

ATOM	X	Y	Z
C	-1.058309	1.305416	2.174675
C	-0.328477	0.263460	1.569115
C	-0.066413	-0.927740	2.277249
C	-0.508963	-1.060142	3.597126
C	-1.203678	-0.002840	4.203857
C	-1.485563	1.176223	3.502610
H	-0.320131	-1.977893	4.147550
H	-1.539354	-0.105887	5.231081
H	-2.039614	1.979675	3.980484

10b-*E*-*Si*

Cartesian coordinates

ATOM	X	Y	Z
C	-1.872108	-0.819541	2.179144
C	-0.685900	-0.237465	1.691057
C	0.384953	0.038506	2.566121
C	0.254364	-0.242188	3.930236
C	-0.942434	-0.790881	4.412139
C	-2.004726	-1.085035	3.547611
H	1.077754	-0.042507	4.610597
H	-1.042541	-1.003668	5.471861
H	-2.920128	-1.525303	3.933512

C	-1.254895	2.388991	1.239983	C	-2.798631	-1.055380	1.096444
O	-1.832463	3.559948	1.560781	O	-4.056576	-1.496043	1.269661
C	-1.154812	3.491689	-0.727727	C	-3.550269	-1.113242	-1.031576
C	-1.640760	4.430397	0.410357	C	-4.706018	-1.371715	-0.026886
H	-2.592372	4.923779	0.207077	H	-5.260734	-2.293415	-0.208208
N	-0.823203	2.259553	0.014627	N	-2.429780	-0.788591	-0.126919
H	-0.235269	3.882689	-1.175323	H	-3.766996	-0.229459	-1.640728
H	-0.894493	5.180961	0.686867	H	-5.405603	-0.533010	0.035744
Rh	0.205466	0.400221	-0.262842	Rh	-0.467631	0.075886	-0.181260
C	0.614181	-1.880429	1.424860	C	1.516276	0.557149	1.829691
O	0.899571	-3.141984	1.778864	O	2.714131	0.823327	2.374256
C	1.549579	-2.671832	-0.481189	C	2.693439	1.195857	0.001997
C	1.336878	-3.809851	0.554301	C	3.595495	1.186732	1.270723
H	2.237995	-4.375435	0.795514	H	4.034445	2.156952	1.509670
N	0.933782	-1.520362	0.213852	N	1.396010	0.746489	0.545581
H	0.941810	-2.869179	-1.367451	H	3.025482	0.421596	-0.695290
H	0.538218	-4.494795	0.258270	H	4.386350	0.434434	1.226056
C	-2.178740	3.263847	-1.866658	C	-3.245932	-2.290336	-1.991031
H	-1.746007	2.482942	-2.504782	H	-2.332859	-2.006907	-2.530278
C	-2.316786	4.536068	-2.718795	C	-4.371600	-2.432406	-3.028438
H	-2.742433	5.367885	-2.142217	H	-5.321970	-2.720600	-2.560254
H	-1.347991	4.863983	-3.114958	H	-4.537216	-1.496706	-3.576203
H	-2.983317	4.358301	-3.569817	H	-4.123298	-3.209255	-3.759682
C	-3.545731	2.768046	-1.372538	C	-2.978447	-3.619321	-1.269120
H	-3.453861	1.865372	-0.760853	H	-2.175852	-3.531723	-0.530372
H	-4.067499	3.530182	-0.779973	H	-3.874195	-3.992903	-0.756981
H	-4.189630	2.526917	-2.225580	H	-2.678493	-4.385681	-1.992465
C	3.009843	-2.414527	-0.916488	C	2.623652	2.537575	-0.763560
H	3.002361	-1.443067	-1.424728	H	1.772686	2.445486	-1.448561
C	3.452248	-3.491444	-1.920091	C	3.903025	2.732889	-1.593446
H	4.466975	-3.290160	-2.282090	H	3.840290	3.650153	-2.189639
H	3.462274	-4.491072	-1.464149	H	4.791474	2.822770	-0.952976
H	2.785830	-3.529628	-2.790007	H	4.070966	1.896008	-2.281960
C	3.999821	-2.303851	0.250454	C	2.352520	3.757090	0.126445
H	3.668413	-1.569595	0.989294	H	1.481065	3.601192	0.766234
H	4.149994	-3.264389	0.760243	H	3.211898	4.007932	0.761643
H	4.978851	-1.977975	-0.117728	H	2.146337	4.633665	-0.496944
C	-1.291556	-0.358216	-1.697692	C	0.360833	-1.664988	-1.248521
H	-2.092323	0.372642	-1.715768	H	-0.492075	-2.331983	-1.321145
C	-1.792437	-1.706353	-1.463376	C	1.464833	-2.430483	-0.672894
O	-1.242432	-2.762317	-1.780634	O	1.309983	-3.415226	0.040776
O	-2.995613	-1.661550	-0.810893	O	2.715917	-1.948999	-1.001581
C	-3.725082	-2.870795	-0.442057	C	3.918557	-2.722767	-0.684822
C	-4.968270	-2.315272	0.262398	C	5.047187	-1.882905	-1.294616

H	-5.623658	-3.133153	0.581930
H	-4.682944	-1.732478	1.144600
H	-5.531950	-1.662439	-0.412433
C	-2.903900	-3.730221	0.528520
H	-3.519256	-4.555120	0.907092
H	-2.026692	-4.144252	0.029815
H	-2.575453	-3.129045	1.383809
C	-4.128706	-3.654884	-1.698734
H	-4.776927	-4.495132	-1.422824
H	-4.685697	-3.007437	-2.385536
H	-3.249251	-4.041393	-2.216034
Si	2.321486	1.475271	0.447182
C	2.303216	3.393015	0.358354
H	2.072531	3.747746	-0.652754
H	1.549633	3.800929	1.043008
H	3.269804	3.824911	0.647398
C	2.969577	1.104422	2.210074
H	3.973522	1.516992	2.373361
H	2.300671	1.564735	2.947566
H	3.008638	0.033324	2.433020
O	3.505136	0.949573	-0.705308
C	4.858382	1.376131	-0.643994
H	4.921845	2.470199	-0.529961
H	5.360541	0.931254	0.230319
C	5.575758	0.956804	-1.920958
H	6.626765	1.270002	-1.897144
H	5.541684	-0.131536	-2.041685
H	5.096027	1.410395	-2.795013
C	-0.210928	-0.176869	-2.743182
H	-0.529046	0.445100	-3.588984
H	0.143472	-1.142497	-3.114091
H	0.720022	0.349743	-2.363640

Total SCF energy -1732.48747944
Gibbs free energy at 298K -1731.83744100
Free energy in solution -1732.45962700

H	6.010927	-2.384879	-1.156000
H	4.883553	-1.737383	-2.367683
H	5.106935	-0.896577	-0.821024
C	3.860422	-4.094420	-1.372410
H	4.809433	-4.623612	-1.226378
H	3.051768	-4.700488	-0.962252
H	3.701798	-3.971469	-2.449924
C	4.107059	-2.859215	0.832607
H	5.084585	-3.308441	1.046221
H	4.074583	-1.876035	1.315908
H	3.322920	-3.480724	1.264947
Si	-1.466794	2.327853	0.078455
C	-3.359506	2.427464	-0.229290
H	-3.632919	2.075891	-1.230942
H	-3.895142	1.813480	0.505017
H	-3.737856	3.452554	-0.126457
C	-1.245378	3.230342	1.754176
H	-1.556267	4.281855	1.699770
H	-1.872117	2.742035	2.510697
H	-0.215311	3.206241	2.123899
O	-0.714317	3.264158	-1.173289
C	-1.080167	4.609822	-1.440757
H	-2.174678	4.714639	-1.508026
H	-0.743326	5.269063	-0.623997
C	-0.446734	5.050513	-2.754616
H	-0.707443	6.091240	-2.983059
H	0.644699	4.970910	-2.701331
H	-0.793380	4.415380	-3.577085
C	0.546630	-0.759690	-2.453862
H	0.108359	-1.171702	-3.372907
H	1.598781	-0.530740	-2.636000
H	0.036741	0.242112	-2.343198

Total SCF energy -1732.47883164
Gibbs free energy at 298K -1731.83132600
Free energy in solution -1732.45171700

11b-*Z*-*Re*

Cartesian coordinates

ATOM	X	Y	Z
C	-1.406912	0.232434	2.041713
C	-0.431125	-0.491051	1.333158
C	-0.069145	-1.791047	1.732443
C	-0.667341	-2.359064	2.863355
C	-1.613186	-1.619783	3.586705

12a-*E*-*Si*

Cartesian coordinates

ATOM	X	Y	Z
C	2.265240	-1.535616	1.737635
C	0.918876	-1.189507	1.563650
C	-0.009610	-1.486974	2.570005
C	0.389356	-2.162279	3.730755
C	1.732795	-2.541871	3.865875

C	-1.991074	-0.331487	3.182220	C	2.682161	-2.226980	2.882948
H	-0.404797	-3.366715	3.173748	H	-0.323342	-2.385188	4.520662
H	-2.069869	-2.056713	4.469268	H	2.048006	-3.073703	4.758659
H	-2.735580	0.224100	3.745809	H	3.724093	-2.504599	3.020596
C	-1.630824	1.527028	1.433285	C	3.050561	-1.012048	0.629784
O	-2.396483	2.477584	1.993089	O	4.378376	-1.179046	0.528225
C	-1.194851	3.298488	0.114985	C	3.526551	0.228504	-1.190955
C	-2.386219	3.593864	1.056018	C	4.755524	-0.610783	-0.760166
H	-3.348887	3.593142	0.538014	H	5.666830	-0.030735	-0.609439
N	-0.993501	1.843062	0.339523	N	2.471241	-0.316404	-0.311187
H	-0.294804	3.786856	0.506626	H	3.263368	0.015590	-2.231628
H	-2.278183	4.510434	1.637371	H	4.962286	-1.445499	-1.437692
Rh	0.323404	0.257334	-0.251719	Rh	0.347532	-0.129617	-0.021302
C	0.861623	-2.365441	0.785029	C	-1.306572	-0.927685	2.216530
O	1.253340	-3.649195	0.798021	O	-2.356391	-0.920102	3.052474
C	2.121198	-2.460669	-1.092429	C	-2.878358	0.112238	0.971451
C	1.932901	-3.875233	-0.471994	C	-3.343887	-0.037349	2.441484
H	2.867195	-4.395447	-0.257117	H	-4.322248	-0.503995	2.560567
N	1.297682	-1.625713	-0.195516	N	-1.475076	-0.350943	1.056724
H	1.664175	-2.425406	-2.088897	H	-2.868196	1.162370	0.666465
H	1.287535	-4.521161	-1.073912	H	-3.320123	0.906685	2.995577
C	-1.346667	3.760806	-1.349987	C	3.697700	1.760978	-1.035712
H	-0.547423	3.245989	-1.899707	H	2.710129	2.195064	-1.220771
C	-1.073746	5.273159	-1.443647	C	4.672495	2.292667	-2.098410
H	-1.825161	5.851284	-0.889251	H	5.690551	1.906068	-1.954422
H	-0.086169	5.536841	-1.046093	H	4.352564	2.021979	-3.112414
H	-1.115360	5.604632	-2.486868	H	4.732860	3.385429	-2.048952
C	-2.685874	3.405581	-2.010749	C	4.107103	2.189318	0.380044
H	-2.936924	2.347553	-1.896485	H	3.359638	1.877572	1.114662
H	-3.508309	4.009104	-1.604448	H	5.085154	1.786243	0.673995
H	-2.634757	3.629602	-3.083226	H	4.176948	3.281550	0.430806
C	3.582007	-1.973157	-1.229231	C	-3.715706	-0.679099	-0.060036
H	3.519114	-0.899633	-1.441270	H	-3.150354	-0.639542	-0.996017
C	4.262096	-2.674924	-2.415350	C	-5.073171	0.008980	-0.274452
H	5.279796	-2.294109	-2.555979	H	-5.647357	-0.507642	-1.051914
H	4.340777	-3.759509	-2.257537	H	-5.687288	0.005205	0.636786
H	3.713149	-2.511964	-3.351005	H	-4.949315	1.051995	-0.590446
C	4.406494	-2.127476	0.055661	C	-3.886320	-2.161412	0.298939
H	3.903546	-1.671346	0.912036	H	-2.917661	-2.650125	0.439534
H	4.614972	-3.178345	0.294890	H	-4.484276	-2.307767	1.207942
H	5.373497	-1.626181	-0.060322	H	-4.401129	-2.685808	-0.513695
C	-0.952283	-0.626887	-1.823261	C	-0.157049	1.373237	-1.664880
H	-0.552865	-1.631472	-1.951776	H	0.829217	1.368604	-2.132499
C	-2.385248	-0.688136	-1.533364	C	-0.192260	2.351040	-0.596338

O	-3.215144	0.199665	-1.711956
O	-2.709242	-1.907529	-0.995853
C	-4.089135	-2.274229	-0.684378
C	-3.945386	-3.701688	-0.143601
H	-4.926011	-4.106223	0.130817
H	-3.498818	-4.357018	-0.899098
H	-3.303589	-3.712232	0.743760
C	-4.937520	-2.269282	-1.963721
H	-5.937199	-2.665593	-1.749786
H	-5.036022	-1.257997	-2.361416
H	-4.475526	-2.905920	-2.727010
C	-4.678570	-1.355969	0.394376
H	-5.670791	-1.720666	0.686839
H	-4.039236	-1.357126	1.283479
H	-4.771152	-0.333522	0.026451
Si	2.238437	1.326234	0.936310
C	2.122146	3.186515	1.402891
H	1.965628	3.821445	0.523430
H	1.293455	3.358738	2.100776
H	3.035570	3.535036	1.901916
C	2.752643	0.504631	2.590682
H	3.727416	0.862761	2.946450
H	2.011276	0.753980	3.360400
H	2.798120	-0.587349	2.529499
O	3.561331	1.207880	-0.186168
C	4.846733	1.742112	0.093101
H	4.774311	2.786509	0.435486
H	5.332921	1.171933	0.902005
C	5.702856	1.684141	-1.166279
H	6.701959	2.095190	-0.976145
H	5.815286	0.650335	-1.511487
H	5.235671	2.261836	-1.971263
H	0.449269	0.908552	-2.565902
C	-0.477896	0.360631	-2.873670
H	-1.236754	1.121258	-3.071204
H	-0.207596	-0.124674	-3.821730

Total SCF energy -1732.47879268
Gibbs free energy at 298K -1731.82996400
Free energy in solution -1732.45042800

C	-1.289556	1.346492	-2.675927
H	-1.336640	2.269573	-3.275194
H	-1.174668	0.502974	-3.362626
H	-2.264257	1.231920	-2.191509
O	0.708376	2.451491	0.267358
O	-1.340704	3.089444	-0.523035
C	-1.491563	4.204767	0.415443
C	-2.872467	4.763702	0.054874
H	-3.110529	5.627998	0.684704
H	-2.898708	5.077857	-0.993453
H	-3.648449	4.004561	0.202537
C	-0.405399	5.256623	0.152538
H	-0.595479	6.148843	0.760467
H	0.582771	4.865597	0.400537
H	-0.415128	5.554055	-0.902022
C	-1.470852	3.725226	1.872917
H	-1.671231	4.571636	2.540861
H	-2.252401	2.975696	2.041563
H	-0.503782	3.290465	2.126743
Si	-0.001401	-1.990407	-1.441018
C	1.242612	-2.012899	-2.889655
H	1.227125	-1.068011	-3.442322
H	2.260999	-2.185540	-2.525087
H	1.005524	-2.818794	-3.596237
C	0.162325	-3.671924	-0.552282
H	-0.001894	-4.507140	-1.245298
H	1.164861	-3.783051	-0.124560
H	-0.555744	-3.768110	0.269148
O	-1.568080	-1.940667	-2.151517
C	-2.075523	-3.028968	-2.913032
H	-1.295504	-3.458420	-3.562244
H	-2.413115	-3.834790	-2.242429
C	-3.236482	-2.545321	-3.772630
H	-3.652984	-3.372906	-4.359854
H	-4.033583	-2.130704	-3.146103
H	-2.903772	-1.760881	-4.460350

Total SCF energy -1732.49106123
Gibbs free energy at 298K -1731.83994500
Free energy in solution -1732.46380300

13b-*Z*-*Re*

Cartesian coordinates

ATOM	X	Y	Z
C	-0.320950	-3.033106	-1.072302

13b-*E*-*Re*

Cartesian coordinates

ATOM	X	Y	Z
C	1.592061	-1.834005	2.028075

C	0.508200	-1.907666	-1.132057	C	0.375933	-1.214708	1.720943
C	1.549184	-1.858776	-2.066886	C	-0.640249	-1.159637	2.682804
C	1.796828	-2.946588	-2.913102	C	-0.468670	-1.763676	3.93515
C	0.989632	-4.089609	-2.799666	C	0.736251	-2.430990	4.203497
C	-0.078833	-4.143763	-1.893535	C	1.779230	-2.464398	3.266015
H	2.591177	-2.911511	-3.654337	H	-1.245252	-1.713407	4.694135
H	1.182701	-4.941771	-3.444604	H	0.873375	-2.912030	5.167425
H	-0.711538	-5.026469	-1.846267	H	2.716608	-2.958275	3.509089
C	-1.406521	-2.785352	-0.132336	C	2.530712	-1.633736	0.929886
O	-2.340821	-3.701824	0.161772	O	3.763676	-2.158453	0.925454
C	-2.772122	-1.623323	1.23488	C	3.376401	-0.787686	-0.984753
C	-3.149027	-3.125491	1.229481	C	4.331852	-1.849295	-0.381931
H	-4.195197	-3.329743	0.997898	H	5.351554	-1.497060	-0.221102
N	-1.516708	-1.622353	0.455481	N	2.193312	-0.906143	-0.102656
H	-2.554055	-1.286333	2.252277	H	3.081861	-1.070674	-1.999573
H	-2.875362	-3.637085	2.157569	H	4.355801	-2.781889	-0.954252
Rh	0.086778	-0.276844	-0.041244	Rh	0.161913	-0.202746	0.003825
C	2.162481	-0.532990	-2.040938	C	-1.734585	-0.331455	2.18501
O	3.053890	-0.123070	-2.953123	O	-2.766775	0.054993	2.948469
C	2.512612	1.610833	-1.402367	C	-2.898737	0.975805	0.751657
C	3.166087	1.325029	-2.777664	C	-3.453048	1.100729	2.193426
H	4.224595	1.580138	-2.841511	H	-4.525063	0.922814	2.285536
N	1.786667	0.344068	-1.150294	N	-1.699604	0.136399	0.965909
H	1.754664	2.394310	-1.47822	H	-2.554836	1.945433	0.382435
H	2.627111	1.790035	-3.608715	H	-3.199858	2.055478	2.664527
C	-3.833503	-0.675518	0.627499	C	3.940716	0.651642	-1.031444
H	-3.353332	0.308328	0.567889	H	3.114429	1.295662	-1.351571
C	-5.042637	-0.557458	1.568565	C	5.048935	0.751171	-2.091674
H	-5.577227	-1.511382	1.672883	H	5.926468	0.141582	-1.83508
H	-4.741243	-0.229124	2.570524	H	4.691540	0.428593	-3.077146
H	-5.760458	0.174437	1.182131	H	5.389797	1.787605	-2.18719
C	-4.261525	-1.074502	-0.792391	C	4.423450	1.160764	0.334108
H	-3.403057	-1.129636	-1.470303	H	3.625511	1.122867	1.083305
H	-4.778062	-2.042841	-0.816643	H	5.279660	0.589428	0.716988
H	-4.955399	-0.330615	-1.199266	H	4.742561	2.205235	0.249448
C	3.498540	1.978892	-0.268675	C	-3.880582	0.378433	-0.283608
H	2.914618	1.939833	0.656978	H	-3.278080	0.150844	-1.169337
C	4.006382	3.416355	-0.463477	C	-4.939983	1.424440	-0.665475
H	4.650486	3.715092	0.371599	H	-5.600093	1.036281	-1.449235
H	4.599948	3.520068	-1.382343	H	-5.576026	1.695092	0.188845
H	3.175307	4.129016	-0.518964	H	-4.477733	2.344378	-1.043236
C	4.662175	0.990614	-0.112356	C	-4.531363	-0.935993	0.168757
H	4.302803	-0.034255	0.019893	H	-3.779993	-1.684752	0.43563
H	5.343056	1.006639	-0.973442	H	-5.201359	-0.798181	1.027376

H	5.257190	1.245741	0.772102
C	-0.374482	1.691920	0.950242
H	0.635548	2.095907	1.041158
C	-1.019017	2.376770	-0.176096
C	-1.095407	1.748419	2.295462
H	-0.447084	1.342447	3.078813
H	-1.359677	2.775766	2.591356
H	-2.030127	1.175523	2.305112
O	-0.453894	2.733909	-1.215553
Si	1.350157	-0.974835	1.818825
C	0.250459	-1.664709	3.214155
H	-0.527774	-0.954840	3.50655
H	-0.227898	-2.596985	2.895414
H	0.852644	-1.890678	4.103588
C	2.619235	-2.337704	1.414272
H	3.235124	-2.563784	2.294542
H	2.108352	-3.259839	1.117104
H	3.289716	-2.052457	0.598292
O	2.207603	0.375305	2.434828
C	3.064632	0.283631	3.567345
H	2.547940	-0.203093	4.409587
H	3.948507	-0.329534	3.330614
C	3.497507	1.684589	3.977967
H	4.155434	1.643576	4.854494
H	4.038290	2.174994	3.161527
H	2.623589	2.296562	4.224022
O	-2.370583	2.563006	0.000228
C	-3.172874	3.319675	-0.961321
C	-3.206950	2.620050	-2.327136
H	-3.928865	3.121898	-2.982961
H	-2.223735	2.638550	-2.79782
H	-3.522661	1.576973	-2.21244
C	-4.567876	3.315827	-0.324925
H	-5.268343	3.890299	-0.941274
H	-4.950889	2.293894	-0.231045
H	-4.535788	3.762514	0.674234
C	-2.650405	4.759097	-1.071033
H	-3.325081	5.352896	-1.699132
H	-2.611862	5.223464	-0.079102
H	-1.651487	4.777299	-1.508498
Total SCF energy		-1732.49045400	
Gibbs free energy at 298K		-1731.84113800	
Free energy in solution		-1732.46259900	

H	-5.132971	-1.355080	-0.645446
C	-0.142130	1.173603	-1.744211
H	-1.229519	1.275926	-1.741632
C	0.483164	2.386110	-1.212238
O	1.554402	2.873370	-1.567583
O	-0.253534	2.935934	-0.171126
C	0.172096	4.163394	0.496983
C	-0.934184	4.400143	1.532421
H	-0.728363	5.308322	2.109574
H	-1.905904	4.518206	1.040171
H	-0.994941	3.556626	2.229477
C	0.217494	5.329133	-0.501462
H	0.416068	6.267677	0.029744
H	0.996920	5.171630	-1.247739
H	-0.746714	5.425524	-1.013675
C	1.519119	3.964223	1.205615
H	1.761047	4.851404	1.803216
H	1.466721	3.103738	1.883633
H	2.316100	3.794043	0.481707
Si	-0.614602	-2.070045	-1.208395
C	0.722895	-2.810185	-2.348945
H	1.111867	-2.078541	-3.06308
H	1.557753	-3.190716	-1.751094
H	0.314867	-3.654653	-2.919203
C	-1.209369	-3.494542	-0.091936
H	-1.639263	-4.299572	-0.702809
H	-0.373143	-3.912305	0.479127
H	-1.971478	-3.170545	0.622444
O	-1.949426	-1.598516	-2.176291
C	-2.396228	-2.377692	-3.28055
H	-1.602061	-2.458747	-4.0381
H	-2.644749	-3.402319	-2.958281
C	-3.623964	-1.719151	-3.894269
H	-3.975891	-2.293441	-4.759707
H	-4.437181	-1.661997	-3.162835
H	-3.385607	-0.702569	-4.224188
H	-0.179918	-0.053041	-3.522852
C	0.378277	0.801913	-3.129867
H	1.441669	0.536290	-3.11387
H	0.276485	1.626781	-3.85223
Total SCF energy		-1732.49134794	
Gibbs free energy at 298K		-1731.84118600	
Free energy in solution		-1732.46354000	

iso-TS

Cartesian coordinates

ATOM	X	Y	Z
C	0.584471	-2.480896	1.861099
C	-0.276673	-1.400077	1.612297
C	-1.141025	-0.921474	2.611342
C	-1.192745	-1.573404	3.848875
C	-0.375918	-2.691240	4.070387
C	0.523934	-3.141629	3.094738
H	-1.846612	-1.208189	4.635959
H	-0.421378	-3.201385	5.027540
H	1.179529	-3.983270	3.300279
C	1.484643	-2.675660	0.736887
O	2.415509	-3.637270	0.684314
C	2.451175	-2.227559	-1.257819
C	3.059699	-3.511055	-0.620448
H	4.135513	-3.449506	-0.447489
N	1.404527	-1.871373	-0.283142
H	1.963566	-2.473342	-2.208431
H	2.833545	-4.420497	-1.182852
Rh	-0.085791	-0.392591	-0.007428
C	-1.772547	0.313970	2.175130
O	-2.492417	1.110594	2.974967
C	-2.132969	2.082124	0.805509
C	-2.723866	2.343835	2.222484
H	-3.799159	2.529433	2.225956
N	-1.555949	0.735463	0.963463
H	-1.298709	2.762124	0.604810
H	-2.214457	3.147530	2.759381
C	3.444574	-1.072697	-1.521139
H	2.830084	-0.231445	-1.867668
C	4.412327	-1.459017	-2.650760
H	5.071959	-2.288534	-2.360931
H	3.877006	-1.758064	-3.560797
H	5.054897	-0.609902	-2.906772
C	4.186966	-0.610477	-0.260859
H	3.480857	-0.261554	0.496759
H	4.820522	-1.400731	0.165268
H	4.842026	0.231884	-0.508131
C	-3.122353	2.196536	-0.375952
H	-2.586785	1.788242	-1.240763
C	-3.438754	3.675138	-0.650667
H	-4.084543	3.773925	-1.530264
H	-3.965892	4.142061	0.193030

13b-*E*-*Si*

Cartesian coordinates

ATOM	X	Y	Z
C	-2.877758	-1.305853	-1.040091
C	-1.486777	-1.487646	-0.932487
C	-0.844621	-2.464105	-1.713342
C	-1.593616	-3.307770	-2.541179
C	-2.988596	-3.159624	-2.585579
C	-3.637990	-2.153526	-1.857220
H	-1.104332	-4.058689	-3.155762
H	-3.573250	-3.818399	-3.220426
H	-4.713799	-2.024459	-1.941967
C	-3.279413	-0.123619	-0.292275
O	-4.548171	0.291934	-0.172951
C	-3.009234	1.763912	0.925733
C	-4.518696	1.453190	0.713373
H	-5.073068	2.253928	0.220845
N	-2.366266	0.600201	0.293525
H	-2.765524	1.752935	1.994015
H	-5.033768	1.169641	1.634969
Rh	-0.413532	-0.175514	0.028567
C	0.601024	-2.323547	-1.591386
O	1.469221	-3.028842	-2.326506
C	2.562722	-1.360928	-0.989066
C	2.796956	-2.490751	-2.032387
H	3.405564	-3.317699	-1.660859
N	1.095943	-1.412777	-0.799954
H	2.781279	-0.378572	-1.417317
H	3.214475	-2.131781	-2.975873
C	-2.497494	3.102074	0.343457
H	-1.405772	3.043103	0.433118
C	-2.998974	4.279966	1.192565
H	-4.093469	4.372704	1.159227
H	-2.701995	4.173856	2.242951
H	-2.582828	5.224048	0.824105
C	-2.847228	3.293311	-1.139105
H	-2.522282	2.441395	-1.745398
H	-3.924518	3.434119	-1.298050
H	-2.346133	4.185330	-1.530796
C	3.377627	-1.468844	0.319488
H	2.971141	-0.688710	0.974115
C	4.848680	-1.125166	0.033328
H	5.429594	-1.122471	0.962195
H	5.314722	-1.859942	-0.638512

H	-2.526085	4.252273	-0.839542	H	4.942213	-0.134538	-0.424726
C	-4.405841	1.374593	-0.200538	C	3.249570	-2.812750	1.045601
H	-4.186309	0.323703	0.004871	H	2.208514	-3.050187	1.271933
H	-5.043752	1.762216	0.604788	H	3.684087	-3.641608	0.471053
H	-4.997524	1.409170	-1.121953	H	3.783884	-2.770738	2.001106
C	0.803247	1.739944	-1.764792	C	2.680512	2.324184	1.317645
H	0.123742	0.873422	-1.839473	H	2.261897	2.329728	2.320684
C	1.491542	1.919244	-0.595808	C	1.841681	1.957317	0.319499
C	0.908287	2.579949	-3.008305	C	4.113725	2.750081	1.166626
H	1.375048	2.047623	-3.853186	H	4.271513	3.797140	1.471452
H	-0.074359	2.924807	-3.364876	H	4.790801	2.146267	1.790017
H	1.519106	3.464745	-2.806969	H	4.444778	2.652634	0.129145
O	1.374067	1.186970	0.478359	O	0.566304	1.660076	0.458659
Si	-1.747228	-1.818035	-1.023984	O	2.379964	1.862742	-0.976452
C	-1.029775	-3.312417	-1.973921	C	1.946260	2.790511	-2.009794
H	-0.298461	-3.001650	-2.728141	C	3.123732	2.826897	-2.992050
H	-0.529517	-3.999159	-1.281145	H	2.896928	3.469679	-3.850521
H	-1.815900	-3.881355	-2.486092	H	4.024064	3.208626	-2.499537
C	-3.131368	-2.535017	0.074775	H	3.339825	1.819826	-3.366363
H	-3.923420	-2.991309	-0.532768	C	1.688418	4.188254	-1.433077
H	-2.722439	-3.316310	0.726604	H	1.425461	4.881613	-2.240516
H	-3.595745	-1.779607	0.715900	H	0.865521	4.169704	-0.712595
O	-2.433586	-0.733770	-2.172155	H	2.578769	4.571301	-0.924857
C	-3.191322	-1.177255	-3.292051	C	0.690745	2.248824	-2.711292
H	-2.606875	-1.887339	-3.897183	H	0.418198	2.881865	-3.565332
H	-4.099020	-1.706311	-2.957893	H	0.871432	1.233505	-3.082718
C	-3.576897	0.025181	-4.142692	H	-0.150023	2.216401	-2.016047
H	-4.155687	-0.291149	-5.018925	Si	-0.673885	-1.639571	1.907462
H	-4.183582	0.728406	-3.562142	C	-2.267477	-1.267594	2.880423
H	-2.680242	0.550942	-4.487396	H	-2.352676	-0.216385	3.170621
O	2.429904	2.935850	-0.580918	H	-3.153867	-1.535890	2.295622
C	2.701002	3.707317	0.618029	H	-2.275739	-1.871032	3.797253
C	3.585120	2.910317	1.588895	C	-0.648714	-3.506543	1.587608
H	3.880267	3.537791	2.439566	H	-0.571274	-4.029875	2.548252
H	3.050798	2.032488	1.954124	H	-1.575334	-3.824495	1.097834
H	4.495726	2.577373	1.078417	H	0.187631	-3.826062	0.961834
C	3.467781	4.923219	0.081724	O	0.663382	-1.355953	2.912340
H	3.773396	5.581715	0.902898	C	0.842118	-0.127674	3.624214
H	4.365380	4.597633	-0.454588	H	0.836759	0.712230	2.919460
H	2.844805	5.496724	-0.612979	H	0.011182	0.015178	4.332745
C	1.397562	4.157743	1.292771	C	2.160880	-0.185922	4.379252
H	1.615433	4.846229	2.117815	H	2.309996	0.733670	4.957718
H	0.757892	4.679411	0.571123	H	2.174208	-1.037106	5.068839
H	0.857616	3.294783	1.690405	H	2.996819	-0.291231	3.680461

Total SCF energy	-1732.46944981
Gibbs free energy at 298K	-1731.82194900
Imaginary frequency	-118.290
Free energy in solution	-1732.44085400

Total SCF energy	-1732.48382048
Gibbs free energy at 298K	-1731.83569600
Free energy in solution	-1732.45417400

Tauto-TS1

Cartesian coordinates

ATOM	X	Y	Z
C	2.099252	-0.158441	2.204725
C	0.818490	-0.490499	1.726506
C	-0.237567	-0.681375	2.640522
C	0.008835	-0.651899	4.017560
C	1.312435	-0.415951	4.477217
C	2.355723	-0.144228	3.581921
H	-0.804592	-0.789013	4.725087
H	1.507793	-0.401713	5.545033
H	3.347637	0.097863	3.954130
C	2.971263	0.223225	1.110127
O	4.287441	0.421914	1.279743
C	3.613106	0.726621	-0.994495
C	4.842298	0.653813	-0.043248
H	5.419474	1.578993	0.000534
N	2.492199	0.364705	-0.095955
H	3.688970	-0.048293	-1.766319
H	5.513428	-0.179500	-0.268374
Rh	0.380204	-0.162483	-0.147473
C	-1.508079	-0.736092	1.941309
O	-2.690037	-0.834070	2.568350
C	-2.948253	-0.616144	0.199000
C	-3.710269	-0.597055	1.552535
H	-4.462518	-1.380322	1.655530
N	-1.538003	-0.602972	0.642970
H	-3.118804	0.317325	-0.343721
H	-4.165188	0.373295	1.771917
C	3.455555	2.087147	-1.715210
H	2.559301	1.998483	-2.339283
C	4.646980	2.313383	-2.662735
H	5.587687	2.458924	-2.115544
H	4.786176	1.470140	-3.351280
H	4.484394	3.212870	-3.266055
C	3.244452	3.269942	-0.761246
H	2.298441	3.179613	-0.220886
H	4.067296	3.371381	-0.040615
H	3.202854	4.204057	-1.333375

Tauto-TS2

Cartesian coordinates

ATOM	X	Y	Z
C	-2.588473	-1.090177	-1.619669
C	-1.188868	-1.087047	-1.452520
C	-0.352253	-1.575530	-2.475448
C	-0.916295	-2.139355	-3.624644
C	-2.312016	-2.203002	-3.748908
C	-3.152716	-1.665684	-2.765204
H	-0.278329	-2.510577	-4.422100
H	-2.748016	-2.647686	-4.638055
H	-4.230974	-1.676703	-2.899600
C	-3.220012	-0.359045	-0.538861
O	-4.543180	-0.174798	-0.423569
C	-3.316001	0.970959	1.287392
C	-4.743314	0.566781	0.817847
H	-5.391146	1.414913	0.590361
N	-2.466888	0.189646	0.372510
H	-3.139683	0.619868	2.310596
H	-5.252124	-0.101623	1.517689
Rh	-0.411154	-0.144518	0.029386
C	1.037528	-1.287610	-2.169133
O	2.053683	-1.521262	-3.012245
C	2.784642	-0.451014	-0.996185
C	3.209670	-0.830573	-2.441404
H	4.058156	-1.513637	-2.496755
N	1.328055	-0.699820	-1.043726
H	2.930148	0.618005	-0.819133
H	3.403613	0.043336	-3.070499
C	-2.997440	2.484608	1.241151
H	-1.930863	2.564974	1.478247
C	-3.804343	3.229239	2.315860
H	-4.883977	3.201186	2.114200
H	-3.638665	2.804507	3.313810
H	-3.510291	4.283843	2.351247
C	-3.189816	3.102055	-0.150184
H	-2.541577	2.616892	-0.885022
H	-4.229979	3.041077	-0.498087
H	-2.919287	4.163584	-0.125849

C	-3.291091	-1.794928	-0.743437	C	3.495973	-1.226406	0.138073
H	-2.520595	-1.783921	-1.522343	H	2.919537	-1.008484	1.043940
C	-4.658596	-1.553388	-1.402872	C	4.922891	-0.686542	0.322874
H	-4.887387	-2.349600	-2.120118	H	5.416767	-1.184237	1.165164
H	-5.469905	-1.541537	-0.661837	H	5.543029	-0.864236	-0.566972
H	-4.683617	-0.599067	-1.942045	H	4.919633	0.390509	0.523621
C	-3.236789	-3.172499	-0.070601	C	3.499150	-2.748557	-0.054989
H	-2.271130	-3.346441	0.409408	H	2.490012	-3.137102	-0.214140
H	-4.027602	-3.302682	0.679430	H	4.127389	-3.060586	-0.899660
H	-3.373548	-3.959643	-0.820564	H	3.897966	-3.238101	0.840446
C	-0.292045	1.363560	-1.646985	C	1.470850	1.618487	1.968349
H	0.667461	1.684297	-2.052707	H	0.654686	1.102307	2.470867
C	-0.808793	2.484139	-0.850141	C	1.190857	2.110781	0.726244
O	-0.122571	3.294809	-0.229937	C	2.769876	1.760902	2.706922
O	-2.186985	2.541916	-0.838113	H	2.632269	2.236296	3.690135
C	-2.895618	3.620714	-0.151238	H	3.248499	0.787954	2.901139
C	-4.368680	3.310059	-0.443482	H	3.476236	2.371324	2.137166
H	-5.014766	4.073963	0.003050	O	0.043283	1.979722	0.111065
H	-4.550818	3.288256	-1.523006	O	2.228714	2.745568	0.048760
H	-4.654322	2.336545	-0.028940	C	1.968393	3.896621	-0.802210
C	-2.519713	4.981002	-0.756280	C	3.358275	4.518883	-0.985625
H	-3.150699	5.766829	-0.324084	H	3.306771	5.390978	-1.647190
H	-1.473267	5.217444	-0.561302	H	3.769149	4.835624	-0.021279
H	-2.684296	4.970107	-1.839798	H	4.047732	3.791106	-1.427720
C	-2.627136	3.575091	1.359393	C	1.028256	4.888165	-0.104052
H	-3.265245	4.303019	1.874853	H	0.933553	5.802613	-0.701377
H	-2.859284	2.580159	1.757807	H	0.035781	4.450207	0.025260
H	-1.581944	3.799926	1.573338	H	1.424368	5.160407	0.880511
Si	0.930364	-2.486215	-0.272222	C	1.403047	3.449921	-2.159251
C	2.748294	-2.803845	-0.752039	H	1.310522	4.309512	-2.834857
H	3.038344	-2.247003	-1.648785	H	2.077280	2.723048	-2.628306
H	3.418044	-2.512371	0.064517	H	0.425724	2.984025	-2.028682
H	2.917500	-3.869910	-0.949978	Si	-0.530833	-2.271304	1.171856
C	0.563675	-3.690560	1.155778	C	-2.099442	-2.437425	2.248938
H	0.631616	-4.728305	0.804209	H	-2.218890	-1.588319	2.930543
H	1.300211	-3.559585	1.956630	H	-2.992710	-2.494003	1.616696
H	-0.428371	-3.551052	1.593727	H	-2.068553	-3.351859	2.854822
O	-0.064349	-2.908448	-1.607420	C	-0.435376	-3.889010	0.168182
C	0.227365	-3.998673	-2.473981	H	-0.332601	-4.752031	0.838658
H	1.208183	-3.858263	-2.953575	H	-1.352509	-4.028305	-0.415742
H	0.276528	-4.941846	-1.905043	H	0.407101	-3.907107	-0.529100
C	-0.857378	-4.093837	-3.537659	O	0.830326	-2.191676	2.216052
H	-0.648703	-4.918985	-4.229231	C	0.954092	-3.006398	3.376351
H	-1.834877	-4.267107	-3.075079	H	0.123201	-2.813703	4.072464

H	-0.910307	-3.162177	-4.110844
C	-1.185422	0.786808	-2.744192
H	-1.436247	1.536245	-3.512933
H	-2.134291	0.407570	-2.356924
H	-0.684403	-0.047880	-3.247814

Total SCF energy -1732.48050273
Gibbs free energy at 298K -1731.83105100
Imaginary frequency -25.370
Free energy in solution -1732.45323600

H	0.910435	-4.074758	3.107203
C	2.278770	-2.700282	4.061254
H	2.390246	-3.301669	4.971642
H	3.117819	-2.922768	3.393427
H	2.329942	-1.640749	4.333006

Total SCF energy -1732.47421572
Gibbs free energy at 298K -1731.82548600
Imaginary frequency -68.080
Free energy in solution -1732.44489900

14a-*E*-*Si*-*Si*

Cartesian coordinates

ATOM	X	Y	Z
C	-3.385314	1.233633	-0.136824
C	-2.575586	0.115847	0.122494
C	-3.127369	-1.172167	0.082229
C	-4.493652	-1.347805	-0.168089
C	-5.299982	-0.219928	-0.375245
C	-4.755805	1.071829	-0.375289
H	-4.923964	-2.344503	-0.215360
H	-6.361493	-0.350807	-0.562281
H	-5.388433	1.932963	-0.573239
C	-2.572961	2.438131	-0.168589
O	-3.065232	3.664028	-0.397919
C	-0.684239	3.680543	-0.121991
C	-1.940715	4.585168	-0.274766
H	-1.930113	5.209512	-1.169915
N	-1.288717	2.344833	0.024572
H	-0.157118	3.920788	0.807205
H	-2.128317	5.211606	0.601630
Rh	-0.659691	0.345658	0.316122
C	-2.073597	-2.164224	0.214319
O	-2.281320	-3.477123	0.031925
C	0.023600	-2.975937	0.421905
C	-0.960467	-4.093473	-0.019636
H	-0.978214	-4.962835	0.639234
N	-0.849253	-1.782622	0.439562
H	0.772818	-2.821290	-0.360931
H	-0.795066	-4.418577	-1.049758
C	0.340388	3.758834	-1.277798
H	1.086821	2.989476	-1.047370
C	1.039384	5.128036	-1.265329
H	0.343298	5.944943	-1.499446
H	1.492696	5.344815	-0.289624

14a-*E*-*Si*-*Re*

Cartesian coordinates

ATOM	X	Y	Z
C	-3.581374	-0.457680	0.158494
C	-2.489332	0.317627	0.571374
C	-2.603679	1.151553	1.695661
C	-3.818787	1.239985	2.383883
C	-4.916545	0.492598	1.933079
C	-4.807567	-0.364288	0.830169
H	-3.910702	1.871125	3.263696
H	-5.862988	0.565287	2.460189
H	-5.659622	-0.957697	0.509894
C	-3.195466	-1.310211	-0.950735
O	-4.049616	-2.143602	-1.565376
C	-1.839072	-2.317658	-2.439036
C	-3.320706	-2.700004	-2.696431
H	-3.509777	-3.774133	-2.714411
N	-1.969244	-1.287140	-1.389999
H	-1.405954	-1.855234	-3.332302
H	-3.726697	-2.243657	-3.604449
Rh	-0.763199	0.118874	-0.282039
C	-1.311460	1.741978	2.006728
O	-1.057181	2.436500	3.125288
C	0.915473	2.095552	1.799779
C	0.391950	2.628048	3.164588
H	0.574225	3.691182	3.328801
N	-0.308742	1.524762	1.207958
H	1.606917	1.262352	1.958792
H	0.767890	2.058298	4.017432
C	-0.929960	-3.495950	-2.014403
H	0.036727	-3.044359	-1.763342
C	-0.714468	-4.451835	-3.198737
H	-1.642830	-4.962427	-3.486873
H	-0.334808	-3.925249	-4.083635

H	1.835014	5.157735	-2.017761	H	0.010743	-5.229376	-2.935018
C	-0.256865	3.431382	-2.652516	C	-1.420824	-4.228100	-0.758218
H	-0.644588	2.409488	-2.670024	H	-1.426840	-3.549499	0.098782
H	-1.053181	4.132337	-2.937939	H	-2.421131	-4.660526	-0.893265
H	0.522234	3.502209	-3.420577	H	-0.741246	-5.054637	-0.520546
C	0.744231	-3.224928	1.766410	C	1.596764	3.146867	0.895207
H	1.220666	-2.274736	2.031668	H	1.689180	2.668725	-0.086071
C	1.832803	-4.295487	1.591153	C	3.000804	3.467852	1.432077
H	2.395475	-4.430372	2.521734	H	3.518974	4.168897	0.767396
H	1.405704	-5.272298	1.325831	H	2.959189	3.935773	2.425501
H	2.546634	-4.020597	0.804873	H	3.616626	2.564327	1.516310
C	-0.207883	-3.579740	2.916610	C	0.770776	4.425583	0.701006
H	-0.994820	-2.828830	3.028211	H	-0.244044	4.198308	0.362985
H	-0.679563	-4.561700	2.781158	H	0.706496	5.025909	1.618058
H	0.345107	-3.616928	3.861651	H	1.235622	5.057413	-0.063593
C	2.101002	0.044461	-2.459537	C	1.999273	-2.682597	0.807178
H	2.199569	1.104497	-2.250077	H	1.630790	-3.254872	-0.039746
C	0.803926	-0.449922	-2.389780	C	1.063914	-1.888632	1.435768
C	3.233620	-0.628909	-3.182283	C	3.360749	-3.030742	1.334183
H	3.361452	-0.241807	-4.206697	H	3.412707	-4.061896	1.721732
H	4.193263	-0.467179	-2.672789	H	4.130916	-2.958441	0.551592
H	3.066542	-1.706952	-3.260744	H	3.648842	-2.356116	2.144644
O	-0.219166	0.178525	-1.963209	O	-0.135833	-1.674492	1.035455
O	0.646894	-1.794469	-2.766062	O	1.492283	-1.223680	2.601245
C	-0.243758	-2.107742	-3.877541	C	0.947492	-1.663467	3.879070
C	0.145539	-3.539483	-4.261762	C	1.890077	-1.039886	4.914380
H	-0.481435	-3.903325	-5.083618	H	1.555768	-1.270595	5.932312
H	1.193665	-3.584663	-4.575345	H	2.909250	-1.419510	4.786914
H	0.015428	-4.214623	-3.408215	H	1.918143	0.049849	4.801635
C	0.013566	-1.153202	-5.053159	C	0.978983	-3.195632	3.993436
H	-0.596822	-1.446946	-5.914818	H	0.636454	-3.499952	4.989240
H	-0.247263	-0.124090	-4.788123	H	0.322843	-3.661467	3.252006
H	1.066680	-1.179449	-5.351460	H	1.993162	-3.578711	3.845711
C	-1.718038	-2.046856	-3.451223	C	-0.487891	-1.151525	4.075553
H	-2.364015	-2.332888	-4.290892	H	-0.875553	-1.475357	5.049799
H	-1.914614	-2.739055	-2.625831	H	-0.520377	-0.057973	4.049201
H	-1.979456	-1.039636	-3.123889	H	-1.138895	-1.530724	3.285833
Si	-0.819660	0.600138	2.693857	Si	-1.312685	1.848727	-1.865843
C	-0.529073	2.405397	3.242404	C	-1.801892	1.143517	-3.574371
H	0.418844	2.781718	2.843624	H	-1.029859	0.469853	-3.961728
H	-1.337788	3.054347	2.887874	H	-2.744832	0.588588	-3.513636
H	-0.493077	2.493835	4.335547	H	-1.941232	1.945643	-4.310130
C	-2.454239	0.041300	3.504580	C	-2.719692	3.040066	-1.368471
H	-2.406060	0.123751	4.598102	H	-2.861964	3.824065	-2.123194

H	-3.282634	0.670892	3.159736
H	-2.705807	-0.995380	3.256704
O	0.462539	-0.333371	3.365118
C	0.677706	-0.412738	4.767936
H	0.527333	0.566633	5.249208
H	-0.045054	-1.109190	5.222312
C	2.099456	-0.890655	5.034209
H	2.286147	-0.968695	6.112339
H	2.266509	-1.875047	4.583368
H	2.824081	-0.192188	4.602740
H	5.827322	3.140886	0.536829
C	5.545466	2.105853	0.361622
C	6.536498	1.132861	0.185980
C	4.200674	1.751543	0.318414
C	6.174527	-0.198517	-0.032074
H	7.586099	1.412307	0.222480
C	3.827188	0.415690	0.092044
H	3.421691	2.492681	0.465486
C	4.827203	-0.554887	-0.078761
H	6.940907	-0.957536	-0.164144
H	4.541865	-1.591006	-0.244953
C	2.407725	0.017531	0.084113
H	2.217023	-1.059276	0.007110
O	1.496954	0.804203	0.429567

Total SCF energy -2078.05962502
Gibbs free energy at 298K -2077.30921700
Free energy in solution -2078.02240700

H	-3.665558	2.494906	-1.272327
H	-2.525293	3.531094	-0.408986
O	0.112188	2.782634	-2.113974
C	0.121411	3.928471	-2.953511
H	-0.447995	3.750034	-3.880000
H	-0.357802	4.778198	-2.441209
C	1.561263	4.278942	-3.306954
H	1.598727	5.173046	-3.941413
H	2.142531	4.473695	-2.399119
H	2.035943	3.449520	-3.841737
H	6.246381	-2.565030	-2.494242
C	5.677804	-1.722486	-2.110314
C	6.327126	-0.530778	-1.777873
C	4.297585	-1.829277	-1.948344
C	5.592019	0.554141	-1.285654
H	7.403241	-0.445625	-1.903483
C	3.554183	-0.746338	-1.451752
H	3.786882	-2.754956	-2.203707
C	4.214133	0.450457	-1.124434
H	6.098486	1.481737	-1.032569
H	3.627717	1.286380	-0.758839
C	2.093187	-0.861926	-1.331950
H	1.652888	-1.789327	-1.719198
O	1.364623	0.081757	-0.988189

Total SCF energy -2078.05224524
Gibbs free energy at 298K -2077.30085500
Free energy in solution -2078.01528900

14TS-*E-Si-Si*

Cartesian coordinates

ATOM	X	Y	Z
C	-3.408497	1.190059	-0.143552
C	-2.584804	0.079317	0.101818
C	-3.119633	-1.214964	0.038675
C	-4.482153	-1.404874	-0.221690
C	-5.302341	-0.284605	-0.415384
C	-4.775539	1.014162	-0.391743
H	-4.899202	-2.406248	-0.286207
H	-6.361067	-0.426562	-0.609999
H	-5.418780	1.869854	-0.578884
C	-2.612155	2.405759	-0.150847
O	-3.120058	3.628638	-0.361323
C	-0.740783	3.672859	-0.075443
C	-2.008984	4.562806	-0.215819

14TS-*E-Si-Re*

Cartesian coordinates

ATOM	X	Y	Z
C	3.592927	0.470552	0.393012
C	2.510368	-0.387316	0.626496
C	2.608716	-1.382513	1.613684
C	3.796683	-1.547583	2.334371
C	4.887703	-0.712078	2.053897
C	4.794585	0.304805	1.094739
H	3.872652	-2.305379	3.109567
H	5.814347	-0.842619	2.604527
H	5.638922	0.963395	0.909741
C	3.224270	1.483788	-0.579682
O	4.090339	2.406650	-1.026462
C	1.914128	2.693668	-1.954976
C	3.398051	3.130393	-2.082288

H	-2.003855	5.204617	-1.098594	H	3.566371	4.195419	-1.916545
N	-1.327396	2.326610	0.046225	N	2.012602	1.521611	-1.058931
H	-0.219047	3.903867	0.858953	H	1.532585	2.358832	-2.924933
H	-2.208666	5.169506	0.671760	H	3.850735	2.835248	-3.033797
Rh	-0.671650	0.331342	0.309623	Rh	0.795783	-0.086853	-0.238214
C	-2.054049	-2.195444	0.164234	C	1.324163	-2.046063	1.776704
O	-2.245543	-3.508729	-0.033312	O	1.055276	-2.918221	2.758442
C	0.050815	-2.985965	0.378721	C	-0.878343	-2.437021	1.418288
C	-0.917898	-4.110493	-0.079239	C	-0.382486	-3.174663	2.696291
H	-0.931383	-4.984848	0.573047	H	-0.517635	-4.256893	2.665014
N	-0.835419	-1.802171	0.400879	N	0.342430	-1.731259	0.983177
H	0.804835	-2.815868	-0.396271	H	-1.615704	-1.670610	1.677514
H	-0.741547	-4.427078	-1.110353	H	-0.820372	-2.782543	3.617337
C	0.285474	3.784796	-1.226762	C	0.965141	3.790552	-1.418148
H	1.040506	3.020821	-1.007096	H	-0.010319	3.304645	-1.306505
C	0.966955	5.162271	-1.188412	C	0.812151	4.914449	-2.455850
H	0.261354	5.974352	-1.410769	H	1.748830	5.468124	-2.601852
H	1.414474	5.367663	-0.207641	H	0.497537	4.525564	-3.432464
H	1.764712	5.215104	-1.937347	H	0.059076	5.638421	-2.126030
C	-0.304194	3.474995	-2.608863	C	1.369015	4.328301	-0.038626
H	-0.682460	2.450208	-2.646006	H	1.345806	3.529839	0.707871
H	-1.106636	4.172735	-2.884638	H	2.367128	4.785789	-0.047716
H	0.476343	3.566774	-3.373216	H	0.663002	5.103601	0.280971
C	0.765357	-3.240449	1.725442	C	-1.483959	-3.349522	0.327896
H	1.229080	-2.287704	2.003376	H	-1.592029	-2.713739	-0.556716
C	1.867379	-4.296449	1.545839	C	-2.874542	-3.835554	0.767425
H	2.425381	-4.434808	2.478704	H	-3.345979	-4.425665	-0.026537
H	1.453507	-5.275293	1.267201	H	-2.819229	-4.476826	1.658167
H	2.583288	-4.004551	0.767660	H	-3.540995	-2.996913	1.002675
C	-0.190113	-3.618547	2.865346	C	-0.582854	-4.530173	-0.057979
H	-0.985659	-2.877318	2.980419	H	0.420439	-4.194307	-0.332838
H	-0.650107	-4.604082	2.716207	H	-0.495026	-5.270605	0.747984
H	0.357332	-3.660226	3.813393	H	-1.001552	-5.050077	-0.926351
C	2.138008	0.140319	-2.399789	C	-2.064965	2.409320	0.792111
H	2.192359	1.204855	-2.197905	H	-1.536953	3.171995	0.227534
C	0.846505	-0.389493	-2.390170	C	-1.201735	1.638727	1.601871
C	3.295027	-0.484151	-3.130274	C	-3.465004	2.761279	1.230932
H	3.386294	-0.106807	-4.162038	H	-3.474507	3.516897	2.032541
H	4.249825	-0.264154	-2.635871	H	-4.046077	3.173682	0.398564
H	3.184350	-1.570615	-3.191939	H	-3.998909	1.882587	1.604073
O	-0.202448	0.199449	-1.983838	O	0.032552	1.484400	1.412229
O	0.746154	-1.728156	-2.795614	O	-1.829804	0.920466	2.614721
C	-0.134080	-2.060049	-3.910826	C	-1.373939	1.081800	3.992670
C	0.308643	-3.471367	-4.311924	C	-2.465521	0.384035	4.810339

H	-0.301415	-3.845987	-5.141541
H	1.359002	-3.474351	-4.621124
H	0.199686	-4.162296	-3.468112
C	0.090465	-1.080529	-5.072550
H	-0.508046	-1.382916	-5.939467
H	-0.207615	-0.065430	-4.792933
H	1.144264	-1.065523	-5.369445
C	-1.609877	-2.059093	-3.486626
H	-2.241925	-2.366272	-4.329344
H	-1.780374	-2.763007	-2.665577
H	-1.912150	-1.065152	-3.154406
Si	-0.848208	0.549651	2.687304
C	-0.571748	2.349340	3.259683
H	0.374289	2.737858	2.868375
H	-1.384610	2.997033	2.912591
H	-0.538753	2.422716	4.353991
C	-2.487018	-0.029293	3.474808
H	-2.446592	0.033729	4.569956
H	-3.315502	0.603137	3.135569
H	-2.732446	-1.062308	3.206339
O	0.431563	-0.386289	3.356923
C	0.642413	-0.474815	4.759965
H	0.484642	0.499987	5.247915
H	-0.077932	-1.178911	5.206375
C	2.066097	-0.946091	5.027627
H	2.249449	-1.030474	6.105859
H	2.240711	-1.926287	4.570609
H	2.787827	-0.240306	4.603390
H	5.757950	3.194382	0.688207
C	5.495837	2.160744	0.477200
C	6.504767	1.205499	0.308480
C	4.157476	1.790779	0.382735
C	6.166199	-0.123945	0.045703
H	7.549060	1.496446	0.385519
C	3.807677	0.457465	0.110952
H	3.364775	2.517878	0.526415
C	4.825495	-0.495318	-0.052321
H	6.945764	-0.870546	-0.080686
H	4.559610	-1.530621	-0.252824
C	2.390596	0.044248	0.051792
H	2.219105	-1.035872	-0.025268
O	1.469198	0.812011	0.429405
Total SCF energy		-2078.05965064	
Gibbs free energy at 298K		-2077.30801200	

H	-2.236607	0.434672	5.880687
H	-3.437954	0.855714	4.636781
H	-2.543275	-0.670759	4.523958
C	-1.311218	2.575729	4.345297
H	-1.048995	2.703452	5.401773
H	-0.552418	3.088418	3.745577
H	-2.278970	3.056341	4.169634
C	-0.010878	0.419115	4.236289
H	0.254616	0.499156	5.297741
H	-0.042891	-0.643032	3.977620
H	0.766667	0.892457	3.635749
Si	1.416711	-1.491143	-2.074524
C	1.911537	-0.473991	-3.613938
H	1.116495	0.220431	-3.905792
H	2.822957	0.102741	-3.422673
H	2.112012	-1.129626	-4.470700
C	2.853987	-2.706187	-1.760807
H	3.005165	-3.360293	-2.629154
H	3.788555	-2.161009	-1.587253
H	2.676919	-3.343995	-0.888880
O	0.029455	-2.404480	-2.502787
C	0.015613	-3.299732	-3.606101
H	0.515269	-2.857254	-4.482368
H	0.562890	-4.222498	-3.353946
C	-1.427613	-3.630893	-3.963589
H	-1.466411	-4.327827	-4.809853
H	-1.939241	-4.091387	-3.111803
H	-1.971899	-2.719804	-4.232597
H	-6.049444	2.591903	-2.828185
C	-5.521298	1.806032	-2.294178
C	-6.199367	0.651754	-1.895342
C	-4.162728	1.948945	-2.011869
C	-5.508265	-0.358650	-1.218551
H	-7.257809	0.537424	-2.114328
C	-3.463327	0.942446	-1.329649
H	-3.633387	2.845764	-2.328338
C	-4.150663	-0.217102	-0.941301
H	-6.030945	-1.261592	-0.912592
H	-3.598664	-1.001102	-0.434427
C	-2.006602	1.087319	-1.075638
H	-1.549522	1.949421	-1.580569
O	-1.294953	0.060252	-0.853321
Total SCF energy		-2078.04984662	
Gibbs free energy at 298K		-2077.29882700	

Imaginary frequency	-48.481
Free energy in solution	-2078.02247800

15TS-*E*-*Re*-*Re*

Cartesian coordinates

ATOM	X	Y	Z
C	2.79572	-2.027401	0.409828
C	2.331695	-0.919593	-0.31168
C	2.917261	-0.596705	-1.543729
C	3.997094	-1.341796	-2.031784
C	4.484712	-2.414869	-1.273021
C	3.884039	-2.774704	-0.059842
H	4.444529	-1.101874	-2.992512
H	5.327311	-2.990831	-1.643284
H	4.249909	-3.630253	0.501308
C	1.972117	-2.245918	1.585777
O	2.239136	-3.202352	2.48675
C	0.365138	-1.863872	3.120976
C	1.176184	-3.138714	3.479673
H	0.593125	-4.059656	3.394464
N	0.941441	-1.4819	1.81221
H	0.603385	-1.062335	3.828784
H	1.647019	-3.098033	4.463479
Rh	0.71223	-0.007389	0.250492
C	2.173047	0.475216	-2.183291
O	2.418359	0.890902	-3.433564
C	0.559259	2.031247	-2.456808
C	1.302921	1.759793	-3.792929
H	1.718491	2.65064	-4.265733
N	1.173675	1.028542	-1.558575
H	-0.498557	1.780073	-2.564466
H	0.690074	1.215073	-4.516887
C	-1.166787	-2.029134	3.125703
H	-1.558783	-1.048027	2.832016
C	-1.663508	-2.319768	4.551445
H	-1.324458	-3.300769	4.910506
H	-1.316504	-1.561751	5.26448
H	-2.758528	-2.327281	4.580024
C	-1.678668	-3.065483	2.1192
H	-1.332757	-2.840195	1.107198
H	-1.356544	-4.083283	2.37621
H	-2.774909	-3.071988	2.110359
C	0.65211	3.477742	-1.92168
H	0.272157	3.435005	-0.895713

Imaginary frequency	-177.263
Free energy in solution	-2078.01354000

15TS-*Z*-*Re*-*Si*

Cartesian coordinates

ATOM	X	Y	Z
C	-3.580663	0.501655	-0.192685
C	-2.552717	-0.389640	0.148975
C	-2.831916	-1.759123	0.260890
C	-4.134184	-2.236366	0.072850
C	-5.158037	-1.327139	-0.226147
C	-4.891440	0.040900	-0.369667
H	-4.349443	-3.298679	0.149538
H	-6.171407	-1.691252	-0.365279
H	-5.690319	0.731478	-0.626076
C	-3.049861	1.845153	-0.332170
O	-3.825730	2.912607	-0.567419
C	-1.513739	3.498399	-0.357581
C	-2.948976	4.074490	-0.529693
H	-3.092983	4.623335	-1.462397
N	-1.771442	2.053404	-0.194681
H	-1.067670	3.870189	0.570688
H	-3.268269	4.698776	0.308999
Rh	-0.717304	0.238189	0.262675
C	-1.607273	-2.500070	0.506094
O	-1.564901	-3.839681	0.522802
C	0.604794	-2.860734	0.783997
C	-0.161117	-4.208798	0.661704
H	-0.080107	-4.848332	1.542623
N	-0.482601	-1.863956	0.662263
H	1.242781	-2.729853	-0.094451
H	0.114809	-4.779738	-0.227620
C	-0.542416	3.825543	-1.511872
H	0.401706	3.342263	-1.236239
C	-0.289913	5.340603	-1.580195
H	-1.187344	5.894238	-1.886454
H	0.038490	5.742882	-0.613312
H	0.491145	5.562273	-2.315482
C	-0.995592	3.252270	-2.861411
H	-1.008401	2.158963	-2.834667
H	-1.992224	3.614495	-3.148208
H	-0.302407	3.560611	-3.652151
C	1.466157	-2.703573	2.057485
H	1.755260	-1.646712	2.091350

C	-0.256167	4.400499	-2.749854	C	2.740170	-3.555394	1.932622
H	-0.241791	5.419217	-2.346144	H	3.390925	-3.407036	2.801526
H	0.069877	4.46301	-3.797379	H	2.505632	-4.627489	1.881834
H	-1.29633	4.053158	-2.743005	H	3.315240	-3.298132	1.034725
C	2.086232	4.018916	-1.856085	C	0.723733	-3.010029	3.364480
H	2.737884	3.357295	-1.278998	H	-0.206800	-2.444360	3.440602
H	2.526516	4.157495	-2.852046	H	0.497578	-4.079062	3.470649
H	2.094216	4.997023	-1.362407	H	1.343508	-2.722600	4.219794
C	-2.429282	-0.234145	-1.681039	C	2.140761	0.021280	-2.558650
H	-1.85972	0.683338	-1.66856	H	2.958269	-0.627999	-2.858452
C	-1.693899	-1.409202	-1.470672	C	0.905111	-0.605891	-2.358737
O	-0.51523	-1.514718	-1.007165	O	-0.195275	-0.050884	-2.091906
O	-2.401945	-2.575285	-1.71068	O	0.976626	-2.012294	-2.362945
C	-1.766308	-3.730093	-2.331311	C	0.269969	-2.723343	-3.424331
C	-2.961353	-4.576236	-2.787574	C	0.955236	-4.093095	-3.470191
H	-2.618902	-5.505308	-3.257084	H	0.470163	-4.744322	-4.206194
H	-3.593651	-4.833467	-1.931014	H	2.011946	-3.988194	-3.737735
H	-3.571716	-4.023577	-3.509289	H	0.898392	-4.583618	-2.491630
C	-0.916865	-4.516345	-1.322486	C	0.440224	-2.001368	-4.769387
H	-0.543034	-5.438011	-1.785884	H	0.002902	-2.604756	-5.572893
H	-0.070338	-3.917727	-0.982953	H	-0.062472	-1.029273	-4.763075
H	-1.522275	-4.795269	-0.453289	H	1.499685	-1.841966	-4.994973
C	-0.926563	-3.294438	-3.540262	C	-1.218760	-2.867696	-3.076542
H	-0.544751	-4.175526	-4.06888	H	-1.750560	-3.387559	-3.883205
H	-1.537761	-2.713026	-4.239715	H	-1.350282	-3.448911	-2.157870
H	-0.07586	-2.685534	-3.22394	H	-1.668282	-1.883794	-2.928711
Si	1.96201	1.579341	1.552228	Si	-1.018046	0.653128	2.619665
C	1.91107	1.264712	3.436653	C	-1.474922	2.463390	3.023656
H	0.8833	1.226581	3.812663	H	-0.737244	3.185048	2.659159
H	2.411505	0.322987	3.688474	H	-2.448481	2.723575	2.593970
H	2.433584	2.062037	3.979996	H	-1.548806	2.584330	4.112223
C	3.820556	1.709956	1.126754	C	-2.341806	-0.412816	3.470858
H	4.295636	2.527454	1.684436	H	-2.257961	-0.297989	4.558158
H	4.334324	0.780393	1.398581	H	-3.343731	-0.088331	3.167588
H	4.000084	1.882399	0.060929	H	-2.255205	-1.476802	3.234853
O	1.237023	3.118437	1.298136	O	0.409571	0.293549	3.492801
C	1.710063	4.292676	1.942714	C	1.511073	1.191442	3.593126
H	1.907538	4.107384	3.010184	H	1.938430	1.383172	2.600381
H	2.661277	4.618176	1.491219	H	1.177742	2.158648	4.000966
C	0.666421	5.394213	1.808053	C	2.560306	0.586640	4.516168
H	1.011395	6.315972	2.292448	H	3.415629	1.264913	4.620634
H	0.469057	5.611454	0.75268	H	2.137722	0.401296	5.509668
H	-0.275241	5.085025	2.273804	H	2.924338	-0.366146	4.116628
H	-4.403476	0.591606	-1.982777	H	3.270260	1.839300	-2.774982

C	-3.762304	-0.20645	-2.379143
H	-4.291911	-1.155347	-2.260902
H	-3.666405	-0.023471	-3.462383
C	-3.591674	1.234779	0.687284
C	-4.84058	0.603134	0.798819
C	-3.533345	2.638195	0.664821
C	-6.009243	1.357388	0.885783
H	-4.888737	-0.483512	0.809597
C	-4.703012	3.38993	0.748685
H	-2.560639	3.115147	0.596291
C	-5.943783	2.753608	0.860233
H	-6.970988	0.858405	0.972223
H	-4.65016	4.475729	0.733986
H	-6.854691	3.342639	0.928582
C	-2.351308	0.4329	0.641556
H	-2.4648	-0.631133	0.872624
O	-1.220871	0.987698	0.713315
Total SCF energy		-2078.05234929	
Gibbs free energy at 298K		-2077.30133900	
Imaginary frequency		-111.037	
Free energy in solution		-2078.01616500	

C	2.242630	1.479905	-2.891765
H	1.603689	2.063750	-2.226770
H	1.934940	1.694202	-3.926985
C	3.733091	0.793009	-0.169303
C	3.978506	2.160220	0.032935
C	4.822876	-0.080395	-0.316618
C	5.286459	2.641658	0.080274
H	3.132485	2.827460	0.161106
C	6.128412	0.401105	-0.269363
H	4.637555	-1.140596	-0.476884
C	6.364536	1.765869	-0.071123
H	5.466437	3.701986	0.238776
H	6.963697	-0.284725	-0.384608
H	7.383338	2.142324	-0.032407
C	2.351125	0.261503	-0.170209
H	2.281996	-0.827715	-0.069217
O	1.368747	0.994282	0.144529
Total SCF energy		-2078.05816613	
Gibbs free energy at 298K		-2077.30489400	
Imaginary frequency		-124.448	
Free energy in solution		-2078.02168600	

15TS-*Z-Re-Re*

Cartesian coordinates

ATOM	X	Y	Z
C	3.590017	-0.007099	0.557826
C	2.414794	-0.768530	0.547787
C	2.385274	-2.011461	1.200232
C	3.529311	-2.503790	1.837636
C	4.708652	-1.745553	1.806308
C	4.749326	-0.495927	1.175239
H	3.505037	-3.458024	2.356943
H	5.601392	-2.127439	2.292159
H	5.664776	0.089535	1.175199
C	3.369054	1.260689	-0.112214
O	4.358773	2.139345	-0.335574
C	2.261425	2.931660	-1.135102
C	3.792970	3.168492	-1.194549
H	4.112429	4.135808	-0.804896
N	2.181191	1.574924	-0.547555
H	1.841111	2.900111	-2.144705
H	4.209298	3.025106	-2.196568
Rh	0.766684	-0.055106	-0.199500
C	1.043693	-2.569328	1.143154

14TS-*Z-Si-Re*

Cartesian coordinates

ATOM	X	Y	Z
C	-0.806869	-3.279989	-0.786244
C	-1.292899	-2.225026	0.002334
C	-2.296864	-2.473915	0.949962
C	-2.821824	-3.760895	1.108589
C	-2.347898	-4.797024	0.291082
C	-1.343597	-4.568042	-0.657581
H	-3.584735	-3.958402	1.856793
H	-2.75937	-5.795573	0.40254
H	-0.979275	-5.382199	-1.278315
C	0.245732	-2.805268	-1.663963
O	0.777868	-3.547591	-2.650962
C	1.801038	-1.418262	-2.50838
C	1.555311	-2.612001	-3.457053
H	2.456878	-3.126746	-3.788525
N	0.6887	-1.583834	-1.542298
H	1.668815	-0.46941	-3.035197
H	0.945214	-2.345363	-4.326568
Rh	-0.524559	-0.445552	-0.146844
C	-2.578313	-1.256826	1.692791

O	0.671663	-3.673011	1.805518	O	-3.328404	-1.227858	2.802623
C	-1.162111	-2.656197	0.636706	C	-2.366635	0.905901	2.304404
C	-0.778778	-3.770302	1.651988	C	-3.118761	0.090745	3.392959
H	-1.001478	-4.781659	1.308769	H	-4.098377	0.491402	3.657596
N	0.122825	-1.945454	0.468977	N	-2.021954	-0.14086	1.322539
H	-1.857237	-1.945807	1.091032	H	-1.427622	1.291292	2.706215
H	-1.215440	-3.619456	2.641673	H	-2.526516	-0.054042	4.300687
C	1.484749	3.990258	-0.321069	C	3.195319	-1.426246	-1.826618
H	0.445624	3.644703	-0.305921	H	3.116784	-0.784734	-0.942401
C	1.511976	5.346796	-1.043939	C	4.2464	-0.828577	-2.775373
H	2.521233	5.777692	-1.073468	H	4.347169	-1.42235	-3.694271
H	1.153281	5.262833	-2.077464	H	3.989592	0.196935	-3.067578
H	0.869643	6.066937	-0.525500	H	5.230528	-0.804006	-2.294677
C	1.961206	4.100519	1.134068	C	3.630598	-2.810785	-1.324114
H	1.794503	3.160268	1.667573	H	2.873028	-3.26676	-0.680337
H	3.024281	4.365887	1.202473	H	3.847163	-3.504925	-2.145419
H	1.401327	4.884593	1.656222	H	4.547302	-2.715544	-0.733594
C	-1.768263	-3.161260	-0.691461	C	-3.159571	2.079247	1.686698
H	-1.778397	-2.291955	-1.356756	H	-2.57284	2.404819	0.820924
C	-3.214740	-3.627283	-0.459098	C	-3.250577	3.241179	2.688394
H	-3.682490	-3.920831	-1.405838	H	-3.758365	4.100857	2.236365
H	-3.261971	-4.498977	0.208688	H	-3.82127	2.964344	3.585798
H	-3.827415	-2.834183	-0.013769	H	-2.256718	3.571865	3.012093
C	-0.938808	-4.256535	-1.375121	C	-4.546848	1.672563	1.171778
H	0.101807	-3.948152	-1.506510	H	-4.479237	0.83916	0.46695
H	-0.953346	-5.202027	-0.816942	H	-5.227826	1.388653	1.985007
H	-1.344263	-4.466437	-2.370865	H	-5.011601	2.512013	0.64277
C	-2.127140	2.076845	1.654466	C	2.124961	1.572686	2.042514
H	-3.157855	1.850344	1.912452	H	3.152925	1.908808	2.130051
C	-1.195216	1.097787	2.048227	C	1.932143	0.202977	1.880769
O	0.045674	1.109129	1.850501	C	1.035336	2.495829	2.503986
O	-1.781115	-0.056671	2.591329	H	0.665521	2.233756	3.508328
C	-1.604893	-0.288924	4.020479	H	1.395782	3.529278	2.549392
C	-2.690212	-1.312790	4.368468	H	0.172929	2.473978	1.824917
H	-2.632307	-1.592784	5.426299	O	0.825571	-0.412739	1.827674
H	-3.684556	-0.900559	4.168533	O	3.119261	-0.523187	1.683034
H	-2.573486	-2.221191	3.767986	C	3.486051	-1.499798	2.701674
C	-1.834992	1.003966	4.819441	C	4.971781	-1.766205	2.437382
H	-1.796908	0.786859	5.893035	H	5.360933	-2.515088	3.136563
H	-1.066985	1.752374	4.599812	H	5.120016	-2.138396	1.418571
H	-2.813971	1.435838	4.588661	H	5.552426	-0.844823	2.552682
C	-0.203593	-0.849626	4.306016	C	2.663489	-2.787713	2.548476
H	-0.082068	-1.042796	5.379109	H	2.983317	-3.534246	3.286574
H	-0.042636	-1.791572	3.772053	H	1.600743	-2.579171	2.684293

H	0.563831	-0.143250	3.982283
Si	1.307095	-0.936805	-2.364377
C	1.950604	0.408504	-3.557757
H	1.231707	1.228178	-3.659769
H	2.902066	0.820811	-3.205781
H	2.125326	-0.007150	-4.558004
C	2.612341	-2.327312	-2.388129
H	2.729218	-2.733890	-3.400994
H	3.587294	-1.942082	-2.068714
H	2.351192	-3.155624	-1.722109
O	-0.147011	-1.542148	-3.039110
C	-0.226174	-2.038457	-4.368715
H	0.307738	-1.378250	-5.069835
H	0.249223	-3.030649	-4.432911
C	-1.689374	-2.132838	-4.780964
H	-1.778219	-2.515140	-5.805287
H	-2.236031	-2.805578	-4.111744
H	-2.162870	-1.146983	-4.730664
H	-2.282479	4.087380	0.830431
C	-1.766108	3.538914	1.630766
H	-0.690466	3.672662	1.504853
H	-2.047802	4.033320	2.573054
C	-3.366569	1.649075	-0.929342
C	-3.971043	2.883798	-1.211488
C	-4.138661	0.480077	-1.020091
C	-5.323085	2.952892	-1.549020
H	-3.374911	3.792384	-1.179232
C	-5.487729	0.549488	-1.355997
H	-3.658829	-0.473608	-0.828224
C	-6.087390	1.786350	-1.618038
H	-5.777416	3.916253	-1.766403
H	-6.076190	-0.362562	-1.419751
H	-7.140230	1.837900	-1.883080
C	-1.920053	1.574380	-0.590540
H	-1.381254	2.531020	-0.630564
O	-1.281085	0.498962	-0.787069
Total SCF energy	-2078.04508245		
Gibbs free energy at 298K	-2077.29212100		
Imaginary frequency	-170.010		
Free energy in solution	-2078.00874800		

H	2.802729	-3.212977	1.549997
C	3.302076	-0.908494	4.108
H	3.682164	-1.60985	4.859693
H	3.848297	0.035112	4.207747
H	2.245718	-0.720483	4.323877
Si	-2.003181	0.115257	-1.947881
C	-1.059204	0.370227	-3.586995
H	-0.19737	1.028411	-3.437948
H	-0.708184	-0.580841	-4.001473
H	-1.705942	0.83456	-4.342214
C	-3.424439	-1.104918	-2.30264
H	-4.072461	-0.730265	-3.105307
H	-3.033112	-2.079204	-2.615994
H	-4.046651	-1.27	-1.416803
O	-2.697785	1.636421	-1.556943
C	-3.670633	2.255495	-2.388175
H	-3.496573	2.02528	-3.45144
H	-4.673061	1.874006	-2.138001
C	-3.621255	3.764817	-2.186461
H	-4.380841	4.263178	-2.80138
H	-3.80536	4.01813	-1.13689
H	-2.63584	4.15482	-2.462433
H	5.005182	4.901892	-0.987655
C	3.936876	4.735258	-0.877124
C	3.05116	5.818017	-0.911939
C	3.449366	3.44355	-0.699472
C	1.677591	5.599638	-0.772418
H	3.431184	6.826746	-1.051139
C	2.07096	3.217424	-0.552058
H	4.134815	2.599633	-0.659793
C	1.186329	4.307071	-0.596577
H	0.988627	6.439769	-0.806536
H	0.121977	4.116565	-0.504746
C	1.558415	1.841018	-0.403141
H	2.283136	1.039606	-0.582588
O	0.326269	1.598417	-0.382097
Total SCF energy	-2078.04840432		
Gibbs free energy at 298K	-2077.29551500		
Imaginary frequency	-24.700		
Free energy in solution	-2078.01178000		

14b-*Si-Si*

Cartesian coordinates

ATOM	X	Y	Z
C	2.608099	-0.005770	0.518339
C	2.996737	1.169359	1.181847
C	4.347763	1.530252	1.259327
C	5.308980	0.704929	0.658682
C	4.937603	-0.449556	-0.045938
C	3.582270	-0.792906	-0.121646
H	4.651191	2.441451	1.768297
H	6.358623	0.975797	0.721976
H	5.693629	-1.058357	-0.535138
Rh	0.712572	-0.409800	0.261445
Si	0.714222	-1.763580	2.237291
C	-2.200693	0.133225	-0.657335
C	-1.945464	0.718094	-2.129831
C	-0.663442	1.535769	-2.137486
H	-1.723766	-0.175330	-2.726325
O	0.438064	1.114475	-1.798719
O	-0.861746	2.800036	-2.559554
C	0.236702	3.758093	-2.780049
C	1.819550	1.896372	1.629980
O	1.888536	3.109102	2.200866
C	-0.371371	2.389182	1.878625
C	0.516312	3.569147	2.368840
H	0.380192	3.815381	3.423452
C	2.936127	-1.871237	-0.853813
O	3.603164	-2.800518	-1.554839
C	1.227602	-3.102748	-1.678381
C	2.598605	-3.711753	-2.092651
H	2.750796	-3.764658	-3.172810
N	0.629951	1.403491	1.423513
N	1.635914	-1.955772	-0.850797
H	0.401768	4.475650	1.769644
H	-0.949297	2.696136	0.998228
H	2.783883	-4.695586	-1.654174
H	0.681109	-3.804671	-1.039817
C	0.283193	-2.699591	-2.832119
H	-0.550502	-2.193757	-2.329812
C	0.913733	-1.711221	-3.822011
H	0.175530	-1.417256	-4.577717
H	1.248779	-0.803282	-3.312838
H	1.764558	-2.147968	-4.362013
C	-0.251527	-3.952060	-3.543352

14b-*Si-Re*

Cartesian coordinates

ATOM	X	Y	Z
C	2.580164	-0.137528	-0.342771
C	3.350499	-0.786185	0.639218
C	4.741043	-0.633116	0.671173
C	5.360769	0.168875	-0.298918
C	4.610133	0.836447	-1.276178
C	3.216364	0.689579	-1.280966
H	5.337077	-1.123631	1.436432
H	6.440530	0.283152	-0.285458
H	5.105378	1.465399	-2.011468
Rh	0.628005	-0.306175	-0.297139
Si	0.791392	-2.125315	-1.852345
O	-1.485467	-0.543647	0.017536
C	-2.268783	0.583437	0.042976
C	-2.251411	1.312045	1.439226
H	-1.929846	1.348291	-0.684488
C	-0.891109	1.908326	1.774224
H	-2.949934	2.158615	1.409969
O	0.191047	1.588384	1.298702
O	-1.025458	2.862871	2.714934
C	0.122303	3.531430	3.357981
C	2.474255	-1.509111	1.548411
O	2.896419	-2.100488	2.675388
C	0.510409	-2.202900	2.435793
C	1.702062	-2.582416	3.363417
H	1.821308	-3.657882	3.508426
C	2.226111	1.309821	-2.143920
O	2.559141	2.058875	-3.210538
C	0.214894	1.981787	-2.884291
C	1.312520	2.295771	-3.926888
H	1.324102	3.327873	-4.279062
N	1.193620	-1.540936	1.309972
N	0.952422	1.140933	-1.914151
H	1.669012	-2.089023	4.337737
H	-0.117157	-1.446677	2.920146
H	1.291368	1.616448	-4.784948
H	-0.589223	1.386732	-3.327264
C	-0.409779	3.241433	-2.230537
H	-1.010692	2.873103	-1.392240
C	0.627401	4.217498	-1.657150
H	0.120831	5.038626	-1.137244
H	1.282886	3.723265	-0.933932

H	-0.742051	-4.637562	-2.841215	H	1.252817	4.667279	-2.438351
H	-0.986812	-3.676145	-4.307547	C	-1.356973	3.939033	-3.219558
H	0.548952	-4.507828	-4.050922	H	-2.138822	3.257541	-3.575618
C	-1.369220	1.819708	2.911697	H	-1.849834	4.794202	-2.743626
H	-1.712389	0.872198	2.481515	H	-0.820473	4.322488	-4.097555
C	-2.574649	2.761416	3.059784	C	-0.413756	-3.361347	2.000500
H	-3.317421	2.331815	3.740925	H	-1.037660	-2.931012	1.208872
H	-2.279431	3.735645	3.474002	C	-1.318638	-3.782595	3.169636
H	-3.068776	2.942598	2.097334	H	-2.019801	-4.562055	2.851086
C	-0.745167	1.503854	4.276983	H	-0.736476	-4.193654	4.006449
H	-1.453680	0.933989	4.885842	H	-1.908034	-2.940234	3.551480
H	0.152703	0.890360	4.176946	C	0.333278	-4.568119	1.418640
H	-0.489809	2.414070	4.835465	H	-0.380062	-5.268400	0.972993
C	0.958283	-3.612056	1.840431	H	1.021769	-4.271054	0.624784
H	0.880863	-4.195435	2.766910	H	0.893643	-5.117820	2.186635
H	0.205110	-3.990347	1.142943	C	0.579587	-1.531919	-3.654212
H	1.948972	-3.793885	1.410030	H	0.528747	-2.403442	-4.319453
C	2.019474	-1.316401	3.542341	H	-0.334342	-0.947063	-3.797291
H	1.843667	-1.906661	4.449790	H	1.433827	-0.922238	-3.967152
H	3.024227	-1.547659	3.171310	C	2.412969	-3.114893	-1.795416
H	2.005790	-0.258820	3.819136	H	2.333015	-3.972984	-2.473594
O	-0.770802	-1.602718	3.057802	H	3.259848	-2.499035	-2.117159
C	-1.971933	-2.210281	2.567337	H	2.640653	-3.496844	-0.796095
C	-3.127339	-1.838043	3.484910	O	-0.396295	-3.308235	-1.561842
H	-1.854137	-3.305544	2.555136	C	-1.761641	-3.111307	-1.940374
H	-2.154246	-1.876069	1.539816	C	-2.578962	-4.310804	-1.482924
H	-4.051548	-2.319581	3.144272	H	-1.833961	-3.016703	-3.035708
H	-2.924977	-2.156419	4.513961	H	-2.133056	-2.186835	-1.486884
H	-3.291355	-0.754978	3.487068	H	-3.625718	-4.197868	-1.790279
C	0.929479	4.091328	-1.455124	H	-2.186531	-5.237484	-1.916854
H	1.653667	4.898840	-1.612120	H	-2.549743	-4.406358	-0.391660
H	0.191806	4.437976	-0.722384	C	0.985538	2.498007	4.090594
H	1.453157	3.223117	-1.053553	H	1.764669	3.012127	4.664736
C	1.215927	3.206768	-3.822390	H	0.374433	1.919743	4.792683
H	1.752055	2.335927	-3.442465	H	1.466932	1.813186	3.390016
H	0.680153	2.924269	-4.735311	C	0.925156	4.330954	2.326898
H	1.945220	3.982023	-4.083073	H	1.437199	3.672381	1.624286
C	-0.500545	4.984552	-3.326683	H	0.264685	5.002412	1.767541
H	-1.237784	5.347290	-2.602907	H	1.672742	4.944178	2.843140
H	0.210844	5.791581	-3.532071	C	-0.561676	4.470455	4.355827
H	-1.024762	4.738423	-4.255658	H	-1.176231	3.903188	5.062232
C	-3.627259	-0.422588	-0.557743	H	0.189743	5.032192	4.921043
C	-3.915904	-1.707031	-1.040016	H	-1.208507	5.183341	3.834146
C	-4.661482	0.313451	0.031679	C	-3.735096	0.297135	-0.324773

C	-5.205466	-2.230804	-0.951797
H	-3.109739	-2.297192	-1.464708
C	-5.954562	-0.208343	0.128675
H	-4.452525	1.307211	0.423769
C	-6.232178	-1.482543	-0.367385
H	-5.410986	-3.228845	-1.332252
H	-6.741536	0.378891	0.596081
H	-7.235931	-1.893326	-0.292925
C	-3.139726	1.455785	-2.751029
H	-3.986309	0.773881	-2.858348
H	-3.463840	2.298680	-2.131062
H	-2.889655	1.853304	-3.739337
O	-1.286488	-0.836181	-0.342602
H	-2.166789	1.016059	0.018712

Total SCF energy -2078.08838525
Gibbs free energy at 298K -2077.33243000
Free energy in solution -2078.05223400

C	-4.550839	1.301997	-0.861853
C	-4.292642	-0.970137	-0.117074
C	-5.886716	1.052372	-1.183087
H	-4.132951	2.292596	-1.038644
C	-5.628569	-1.225708	-0.433948
H	-3.656196	-1.750048	0.286943
C	-6.431721	-0.215649	-0.968718
H	-6.499823	1.845014	-1.605953
H	-6.043229	-2.217011	-0.265225
H	-7.470258	-0.415189	-1.220764
C	-2.689484	0.380993	2.587166
H	-3.733582	0.087429	2.446856
H	-2.081451	-0.526906	2.577041
H	-2.596697	0.874891	3.559462

Total SCF energy -2078.08612419
Gibbs free energy at 298K -2077.32910200
Free energy in solution -2078.05139000

15b-*Re-Re*

Cartesian coordinates

ATOM	X	Y	Z
C	2.583500	-0.501228	-0.261281
C	3.119812	-1.370168	0.710438
C	4.504629	-1.468083	0.883963
C	5.351105	-0.694189	0.075391
C	4.834115	0.206221	-0.866458
C	3.444917	0.312169	-1.015917
H	4.924122	-2.125785	1.640793
H	6.426712	-0.776532	0.198768
H	5.504635	0.823916	-1.458171
Rh	0.645700	-0.273195	-0.358297
Si	0.763736	-1.923461	-2.101380
O	-1.321145	0.071050	0.242134
C	-2.213939	1.111101	0.036921
C	-2.494874	1.826151	1.402910
H	-1.819130	1.885530	-0.645199
C	-1.174508	2.268330	2.010797
O	-0.419441	3.066450	1.484235
O	-0.975256	1.716935	3.227701
C	0.182143	2.077048	4.064724
C	2.040543	-1.968388	1.483280
O	2.224719	-2.687822	2.599780
C	-0.102196	-2.271233	2.165624
C	0.901799	-2.866324	3.196128

15b-*Re-Si*

Cartesian coordinates

ATOM	X	Y	Z
C	3.584524	-0.712434	0.166002
C	2.513453	-0.033301	0.774076
C	2.786277	1.048678	1.625489
C	4.105628	1.420700	1.912179
C	5.158665	0.698449	1.333993
C	4.910031	-0.360633	0.449542
H	4.314379	2.263384	2.566174
H	6.183939	0.977094	1.558218
H	5.737174	-0.889463	-0.017024
C	3.070662	-1.700522	-0.767004
O	3.851502	-2.520497	-1.485503
C	1.524194	-2.843969	-1.955985
C	2.954840	-3.381811	-2.247604
H	3.247869	-3.311867	-3.297225
N	1.782830	-1.808918	-0.939817
H	0.912111	-3.627744	-1.499582
H	3.110867	-4.405659	-1.897741
Rh	0.672999	-0.439899	0.234904
C	1.547034	1.693377	2.024606
O	1.526523	2.823673	2.750018
C	-0.666095	2.104215	2.146091
C	0.145261	3.281022	2.753320
H	-0.121395	3.522205	3.783307

H	0.768676	-3.933599	3.381289	N	0.399126	1.216612	1.631134
C	2.664426	1.227068	-1.830046	H	-1.252362	2.456305	1.290099
O	3.213768	2.059260	-2.729815	H	0.101754	4.190128	2.146215
C	0.868180	2.374017	-2.550359	C	0.746481	-2.296430	-3.171576
C	2.094304	2.651420	-3.452912	H	-0.175320	-1.891170	-2.738119
H	2.319381	3.708121	-3.599667	C	0.379531	-3.439904	-4.129890
N	0.806227	-1.715250	1.147938	H	1.268639	-3.890459	-4.592167
N	1.364609	1.266078	-1.703047	H	-0.170820	-4.236997	-3.615002
H	0.906312	-2.332866	4.150571	H	-0.254492	-3.070006	-4.943307
H	-0.652641	-1.428595	2.597026	C	1.479842	-1.159170	-3.894463
H	2.031769	2.150646	-4.424284	H	1.667406	-0.320622	-3.217239
H	0.022800	2.011309	-3.143933	H	2.437141	-1.486600	-4.321697
C	0.399464	3.593581	-1.718945	H	0.871206	-0.786230	-4.726172
H	-0.316934	3.212023	-0.985866	C	-1.635322	1.396587	3.120655
C	1.524026	4.263183	-0.916960	H	-1.939214	0.475736	2.612505
H	1.101178	5.042658	-0.275591	C	-2.881227	2.265739	3.351559
H	2.026294	3.546977	-0.259783	H	-3.598082	1.747065	3.997774
H	2.277459	4.734594	-1.561829	H	-2.630071	3.215963	3.842960
C	-0.325399	4.602784	-2.623027	H	-3.391359	2.499528	2.409006
H	-1.164394	4.138523	-3.156595	C	-0.986593	0.985475	4.448622
H	-0.726026	5.429876	-2.026937	H	-0.079018	0.399312	4.285899
H	0.346686	5.039803	-3.373889	H	-0.737762	1.851577	5.075789
C	-1.145159	-3.257416	1.594878	H	-1.675928	0.354992	5.018933
H	-1.652591	-2.698448	0.800885	C	-1.915928	1.193112	-1.939446
C	-2.180551	-3.604852	2.677202	H	-2.709379	1.947766	-1.895518
H	-2.983005	-4.221755	2.257579	C	-0.600638	1.948204	-1.843647
H	-1.732985	-4.175466	3.502900	O	0.485320	1.483823	-1.523061
H	-2.638396	-2.703453	3.102862	O	-0.774000	3.233335	-2.222366
C	-0.537081	-4.521904	0.975481	C	0.347163	4.177763	-2.386268
H	-1.329456	-5.145452	0.546926	C	-0.358494	5.443401	-2.882566
H	0.151963	-4.276829	0.164598	H	0.370512	6.245000	-3.042711
H	-0.008625	-5.136027	1.716852	H	-0.876510	5.251165	-3.827643
C	0.911119	-1.100041	-3.814287	H	-1.096957	5.786742	-2.150646
H	0.788444	-1.865168	-4.591480	C	1.329071	3.657259	-3.441534
H	0.154801	-0.326729	-3.978767	H	2.076497	4.429286	-3.656865
H	1.899754	-0.646383	-3.942690	H	1.843736	2.759050	-3.097111
C	2.124616	-3.237308	-1.981736	H	0.799775	3.428380	-4.372968
H	1.964432	-3.981430	-2.771243	C	1.026835	4.430927	-1.036324
H	3.118334	-2.798292	-2.116972	H	1.771736	5.227909	-1.142112
H	2.116284	-3.760632	-1.021600	H	0.286513	4.758210	-0.296910
O	-0.654375	-2.853051	-2.069425	H	1.525415	3.532473	-0.669859
C	-1.950700	-2.318676	-2.345428	Si	0.461236	-2.073225	1.966165
C	-2.947805	-3.464383	-2.429689	C	0.588935	-3.849945	1.288425
H	-1.938221	-1.765671	-3.297885	H	-0.114417	-4.031785	0.470471

H	-2.229825	-1.614646	-1.555179	H	1.601968	-4.056039	0.926360
H	-3.954324	-3.074607	-2.619595	H	0.367594	-4.565223	2.091080
H	-2.679316	-4.157745	-3.234485	C	1.716854	-1.928342	3.382333
H	-2.967019	-4.025899	-1.488994	H	1.489923	-2.677007	4.150973
C	1.494033	1.702484	3.366442	H	2.734058	-2.106169	3.015968
H	2.330391	1.834212	4.063083	H	1.704438	-0.942690	3.855757
H	1.473395	0.654206	3.051292	O	-1.049017	-1.934004	2.745763
H	1.664627	2.324804	2.487204	C	-2.248557	-2.468245	2.182436
C	0.124465	3.567731	4.420137	H	-2.458901	-1.978413	1.225422
H	0.243868	4.187841	3.530209	H	-2.122906	-3.543736	1.982467
H	-0.832182	3.810254	4.896298	C	-3.393750	-2.269970	3.165265
H	0.926845	3.809728	5.126578	H	-4.320325	-2.690254	2.756825
C	-0.030402	1.218213	5.314930	H	-3.175605	-2.763832	4.118858
H	-0.011169	0.152690	5.060635	H	-3.561127	-1.205518	3.361989
H	0.758982	1.413507	6.048800	H	-2.952322	0.027596	-3.450453
H	-0.997655	1.441347	5.776814	C	-1.984031	0.520432	-3.324308
C	-3.533962	0.617598	-0.560543	H	-1.199654	-0.230738	-3.425527
C	-4.091399	1.215466	-1.696605	H	-1.867871	1.260716	-4.124132
C	-4.217192	-0.457470	0.027613	C	-3.578873	-0.353464	-0.840942
C	-5.297901	0.757118	-2.235211	C	-3.815533	-1.676496	-1.231076
H	-3.573949	2.049927	-2.166673	C	-4.680010	0.460668	-0.542171
C	-5.423172	-0.915942	-0.500862	C	-5.118083	-2.171542	-1.327216
H	-3.782312	-0.942751	0.897026	H	-2.956369	-2.306307	-1.436972
C	-5.969222	-0.309825	-1.637433	C	-5.984064	-0.029101	-0.634898
H	-5.710723	1.233827	-3.121144	H	-4.516133	1.489436	-0.223173
H	-5.939184	-1.748879	-0.029038	C	-6.208014	-1.350107	-1.031034
H	-6.908487	-0.667617	-2.051449	H	-5.282817	-3.203251	-1.630098
C	-3.415437	3.052527	1.277748	H	-6.824327	0.617049	-0.391599
H	-2.958982	3.811870	0.633511	H	-7.221894	-1.736199	-1.101113
H	-4.379480	2.766838	0.847293	C	-2.138559	0.182978	-0.743222
H	-3.602330	3.510487	2.256224	H	-2.123780	0.820909	0.164838
H	-2.947382	1.088906	2.073076	O	-1.210642	-0.825812	-0.685339

Total SCF energy	-2078.08901263	Total SCF energy	-2078.08959296
Gibbs free energy at 298K	-2077.33497700	Gibbs free energy at 298K	-2077.33327700
Free energy in solution	-2078.05134400	Free energy in solution	-2078.05315800