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Supporting Information

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Substituent Effects on Reaction Barriers, Reactant Preorganization Energies, and Ligand Exchange Energies Control Reactivities in Rh(I)-Catalyzed (5+2) Cycloadditions of Substituted Vinylcyclopropanes with Alkynes

Supporting Information

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Figure S1. The energy surface of the (5+2) cycloaddition between 1-methyl-1-(1-propenyl)-cyclopropane (**1b**, R = Me) and acetylene. Bond lengths are in Å.

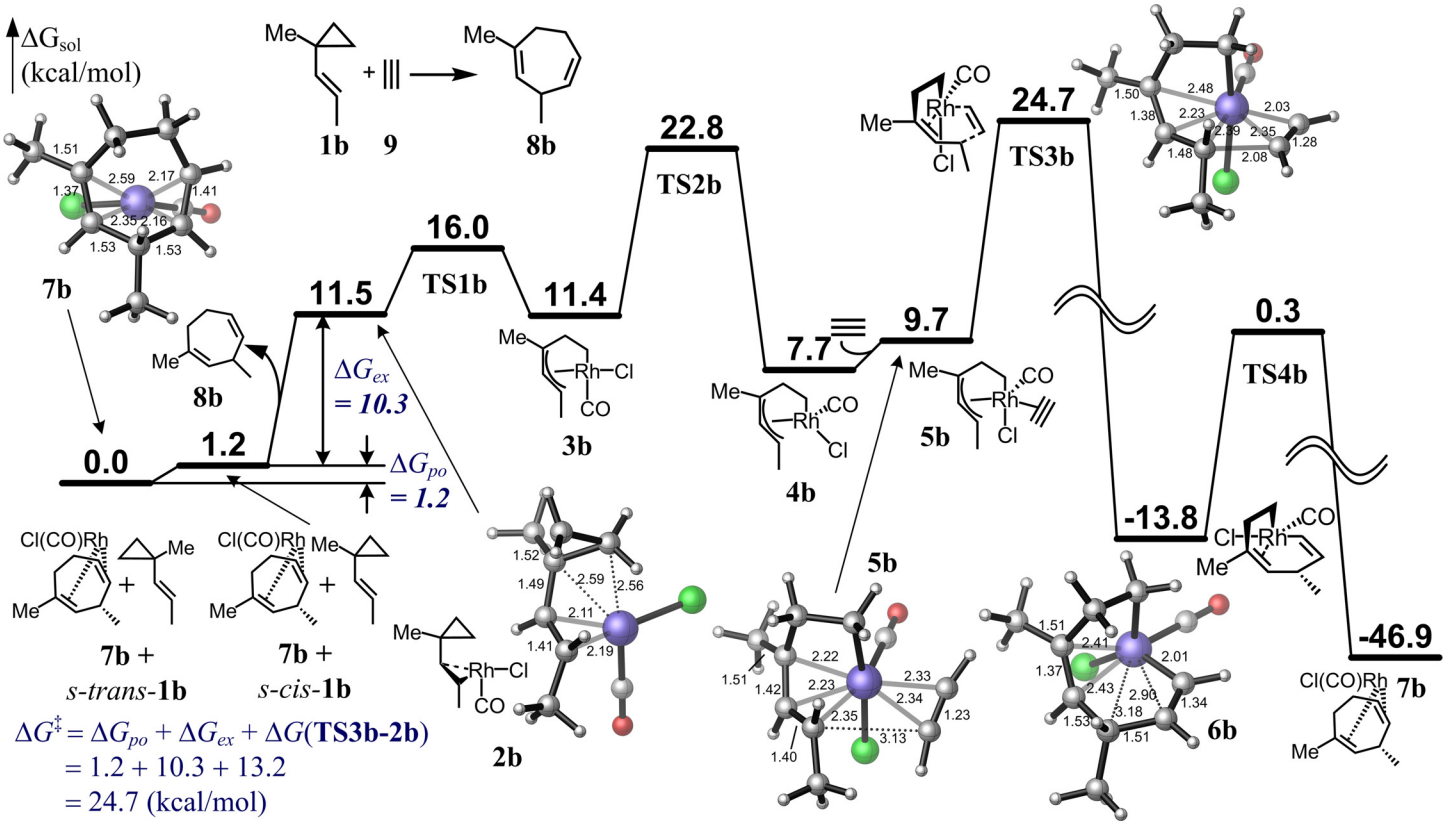


Figure S2. The energy surface of the (5+2) cycloaddition between 1-isopropyl-1-(1-propenyl)-cyclopropane (**1c**, R = *i*-Pr) and acetylene. Bond lengths are in Å.

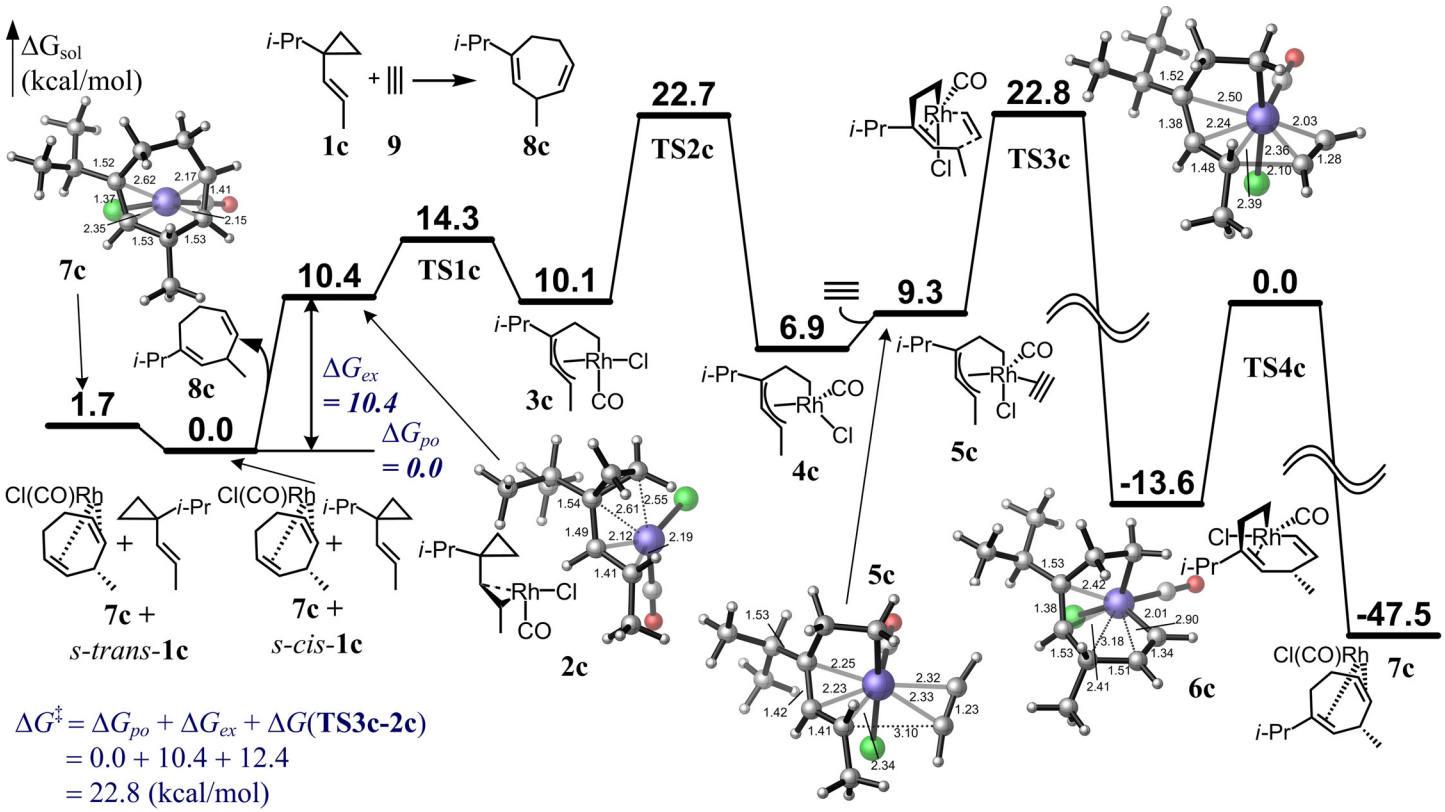
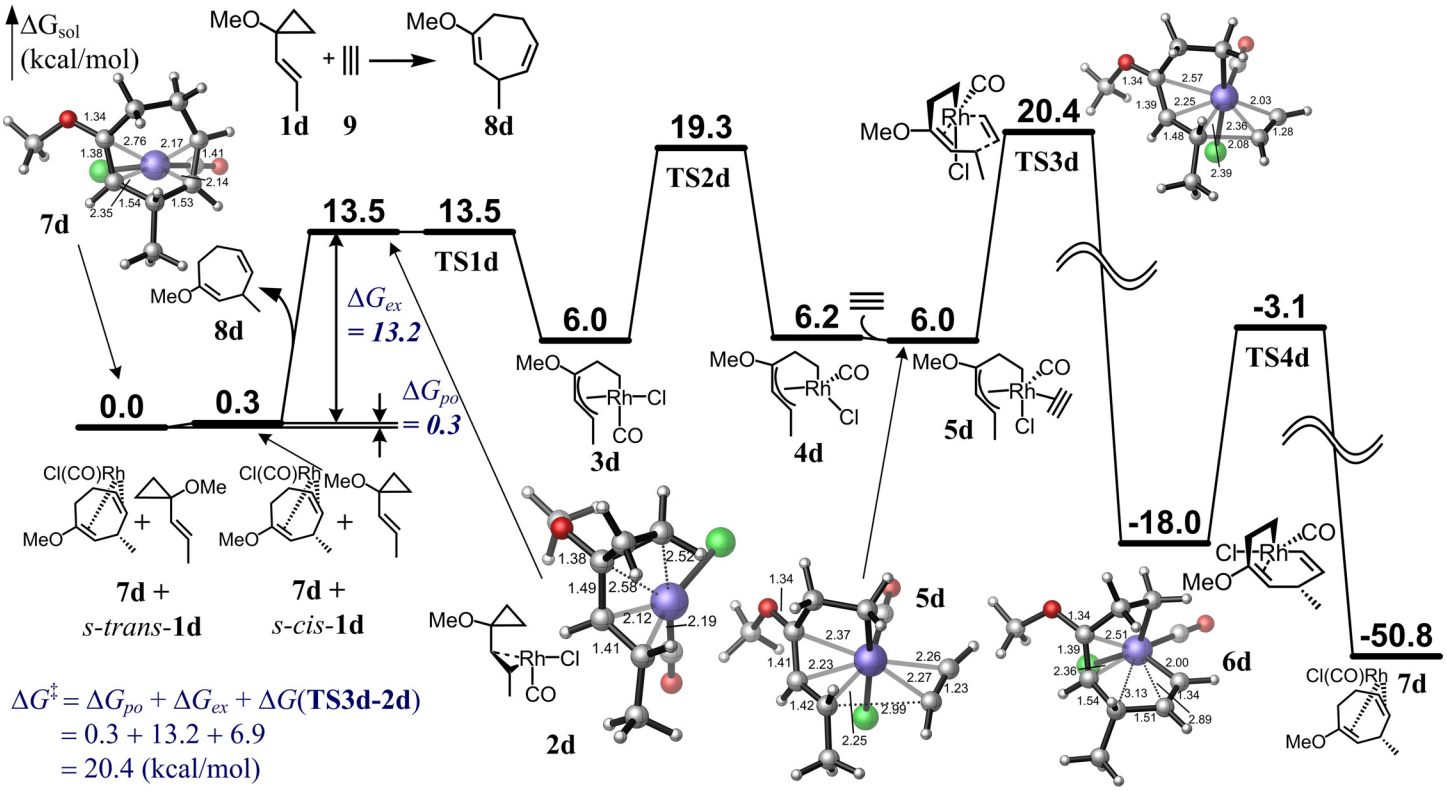


Figure S3. The energy surface of the (5+2) cycloaddition between 1-methoxy-1-(1-propenyl)-cyclopropane (**1d**, R = OMe) and acetylene. Bond lengths are in Å.



Computational Details

All geometry optimizations and frequency calculations were performed with the B3LYP[1,2] functional implemented in Gaussian 03.[3] The SDD basis set was used on rhodium and the 6-31G(d) basis set for other atoms. All free energies reported involve solvation free energy correction, computed using the CPCM[4,5] polarizable conductor calculation model as implemented in Gaussian 03. Dichloromethane (CH_2Cl_2) was specified as solvent. Figures for the transition state structures are prepared with CYLview.[6]

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

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

s-cis-**1a**

Total SCF energy: -234.60415836 a.u.
Enthalpy at 298K: -234.452892 a.u.
Gibbs free energy at 298K: -234.491218 a.u.
Total free energy in solution at 298K: -234.486898 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.339948	0.333669	-0.072961
C	0.411034	-0.607443	-0.269507
C	-1.039708	-0.377563	-0.515609
C	-1.742866	0.893034	-0.108604
C	-2.029473	-0.386805	0.637556
H	1.044099	1.382670	-0.110057
H	-1.169746	1.657437	0.408058
H	-2.507569	1.288021	-0.771938
H	-1.624067	-0.484192	1.641134
H	-2.989620	-0.874597	0.490203
H	0.717975	-1.655966	-0.248616
H	-1.413516	-0.847397	-1.426339
C	2.793562	0.065949	0.197213
H	3.010474	-1.007840	0.205834
H	3.433090	0.535495	-0.562834
H	3.103901	0.481324	1.166030

s-trans-**1a**

Total SCF energy: -234.60654290 a.u.
Enthalpy at 298K: -234.455378 a.u.
Gibbs free energy at 298K: -234.493602 a.u.
Total free energy in solution at 298K: -234.489699 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.569202	-0.000085	0.435911
C	0.392807	0.000116	-0.200915
C	-0.933217	-0.000032	0.455471
H	-0.901399	-0.000025	1.543518
C	-2.096316	-0.751088	-0.171850
C	-2.096193	0.751140	-0.171748
H	1.574251	-0.000453	1.527527
H	-1.913465	-1.264822	-1.112383
H	-2.780832	-1.272396	0.491986
H	-1.913352	1.264947	-1.112232
H	-2.780607	1.272459	0.492179
H	0.382562	-0.000418	-1.293675
C	2.914078	0.000000	-0.233416
H	3.503268	0.883680	0.048971
H	3.508081	-0.877319	0.058422
H	2.819332	-0.005954	-1.325030

s-cis-**1b**

Total SCF energy: -273.91971993 a.u.
Enthalpy at 298K: -273.739146 a.u.
Gibbs free energy at 298K: -273.780624 a.u.
Total free energy in solution at 298K: -273.773709 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.624136	-0.181934	-0.301158
C	-0.590205	0.349396	0.358108
C	0.860357	0.170502	0.041797
C	1.330608	-1.068595	-0.682963
C	1.622895	-0.910307	0.791244
H	-1.429902	-0.815672	-1.167256
H	0.598467	-1.815929	-0.974080
H	2.153931	-0.961998	-1.384971
H	1.067299	-1.535773	1.484845
H	2.644130	-0.696128	1.098455
H	-0.794757	1.000186	1.212728
C	1.598243	1.476342	-0.228650
H	1.496795	2.168978	0.617064
H	2.668498	1.301568	-0.388867
H	1.198719	1.976580	-1.119156
C	-3.069669	0.024027	0.054132
H	-3.624675	0.473489	-0.780814
H	-3.565902	-0.929874	0.281024
H	-3.181157	0.677984	0.925976

s-trans-**1b**

Total SCF energy: -273.92156896 a.u.
Enthalpy at 298K: -273.740896 a.u.
Gibbs free energy at 298K: -273.781865 a.u.
Total free energy in solution at 298K: -273.775605 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.696139	0.303097	0.000213
C	0.570184	-0.419706	-0.000558
C	-0.824254	0.098436	-0.000267
C	-1.856617	-0.733758	0.751583
C	-1.857249	-0.733954	-0.750971
H	1.635696	1.391132	0.001226
H	-1.513183	-1.626289	1.268328
H	-2.649343	-0.199653	1.269625
H	-1.514469	-1.626745	-1.267720
H	-2.650473	-0.199999	-1.268416
H	0.655565	-1.509037	-0.001267
C	-1.005611	1.605337	-0.000205
H	-0.547844	2.060898	0.886497
H	-0.548521	2.060739	-0.887334
H	-2.068591	1.870057	0.000202
C	3.082800	-0.277077	0.000010
H	3.060430	-1.372579	-0.000701
H	3.654388	0.049195	-0.880060
H	3.653993	0.048029	0.880799

s-cis-**1c**

Total SCF energy: -352.54524747 a.u.
Enthalpy at 298K: -352.304954 a.u.
Gibbs free energy at 298K: -352.352453 a.u.

Total free energy in solution at 298K: -352.343205 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.047370	-0.074644	0.258557
C	-0.921528	-0.057093	-0.462599
C	0.380497	0.562025	-0.058419
C	0.371249	1.793849	0.817689
C	0.713659	1.921458	-0.648321
H	-2.051013	0.393599	1.243540
H	-0.581524	2.194465	1.150771
H	1.174877	1.906467	1.541645
H	-0.020323	2.389361	-1.299209
H	1.747485	2.120780	-0.922409
H	-0.929024	-0.538228	-1.443122
C	1.560867	-0.411421	0.125176
C	1.325299	-1.372542	1.300041
H	0.453960	-2.011106	1.114489
H	2.194587	-2.022876	1.455411
H	1.142533	-0.822918	2.230723
C	-3.342808	-0.695948	-0.181869
H	-4.149572	0.048911	-0.224456
H	-3.253596	-1.154402	-1.172820
H	-3.671952	-1.471631	0.523105
C	1.889563	-1.181115	-1.164596
H	1.083550	-1.874197	-1.433325
H	2.043331	-0.498217	-2.008439
H	2.802848	-1.774740	-1.039463
H	2.437273	0.207317	0.369610

s-trans-**1c**

Total SCF energy: -352.54250620 a.u.
Enthalpy at 298K: -352.301960 a.u.
Gibbs free energy at 298K: -352.348614 a.u.
Total free energy in solution at 298K: -352.340552 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-2.038565	-0.412253	-0.250609
C	-1.172191	0.557990	0.064072
C	0.320188	0.530409	0.009381
C	1.011502	1.469065	0.991972
C	0.943656	1.844716	-0.458885
H	-1.674157	-1.382580	-0.585442
H	0.392190	2.006797	1.705473
H	1.974192	1.160787	1.392200
H	0.264948	2.638730	-0.759415
H	1.859268	1.807133	-1.039775
H	-1.586018	1.513833	0.395223
C	0.979900	-0.823231	-0.310855
H	0.393213	-1.275931	-1.122500
C	0.909672	-1.762356	0.908249
H	-0.110028	-1.844615	1.296059
H	1.259352	-2.768599	0.647688
H	1.544856	-1.388033	1.720573
C	2.425983	-0.732977	-0.823204
H	2.822311	-1.740603	-0.993777
H	2.492609	-0.188574	-1.770832
H	3.091149	-0.243429	-0.100507
C	-3.533789	-0.268572	-0.179454
H	-4.000164	-0.438935	-1.159857
H	-3.975907	-1.003159	0.507978
H	-3.825946	0.730438	0.162915

s-cis-**1d**

Total SCF energy: -349.12007910 a.u.
Enthalpy at 298K: -348.933964 a.u.
Gibbs free energy at 298K: -348.978333 a.u.
Total free energy in solution at 298K: -348.972532 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.806002	-0.069684	0.328362
C	0.767962	0.039291	-0.506336
C	-0.654823	-0.295805	-0.204498
C	-1.052821	-1.211692	0.930252
C	-1.193075	-1.669349	-0.507317
H	1.631502	-0.422597	1.345470
H	-0.283544	-1.668430	1.545826
H	-1.964718	-0.956193	1.462039
H	-0.498977	-2.417097	-0.880346
H	-2.193298	-1.711393	-0.928955
H	0.931209	0.411887	-1.519639
O	-1.567796	0.728472	-0.535248
C	-1.484950	1.861719	0.314376
H	-2.233626	2.574184	-0.042017
H	-1.705414	1.600423	1.360306
H	-0.492178	2.331184	0.275979
C	3.230791	0.250733	-0.023492
H	3.874472	-0.634052	0.076965
H	3.319211	0.618447	-1.051307
H	3.643211	1.014583	0.649572

s-trans-**1d**

Total SCF energy: -349.12099350 a.u.
Enthalpy at 298K: -348.934831 a.u.
Gibbs free energy at 298K: -348.978572 a.u.
Total free energy in solution at 298K: -348.973048 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.783456	0.123640	-0.208569
C	0.744395	-0.601058	0.218001
C	-0.684257	-0.309881	-0.084224
C	-1.770622	-0.926355	0.781833
C	-1.553331	-1.423008	-0.625615
H	1.585564	0.999971	-0.824785
H	-1.473090	-1.557162	1.615841
H	-2.653658	-0.321043	0.965798
H	-1.100081	-2.398646	-0.777820
H	-2.278876	-1.130922	-1.378951
H	0.920932	-1.491921	0.823091
O	-0.957799	0.947420	-0.648261
C	-0.957004	2.016868	0.288238
H	-1.171456	2.925635	-0.280279
H	-1.733112	1.881466	1.054991
H	0.014100	2.123396	0.788266
C	3.223760	-0.184973	0.084780

H	3.794829	-0.334656	-0.841893
H	3.710867	0.642008	0.619965
H	3.328000	-1.088887	0.695198

2a

Total SCF energy: -918.80071296 a.u.
Enthalpy at 298K: -918.632660 a.u.
Gibbs free energy at 298K: -918.685031 a.u.
Total free energy in solution at 298K: -918.691558 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	0.354288	-0.133513	-0.015538
C	-1.885040	-1.425047	-0.323133
C	-2.050169	-0.345440	0.830890
C	-1.300446	0.936451	0.743844
C	-0.984877	1.545943	-0.483816
H	-1.477405	1.190280	-1.390643
H	-1.131938	1.468906	1.677336
C	-3.193894	-0.736232	-0.060605
H	-3.988325	-1.323349	0.390634
H	-3.532034	-0.007447	-0.791923
H	-1.394267	-1.186028	-1.269340
H	-1.738715	-2.449938	-0.001811
C	1.830066	0.879742	0.257824
O	2.764594	1.530240	0.450074
Cl	1.566947	-2.120385	-0.223192
C	-0.471991	2.962271	-0.582081
H	0.242299	3.071383	-1.404773
H	-1.304517	3.651883	-0.778177
H	0.018965	3.281843	0.342962
H	-2.053765	-0.790969	1.821087

2b

Total SCF energy: -958.11636549 a.u.
Enthalpy at 298K: -957.919025 a.u.
Gibbs free energy at 298K: -957.974161 a.u.
Total free energy in solution at 298K: -957.976725 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	0.485092	-0.151337	-0.106354
C	-1.823986	-1.001682	-0.805898
C	-2.048360	0.019974	0.399768
C	-1.070475	1.145354	0.503263
C	-0.472167	1.757465	-0.613253
H	-0.872286	1.550926	-1.607346
H	-0.951375	1.590771	1.489383
C	-3.017696	-0.085442	-0.740665
H	-3.979738	-0.540461	-0.520500
H	-3.062823	0.730157	-1.456895
H	-1.123985	-0.813606	-1.625882
H	-1.933676	-2.053074	-0.564743
C	2.042335	0.571767	0.475149
O	3.026150	1.035054	0.863564
Cl	1.387885	-2.301993	-0.299969
C	-2.456059	-0.600003	1.727411
H	-3.048919	0.116898	2.308686
H	-3.068560	-1.494016	1.574682
H	-1.579509	-0.886070	2.317083
C	0.278162	3.064248	-0.518494
H	1.114857	3.095656	-1.224142
H	-0.389568	3.901201	-0.765552
H	0.672694	3.235174	0.488441

2c

Total SCF energy: -1036.74116322 a.u.
Enthalpy at 298K: -1036.484248 a.u.
Gibbs free energy at 298K: -1036.545348 a.u.
Total free energy in solution at 298K: -1036.545301 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	0.846369	-0.101864	-0.169457
C	-1.163971	-0.841650	-1.550356
C	-1.750661	0.088622	-0.394847
C	-0.833184	1.156210	0.108505
C	0.055987	1.867585	-0.718195
H	-0.040795	1.778478	-1.801290
H	-0.993976	1.497696	1.128352
C	-2.291779	0.124202	-1.795193
H	-3.281583	-0.300075	-1.942270
H	-2.085593	0.993525	-2.413366
H	-0.231112	-0.625806	-2.084473
H	-1.366253	-1.903161	-1.458827
C	2.175150	0.535397	0.887953
O	3.009248	0.941694	1.575477
Cl	1.811182	-2.233511	-0.327051
C	-2.630340	-0.623107	0.647402
H	-3.136711	-1.438286	0.111482
C	-1.842632	-1.255301	1.804820
H	-1.074278	-1.945553	1.442192
H	-1.344690	-0.496966	2.420097
H	-2.523695	-1.812218	2.458946
C	-3.722183	0.330181	1.165837
H	-4.306875	0.759225	0.344244
H	-4.411107	-0.204367	1.828915
H	-3.291824	1.158924	1.741267
C	0.738139	3.139034	-0.272655
H	1.741325	3.225383	-0.702838
H	0.162194	4.012776	-0.607781
H	0.827136	3.193363	0.817320

2d

Total SCF energy: -1033.31547099 a.u.
Enthalpy at 298K: -1033.112883 a.u.
Gibbs free energy at 298K: -1033.170686 a.u.
Total free energy in solution at 298K: -1033.172509 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	0.561165	-0.136273	-0.195003
C	-1.694555	-0.600282	-1.220161
C	-1.955117	0.351107	0.081653
C	-0.862411	1.295847	0.437102
C	-0.067464	1.932711	-0.534083

H	-0.380334	1.899484	-1.578836
H	-0.820401	1.610635	1.477358
C	-2.773321	0.454426	-1.156056
H	-3.794420	0.099824	-1.054691
H	-2.653041	1.337750	-1.776457
H	-0.904313	-0.442771	-1.960400
H	-1.971648	-1.638162	-1.076343
C	2.142492	0.286467	0.601120
O	3.134332	0.557165	1.125728
Cl	1.210974	-2.358589	-0.578774
O	-2.630072	-0.263886	1.118143
C	-1.862159	-1.059367	2.027499
H	-1.157045	-0.451544	2.606439
H	-2.587889	-1.511763	2.706247
H	-1.307361	-1.841004	1.495551
C	0.828444	3.102059	-0.203919
H	1.728901	3.100247	-0.826900
H	0.301022	4.046997	-0.393770
H	1.138001	3.094584	0.846215

3a

Total SCF energy: -918.79553823 a.u.
Enthalpy at 298K: -918.628254 a.u.
Gibbs free energy at 298K: -918.680902 a.u.
Total free energy in solution at 298K: -918.685276 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.187240	-1.712934	0.356035
C	2.362685	-1.255121	-0.519263
C	1.792254	-0.014317	-1.199204
C	1.502600	1.173772	-0.506838
C	1.232525	1.130053	0.896813
Rh	-0.155079	-0.181144	-0.105730
C	-1.517197	1.173681	-0.745568
O	-2.359478	1.829601	-1.159635
Cl	-1.895615	-1.555672	0.625883
H	1.822010	0.454549	1.513078
H	1.239109	2.065191	-1.073359
H	0.733340	-2.650531	0.032861
H	1.395992	-1.754200	1.428849
H	3.274266	-1.011056	0.041324
H	2.638014	-1.997316	-1.274710
C	0.694639	2.325849	1.635219
H	0.061339	2.013271	2.471602
H	1.524949	2.913024	2.054236
H	0.108011	2.981826	0.984016
H	1.754309	0.020458	-2.286154

3b

Total SCF energy: -958.11604401 a.u.
Enthalpy at 298K: -957.919345 a.u.
Gibbs free energy at 298K: -957.975305 a.u.
Total free energy in solution at 298K: -957.976910 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.870925	-1.696984	-0.842511
C	-2.254140	-1.235263	-0.366540
C	-1.916212	-0.038163	0.527385
C	-1.432994	1.159065	-0.037774
C	-0.789345	1.155954	-1.313350
Rh	0.287279	-0.174915	-0.004509
C	1.410009	1.166756	0.994130
O	2.095818	1.828301	1.630609
Cl	2.157740	-1.563851	-0.212222
H	-1.176510	0.496560	-2.087217
H	-1.340579	2.037352	0.599792
H	-0.543226	-2.635047	-0.392257
H	-0.747201	-1.748131	-1.928040
H	-2.927190	-0.932074	-1.178454
H	-2.780550	-1.997955	0.217240
C	-2.345811	-0.080108	1.967822
H	-3.444719	-0.081204	2.021530
H	-2.003424	-1.002909	2.449093
H	-1.971476	0.772328	2.542890
C	-0.086198	2.376109	-1.844804
H	0.763417	2.089659	-2.473306
H	-0.772488	2.965232	-2.470574
H	0.281949	3.022212	-1.041036

3c

Total SCF energy: -1036.74100475 a.u.
Enthalpy at 298K: -1036.484414 a.u.
Gibbs free energy at 298K: -1036.546609 a.u.
Total free energy in solution at 298K: -1036.545782 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.229238	-0.886552	-1.828266
C	-1.640881	-0.316437	-1.642419
C	-1.564250	0.309400	-0.245403
C	-0.796968	1.476715	-0.047935
C	0.273607	1.813291	-0.931419
Rh	0.663327	-0.134273	-0.097227
C	1.435920	0.403702	1.683247
O	1.879328	0.578848	2.725475
Cl	2.338198	-1.752792	-0.325307
H	0.150711	1.617399	-1.994509
H	-0.872061	1.992708	0.908640
H	-0.185004	-1.974744	-1.762051
H	0.290678	-0.551370	-2.730361
H	-1.912544	0.442856	-2.386256
H	-2.418032	-1.085312	-1.679250
C	-2.521727	-0.140836	0.844974
H	-2.229557	0.369013	1.773363
C	-3.954558	0.314060	0.487721
H	-4.306096	-0.164469	-0.433594
H	-4.645773	0.037146	1.291620
H	-4.011003	1.399680	0.350403
C	-2.475809	-1.655524	1.112877
H	-2.787444	-2.234186	0.236207
H	-1.468647	-1.980833	1.392903
H	-3.157248	-1.907121	1.933315
C	1.224841	2.938557	-0.622668
H	2.218480	2.730589	-1.033027
H	0.868912	3.871247	-1.084444
H	1.325292	3.108084	0.454412

3d

Total SCF energy: -1033.32620712 a.u.
Enthalpy at 298K: -1033.123176 a.u.
Gibbs free energy at 298K: -1033.181517 a.u.
Total free energy in solution at 298K: -1033.184444 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.232035	-2.043695	0.457840
C	1.740266	-1.808417	0.631321
C	1.947144	-0.399092	0.114666
C	1.353380	0.719779	0.725746
C	0.344978	0.554705	1.738094
Rh	-0.511812	-0.148461	-0.059931
C	-1.206486	1.576515	-0.747805
O	-1.625380	2.523813	-1.243952
Cl	-2.534450	-1.193003	-0.608002
H	0.406979	-0.322767	2.379928
H	1.592273	1.717709	0.372065
H	0.008419	-2.696412	-0.388336
H	-0.266172	-2.426724	1.352735
H	2.077969	-1.869093	1.673161
H	2.364768	-2.488449	0.044580
O	2.774300	-0.328813	-0.927943
C	2.984148	0.920976	-1.599177
H	3.482727	1.639851	-0.940509
H	3.628431	0.690443	-2.447197
H	2.029606	1.324726	-1.952454
C	-0.256033	1.754191	2.424776
H	-1.278809	1.537112	2.749497
H	0.326412	2.013463	3.321079
H	-0.283370	2.632146	1.770780

4a

Total SCF energy: -918.80490586 a.u.
Enthalpy at 298K: -918.637170 a.u.
Gibbs free energy at 298K: -918.689400 a.u.
Total free energy in solution at 298K: -918.694980 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.502202	-1.104745	1.507714
C	0.041379	-2.397351	0.904341
C	0.354058	-1.978926	-0.536466
C	1.479168	-1.165137	-0.852897
C	2.047941	-0.269739	0.059804
Rh	-0.250245	0.089830	-0.171052
Cl	-0.079084	2.363691	0.506476
C	-2.110100	0.090338	-0.480419
O	-3.240861	0.090660	-0.690477
H	2.012490	-0.502675	1.122558
H	1.726607	-1.040489	-1.908066
H	-1.548222	-1.143896	1.808791
H	0.100082	-0.622444	2.280513
H	0.931276	-2.775219	1.425032
H	-0.709810	-3.192806	0.908173
C	3.051562	0.779507	-0.334256
H	2.786467	1.742555	0.115947
H	4.056532	0.508494	0.015527
H	3.090807	0.912143	-1.420864
H	-0.084708	-2.559742	-1.343465

4b

Total SCF energy: -958.12179706 a.u.
Enthalpy at 298K: -957.924576 a.u.
Gibbs free energy at 298K: -957.980129 a.u.
Total free energy in solution at 298K: -957.982707 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.664100	0.331991	1.763556
C	-1.904324	-0.491804	1.430591
C	-1.772822	-0.717021	-0.085708
C	-0.814087	-1.656324	-0.566082
C	0.339126	-2.016650	0.145368
Rh	0.211551	0.275453	-0.113562
Cl	2.565765	0.550501	0.127873
C	-0.190653	2.101947	-0.392825
O	-0.442629	3.208626	-0.580757
H	0.310533	-2.022442	1.233460
H	-0.849247	-1.900395	-1.629609
H	-0.869986	1.357075	2.069281
H	0.072703	-0.122366	2.429399
H	-1.947008	-1.442566	1.978231
H	-2.826318	0.056860	1.648968
C	-2.950252	-0.339265	-0.954173
H	-3.806341	-0.995684	-0.737347
H	-3.275207	0.688383	-0.762148
H	-2.718232	-0.429726	-2.020272
C	1.463287	-2.808392	-0.467929
H	2.428443	-2.370754	-0.191034
H	1.448310	-3.847164	-0.111714
H	1.398529	-2.821002	-1.561483

4c

Total SCF energy: -1036.74647047 a.u.
Enthalpy at 298K: -1036.489511 a.u.
Gibbs free energy at 298K: -1036.551217 a.u.
Total free energy in solution at 298K: -1036.550888 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.195161	-0.384188	1.949610
C	1.233260	0.143496	1.866145
C	1.456539	0.323847	0.352070
C	0.825451	1.422917	-0.300276
C	-0.338997	2.042474	0.178699
Rh	-0.659966	-0.228356	-0.060300
Cl	-3.023620	0.014829	-0.242065
C	-0.624384	-2.110290	-0.250625
O	-0.598248	-3.253649	-0.377165
H	-0.514572	2.089339	1.251842
H	1.100747	1.619923	-1.336179
H	-0.277230	-1.415293	2.291457
H	-0.929683	0.244025	2.457895

H	1.371823	1.085392	2.412850
H	1.952371	-0.578750	2.266422
C	2.693834	-0.342884	-0.243264
H	2.726211	-1.361656	0.167972
C	3.964698	0.390000	0.242313
H	4.010239	0.450542	1.335329
H	4.864334	-0.133712	-0.100670
H	3.997766	1.412561	-0.153287
C	2.695355	-0.466036	-1.773581
H	1.791472	-0.967601	-2.136537
H	2.765210	0.511386	-2.266056
H	3.562016	-1.051421	-2.099820
C	-1.129963	3.029223	-0.638842
H	-2.202041	2.825886	-0.544305
H	-0.948750	4.055946	-0.293210
H	-0.867738	2.975171	-1.701274

4d

Total SCF energy: -1033.32598501 a.u.
Enthalpy at 298K: -1033.122860 a.u.
Gibbs free energy at 298K: -1033.181117 a.u.
Total free energy in solution at 298K: -1033.184101 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.025304	-0.452784	1.888064
C	1.406051	0.080573	1.915006
C	1.732359	0.391949	0.459178
C	1.075851	1.424015	-0.247357
C	-0.166021	1.963919	0.188619
Rh	-0.445335	-0.205258	-0.121834
Cl	-2.817790	-0.059984	-0.138604
C	-0.334667	-2.095325	-0.447219
O	-0.277913	-3.225920	-0.650764
H	-0.338624	2.064474	1.259603
H	1.416289	1.660581	-1.253177
H	-0.111719	-1.502596	2.165431
H	-0.771975	0.140449	2.418644
H	1.517036	0.978449	2.537020
H	2.120095	-0.667036	2.270870
O	2.884103	-0.196068	0.053010
C	3.303692	-0.036927	-1.298922
H	3.565266	1.005487	-1.517793
H	4.189665	-0.662831	-1.410732
H	2.520406	-0.378272	-1.988132
C	-0.928663	2.952416	-0.661291
H	-2.005591	2.818453	-0.520113
H	-0.675509	3.986621	-0.389294
H	-0.712116	2.821432	-1.727963

5a

Total SCF energy: -996.14157085 a.u.
Enthalpy at 298K: -995.941438 a.u.
Gibbs free energy at 298K: -996.000242 a.u.
Total free energy in solution at 298K: -996.008720 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.494150	-1.362027	1.886124
C	0.579572	-0.897756	2.254983
Rh	0.254438	-0.015939	0.126913
C	2.077973	-0.303550	-0.294181
O	3.170996	-0.502608	-0.585944
C	-1.991428	0.751334	0.069568
C	-1.335282	0.903936	-1.157660
C	-0.108414	1.610654	-1.286356
C	0.317540	2.692070	-0.291805
C	0.633909	1.880885	0.973378
Cl	-0.271642	-2.134541	-1.141071
H	1.667626	1.988125	1.307814
H	-0.040526	2.052037	1.816645
H	-1.617862	0.242609	-1.973588
H	-1.893385	1.529585	0.822643
H	1.203064	3.211292	-0.671863
H	-0.467032	3.447757	-0.151596
H	1.469080	-0.636770	2.787708
H	-1.398833	-1.898041	1.696212
C	-3.180964	-0.161498	0.216906
H	-3.320688	-0.466582	1.259962
H	-4.102256	0.355933	-0.085426
H	-3.069466	-1.057388	-0.401542
H	0.377974	1.572479	-2.258015

5b

Total SCF energy: -1035.45940785 a.u.
Enthalpy at 298K: -1035.229825 a.u.
Gibbs free energy at 298K: -1035.291822 a.u.
Total free energy in solution at 298K: -1035.297168 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.015165	-1.064088	-1.187663
C	1.115756	-1.661440	-1.769602
Rh	0.020961	-0.300996	-0.224884
C	-1.224394	-1.690231	0.117482
O	-1.972945	-2.526142	0.365963
C	1.073804	1.797208	-0.319955
C	0.073250	1.747427	0.660810
C	-1.278073	1.394008	0.384660
C	-1.828411	1.560400	-1.038907
C	-1.102233	0.466012	-1.833822
Cl	1.247497	-0.994329	1.871837
H	-1.781279	-0.276055	-2.258439
H	-0.430365	0.828816	-2.616391
H	0.386875	1.725071	1.702709
H	0.804145	2.062127	-1.339560
H	-2.912651	1.406008	-1.032633
H	-1.650408	2.575534	-1.418670
H	0.529438	-2.294382	-2.400997
H	2.913125	-0.686373	-0.748897
C	-2.256630	1.305746	1.531641
H	-2.720713	2.289477	1.697395
H	-3.066113	0.601773	1.314422
H	-1.767560	0.994773	2.459278
C	2.519134	2.011113	0.052256
H	3.189346	1.677857	-0.747917
H	2.722151	3.080149	0.206615
H	2.772654	1.475812	0.972538

5c

Total SCF energy: -1114.08370714 a.u.
Enthalpy at 298K: -1113.794367 a.u.
Gibbs free energy at 298K: -1113.862073 a.u.
Total free energy in solution at 298K: -1113.864683 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.891725	0.347664	-0.387124
C	2.767155	-0.688316	-1.033280
Rh	0.639264	-0.233374	-0.226914
C	0.334269	-2.097132	-0.021720
O	0.146016	-3.219720	0.138050
C	0.318041	2.074419	-0.391475
C	-0.788593	1.432648	0.191100
C	-1.511610	0.387850	-0.445431
C	-1.433912	0.246576	-1.974418
C	0.002595	-0.222372	-2.231750
Cl	1.212913	-0.137267	2.232468
H	0.053121	-1.214032	-2.685898
H	0.620934	0.470267	-2.809225
H	-0.939367	1.572726	1.258299
H	0.360187	2.177977	-1.473313
H	-2.165325	-0.496485	-2.309333
H	-1.685237	1.190863	-2.475452
H	2.920985	-1.561167	-1.631315
H	3.203105	1.200284	0.176227
C	-2.689038	-0.288414	0.251461
H	-2.736577	-1.313996	-0.141165
C	-3.996964	0.420788	-0.171470
H	-4.124962	0.444085	-1.259158
H	-4.861270	-0.099618	0.256171
H	-4.012360	1.454651	0.194641
C	-2.595254	-0.371681	1.781291
H	-1.638625	-0.784994	2.114025
H	-2.712109	0.614209	2.247510
H	-3.403034	-1.005545	2.164027
C	1.128584	3.075819	0.392747
H	2.111361	3.239788	-0.063442
H	0.623341	4.051885	0.406177
H	1.269299	2.745148	1.426387

5d

Total SCF energy: -1110.66868687 a.u.
Enthalpy at 298K: -1110.432944 a.u.
Gibbs free energy at 298K: -1110.496851 a.u.
Total free energy in solution at 298K: -1110.501964 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	2.613143	0.083343	-0.752135
C	2.426206	-1.133533	-0.835484
Rh	0.438118	-0.259609	-0.216753
C	-0.179212	-2.055190	0.111121
O	-0.524803	-3.126815	0.337693
C	0.339028	1.986192	-0.391249
C	-0.858792	1.500156	0.198783
C	-1.741653	0.638719	-0.487053
C	-1.648132	0.398145	-1.986818
C	-0.263410	-0.234081	-2.203317
Cl	1.054302	-0.173058	2.238489
H	-0.327132	-1.241373	-2.619215
H	0.410413	0.364250	-2.822101
H	-1.002078	1.659626	1.262224
H	0.347716	2.149082	-1.467686
H	-2.464674	-0.272376	-2.269308
H	-1.794474	1.340742	-2.530480
H	2.588003	-2.183079	-0.967227
H	3.068757	1.049682	-0.710078
O	-2.849871	0.120228	0.066120
C	-3.028651	0.202380	1.488386
H	-3.194938	1.239705	1.799741
H	-3.917299	-0.391148	1.703383
H	-2.157568	-0.212002	2.007936
C	1.239633	2.902070	0.403569
H	2.218886	3.014592	-0.075056
H	0.803568	3.909358	0.464699
H	1.390833	2.520809	1.417405

6a

Total SCF energy: -996.19140225 a.u.
Enthalpy at 298K: -995.987665 a.u.
Gibbs free energy at 298K: -996.043766 a.u.
Total free energy in solution at 298K: -996.047713 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	0.575950	-0.055427	-0.093497
C	-0.934248	1.010314	1.344973
C	-1.640763	0.955955	0.176365
C	-2.652984	-0.113466	-0.219738
C	-1.969309	-1.393924	-0.648861
C	-0.643880	-1.581808	-0.595889
C	0.424997	-0.890596	1.823431
C	-0.808061	-0.138305	2.331505
H	-0.678578	0.231916	3.355544
H	-1.694261	-0.779130	2.303425
H	1.357609	-0.580984	2.302214
H	0.325579	-1.975788	1.830136
H	-1.588553	1.831550	-0.470500
H	-3.278997	-0.335850	0.660504
H	-2.622911	-2.176075	-1.045030
H	-0.224345	-2.542957	-0.893841
Cl	1.665958	2.063267	-0.498401
C	2.104326	-1.029448	-0.537317
O	3.035308	-1.655326	-0.778284
C	-3.590338	0.418497	-1.322558
H	-4.342918	-0.333024	-1.583668
H	-4.115957	1.321943	-0.992925
H	-3.024547	0.659540	-2.229866
H	-0.372048	1.916818	1.558989

6b

Total SCF energy: -1035.50829253 a.u.
Enthalpy at 298K: -1035.275258 a.u.

Gibbs free energy at 298K: -1035.333915 a.u.
Total free energy in solution at 298K: -1035.334680 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	0.630708	-0.135920	-0.022890
C	-1.150838	1.231217	0.855805
C	-1.657007	0.631657	-0.270507
C	-2.498725	-0.643952	-0.325436
C	-1.679761	-1.891839	-0.086688
C	-0.361168	-1.875296	0.129517
C	0.346153	-0.182803	2.063205
C	-1.030739	0.476662	2.175475
H	-1.105122	1.157711	3.033031
H	-1.815597	-0.278724	2.270003
H	1.157669	0.455235	2.427529
H	0.406879	-1.169211	2.524238
H	-1.645993	1.224864	-1.184426
H	-3.265111	-0.579830	0.465543
H	-2.216317	-2.842928	-0.137205
H	0.189182	-2.795904	0.318242
Cl	1.404713	1.423956	-1.689628
C	2.285206	-0.996155	0.040062
O	3.292298	-1.542595	0.106654
C	-0.706281	2.673203	0.857364
H	-1.472244	3.265861	1.379413
H	0.233478	2.810924	1.402979
H	-0.579685	3.067541	-0.152606
C	-3.244927	-0.725648	-1.673436
H	-3.870938	-1.623477	-1.713797
H	-3.894158	0.145549	-1.818591
H	-2.533877	-0.769981	-2.505998

6c

Total SCF energy: -1114.13181415 a.u.
Enthalpy at 298K: -1113.838889 a.u.
Gibbs free energy at 298K: -1113.903140 a.u.
Total free energy in solution at 298K: -1113.901165 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	0.872074	-0.089912	0.001533
C	-1.516984	-0.124238	-0.357894
C	-1.254087	0.931693	0.483096
C	-1.094488	2.402263	0.091436
C	0.254923	2.696743	-0.520134
C	1.190307	1.761519	-0.705746
C	0.227752	-0.355405	-1.986987
C	-1.256043	-0.000189	-1.855997
H	-1.900596	-0.667410	-2.439968
H	-1.438966	1.023904	-2.194903
H	0.398485	-1.422455	-2.155806
H	0.760304	0.233756	-2.734298
H	-1.407978	0.751448	1.547004
H	-1.870484	2.643945	-0.654567
H	2.144353	2.000885	-1.172966
Cl	0.874397	-1.255984	2.114277
C	2.637738	-0.589874	-0.349696
O	3.719442	-0.884003	-0.596056
C	-2.167483	-1.393441	0.184971
H	-1.985948	-1.414890	1.265225
C	-1.641181	-2.711778	-0.404545
H	-2.184284	-3.552353	0.041332
H	-1.788085	-2.767846	-1.490008
H	-0.579244	-2.851496	-0.183009
C	-3.692752	-1.269440	-0.042574
H	-4.202195	-2.145138	0.374971
H	-4.100182	-0.375289	0.441343
H	-3.939543	-1.221225	-1.110427
C	-1.351703	3.302278	1.317969
H	-1.267388	4.359663	1.044778
H	-2.356444	3.137913	1.724193
H	-0.621033	3.096410	2.108178
H	0.459627	3.739166	-0.777700

6d

Total SCF energy: -1110.71987299 a.u.
Enthalpy at 298K: -1110.480468 a.u.
Gibbs free energy at 298K: -1110.541234 a.u.
Total free energy in solution at 298K: -1110.540277 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	0.748673	-0.071309	-0.020853
C	-1.465889	0.599571	0.949296
C	-1.599924	-0.047978	-0.267884
C	-1.998076	-1.527408	-0.413630
C	-0.847559	-2.470881	-0.160496
C	0.394483	-2.040651	0.081045
C	0.468181	-0.255371	2.061322
C	-1.049353	-0.127614	2.211471
H	-1.351552	0.443159	3.096180
H	-1.523871	-1.111919	2.245753
H	0.995108	0.622783	2.447090
H	0.875324	-1.165364	2.503975
H	-1.815947	0.568986	-1.135354
H	-2.796705	-1.750062	0.313826
H	-1.061279	-3.540880	-0.226399
H	1.212175	-2.732722	0.277128
Cl	0.998597	1.635583	-1.721704
C	2.598526	-0.310928	0.108599
O	3.728337	-0.491882	0.204962
O	-1.563583	1.918237	1.149518
C	-1.937026	2.789070	0.064789
H	-2.047464	3.774167	0.518161
H	-1.152165	2.802437	-0.695136
H	-2.890564	2.465869	-0.367184
C	-2.595519	-1.760636	-1.817243
H	-2.895946	-2.806847	-1.939172
H	-3.480347	-1.133449	-1.977876
H	-1.858335	-1.526028	-2.593120

7a

Total SCF energy: -996.24525196 a.u.
Enthalpy at 298K: -996.039536 a.u.
Gibbs free energy at 298K: -996.093769 a.u.
Total free energy in solution at 298K: -996.099727 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.891326	-1.319990	-0.312241
O	2.696289	-2.122655	-0.488971
Rh	0.558917	-0.046238	-0.025554
Cl	2.127296	1.537405	0.726204
C	-1.078856	1.659810	-0.227789
C	-1.519836	1.421477	-1.655230
C	-1.799045	-0.052326	-2.024465
C	-0.947778	-1.060182	-1.257471
C	-1.170719	-1.332907	0.105013
C	-2.087527	-0.426930	0.922484
C	-1.358640	0.920100	0.891477
H	-2.404568	2.042213	-1.865802
H	-0.724244	1.808549	-2.302390
H	-2.858198	-0.289249	-1.847424
H	-1.634345	-0.180890	-3.098600
H	-0.913885	-2.305656	0.519986
H	-3.074623	-0.340696	0.441359
H	-0.561462	2.602799	-0.061888
H	-1.045872	1.329459	1.850618
C	-2.288040	-0.929257	2.355095
H	-2.912519	-0.236519	2.929693
H	-2.780480	-1.907709	2.356980
H	-1.326406	-1.029860	2.871583
H	-0.494285	-1.845169	-1.859105

7b

Total SCF energy: -1035.56256697 a.u.
Enthalpy at 298K: -1035.327205 a.u.
Gibbs free energy at 298K: -1035.384491 a.u.
Total free energy in solution at 298K: -1035.387400 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	-0.651928	-0.055730	-0.049740
C	0.554786	-1.368039	-1.282842
C	1.473044	-0.496071	-2.117732
C	2.335574	0.517287	-1.335654
C	1.647038	1.141983	-0.127929
C	1.412570	0.381847	0.986363
C	1.711072	-1.118849	1.031299
C	0.692727	-1.735665	0.071345
H	2.130800	-1.140435	-2.721932
H	0.845637	0.047765	-2.834859
H	3.250579	0.021026	-0.985061
H	2.657771	1.307799	-2.021022
H	1.081710	0.866899	1.903223
H	2.738150	-1.312564	0.681384
H	-0.060258	-2.030553	-1.891743
H	0.201075	-2.647906	0.405331
C	1.573161	-1.686816	2.448140
H	1.776831	-2.763263	2.456480
H	2.280491	-1.204396	3.131621
H	0.560595	-1.527023	2.836051
C	-2.242478	-0.916727	-0.425263
O	-3.220707	-1.482662	-0.649354
Cl	-1.794387	1.855037	0.718569
C	1.477074	2.638050	-0.131883
H	0.926686	2.991003	0.741787
H	2.468866	3.112721	-0.151294
H	0.940644	2.970470	-1.027571

7c

Total SCF energy: -1114.18691714 a.u.
Enthalpy at 298K: -1113.891896 a.u.
Gibbs free energy at 298K: -1113.955211 a.u.
Total free energy in solution at 298K: -1113.955154 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	-0.898244	-0.264043	0.023373
C	-0.740709	1.357271	1.459696
C	0.583668	1.212770	2.183980
C	1.836229	1.146604	1.287120
C	1.650640	0.347679	0.002052
C	0.881804	0.876073	-1.001583
C	0.115947	2.193875	-0.848107
C	-0.978656	1.880751	0.172239
H	0.694408	2.045180	2.896886
H	0.529977	0.301574	2.792670
H	2.136289	2.166427	1.011860
H	2.662480	0.733478	1.871667
H	0.883751	0.398514	-1.980649
H	0.786113	2.981583	-0.466690
H	-1.591126	1.377009	2.141099
H	-1.968796	2.280899	-0.040322
C	-0.469455	2.670025	-2.182292
H	-1.024366	3.605728	-2.052224
H	0.326295	2.848925	-2.913807
H	-1.153002	1.920957	-2.598069
C	-2.632982	-0.699709	0.482089
O	-3.725221	-0.937021	0.762407
Cl	-0.609561	-2.322489	-1.089916
C	2.531838	-0.869339	-0.241017
H	2.144183	-1.373945	-1.132633
C	3.975266	-0.405574	-0.540633
H	4.420983	0.117079	0.314616
H	4.605565	-1.274678	-0.760039
H	4.009459	0.266794	-1.405085
C	2.510355	-1.887901	0.911563
H	1.497421	-2.260995	1.086064
H	3.143150	-2.744975	0.655480
H	2.898846	-1.464292	1.846069

7d

Total SCF energy: -1110.77297390 a.u.
Enthalpy at 298K: -1110.531357 a.u.
Gibbs free energy at 298K: -1110.590646 a.u.
Total free energy in solution at 298K: -1110.592616 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Rh	-0.784340	0.102178	-0.037738
C	-0.325371	-1.798177	-0.973165
C	0.810054	-1.607367	-1.962419
C	2.125943	-1.028216	-1.405902
C	1.949725	0.073885	-0.384285

C	1.373904	-0.160279	0.845250
C	0.981309	-1.590904	1.254127
C	-0.262538	-1.916979	0.431474
H	1.027916	-2.573986	-2.442264
H	0.447128	-0.949937	-2.762161
H	2.709277	-1.827763	-0.930314
H	2.731004	-0.636016	-2.227197
H	1.417894	0.597640	1.621063
H	1.796415	-2.296381	1.023257
H	-1.204606	-2.239881	-1.442003
H	-1.059943	-2.459586	0.936999
O	2.514783	1.215262	-0.787465
C	2.599588	2.325137	0.125131
H	3.169971	2.035038	1.015391
H	3.133705	3.102785	-0.420961
H	1.598977	2.668244	0.397683
C	0.700225	-1.677511	2.759194
H	0.410048	-2.695865	3.040670
H	1.591157	-1.408515	3.337302
H	-0.111179	-0.998272	3.043929
C	-2.592690	-0.041840	-0.368777
O	-3.723627	-0.164088	-0.558347
Cl	-0.991329	2.424036	0.373504

8a

Total SCF energy: -312.02878029 a.u.
Enthalpy at 298K: -311.839774 a.u.
Gibbs free energy at 298K: -311.881181 a.u.
Total free energy in solution at 298K: -311.879313 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-0.837032	1.567195	-0.090615
C	-1.956293	0.555255	-0.067555
C	-1.615060	-0.790837	0.594279
C	-0.585439	-1.612519	-0.144300
C	0.611456	-1.210370	-0.582615
C	1.305504	0.123992	-0.427775
C	0.480520	1.373597	-0.218491
H	-2.807893	0.998938	0.465501
H	-2.311812	0.369959	-1.092322
H	-1.275809	-0.598394	1.622326
H	-2.537335	-1.377604	0.685174
H	1.231694	-1.957229	-1.080820
H	-1.162113	2.603520	0.008224
H	1.102313	2.270902	-0.195405
H	-0.855739	-2.651420	-0.333262
C	2.391679	0.010443	0.675675
H	3.072523	-0.823337	0.469750
H	2.988341	0.928668	0.735174
H	1.928155	-0.161170	1.652895
H	1.855664	0.296631	-1.368846

8b

Total SCF energy: -351.34682373 a.u.
Enthalpy at 298K: -351.128768 a.u.
Gibbs free energy at 298K: -351.172680 a.u.
Total free energy in solution at 298K: -351.167875 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	0.457041	1.915946	-0.395460
C	-1.021075	1.785123	-0.116509
C	-1.434084	0.582732	0.751483
C	-1.139426	-0.747880	0.085460
C	0.122960	-1.155453	-0.091561
C	1.354693	-0.389232	0.362981
C	1.438702	1.030367	-0.188034
H	-1.358265	2.710290	0.374687
H	-1.566808	1.751389	-1.073064
H	-0.906615	0.648508	1.713691
H	-2.504242	0.661240	0.979416
H	0.305609	-2.106275	-0.593626
H	1.321912	-0.314371	1.464575
H	2.450929	1.354333	-0.434676
C	2.634666	-1.168399	0.011484
H	3.526635	-0.656433	0.390004
H	2.612379	-2.174087	0.446195
H	2.741649	-1.272316	-1.075391
C	-2.320625	-1.553707	-0.391714
H	-2.935339	-0.978448	-1.098914
H	-2.009347	-2.477907	-0.889482
H	-2.981416	-1.822966	0.444730
H	0.745805	2.880057	-0.816936

8c

Total SCF energy: -429.97127283 a.u.
Enthalpy at 298K: -429.693333 a.u.
Gibbs free energy at 298K: -429.743252 a.u.
Total free energy in solution at 298K: -429.736439 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	-1.721883	1.774521	0.211399
C	-0.298029	2.089830	-0.176946
C	0.636366	-0.287213	-0.129626
C	-0.427920	-1.043688	0.168020
C	-1.854023	-0.758643	-0.275458
C	-2.372267	0.606415	0.162542
H	-0.308889	2.999489	-0.796646
H	0.266593	2.364975	0.727571
H	-0.283759	-1.945312	0.765324
H	-1.876331	-0.783070	-1.379599
H	-3.420028	0.613300	0.466604
C	-2.803212	-1.867482	0.211800
H	-3.822995	-1.705302	-0.155304
H	-2.469964	-2.850664	-0.139177
H	-2.840253	-1.894854	1.307926
C	2.031122	-0.674362	0.339949
H	1.924687	-1.585533	0.944541
H	-2.284313	2.637005	0.572588
C	2.667154	0.403673	1.239442
H	3.648183	0.073437	1.602169
H	2.819291	1.344580	0.696200
H	2.036418	0.614890	2.110099
C	2.960442	-1.015507	-0.842557
H	3.943228	-1.340057	-0.479563
H	2.539343	-1.821032	-1.454211

H	3.121875	-0.147992	-1.494084
C	0.459419	0.985547	-0.938552
H	1.432180	1.383668	-1.248814
H	-0.088285	0.763936	-1.865694

8d

Total SCF energy: -426.55346415 a.u.
Enthalpy at 298K: -426.328771 a.u.
Gibbs free energy at 298K: -426.375784 a.u.
Total free energy in solution at 298K: -426.371544 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.992755	1.240073	-0.431337
C	0.781758	2.050759	-0.042882
C	-0.230216	1.322643	0.855333
C	-0.948993	0.186899	0.169107
C	-0.363300	-0.884401	-0.387064
C	1.116553	-1.213416	-0.394346
C	2.118065	-0.086840	-0.547378
H	1.128658	2.949151	0.485925
H	0.268077	2.419469	-0.943802
H	0.291560	0.949969	1.746394
H	-0.989618	2.031002	1.201240
H	-0.987592	-1.651135	-0.836931
H	3.113178	-0.455558	-0.803767
H	2.886417	1.831670	-0.633556
C	1.494091	-2.102700	0.820722
H	0.863195	-2.998213	0.856075
H	2.541373	-2.425473	0.766423
H	1.355764	-1.552769	1.757743
H	1.275060	-1.844643	-1.283123
O	-2.302916	0.415319	0.189986
C	-3.153370	-0.547865	-0.403806
H	-4.171708	-0.174738	-0.275651
H	-2.938220	-0.666547	-1.474574
H	-3.056858	-1.525645	0.087621

9

Total SCF energy: -77.32380182 a.u.
Enthalpy at 298K: -77.293271 a.u.
Gibbs free energy at 298K: -77.316163 a.u.
Total free energy in solution at 298K: -77.317573 a.u.

Cartesian coordinates

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

TS1a

Total SCF energy: -918.78685502 a.u.
Enthalpy at 298K: -918.620816 a.u.
Gibbs free energy at 298K: -918.671793 a.u.
Total free energy in solution at 298K: -918.679404 a.u.
Imaginary frequency: -239.4277 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-1.058533	-1.820866	-0.481102
C	-1.756694	-0.662052	1.031112
Rh	0.235274	-0.084149	-0.013581
C	-1.441565	1.235498	-0.527712
H	-0.512489	-2.692283	-0.135376
H	-0.956556	-1.620913	-1.551572
C	-1.547784	0.737393	0.794134
H	-1.370941	1.386138	1.648321
H	-1.928539	0.685226	-1.332674
Cl	2.054067	-1.577881	-0.279070
C	-2.437165	-1.615876	0.107040
H	-3.162460	-1.152295	-0.563774
H	-2.879902	-2.481914	0.600658
C	1.501524	1.312665	0.329892
O	2.273179	2.120837	0.598165
C	-1.231642	2.698832	-0.820257
H	-0.612798	2.835940	-1.713289
H	-2.195578	3.190750	-1.012368
H	-0.747595	3.216916	0.014121
H	-1.493901	-1.037170	2.017299

TS1b

Total SCF energy: -958.10641465 a.u.
Enthalpy at 298K: -957.910878 a.u.
Gibbs free energy at 298K: -957.964844 a.u.
Total free energy in solution at 298K: -957.969478 a.u.
Imaginary frequency: -220.8227 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-1.468904	-1.098319	-0.992218
C	-1.931507	0.101438	0.542357
Rh	0.347066	-0.129811	-0.125943
C	-0.540894	1.794225	-0.663557
H	-1.428576	-2.137804	-0.683871
H	-1.056774	-0.908188	-1.987027
C	-1.091307	1.275777	0.534084
H	-0.850321	1.728887	1.493181
H	-1.037011	1.570763	-1.607753
Cl	1.381799	-2.256137	-0.312672
C	-2.729150	-0.340242	-0.638083
H	-3.000697	0.453852	-1.334702
H	-3.602889	-0.946288	-0.392424
C	1.976467	0.576923	0.547281
O	2.951165	0.980813	1.006324
C	-2.204841	-0.590204	1.854504
H	-3.171702	-0.236184	2.241840
H	-2.284478	-1.672996	1.720497
H	-1.428403	-0.393043	2.597402
C	0.273697	3.062898	-0.686528
H	1.059172	3.011316	-1.447889
H	-0.365232	3.922271	-0.934290
H	0.747674	3.261781	0.280255

TS1c

Total SCF energy: -1036.73458679 a.u.
Enthalpy at 298K: -1036.478806 a.u.
Gibbs free energy at 298K: -1036.539696 a.u.
Total free energy in solution at 298K: -1036.539108 a.u.
Imaginary frequency: -250.0959 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-0.034646	-2.137159	0.126945
C	1.579554	-0.370564	0.193695
Rh	-0.686141	-0.165868	-0.070975
C	-0.068015	0.084890	1.972578
H	-0.218237	-2.628900	-0.829691
H	-0.577264	-2.661237	0.918972
C	1.004984	0.512016	1.128476
H	1.219455	1.576186	1.060227
H	-0.051320	-0.931127	2.361153
Cl	-2.609973	-0.979112	-1.127077
C	1.448567	-1.884039	0.412674
H	1.754272	-2.155375	1.430654
H	2.112588	-2.421033	-0.273130
C	-1.284365	1.713761	-0.471852
O	-1.667397	2.737476	-0.816877
C	2.576484	0.086848	-0.860034
H	2.482492	-0.629355	-1.685984
C	2.388928	1.513548	-1.435111
H	2.149891	1.472393	-2.502104
H	1.579397	2.068623	-0.954396
H	3.301035	2.109723	-1.325702
C	3.999729	-0.094721	-0.272953
H	4.163103	-1.110351	0.102671
H	4.749908	0.103041	-1.046257
H	4.169485	0.606425	0.552714
C	-0.815235	1.058407	2.844578
H	-1.857183	0.745932	2.969685
H	-0.361520	1.094238	3.845905
H	-0.806950	2.072054	2.430525

TS1d

Total SCF energy: -1033.31419655 a.u.
Enthalpy at 298K: -1033.112862 a.u.
Gibbs free energy at 298K: -1033.169231 a.u.
Total free energy in solution at 298K: -1033.172549 a.u.
Imaginary frequency: -165.5489 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-1.466119	-0.713307	-1.325399
C	-1.944879	0.351912	0.089192
Rh	0.508623	-0.128080	-0.211037
C	-0.102209	1.923304	-0.601780
H	-1.659046	-1.758387	-1.112300
H	-0.776201	-0.525573	-2.152905
C	-0.891203	1.321070	0.405062
H	-0.819841	1.656276	1.436319
H	-0.442773	1.878516	-1.636586
Cl	1.207879	-2.372680	-0.477588
C	-2.636623	0.239376	-1.210679
H	-2.607440	1.116560	-1.853310
H	-3.625094	-0.210172	-1.147707
C	2.111979	0.303556	0.619721
O	3.093104	0.565679	1.165806
O	-2.572937	-0.331684	1.074587
C	-1.830170	-0.770722	2.223124
H	-1.567799	0.070217	2.874133
H	-2.500225	-1.444515	2.758593
H	-0.923877	-1.299593	1.909311
C	0.800000	3.097395	-0.309424
H	1.689929	3.077570	-0.947198
H	0.274985	4.041845	-0.509484
H	1.129421	3.108934	0.734752

TS2a

Total SCF energy: -918.77792994 a.u.
Enthalpy at 298K: -918.612093 a.u.
Gibbs free energy at 298K: -918.664114 a.u.
Total free energy in solution at 298K: -918.667918 a.u.
Imaginary frequency: -232.8964 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-0.806232	-0.108052	1.821205
C	-1.742913	1.076862	1.584857
C	-1.403739	1.522411	0.163313
C	-1.560616	0.666131	-0.938015
C	-1.593558	-0.759654	-0.720458
Rh	0.251043	0.014443	0.027161
Cl	1.624469	-1.778903	0.617000
C	1.687983	1.362444	-0.682605
O	2.130864	2.374259	-0.986767
H	-2.213927	-1.141027	0.088612
H	-1.446966	1.062791	-1.945581
H	-2.808095	0.823921	1.681513
H	-1.538969	1.894253	2.283340
H	-0.017628	0.068835	2.555219
H	-1.273543	-1.078304	1.994049
C	-1.444524	-1.713307	-1.879596
H	-1.050701	-2.674955	-1.538771
H	-2.423745	-1.897031	-2.347416
H	-0.770748	-1.321112	-2.649137
H	-1.233887	2.578962	-0.031139

TS2b

Total SCF energy: -958.09694573 a.u.
Enthalpy at 298K: -957.901608 a.u.
Gibbs free energy at 298K: -957.956780 a.u.
Total free energy in solution at 298K: -957.958745 a.u.
Imaginary frequency: -239.3193 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-0.064438	-0.780244	1.813596
C	-1.549962	-1.058787	1.595275
C	-1.842345	-0.511125	0.192469
C	-1.162984	-1.049958	-0.913611
C	0.068466	-1.777955	-0.722328
Rh	0.328077	0.199740	0.020599

Cl	2.572684	0.492796	0.600347
C	-0.135199	2.118028	-0.659051
O	-0.797075	3.009397	-0.945029
H	0.111708	-2.513544	0.079183
H	-1.470791	-0.756116	-1.916477
H	-1.811396	-2.124360	1.660015
H	-2.168709	-0.531441	2.329179
H	0.148385	0.001674	2.545451
H	0.575237	-1.645819	1.991196
C	-3.066313	0.345755	0.006304
H	-3.967150	-0.246081	0.225214
H	-3.068162	1.194429	0.699274
H	-3.154181	0.731076	-1.014352
C	0.946650	-2.109000	-1.903621
H	1.982881	-2.252800	-1.584973
H	0.608071	-3.041506	-2.380466
H	0.928382	-1.316806	-2.660092

TS2c

Total SCF energy: -1036.72018317 a.u.
Enthalpy at 298K: -1036.465109 a.u.
Gibbs free energy at 298K: -1036.526556 a.u.
Total free energy in solution at 298K: -1036.525666 a.u.
Imaginary frequency: -261.0977 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-0.391629	-1.114916	-1.681601
C	1.114861	-1.293556	-1.510774
C	1.472391	-0.529959	-0.225359
C	0.851089	-0.903954	0.977092
C	-0.359712	-1.690803	0.956408
Rh	-0.733558	0.140131	-0.062145
Cl	-3.024935	0.221323	-0.558862
C	-0.534379	2.192450	0.262632
O	-0.211508	3.289321	0.303811
H	-0.405595	-2.546769	0.285434
H	1.179425	-0.456439	1.912031
H	1.423414	-2.346145	-1.439538
H	1.661274	-0.857381	-2.353903
H	-0.679946	-0.472328	-2.516462
H	-0.994480	-2.023996	-1.684525
C	2.714665	0.347904	-0.265272
H	2.603748	1.011469	-1.135672
C	3.957789	-0.537518	-0.523090
H	3.855496	-1.140116	-1.431240
H	4.849373	0.089160	-0.636369
H	4.128252	-1.218695	0.319382
C	2.947781	1.224947	0.972269
H	3.170385	0.621025	1.860074
H	3.808827	1.880558	0.803548
H	2.086236	1.860793	1.198170
C	-1.174113	-1.865131	2.214777
H	-2.218052	-2.081296	1.970438
H	-0.785400	-2.708765	2.805719
H	-1.149327	-0.970793	2.847095

TS2d

Total SCF energy: -1033.30449105 a.u.
Enthalpy at 298K: -1033.102989 a.u.
Gibbs free energy at 298K: -1033.160890 a.u.
Total free energy in solution at 298K: -1033.163294 a.u.
Imaginary frequency: -252.4533 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-0.416194	-0.888058	-1.771166
C	1.072108	-1.244881	-1.773158
C	1.636391	-0.704794	-0.469282
C	1.074246	-1.031210	0.773198
C	-0.211240	-1.697511	0.817771
Rh	-0.560423	0.204024	-0.009145
Cl	-2.843683	0.528237	-0.373150
C	0.040080	2.135672	0.466713
O	0.786054	2.999941	0.596020
H	-0.392113	-2.499979	0.103345
H	1.545895	-0.696661	1.692029
H	1.266705	-2.324256	-1.844724
H	1.609255	-0.761833	-2.594359
H	-0.693012	-0.151725	-2.528031
H	-1.103895	-1.734404	-1.806388
O	2.794003	-0.042539	-0.634573
C	3.501306	0.439296	0.510924
H	3.795779	-0.389117	1.165389
H	4.390739	0.933398	0.119679
H	2.895519	1.161780	1.067931
C	-0.893379	-1.912924	2.147555
H	-1.969612	-2.047215	2.006623
H	-0.502394	-2.816941	2.639282
H	-0.741592	-1.066923	2.827412

TS3a

Total SCF energy: -996.11708245 a.u.
Enthalpy at 298K: -995.917327 a.u.
Gibbs free energy at 298K: -995.972339 a.u.
Total free energy in solution at 298K: -995.983518 a.u.
Imaginary frequency: -287.1716 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-1.162191	-0.524353	1.809374
C	-1.989847	0.342988	0.113346
C	-1.321698	0.609509	-1.181443
C	-0.455993	1.650629	-1.446829
C	-0.095495	2.733681	-0.439735
C	0.495889	1.996456	0.773724
C	0.087511	-0.717904	1.990041
Rh	0.387480	-0.011575	0.109066
Cl	0.131581	-2.274074	-0.925941
C	2.222829	-0.158718	-0.041042
O	3.365386	-0.268157	-0.126306
H	0.778357	-1.110539	2.718941
H	-2.129718	-0.707295	2.243019
H	-0.102904	2.083510	1.684160
H	1.519698	2.304789	0.990655
H	-2.216369	1.249014	0.675423
H	-1.501012	-0.121856	-1.964872
H	-0.978165	3.340437	-0.190551

H	0.632982	3.414210	-0.891184
C	-3.148303	-0.634854	-0.031088
H	-3.702988	-0.764263	0.903292
H	-3.852333	-0.256269	-0.782056
H	-2.778641	-1.610315	-0.362887
H	-0.061682	1.719353	-2.458561

TS3b

Total SCF energy: -1035.43687582 a.u.
Enthalpy at 298K: -1035.207475 a.u.
Gibbs free energy at 298K: -1035.265631 a.u.
Total free energy in solution at 298K: -1035.273302 a.u.
Imaginary frequency: -268.1338 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	1.242585	-1.391760	-1.489119
C	1.975766	0.177147	-0.329668
C	1.265164	0.956404	0.709952
C	0.386118	2.003596	0.497299
C	0.058019	2.477718	-0.917467
C	-0.511717	1.263035	-1.670950
C	0.006319	-1.696610	-1.587110
Rh	-0.371102	-0.255792	-0.205201
Cl	-0.081879	-1.829520	1.716418
C	-2.204369	-0.376749	-0.028431
O	-3.347574	-0.464261	0.081842
H	-0.651871	-2.394530	-2.079220
H	2.230213	-1.698869	-1.785380
H	0.086054	0.956961	-2.533634
H	-1.540671	1.426725	-1.995371
H	2.187350	0.751332	-1.231495
H	1.450610	0.646322	1.735152
H	0.957244	2.894511	-1.393896
H	-0.668599	3.295293	-0.863599
C	-0.164580	2.785839	1.659126
H	0.271010	3.795771	1.659343
H	-1.249527	2.911268	1.572693
H	0.056100	2.312007	2.619514
C	3.167575	-0.579971	0.241547
H	3.750851	-1.084406	-0.534952
H	3.836787	0.125706	0.748901
H	2.831275	-1.323423	0.971052

TS3c

Total SCF energy: -1114.06185294 a.u.
Enthalpy at 298K: -1113.772678 a.u.
Gibbs free energy at 298K: -1113.837390 a.u.
Total free energy in solution at 298K: -1113.843131 a.u.
Imaginary frequency: -263.0305 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	2.271689	1.163777	-1.018956
C	0.499811	2.018464	-0.297304
C	-0.610311	1.357734	0.423346
C	-1.630889	0.607041	-0.134978
C	-1.681408	0.392135	-1.646758
C	-0.370501	-0.312604	-2.038354
C	2.478396	-0.092898	-1.097506
Rh	0.674098	-0.364227	-0.201398
Cl	1.647740	-0.298343	2.102442
C	0.606208	-2.207139	-0.113188
O	0.589030	-3.357743	-0.058504
H	3.222254	-0.808094	-1.409736
H	2.728746	2.127130	-1.160084
H	0.231945	0.245921	-2.759702
H	-0.549480	-1.315668	-2.429616
H	0.239888	2.323519	-1.310879
H	-0.600405	1.478815	1.503880
H	-1.810133	1.357578	-2.156274
H	-2.555388	-0.210423	-1.910839
C	-2.778773	0.137657	0.742233
H	-2.503240	0.348488	1.783151
C	-3.059323	-1.371952	0.635514
H	-2.186611	-1.955703	0.943549
H	-3.896708	-1.641904	1.288679
H	-3.329355	-1.667951	-0.384891
C	-4.047625	0.956910	0.413268
H	-3.875088	2.031553	0.538175
H	-4.383805	0.782754	-0.615656
H	-4.864356	0.664257	1.082461
C	1.170900	3.093375	0.547095
H	1.931063	3.648368	-0.011202
H	0.416705	3.816097	0.882087
H	1.636698	2.644255	1.429886

TS3d

Total SCF energy: -1110.64861984 a.u.
Enthalpy at 298K: -1110.412929 a.u.
Gibbs free energy at 298K: -1110.473436 a.u.
Total free energy in solution at 298K: -1110.479143 a.u.
Imaginary frequency: -260.8434 cm^{-1}

Cartesian coordinates

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

H	-2.245100	-0.605550	2.126933
C	0.225873	3.185518	0.309712
H	0.904723	3.850269	-0.232586
H	-0.690347	3.750464	0.521117
H	0.690305	2.906183	1.260577
H	-0.357330	2.118324	-1.539475

TS4a

Total SCF energy: -996.16615910 a.u.
Enthalpy at 298K: -995.963707 a.u.
Gibbs free energy at 298K: -996.017890 a.u.
Total free energy in solution at 298K: -996.024057 a.u.
Imaginary frequency: -429.8493 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-0.666789	-1.345242	-0.978759
C	-0.297383	-1.993179	0.793390
Rh	0.609188	-0.058141	0.040901
C	-1.874620	-0.796356	-1.239630
C	-2.503630	0.318863	-0.430032
C	-1.529968	0.865458	0.610190
C	-1.037301	0.154106	1.670475
C	-1.253877	-1.344956	1.800926
C	2.182184	-0.640634	-0.787447
Cl	1.631625	2.029067	0.435374
H	-1.337034	1.935804	0.583088
H	-3.391422	-0.071705	0.097748
H	-2.417335	-1.108134	-2.133704
H	-0.279363	-2.109112	-1.647932
H	-0.642282	-2.957298	0.419244
H	0.700665	-2.164760	1.213624
H	-1.031297	-1.688396	2.816867
H	-2.294094	-1.610783	1.580131
O	3.151366	-0.998707	-1.291032
C	-2.990839	1.449718	-1.358615
H	-3.699788	1.064952	-2.099578
H	-3.495536	2.235225	-0.784691
H	-2.147363	1.899781	-1.893603
H	-0.493831	0.679628	2.452182

TS4b

Total SCF energy: -1035.48407010 a.u.
Enthalpy at 298K: -1035.252058 a.u.
Gibbs free energy at 298K: -1035.309176 a.u.
Total free energy in solution at 298K: -1035.312135 a.u.
Imaginary frequency: -433.4670 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-0.500623	-1.843060	0.146608
C	-0.300609	-1.020712	1.866433
Rh	0.639538	-0.112865	0.016136
C	-1.682958	-1.727673	-0.496777
C	-2.383774	-0.411711	-0.755881
C	-1.548624	0.787270	-0.303715
C	-1.207104	1.072627	0.995093
C	-1.413362	0.008263	2.069895
C	2.286308	-0.984344	-0.047979
Cl	1.591137	1.671982	-1.201552
H	-1.395821	1.569406	-1.045145
H	-3.339292	-0.395992	-0.201661
H	-2.141525	-2.615808	-0.935000
H	-0.038033	-2.821993	0.239663
H	-0.535115	-2.003793	2.275665
H	0.639582	-0.710309	2.339515
H	-1.353569	0.445720	3.073139
H	-2.399084	-0.460184	1.970611
O	3.300718	-1.524976	-0.088188
C	-0.737487	2.437583	1.430747
H	-0.444388	3.056552	0.580436
H	-1.556062	2.937075	1.970551
H	0.112864	2.371811	2.118115
C	-2.732168	-0.280369	-2.253210
H	-3.343460	-1.126647	-2.584860
H	-3.297678	0.639216	-2.442863
H	-1.820312	-0.257293	-2.859695

TS4c

Total SCF energy: -1114.10835565 a.u.
Enthalpy at 298K: -1113.816627 a.u.
Gibbs free energy at 298K: -1113.879833 a.u.
Total free energy in solution at 298K: -1113.879529 a.u.
Imaginary frequency: -433.7582 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	0.982029	1.596502	-1.118577
C	0.013514	0.259546	-2.097190
Rh	0.844593	-0.164664	-0.031323
C	0.291561	2.605047	-0.544125
C	-0.889982	2.400891	0.378901
C	-1.145564	0.920809	0.674411
C	-1.550512	-0.021543	-0.241410
C	-1.467890	0.325854	-1.725923
C	2.570313	-0.754327	-0.429743
Cl	0.952630	-1.383740	1.990081
H	-1.227894	0.657322	1.727899
H	-1.795743	2.820962	-0.094366
H	0.636944	3.632199	-0.673416
H	1.854759	1.822468	-1.725362
H	0.267754	0.842034	-2.983245
H	0.341712	-0.767097	-2.300319
H	-2.046217	-0.372848	-2.339071
H	-1.866889	1.330071	-1.909005
O	3.634413	-1.114917	-0.675995
C	-2.236512	-1.308228	0.202359
H	-1.986420	-1.455044	1.259029
C	-3.765341	-1.106443	0.092085
H	-4.076387	-0.936684	-0.946418
H	-4.286491	-2.001623	0.449825
H	-4.102694	-0.253732	0.691408
C	-1.799054	-2.570214	-0.558651
H	-2.028091	-2.507610	-1.629966
H	-0.726946	-2.749893	-0.438010
H	-2.333522	-3.441181	-0.163194
C	-0.675195	3.173453	1.697283
H	-0.508251	4.238012	1.500368

H	-1.552300	3.084153	2.348614
H	0.195765	2.783210	2.234844

TS4d

Total SCF energy: -1110.69423667 a.u.
Enthalpy at 298K: -1110.455873 a.u.
Gibbs free energy at 298K: -1110.515048 a.u.
Total free energy in solution at 298K: -1110.516464 a.u.
Imaginary frequency: -434.3869 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
C	-0.181268	-2.029695	-0.331036
C	0.029172	-1.027819	-1.937000
Rh	-0.745147	-0.057825	-0.028400
C	0.918532	-2.342740	0.389319
C	1.930068	-1.322442	0.860059
C	1.555655	0.111323	0.453118
C	1.559288	0.537462	-0.861265
C	1.443683	-0.454683	-2.001237
C	-2.573271	-0.327625	-0.240249
Cl	-1.230262	1.752123	1.419409
H	1.644777	0.858885	1.234995
H	2.919383	-1.568838	0.435197
H	1.058594	-3.367114	0.738573
H	-0.905710	-2.803665	-0.569126
H	-0.072429	-1.977533	-2.462883
H	-0.695114	-0.345788	-2.399768
H	1.622997	0.055155	-2.952591
H	2.194058	-1.244323	-1.885926
O	-3.704404	-0.504185	-0.363538
O	1.650720	1.800794	-1.294603
C	1.789142	2.868477	-0.340545
H	2.678386	2.708845	0.279808
H	1.909789	3.771616	-0.938897
H	0.893391	2.936834	0.282314
C	2.076474	-1.399364	2.394651
H	2.350327	-2.412866	2.707358
H	2.857978	-0.715079	2.745611
H	1.134267	-1.130319	2.883627