Supporting information to
"Mechanism for C-H Bond Activation in Ethylene in the Gas Phase vs. in Solution - Vinylic or Agostic? Revisisting the Case of Protonated Cp*Rh(C2H4)2"

by E. Fooladi, A. Krapp, O. Sekiguchi, M. Tilset, E. Uggerud

Department of Chemistry and Center for Theortical and Computational Chemistry,
University of Oslo, P.O.Box 1033 Blindern, N-0315 Oslo, Norway
mats.tilset@kjemi.uio.no

Optimized structures and their electronic energies (E) and the zero-point energies (ZPE) at BP86/def2-TZVPP
Numbering as in the text, cartesian coordinates in Angstrom

Structure 10
E=-658.6256477 ZPE=0.3261741

Rh	0.505608	-0.166115	-0.392358
C	-1.754634	0.188586	-0.689065
C	-1.056515	1.415405	-0.270800
C	-0.540147	1.214312	1.053349
C	-0.798877	-0.157011	1.412612
C	-1.596812	-0.769414	0.337824
C	0.086626	2.251234	1.925108
C	-0.570172	-0.755598	2.762705
C	-2.197801	-2.136244	0.393554
C	-2.566721	0.046050	-1.937460
C	-1.083872	2.716714	-1.006746
H	0.621326	3.009853	1.342193
H	-0.694782	2.766904	2.504949
H	0.787318	1.814726	2.646895
H	0.350820	-0.387434	3.229000
H	-1.405076	-0.481866	3.427672
H	-0.531272	-1.850476	2.733561
H	-1.508470	-2.879247	0.815771
H	-3.088286	-2.128575	1.041447
H	-2.515331	-2.486085	-0.595156
H	-2.658081	-0.999906	-2.251553
H	-3.585117	0.428365	-1.765481
H	-2.145831	0.617913	-2.772643
H	-1.130043	2.578441	-2.092876
H	-1.981280	3.284198	-0.712709
H	-0.212067	3.338165	-0.772805
C	1.519343	-2.054662	0.330117
C	1.258579	-2.198739	-1.026213
H	2.062164	-2.062907	-1.749821
H	2.518559	-1.805849	0.680149
H	3.489974	0.541818	-1.682596
C	3.434202	0.791580	-0.621052
C	2.357156	0.598654	0.140076
H	2.389640	0.864090	1.201773
H	4.342340	1.222745	-0.189440
H	0.393160	-2.760788	-1.376788
H	0.850299	-2.498088	1.065981
H	1.157546	0.584449	-1.796253
H	0.797984	-0.140486	-2.099199

Structure 11
E=-657.4372452 ZPE=0.3089999

Rh	-0.582117	-0.148437	-0.168642
C	1.481547	0.361873	-0.990462
C	1.655870	-0.741485	-0.125387
C	1.104038	-0.364720	1.173087

C	0.732173	1.050498	1.128728
C	0.904420	1.484405	-0.216692
C	1.157859	-1.193205	2.410319
C	0.313991	1.879752	2.297122
C	0.706559	2.865610	-0.749460
C	1.870195	0.450018	-2.427603
C	2.311841	-2.046332	-0.444665
H	1.112857	-2.266823	2.195543
H	2.115445	-1.007246	2.925330
H	0.357353	-0.936447	3.113790
H	-0.245773	1.295696	3.036853
H	1.204962	2.284951	2.802482
H	-0.302228	2.734559	1.994028
H	0.022193	3.452186	-0.126649
H	1.671284	3.397337	-0.772248
H	0.317454	2.858466	-1.774965
H	1.123844	0.994845	-3.019771
H	2.818383	1.003668	-2.524436
H	2.016706	-0.538377	-2.876764
H	2.272995	-2.276295	-1.515830
H	3.373921	-2.012432	-0.155774
H	1.861544	-2.884291	0.102612
C	-2.256759	0.849917	0.172848
C	-3.242906	0.632044	-0.715473
H	-1.797772	-2.014321	-1.751044
C	-1.215854	-2.162444	-0.838458
C	-1.797918	-1.971408	0.408559
H	-1.339422	-2.386877	1.305666
H	-0.310863	-2.757481	-0.953073
H	-2.841573	-1.684370	0.507165
H	-2.253550	1.740471	0.809904
H	-3.995123	1.400042	-0.926678
H	-3.337699	-0.284725	-1.302042

Structure 12
E=-579.6238056 ZPE=0.265522

C	0.618774	-1.196217	0.847892
C	-0.045447	0.003230	1.387802
C	0.622496	1.198307	0.844015
C	1.521158	0.736236	-0.138159
C	1.519664	-0.740846	-0.135134
Rh	-0.584605	0.000093	-0.615487
C	-2.489915	-0.720945	-1.077527
C	-2.490961	0.719177	-1.076422
C	-1.002273	0.006494	2.537808
C	0.402131	2.607185	1.300084
C	2.402202	1.571466	-1.014270
C	2.399392	-1.581832	-1.007017
C	0.393434	-2.602611	1.309126
H	2.054788	2.610884	-1.063203
H	3.440039	1.583748	-0.640537
H	2.438226	1.183251	-2.041606
H	2.437198	-1.198118	-2.035973
H	3.436913	-1.595164	-0.632418
H	2.049467	-2.620596	-1.051895
H	0.663167	-3.330078	0.532929
H	0.999022	-2.832810	2.202373
H	-0.657165	-2.779962	1.573375
H	-1.647669	-0.880655	2.529054
H	-0.451411	0.006956	3.493915
H	-1.644756	0.895731	2.526516
H	-0.647769	2.789216	1.563925
H	1.008824	2.838795	2.192222
H	0.674110	3.330758	0.521030
H	-2.985555	-1.283390	-0.283361

H	-2.987370	1.279536	-0.281256
H	-2.487389	-1.247445	-2.039672
H	-2.489370	1.247277	-2.037677

Structure 13
E=-580.0091405 ZPE=0.2787544

C	-0.270999	1.293113	0.245189
C	-0.196185	0.260699	1.273834
C	-1.000718	-0.861755	0.819856
C	-1.510154	-0.534850	-0.460850
C	-1.431639	0.974616	-0.686703
Rh	0.730687	-0.368122	-0.519584
C	2.716845	0.254944	-1.089554
C	2.814585	-0.550264	0.048558
C	0.450307	0.388112	2.611340
C	-1.198194	-2.140368	1.564954
C	-2.293620	-1.429459	-1.361516
C	-2.750834	1.723718	-0.372750
C	0.323114	2.657498	0.340604
H	-3.548223	1.395276	-1.050493
H	-3.067007	1.534173	0.661261
H	-2.617509	2.803869	-0.511002
H	0.493536	3.090443	-0.653414
H	-0.377634	3.328075	0.867053
H	1.266546	2.672198	0.899071
H	1.275539	1.109533	2.600564
H	-0.290511	0.755672	3.340248
H	0.826035	-0.572123	2.984017
H	-0.323805	-2.404238	2.171521
H	-2.055122	-2.041308	2.250654
H	-1.420991	-2.976274	0.891500
H	-2.096750	-2.491922	-1.178399
H	-3.374154	-1.264821	-1.213126
H	-2.087873	-1.210082	-2.418538
H	3.030445	-1.619527	-0.043421
H	2.874890	-0.183356	-2.081501
H	3.010799	-0.123169	1.031771
H	2.843479	1.335454	-1.031927
H	-1.157645	1.211606	-1.732319

Structure 14
E=-578.7937617 ZPE=0.2567608

Rh	0.466010	-0.091282	-0.690037
C	-1.709080	-0.196635	-0.156563
C	-1.237889	1.074797	0.284781
C	-0.103638	0.853478	1.154687
C	0.079389	-0.588793	1.305251
C	-1.034804	-1.263911	0.606389
C	0.639419	1.905578	1.904799
C	1.027875	-1.251816	2.242540
C	-1.216404	-2.606205	0.471778
C	-2.816226	-0.439268	-1.126360
C	-1.800087	2.404503	-0.088939
H	0.713435	2.841412	1.338941
H	0.106004	2.129890	2.843089
H	1.649426	1.579628	2.178310
H	1.949594	-0.673801	2.374485
H	0.553242	-1.343675	3.233812
H	1.293176	-2.262185	1.910726
H	-0.621975	-3.319716	1.039396
H	-1.985169	-3.012036	-0.183560
H	-2.630149	-1.331180	-1.738616
H	-3.759253	-0.612809	-0.582923
H	-2.974594	0.413420	-1.795993
H	-2.278754	2.384419	-1.074937

H	-2.572381	2.699300	0.639961
H	-1.035733	3.190069	-0.088753
C	2.369185	0.821175	-1.103798
C	2.500632	-0.573094	-1.193551
H	2.452046	-1.062845	-2.172058
H	3.004732	-1.145439	-0.415282
H	2.768667	1.374892	-0.254426
H	2.206989	1.419503	-2.006583

Structure 15
E=-579.9698351 ZPE=0.2714225

Rh	-0.322280	-0.184584	-0.800702
C	1.802865	-0.027929	0.070586
C	0.946923	-1.043346	0.684941
C	-0.172714	-0.368220	1.354894
C	-0.083015	1.014246	1.013668
C	1.153250	1.215432	0.218008
C	-1.142995	-1.013678	2.286989
C	-0.957016	2.115224	1.509059
C	1.617665	2.541203	-0.277402
C	3.118648	-0.291900	-0.589722
C	1.268296	-2.491032	0.800728
H	-1.366907	-2.045742	1.995067
H	-0.708864	-1.041849	3.299217
H	-2.088378	-0.464036	2.343267
H	-1.929783	1.744818	1.851160
H	-0.474044	2.606298	2.369799
H	-1.121118	2.890020	0.749617
H	0.788846	3.143036	-0.672327
H	2.058997	3.115898	0.553544
H	2.381768	2.446984	-1.056425
H	3.372152	0.478970	-1.326179
H	3.919343	-0.301864	0.166044
H	3.140423	-1.265707	-1.093408
H	1.858639	-2.852580	-0.049003
H	1.871794	-2.655614	1.710169
H	0.366110	-3.106283	0.893001
C	-2.275594	-0.632025	-1.060453
C	-3.225485	0.251221	-0.711267
H	-4.261753	0.118319	-1.040080
H	-3.029495	1.156863	-0.134149
H	-2.565844	-1.514930	-1.639450
H	0.378971	-0.720387	-2.326497
H	-0.393250	-1.041099	-2.361930

Structure 2
E=-658.6801839 ZPE=0.3317815

Rh	0.617432	-0.108715	-0.196512
C	-1.120472	-0.812816	0.909695
C	-1.595571	-0.669758	-0.465701
C	-1.451348	0.695414	-0.828249
C	-0.910946	1.424586	0.315791
C	-0.760774	0.499212	1.411361
C	-1.853488	1.309669	-2.129400
C	-0.749588	2.909668	0.389118
C	-0.427990	0.836172	2.829499
C	-1.229003	-2.058213	1.727286
C	-2.229394	-1.747245	-1.285481
H	-1.805313	0.590245	-2.954965
H	-2.894167	1.665740	-2.065554
H	-1.234819	2.177449	-2.387274
H	-0.430541	3.340556	-0.567869
H	-1.712220	3.377790	0.648029
H	-0.030528	3.209632	1.160509
H	0.188245	1.739086	2.906258

H	-1.354709	1.022995	3.394959
H	0.102936	0.019477	3.331723
H	-0.565605	-2.040202	2.599273
H	-2.259898	-2.158004	2.102883
H	-1.013843	-2.961687	1.143618
H	-1.849868	-2.743354	-1.028008
H	-3.315631	-1.764422	-1.103230
H	-2.080767	-1.590857	-2.360335
C	2.390513	1.075619	-1.124693
C	2.280977	1.053766	0.353266
H	3.067780	0.543403	0.906211
H	1.965033	1.982355	0.831439
H	1.513854	0.456974	-1.669449
H	2.245721	2.056920	-1.589458
H	3.267012	0.557409	-1.530541
C	1.908368	-1.830826	0.288760
C	1.339565	-2.042481	-0.973269
H	1.931995	-1.890833	-1.876202
H	0.479828	-2.699148	-1.100943
H	1.503408	-2.322587	1.172556
H	2.952568	-1.533349	0.371515

Structure 3
-580.017819 0.2771196

Rh	-0.592534	-0.052878	-0.508190
C	1.065336	1.207534	0.050029
C	1.669127	-0.053200	-0.450110
C	1.220836	-1.112250	0.359347
C	0.292342	-0.544442	1.350429
C	0.283359	0.914518	1.209726
C	1.602318	-2.554827	0.268410
C	-0.365878	-1.313737	2.440246
C	-0.347137	1.888353	2.151190
C	1.348511	2.557344	-0.516247
C	2.601770	-0.132952	-1.611283
H	1.951859	-2.823831	-0.734770
H	2.419927	-2.773784	0.972979
H	0.767623	-3.217675	0.526907
H	-0.651038	-2.321813	2.116138
H	0.343610	-1.433415	3.277131
H	-1.251090	-0.801279	2.833521
H	-1.263135	1.490643	2.603256
H	0.351467	2.116829	2.971637
H	-0.595150	2.833844	1.655830
H	0.600649	3.296890	-0.210002
H	2.331615	2.909703	-0.162297
H	1.393175	2.539359	-1.612527
H	2.289335	0.522789	-2.434415
H	3.608767	0.197085	-1.308325
H	2.690775	-1.154010	-1.998363
C	-2.629298	-0.872409	-1.259009
C	-2.564145	0.501400	-0.686737
H	-2.655346	1.324195	-1.406318
H	-3.105514	0.698546	0.239455
H	-1.545290	-1.402332	-1.299035
H	-3.192414	-1.607325	-0.675349
H	-2.888658	-0.926895	-2.322821

Structure 4
E=-658.6481636 ZPE=0.3297078

Rh	-0.492398	-0.225619	0.006083
C	0.997473	0.959000	1.047226
C	0.964836	1.512085	-0.321734
C	1.296382	0.477734	-1.217323
C	1.545456	-0.743890	-0.426571

C	1.448023	-0.406351	0.979118
C	1.440776	0.579811	-2.701425
C	2.052726	-2.033149	-0.984354
C	1.824148	-1.281262	2.131166
C	0.808280	1.758202	2.295554
C	0.681425	2.939289	-0.659152
H	0.858887	1.411852	-3.113842
H	2.496668	0.752807	-2.963313
H	1.131270	-0.340676	-3.210689
H	1.630607	-2.249686	-1.973071
H	3.146779	-1.978511	-1.106142
H	1.843044	-2.880431	-0.321259
H	1.659490	-2.343445	1.914556
H	2.894762	-1.156798	2.357808
H	1.263816	-1.027001	3.037939
H	0.513262	1.130385	3.144129
H	1.756149	2.252618	2.563729
H	0.057995	2.548241	2.172510
H	-0.063832	3.384942	0.012234
H	1.598531	3.540130	-0.552459
H	0.331006	3.057325	-1.691107
C	-1.770301	-2.028555	-0.761409
C	-1.461231	-1.929946	0.694289
H	-2.306113	-1.733607	1.359202
H	-0.783720	-2.681055	1.104123
H	-1.426464	-1.062937	-1.363738
H	-1.254297	-2.836757	-1.288801
H	-2.838717	-2.003245	-1.010924
C	-2.459885	1.190841	0.146041
C	-3.684712	0.737158	-0.155928
H	-4.060943	-0.215672	0.217916
H	-4.365395	1.316940	-0.780574
H	-2.122201	2.173216	-0.178750
H	-1.903062	0.708401	1.003819

Structure 5
E=-658.6431717 ZPE=0.3294267

Rh	-0.473638	-0.243289	-0.117770
C	0.798368	0.843028	1.218539
C	0.665344	1.579698	-0.018408
C	1.185036	0.728624	-1.063187
C	1.807394	-0.457388	-0.432868
C	1.574383	-0.386549	0.948843
C	1.295599	1.081317	-2.508864
C	2.563296	-1.508010	-1.178012
C	2.026315	-1.347103	1.999329
C	0.433365	1.340260	2.576605
C	0.159777	2.975313	-0.173343
H	0.513269	1.782292	-2.820640
H	2.267449	1.566837	-2.696624
H	1.246746	0.195797	-3.153908
H	2.091105	-1.751818	-2.138213
H	3.579290	-1.148632	-1.406076
H	2.664006	-2.432941	-0.599292
H	2.304562	-2.319396	1.577417
H	2.912252	-0.947358	2.517444
H	1.258511	-1.510827	2.766511
H	0.188081	0.521504	3.263518
H	1.290849	1.881250	3.010423
H	-0.412279	2.035790	2.544275
H	-0.597519	3.221461	0.578582
H	0.998032	3.679798	-0.055027
H	-0.277860	3.146298	-1.163413
C	-1.753599	-2.217033	-0.949409
C	-1.745684	-2.220895	0.582247

H	-2.738409	-2.492882	0.965905
H	-1.001030	-2.897862	1.010299
H	-0.982255	-1.554020	-1.470380
H	-1.482216	-3.207982	-1.336342
H	-2.719148	-1.905218	-1.356392
C	-2.191433	0.777149	-0.528086
C	-3.243331	0.968123	0.272031
H	-3.310536	0.578945	1.290736
H	-4.106119	1.551064	-0.065484
H	-2.193354	1.220580	-1.532737
H	-1.628704	-1.203856	1.096575

Structure 6
E=-578.7885965 ZPE=0.2550008

Rh	0.672302	-0.000392	-0.458184
C	-0.620229	-1.159358	0.800249
C	-1.477166	-0.706087	-0.304364
C	-1.477102	0.705650	-0.305558
C	-0.620150	1.160732	0.798319
C	-0.143617	0.001277	1.523647
C	-2.217001	1.609864	-1.236078
C	-0.404272	2.584104	1.180094
C	0.602878	0.002320	2.818595
C	-0.404393	-2.582092	1.184411
C	-2.217154	-1.611815	-1.233343
H	-2.498207	1.102115	-2.165371
H	-3.144802	1.960776	-0.757104
H	-1.633172	2.501872	-1.495146
H	-0.373703	3.244483	0.305274
H	-1.243263	2.921072	1.811955
H	0.517357	2.720602	1.756488
H	1.237335	0.889662	2.923672
H	-0.109832	0.002950	3.658219
H	1.237407	-0.884804	2.925069
H	0.517418	-2.717700	1.760725
H	-1.243203	-2.917864	1.817150
H	-0.374200	-3.243985	0.310726
H	-1.633498	-2.504424	-1.490720
H	-3.145097	-1.961643	-0.753854
H	-2.498119	-1.105687	-2.163593
C	2.392673	-0.001778	-1.845385
C	2.622695	-0.000324	-0.531961
H	3.550700	0.000365	0.036355
H	3.060679	-0.002719	-2.711730
H	1.299624	-0.002395	-2.241568

Structure 7
E=-658.6425551 ZPE=0.3278506

Rh	-0.514992	-0.216011	-0.160329
C	0.965440	0.968463	1.145082
C	0.853939	1.528480	-0.212065
C	1.306991	0.537951	-1.141473
C	1.588122	-0.672510	-0.382129
C	1.440330	-0.361359	1.043096
C	1.555525	0.730762	-2.603609
C	2.185694	-1.925361	-0.932036
C	1.825457	-1.264062	2.170320
C	0.712693	1.732670	2.404533
C	0.523994	2.952288	-0.527333
H	0.908506	1.504353	-3.031094
H	2.599381	1.046890	-2.756954
H	1.404896	-0.193047	-3.172849
H	1.909557	-2.086914	-1.980254
H	3.285044	-1.860893	-0.888627
H	1.893755	-2.811314	-0.355256

H	1.700449	-2.323683	1.916644
H	2.890233	-1.119564	2.412816
H	1.251636	-1.057550	3.081110
H	0.476658	1.073066	3.247392
H	1.612333	2.306886	2.678121
H	-0.103739	2.456552	2.292875
H	-0.217975	3.368314	0.165254
H	1.427883	3.575700	-0.438571
H	0.145323	3.067926	-1.549311
C	-1.485387	-2.141911	-0.677103
C	-1.347482	-2.054360	0.713357
H	-2.205482	-1.805244	1.339646
H	-0.547172	-2.585558	1.226735
H	-1.168004	-0.184150	-1.585319
H	-0.785702	-2.733246	-1.266463
H	-2.452658	-1.972657	-1.146488
C	-2.622699	1.029417	0.149503
C	-3.810579	0.441673	-0.055598
H	-4.041532	-0.553779	0.324490
H	-4.602381	0.946467	-0.610309
H	-2.415096	2.038034	-0.200787
H	-1.943514	0.611056	0.944719

Structure 8
E=-658.6746676 ZPE=0.3304107

Rh	0.649554	-0.040411	-0.243679
C	-1.456945	0.095002	-1.003403
C	-1.173496	1.239938	-0.173663
C	-0.956399	0.765909	1.190379
C	-1.044163	-0.657579	1.182856
C	-1.322217	-1.085337	-0.182295
C	-0.833199	1.634998	2.400948
C	-1.013676	-1.551612	2.380540
C	-1.634208	-2.486122	-0.603009
C	-1.938675	0.128757	-2.420271
C	-1.297197	2.673536	-0.582292
H	-0.382171	2.607899	2.172433
H	-1.835641	1.837857	2.810201
H	-0.245892	1.159603	3.194909
H	-0.391875	-1.144523	3.186142
H	-2.033527	-1.667258	2.780456
H	-0.653771	-2.559115	2.138898
H	-1.048209	-3.226618	-0.044794
H	-2.696001	-2.706644	-0.410896
H	-1.457417	-2.641509	-1.673507
H	-1.665901	-0.778559	-2.970393
H	-3.037449	0.201469	-2.428998
H	-1.547827	0.992398	-2.969406
H	-1.135561	2.806590	-1.657905
H	-2.308921	3.043615	-0.353758
H	-0.591898	3.320451	-0.045823
C	2.050324	-1.552423	0.583361
C	1.880574	-1.818442	-0.778858
H	2.668942	-1.564835	-1.486022
H	2.974202	-1.099028	0.937602
H	3.039025	0.922481	-1.337377
C	2.201042	1.431981	-0.862863
C	2.096574	1.460287	0.531137
H	1.517894	2.243047	1.019160
H	1.726467	2.200032	-1.472125
H	1.191593	-2.590292	-1.119599
H	1.492748	-2.109673	1.334780
H	2.850029	0.989046	1.157884
H	0.991195	-0.091294	-1.771707

Structure ethan
E=-79.8598582 ZPE=0.0725702

C	0.000000	0.764570	0.000000
C	0.000000	-0.764570	0.000000
H	1.022455	-1.167320	0.000000
H	-0.511274	-1.167219	0.885482
H	-0.511274	-1.167219	-0.885482
H	-1.022455	1.167320	0.000000
H	0.511274	1.167219	0.885482
H	0.511274	1.167219	-0.885482

Structure ethen
E=-78.6201659 ZPE=0.049579

C	0.000000	0.000000	0.666436
C	0.000000	0.000000	-0.666436
H	0.000000	0.927857	1.240174
H	0.000000	-0.927857	1.240174
H	0.000000	-0.927857	-1.240174
H	0.000000	0.927857	-1.240174

Structure h2
E=-1.177727 ZPE=0.0098394

H	0.000000	0.000000	0.000000
H	0.000000	0.000000	0.750300

Structure TS_10_11
E=-658.6110555 ZPE=0.321181

Rh	0.556373	-0.102920	-0.251251
C	-1.700496	0.025566	-0.781061
C	-1.177473	1.323583	-0.299464
C	-0.735278	1.165464	1.043285
C	-0.850879	-0.250489	1.363761
C	-1.535149	-0.922498	0.244871
C	-0.290983	2.241828	1.975986
C	-0.616502	-0.847031	2.709412
C	-2.002560	-2.341261	0.256372
C	-2.380185	-0.175683	-2.095378
C	-1.267017	2.607436	-1.054609
H	0.167710	3.085044	1.445427
H	-1.160196	2.637937	2.524032
H	0.423408	1.873085	2.721617
H	0.222275	-0.372875	3.231732
H	-1.516576	-0.697389	3.329070
H	-0.437389	-1.927209	2.662631
H	-1.295373	-3.009097	0.764970
H	-2.956583	-2.417340	0.801420
H	-2.173446	-2.727556	-0.754967
H	-2.397414	-1.229913	-2.393968
H	-3.426603	0.163397	-2.030289
H	-1.908189	0.403217	-2.898064
H	-1.137416	2.463755	-2.133436
H	-2.265824	3.050100	-0.906592
H	-0.529406	3.340363	-0.709053
C	1.834279	-1.867731	0.348709
C	1.364736	-2.048294	-0.945002
H	2.009443	-1.829963	-1.798585
H	2.845947	-1.519863	0.539526
H	3.524064	-0.031002	-1.280048
C	3.338787	0.813314	-0.611795
C	2.219037	0.958242	0.111315
H	2.127705	1.800610	0.806264
H	4.123659	1.576353	-0.592538
H	0.510419	-2.692339	-1.151798
H	1.334931	-2.345040	1.191464
H	0.664336	0.152615	-2.934487

H	1.011839	0.789845	-2.726437

Structure TS_12_13
E=-579.9918842 ZPE=0.2743735

C	0.128636	-0.574944	1.279029
C	0.231203	0.888039	1.218439
C	1.142670	1.222078	0.180412
C	1.604888	-0.010521	-0.426192
C	1.077530	-1.166911	0.298108
Rh	-0.607046	-0.091492	-0.622384
C	-2.590458	-0.740522	-1.097039
C	-2.598428	0.643768	-0.807357
C	-0.449737	1.825893	2.158441
C	1.584124	2.591309	-0.220810
C	2.556088	-0.100355	-1.570448
C	1.781470	-2.494960	0.455461
C	-0.607907	-1.352639	2.312944
H	2.214907	-2.838845	-0.490481
H	2.598285	-2.382367	1.183501
H	1.103179	-3.273756	0.821643
H	-0.892879	-2.346768	1.949358
H	0.044632	-1.497510	3.191002
H	-1.508116	-0.831870	2.658040
H	-1.438036	1.458746	2.459468
H	0.150103	1.929795	3.076820
H	-0.570346	2.825073	1.725928
H	0.871450	3.359918	0.097405
H	2.554462	2.826060	0.244714
H	1.720777	2.676894	-1.305905
H	2.419764	0.719898	-2.285979
H	3.592395	-0.033764	-1.199107
H	2.460822	-1.052300	-2.105908
H	-2.616022	1.368932	-1.627096
H	-2.601950	-1.078811	-2.136752
H	-2.991250	1.017745	0.138531
H	-2.974901	-1.468533	-0.383157
H	0.019347	-1.642830	-0.690685

Structure TS_2_4
E=-658.6478264 ZPE=0.3292008

Rh	-0.501852	-0.230559	0.006418
C	1.007011	0.902862	1.071320
C	0.971253	1.507713	-0.277675
C	1.281758	0.508347	-1.217082
C	1.518531	-0.745512	-0.476923
C	1.437423	-0.463847	0.944897
C	1.415540	0.669135	-2.697277
C	2.001199	-2.017639	-1.090745
C	1.816545	-1.388496	2.056287
C	0.851495	1.660415	2.350022
C	0.711040	2.951496	-0.556650
H	0.838835	1.523419	-3.069915
H	2.470493	0.842150	-2.962850
H	1.090433	-0.225847	-3.241300
H	1.558279	-2.193906	-2.078491
H	3.093173	-1.965829	-1.232878
H	1.798581	-2.887290	-0.455255
H	1.643811	-2.439607	1.796332
H	2.889343	-1.279902	2.280569
H	1.263137	-1.170086	2.976629
H	0.574087	1.006040	3.184346
H	1.807447	2.142371	2.612441
H	0.102327	2.457351	2.271688
H	0.001433	3.392537	0.154646
H	1.647275	3.524234	-0.460109

H	0.332052	3.115198	-1.572243
C	-1.801761	-2.038835	-0.741421
C	-1.508605	-1.897861	0.716969
H	-2.361799	-1.663925	1.360037
H	-0.859309	-2.654544	1.160847
H	-1.452376	-1.091589	-1.360821
H	-1.279537	-2.863239	-1.236580
H	-2.867437	-2.030353	-1.003434
C	-2.410578	1.301908	0.237245
C	-3.558506	0.803260	-0.248736
H	-3.972176	-0.141651	0.104616
H	-4.134669	1.333195	-1.008339
H	-2.042767	2.277407	-0.075608
H	-1.951380	0.851342	1.145465

Structure TS_2_8
E=-658.6730498 ZPE=0.3299916

Rh	0.637334	-0.111878	-0.210900
C	-1.144150	-0.632250	1.084866
C	-1.492525	-0.837437	-0.319312
C	-1.418105	0.429365	-0.986549
C	-0.974387	1.411408	-0.019151
C	-0.848754	0.753674	1.273319
C	-1.837491	0.711773	-2.395099
C	-0.874581	2.884834	-0.256364
C	-0.594944	1.431093	2.582580
C	-1.256854	-1.665829	2.158504
C	-2.022248	-2.109589	-0.898933
H	-1.691235	-0.155071	-3.049335
H	-2.909013	0.964619	-2.417488
H	-1.293990	1.560475	-2.825423
H	-0.623715	3.118939	-1.297528
H	-1.841907	3.364354	-0.039051
H	-0.130750	3.360967	0.394161
H	0.010870	2.338085	2.472421
H	-1.552362	1.736447	3.033320
H	-0.092393	0.769057	3.297109
H	-0.627232	-1.431871	3.024517
H	-2.298299	-1.716573	2.513728
H	-0.995740	-2.669399	1.800408
H	-1.579791	-2.996887	-0.429577
H	-3.109211	-2.169317	-0.731094
H	-1.854840	-2.170774	-1.980426
C	2.389882	1.079733	-0.919268
C	2.273087	1.144276	0.493334
H	2.976541	0.605252	1.123662
H	1.839825	2.035210	0.946686
H	2.099361	1.942144	-1.520328
H	3.189929	0.478688	-1.355680
C	1.858012	-1.816469	0.504789
C	1.516120	-2.053193	-0.831001
H	2.259905	-1.925001	-1.616274
H	0.688614	-2.711697	-1.091636
H	1.304143	-2.288192	1.315293
H	2.870259	-1.506979	0.760450
H	1.242612	0.113709	-1.667688

Structure TS_3_12
E=-580.011449 ZPE=0.2747707

Rh	0.582481	-0.185248	-0.523932
C	-0.374003	-0.550284	1.341963
C	-1.325529	-0.979686	0.320369
C	-1.604037	0.155864	-0.480493
C	-0.918106	1.337585	0.106207
C	-0.202317	0.911987	1.246261

C	-2.491581	0.214325	-1.675551
C	-1.054296	2.729999	-0.410801
C	0.546551	1.756292	2.224636
C	0.164467	-1.403414	2.434055
C	-1.905851	-2.351507	0.185479
H	-2.662103	-0.776436	-2.110426
H	-3.473149	0.627840	-1.390306
H	-2.085550	0.873054	-2.454209
H	-1.032802	2.764604	-1.507601
H	-2.023330	3.151787	-0.098011
H	-0.266715	3.388510	-0.028599
H	0.862228	2.709528	1.786430
H	-0.098122	1.985414	3.087883
H	1.436241	1.246292	2.613014
H	1.133177	-1.044486	2.800539
H	-0.535060	-1.375771	3.287713
H	0.262555	-2.451757	2.129886
H	-1.197617	-3.129633	0.492235
H	-2.795650	-2.444648	0.827265
H	-2.216663	-2.563773	-0.843537
C	2.556707	-0.908214	-1.235474
C	2.622129	0.402968	-0.676809
H	3.069680	0.559436	0.304359
H	2.965999	-1.756687	-0.685604
H	2.689366	1.258765	-1.353845
H	2.615089	-1.023219	-2.320493
H	1.055988	-1.558146	-1.238794

Structure TS_4_5
E=-658.6218607 ZPE=0.3260434

Rh	0.492349	-0.346994	-0.211199
C	-0.833981	1.228906	-0.823305
C	-0.451219	1.569750	0.534902
C	-0.951236	0.535860	1.386916
C	-1.709997	-0.420919	0.587051
C	-1.661897	0.009375	-0.764475
C	-0.818486	0.489086	2.873593
C	-2.489557	-1.576046	1.132544
C	-2.401313	-0.582817	-1.919823
C	-0.675732	2.115092	-2.015556
C	0.253396	2.816222	0.961907
H	0.078289	1.011215	3.225770
H	-1.687080	0.990283	3.331127
H	-0.804643	-0.537477	3.258687
H	-1.977180	-2.064082	1.971338
H	-3.465196	-1.232863	1.510976
H	-2.690234	-2.334149	0.366430
H	-2.582256	-1.656099	-1.790225
H	-3.384394	-0.094899	-2.015118
H	-1.872219	-0.433556	-2.867871
H	-0.700239	1.551302	-2.954901
H	-1.501220	2.843916	-2.044928
H	0.259884	2.684992	-1.979065
H	0.957876	3.166780	0.199346
H	-0.479666	3.619397	1.135267
H	0.813707	2.671533	1.892638
C	1.530500	-2.316841	0.544017
C	1.026218	-2.308868	-0.855468
H	1.785891	-2.421746	-1.628921
H	0.125861	-2.889056	-1.062070
H	1.456456	-1.266363	1.085436
H	0.964940	-2.966000	1.219521
H	2.613142	-2.469342	0.619943
C	2.315214	0.560097	-0.559475
C	3.371704	0.534517	0.254526

H	4.277146	1.092679	-0.003382
H	3.413813	-0.012756	1.198727
H	2.370291	1.132460	-1.489759
H	0.849642	-0.691930	-1.699118

Structure TS_4_7
E=-658.6400092 ZPE=0.3268249

Rh	-0.497345	-0.242674	-0.088027
C	0.978411	0.978647	1.111511
C	0.856543	1.534551	-0.250494
C	1.283051	0.545459	-1.178682
C	1.591600	-0.663231	-0.416430
C	1.470849	-0.348970	1.007649
C	1.471065	0.718464	-2.652619
C	2.187587	-1.912197	-0.977709
C	1.879905	-1.243711	2.133093
C	0.751873	1.753049	2.370354
C	0.491802	2.949239	-0.565084
H	0.797672	1.477564	-3.066012
H	2.502974	1.043603	-2.858411
H	1.307949	-0.216205	-3.200853
H	1.846018	-2.108974	-2.000643
H	3.284696	-1.814062	-1.014798
H	1.964531	-2.790311	-0.360352
H	1.730438	-2.304282	1.897089
H	2.953214	-1.109916	2.341224
H	1.335550	-1.017410	3.056865
H	0.534806	1.099579	3.222889
H	1.655939	2.331441	2.619490
H	-0.069484	2.473138	2.271434
H	-0.255405	3.350302	0.131084
H	1.381903	3.592723	-0.479629
H	0.107266	3.056891	-1.585970
C	-1.582162	-2.084211	-0.703254
C	-1.371066	-2.050976	0.701814
H	-2.210264	-1.837762	1.365306
H	-0.590322	-2.668530	1.144352
H	-0.952732	-2.720547	-1.325674
H	-2.592452	-1.942875	-1.090736
C	-2.582974	1.052622	0.114506
C	-3.797169	0.506485	-0.040941
H	-4.067640	-0.448610	0.410513
H	-4.573643	1.008287	-0.619468
H	-2.337278	2.029171	-0.296763
H	-1.918288	0.651820	0.935046
H	-1.230804	-0.626046	-1.457029

Structure TS_7_7'
E=-658.6305422 ZPE=0.3265361

Rh	0.551218	-0.145070	-0.012754
C	-1.210000	0.944254	-1.008947
C	-0.946063	1.468303	0.328810
C	-1.180474	0.414977	1.283891
C	-1.480255	-0.782034	0.530559
C	-1.535305	-0.435448	-0.889512
C	-1.207023	0.545995	2.773509
C	-1.896058	-2.096656	1.105922
C	-1.990028	-1.342217	-1.987924
C	-1.207503	1.748039	-2.269142
C	-0.675544	2.904027	0.651308
H	-0.565691	1.361278	3.126925
H	-2.232464	0.763153	3.112322
H	-0.887787	-0.377007	3.271204
H	-1.485778	-2.257562	2.109295
H	-2.993798	-2.127762	1.192862

H	-1.603168	-2.940352	0.469222
H	-1.721777	-2.389168	-1.801819
H	-3.087666	-1.304602	-2.072377
H	-1.576874	-1.050748	-2.960440
H	-0.977041	1.134013	-3.147519
H	-2.203641	2.190271	-2.430819
H	-0.491452	2.577368	-2.229579
H	-0.069930	3.394574	-0.121195
H	-1.623402	3.460970	0.713854
H	-0.165853	3.019760	1.615038
C	1.575755	-1.986053	0.608797
C	1.431982	-2.001563	-0.786702
H	2.278803	-1.774036	-1.436232
H	0.649250	-2.594953	-1.258251
H	1.763339	0.391002	0.954871
H	0.903560	-2.566539	1.239475
H	2.539324	-1.751668	1.063150
C	2.498605	1.013016	-0.128579
C	3.802116	0.586341	-0.139680
H	4.082914	-0.440052	-0.372287
H	4.607731	1.278171	0.101781
H	2.314374	2.075852	0.034149
H	1.861001	0.570316	-1.033559

Structure TS_9_10
E=-658.6408569 ZPE=0.3268657

Rh	0.352816	-0.341765	-0.450543
C	-1.666276	0.457723	-0.659409
C	-0.801630	1.543933	-0.299966
C	-0.301984	1.291394	1.059541
C	-0.813641	0.053256	1.513158
C	-1.609942	-0.517579	0.423740
C	0.526048	2.249508	1.848413
C	-0.669815	-0.527311	2.883026
C	-2.441557	-1.753476	0.522792
C	-2.563921	0.384355	-1.853284
C	-0.617359	2.817035	-1.062368
H	1.226147	2.809502	1.217591
H	-0.131800	2.992267	2.327978
H	1.094122	1.751516	2.641789
H	0.258739	-0.208307	3.370086
H	-1.505614	-0.193317	3.518219
H	-0.694759	-1.623586	2.876708
H	-1.948479	-2.541964	1.104417
H	-3.386693	-1.518001	1.038516
H	-2.699849	-2.156864	-0.462618
H	-2.729500	-0.647427	-2.182574
H	-3.546352	0.810063	-1.594570
H	-2.168089	0.954022	-2.700846
H	-0.772458	2.673647	-2.137546
H	-1.344064	3.570732	-0.719655
H	0.380663	3.248010	-0.916960
C	1.212852	-2.210832	0.357017
C	0.886877	-2.431894	-0.984164
H	1.664657	-2.449031	-1.746838
H	2.245079	-2.046732	0.660521
H	3.947036	-0.812608	-0.099412
C	3.687565	0.245737	-0.073874
C	2.606567	0.735298	-0.692916
H	2.392676	1.802159	-0.713566
H	4.375259	0.899626	0.464133
H	-0.028126	-2.956294	-1.255666
H	0.549454	-2.556595	1.148298
H	2.048576	0.113005	-1.443763
H	0.293940	-0.557280	-2.010024