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

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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
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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
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H -2.658081 -0.999906 -2.251553
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### Structure 13

**E=−580.0091405 ZPE=0.2787544**

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C    1.153250   1.215432   0.218008
C   -1.142995  -1.013678  2.286989
C   -0.957016   2.115224  1.509059
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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
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C    -3.225485   0.251221  -0.711267
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H   -3.029495   1.156863  -0.134149
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Structure 2
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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
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C  -0.974387   1.411408  -0.019151
C  -0.848754   0.753674  1.273319
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C  -2.022248  -2.109589  -0.898933
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H  -2.909013   0.964619  -2.417488
H  -1.293990   1.560475  -2.825423
H  -0.623715   3.118939  -1.297528
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H  -0.130750   3.360967  0.394161
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H  -0.995740  -2.669399  1.800408
H  -1.579791  -2.996887  -0.429577
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C  -2.273087   1.144276   0.493334
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E=-580.011449  ZPE=0.2747707

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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
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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
C  -0.782899   1.011215   3.225770
C  -1.687080    0.990283   3.331127
C  -0.804643   -0.537477   3.258687
C  -1.977180  -2.064082   1.971338
C  -3.465196  -1.232863   1.510976
C  -2.690234  -2.334149   0.366430
C  -2.582256  -1.656099  -1.790225
C  -3.384394   -0.094899  -2.015118
C  -1.872219   -0.433556  -2.867871
C  -0.700239   1.551302  -2.954901
C  -1.501220   2.843916  -2.044928
C  -0.259884   2.684992  -1.979065
C  -0.957876   3.166780   0.193946
C  -0.479666   3.619397   1.135267
C  -0.813707   2.671533   1.892638
C  -1.530500  -2.316841   0.544017
C  -1.026218  -2.308868  -0.855468
C  -1.785891  -2.421746  -1.628921
C  -0.125861   -2.889056  -1.062070
C  -1.456456  -1.266363   1.085436
C  -0.964940   -2.966000   1.219521
C  -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
C 0.797672 1.477564 -3.060612
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

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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
C 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 -0.462168
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