

Supplementary Information

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1. Computational Details and References

All DFT calculations were performed with the Gaussian 09 program package.^[1] The geometry optimization of all the minima and transition states involved was carried out at the M06-2X level of theory^[2] with the 6-31G(d) basis set.^[3] The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum or a transition state and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K. A quasiharmonic correction was applied during the entropy calculation by setting all positive frequencies that are less than 100 cm⁻¹ to 100 cm⁻¹.^[4] Solvent effects in dichloroethane (DCE) were computed at the M06-2X/6-311+G(d,p) level using the gas-phase optimized structures. Solvation energies were evaluated by a self-consistent reaction field (SCRF) using the CPCM model,^[5] where UFF radii were used.

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- [1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, *Gaussian 09*, Revision C.01, Gaussian Inc.: Wallingford CT, **2010**.
- [2] (a) Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215; (b) Y. Zhao, D. G. Truhlar, *Acc. Chem. Res.* **2008**, *41*, 157.
- [3] W. J. Hehre, L. Radom, P. v. R. Schleyer, J. A. Pople, *Ab Initio Molecular Orbital Theory*, Wiley: New York, **1986**.
- [4] (a) Y. Zhao, D. G. Truhlar, *Phys. Chem. Chem. Phys.* **2008**, *10*, 2813; (b) R. F. Ribeiro, A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2011**, *115*, 14556.
- [5] (a) V. Barone, M. Cossi, *J. Phys. Chem. A* **1998**, *102*, 1995; (b) M. Cossi, N. Rega, G. Scalmani, V. Barone, *J. Comput. Chem.* **2003**, *24*, 669.

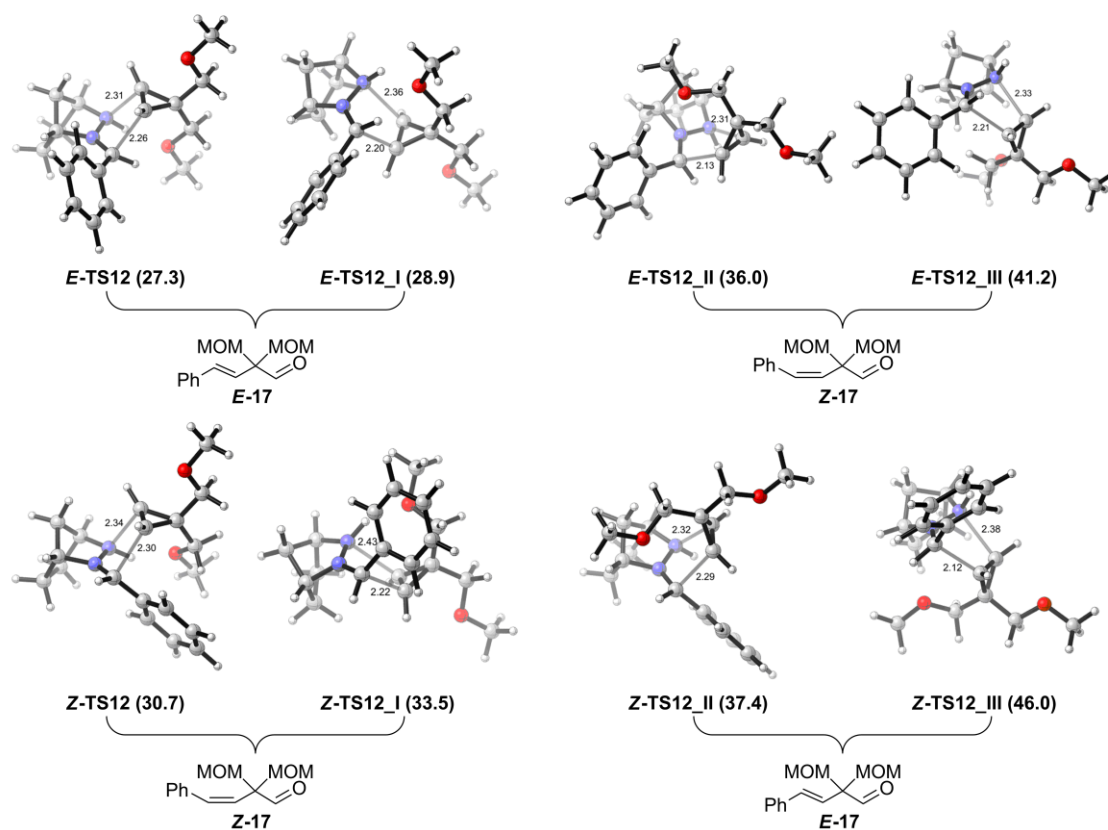


Fig. S1 Optimized transition-state structures of eight possible (3+2) cycloadditions of cyclopropene **11** with hydrazonium **E-10** or **Z-10** (The data in parentheses are free energies in dichloroethane, in kcal mol⁻¹; distances are in Å; atoms distant from the observer are “fogged out”) and the metathesis product **E-17** or **Z-17** subsequently generated (MOM = methoxymethyl).

2. Coordinates and Energies of Stationary Points

PhCHO

$G_{\text{DCE}} = -345.441617$ Hartree

O	-2.830111	-0.397430	0.000031
C	-1.989820	0.470528	-0.000034
C	-0.528728	0.216593	-0.000016
C	0.361046	1.290350	-0.000004
C	1.732647	1.056288	0.000008
C	2.208125	-0.253015	0.000010
C	1.318364	-1.328955	-0.000001
C	-0.050126	-1.096073	-0.000014
H	-2.278759	1.542822	0.000043
H	-0.025035	2.307501	-0.000006
H	2.428407	1.889247	0.000017
H	3.278196	-0.437784	0.000021
H	1.697484	-2.346083	0.000001
H	-0.768459	-1.910559	-0.000023

9

$G_{\text{DCE}} = -306.619959$ Hartree

C	1.271450	0.780725	-0.515181
C	0.081900	1.124170	0.382745
C	0.082683	-1.124777	0.381642
C	1.271735	-0.779500	-0.516012
H	1.204286	1.228206	-1.511873
H	2.176497	1.188303	-0.056500
H	1.205111	-1.226169	-1.513026
H	2.176886	-1.187166	-0.057340
C	0.033250	-0.000870	1.413470
H	-0.837108	-0.001487	2.077827
H	0.937408	-0.001018	2.029981
H	-0.052590	2.158620	0.704702
H	-0.051483	-2.159747	0.702139
N	-1.196185	0.739092	-0.454571
H	-1.162533	1.099535	-1.423579
N	-1.195972	-0.738879	-0.455110
H	-2.067441	-1.087707	-0.020485
H	-2.067866	1.087017	-0.019611
H	-1.162176	-1.098366	-1.424458

H₃O⁺

$G_{\text{DCE}} = -76.7912195$ Hartree

O	-0.000040	-0.000067	-0.076160
H	0.156699	0.933594	0.202980
H	0.730635	-0.602066	0.203113
H	-0.887015	-0.330994	0.203190

Z-10

$G_{\text{DCE}} = -575.283303$ Hartree

C	2.887848	-1.079868	0.815985
C	2.237077	-0.933278	-0.572490
C	2.590387	1.176213	0.015571
C	3.134376	0.401927	1.230262
H	2.247578	-1.627809	1.511109
H	3.822521	-1.636138	0.711443
H	2.616046	0.675995	2.153182
H	4.196658	0.610640	1.376197
C	2.968239	0.275914	-1.164526
H	2.565447	0.615098	-2.120425
H	4.042802	0.101875	-1.238745
H	2.127381	-1.834512	-1.174187
H	2.854978	2.230004	-0.055127
N	1.109034	1.042530	-0.042385
H	0.639019	1.267406	0.838534
N	0.902137	-0.315623	-0.329458
C	-0.240190	-0.915849	-0.379036
C	-1.560753	-0.366777	-0.156510
C	-2.585518	-1.309549	0.045809
C	-1.872292	1.006951	-0.184100
C	-3.890894	-0.891970	0.251238
H	-2.349492	-2.370336	0.045243
C	-3.186161	1.411457	0.000052
H	-1.108325	1.745347	-0.397025
C	-4.190438	0.469653	0.229182
H	-4.674142	-1.623292	0.416976
H	-3.431358	2.467363	-0.036588
H	-5.213003	0.799785	0.381778
H	-0.164388	-1.978729	-0.598095

E-10

$G_{\text{DCE}} = -575.280532$ Hartree

C	2.018658	1.497355	-0.406378
C	1.333909	0.588716	0.633514
C	3.191421	-0.537450	0.154509
C	3.327226	0.713107	-0.732981
H	1.390130	1.668048	-1.284247
H	2.226103	2.467555	0.051169
H	3.413226	0.456032	-1.792311
H	4.217483	1.284788	-0.461208
C	2.523398	0.011950	1.414532
H	2.244391	-0.758346	2.135833
H	3.103423	0.799721	1.898130
H	0.495270	0.993919	1.195506
H	4.085583	-1.144561	0.288131
N	2.090491	-1.396515	-0.355679
H	2.154220	-1.554313	-1.362000
N	0.920947	-0.640777	-0.095002
C	-0.249624	-1.114033	-0.360668
H	-0.239440	-2.134631	-0.743152
C	-1.527502	-0.450434	-0.189603
C	-2.644463	-1.284461	-0.017601
C	-1.697281	0.944329	-0.230098
C	-3.903073	-0.731240	0.171057
H	-2.517700	-2.363610	-0.016405
C	-2.961330	1.487936	-0.059533
H	-0.858308	1.598940	-0.443766
C	-4.059951	0.653485	0.154090
H	-4.760897	-1.377768	0.320388
H	-3.096208	2.563093	-0.105540
H	-5.045664	1.086613	0.289208

11

$G_{\text{DCE}} = -424.079154$ Hartree

C	-0.647387	0.000115	1.515300
C	0.647387	-0.000115	1.515300
C	0.000000	0.000000	0.171534
H	-1.579979	0.000295	2.057080
H	1.579979	-0.000295	2.057080
C	-0.000207	-1.257623	-0.687564

H	0.887273	-1.265039	-1.346827
H	-0.888009	-1.265043	-1.346390
C	-0.000387	-3.583706	-0.598681
H	-0.000199	-4.409037	0.115997
H	-0.892444	-3.662048	-1.238361
H	0.891177	-3.662213	-1.239024
C	0.000207	1.257623	-0.687564
H	-0.887273	1.265039	-1.346827
H	0.888009	1.265043	-1.346390
C	0.000387	3.583706	-0.598681
H	0.000199	4.409037	0.115997
H	0.892444	3.662048	-1.238361
H	-0.891177	3.662213	-1.239024
O	0.000000	2.390412	0.138574
O	0.000000	-2.390412	0.138574

***E*-TS12 (TS-C-1)**

$G_{\text{DCE}} = -999.325303$ Hartree

C	2.797937	2.493804	-0.469487
C	2.038389	1.337744	-1.155439
C	0.516927	2.951316	-1.106447
C	1.726167	3.621763	-0.419789
H	3.167639	2.200222	0.514865
H	3.656434	2.774329	-1.084628
H	1.485142	3.935679	0.598784
H	2.038091	4.508053	-0.977369
C	1.176910	2.077486	-2.182521
H	0.472782	1.435072	-2.716261
H	1.781973	2.653107	-2.884844
H	2.634393	0.486622	-1.469395
H	-0.303617	3.601555	-1.406790
N	0.007817	1.876781	-0.230334
N	0.995708	0.936070	-0.171318
C	0.824104	-0.176423	0.525426
C	1.746165	-1.317417	0.393928
C	2.031832	-1.887269	-0.853735
C	2.297715	-1.875785	1.551080
C	2.887299	-2.978115	-0.942566
H	1.555981	-1.494278	-1.750017
C	3.160382	-2.962772	1.457842
H	2.058007	-1.451583	2.522354
C	3.458206	-3.511101	0.212886

H	3.097964	-3.422096	-1.909846
H	3.593888	-3.385641	2.357912
H	4.124646	-4.364552	0.142852
H	0.244429	-0.071526	1.436518
H	-0.423935	2.080333	0.675351
C	-1.674477	0.418841	-0.842583
H	-1.884403	0.974322	-1.745294
C	-1.166463	-0.732375	-0.389033
C	-2.415240	-0.227242	0.274456
H	-0.811285	-1.676785	-0.777861
C	-3.735549	-0.914363	-0.075927
H	-4.560117	-0.180824	-0.042434
H	-3.962403	-1.694380	0.672457
C	-4.800869	-2.123794	-1.763548
H	-4.616719	-2.528739	-2.759146
H	-5.057106	-2.944720	-1.080044
H	-5.646261	-1.423602	-1.806911
C	-2.493272	0.312103	1.696529
H	-2.521175	-0.528014	2.407918
H	-3.435328	0.871320	1.813844
C	-1.520274	1.662299	3.354217
H	-0.651021	2.294656	3.541159
H	-2.435063	2.255691	3.469292
H	-1.533619	0.838522	4.077699
O	-3.619165	-1.470555	-1.354070
O	-1.409502	1.164943	2.029028

***E*-TS12_I**

$G_{\text{DCE}} = -999.322692$ Hartree

C	-1.167425	2.092573	-1.998180
C	-1.872292	1.889995	-0.633962
C	-0.232367	3.300354	-0.151319
C	-0.106656	3.186310	-1.679449
H	-0.710459	1.163923	-2.351562
H	-1.891331	2.422306	-2.746801
H	0.899956	2.917545	-1.999288
H	-0.361935	4.143264	-2.141492
C	-1.758787	3.273269	0.024986
H	-2.091152	3.280178	1.064977
H	-2.263642	4.056105	-0.544351
H	-2.840352	1.394358	-0.637592
H	0.332831	4.096231	0.330551

N	0.159513	1.973074	0.398815
N	-0.934960	1.166256	0.258173
C	-0.871386	-0.110518	0.611568
C	-1.942646	-1.069016	0.296114
C	-2.376436	-1.920334	1.318336
C	-2.495876	-1.191934	-0.985438
C	-3.377998	-2.853090	1.075534
H	-1.933798	-1.841314	2.307600
C	-3.492033	-2.130107	-1.226452
H	-2.127859	-0.574920	-1.801235
C	-3.938455	-2.955793	-0.195369
H	-3.716785	-3.502414	1.875797
H	-3.913257	-2.226491	-2.221560
H	-4.715212	-3.688892	-0.386677
C	1.648742	0.467532	-0.643421
C	0.933528	-0.657870	-0.516417
C	2.233920	-0.578690	0.234949
C	2.369472	-0.474830	1.748968
H	3.411368	-0.210087	1.989227
H	2.168153	-1.455326	2.208569
C	1.693681	0.594741	3.727130
H	0.989934	1.340583	4.098912
H	1.495960	-0.367679	4.214246
H	2.717395	0.910576	3.960084
C	3.421410	-1.362830	-0.324529
H	3.486248	-2.347013	0.172973
H	4.361158	-0.825458	-0.108375
C	4.280693	-2.258851	-2.300625
H	4.061110	-2.319333	-3.367001
H	5.253578	-1.769591	-2.157451
H	4.330504	-3.273182	-1.881925
O	1.508435	0.495110	2.323010
O	3.241978	-1.513139	-1.703435
H	-0.267807	-0.299336	1.492579
H	0.626230	1.881944	1.302766
H	0.445024	-1.378843	-1.158452
H	1.984443	1.196324	-1.364557

E-TS12_II

$G_{\text{DCE}} = -999.311424$ Hartree

C	-2.681051	2.440909	-0.404560
C	-1.643649	1.620145	0.392261

C	-0.374505	3.165737	-0.575564
C	-1.780225	3.485690	-1.132175
H	-3.254616	1.811649	-1.087851
H	-3.379298	2.919807	0.286523
H	-1.818238	3.395358	-2.221606
H	-2.058240	4.511545	-0.879394
C	-0.671786	2.714981	0.852854
H	0.206184	2.341421	1.373745
H	-1.180087	3.485601	1.435501
H	-2.017867	0.900426	1.115451
H	0.400993	3.914304	-0.728455
N	0.067651	1.858416	-1.142572
N	-0.840888	0.948310	-0.657989
C	-0.722229	-0.318261	-1.042905
C	-1.623224	-1.384401	-0.552617
C	-1.696973	-1.768805	0.789931
C	-2.416523	-2.032871	-1.506630
C	-2.583906	-2.768936	1.172047
H	-1.020262	-1.315852	1.504910
C	-3.306975	-3.026542	-1.116437
H	-2.343756	-1.753677	-2.554792
C	-3.394346	-3.391749	0.224677
H	-2.632510	-3.074634	2.212168
H	-3.925186	-3.519179	-1.859439
H	-4.082455	-4.173504	0.529859
H	-0.430186	-0.421341	-2.087763
H	0.095489	1.847573	-2.164230
C	1.930423	0.506680	-0.985448
C	1.352639	-0.695626	-0.768326
C	2.273763	-0.165658	0.292850
C	3.689798	-0.742612	0.350084
C	5.435862	-1.523579	-0.988719
H	5.685700	-1.694931	-2.036118
H	6.165548	-0.830554	-0.549040
H	5.479147	-2.476603	-0.444684
C	1.849526	0.270025	1.688986
C	0.101696	0.429857	3.227091
H	-0.980738	0.300847	3.308485
H	0.598527	-0.263339	3.917543
H	0.363804	1.458731	3.511625
O	4.133241	-0.979761	-0.954725
O	0.462276	0.157305	1.887613
H	2.439681	1.083443	-1.743772
H	1.320453	-1.632708	-1.309925

H	2.370763	-0.368310	2.421054
H	2.179058	1.306277	1.876631
H	4.358552	-0.033840	0.870683
H	3.678188	-1.675851	0.939315

***E*-TS12_III**

$G_{\text{DCE}} = -999.303098$ Hartree

C	0.794610	2.296494	1.186205
C	1.740056	1.879511	0.046391
C	0.232149	3.134065	-0.995016
C	-0.290327	3.128896	0.449833
H	0.379603	1.460071	1.739378
H	1.373144	2.904808	1.887081
H	-1.273784	2.660051	0.524162
H	-0.353937	4.150168	0.832331
C	1.760017	3.161663	-0.808465
H	2.324593	3.063777	-1.738942
H	2.104170	4.030758	-0.244276
H	2.683508	1.419490	0.331585
H	-0.220709	3.852109	-1.676926
N	0.031351	1.745856	-1.511812
N	1.040529	1.004581	-0.943936
C	1.106446	-0.289182	-1.223885
C	2.086954	-1.157540	-0.518364
C	3.455029	-0.930390	-0.713624
C	1.666345	-2.220182	0.283067
C	4.391315	-1.749004	-0.092371
H	3.784599	-0.122592	-1.362876
C	2.609751	-3.038018	0.899438
H	0.605428	-2.405592	0.418867
C	3.968959	-2.802087	0.716489
H	5.449961	-1.569286	-0.247737
H	2.279463	-3.863028	1.521785
H	4.700809	-3.443149	1.196847
H	0.870483	-0.529215	-2.258786
C	-1.672043	0.183309	-1.196192
C	-0.988226	-0.975393	-1.161292
C	-1.868029	-0.655489	0.018104
C	-1.263160	-0.401794	1.379737
C	-1.710232	0.783447	3.358990
H	-2.176313	1.707995	3.701418
H	-2.204166	-0.072160	3.837496

H	-0.650074	0.783374	3.651085
C	-3.246917	-1.298715	0.126864
C	-5.083487	-1.981035	-1.145415
H	-5.427309	-2.023823	-2.179236
H	-5.057728	-2.996989	-0.728761
H	-5.781253	-1.373299	-0.554070
O	-1.862058	0.733626	1.954298
O	-3.793910	-1.406432	-1.157572
H	-3.152690	-2.292125	0.599564
H	-3.878251	-0.674973	0.780216
H	-1.449504	-1.287542	2.010729
H	-0.171326	-0.289393	1.308478
H	-0.871857	-1.817818	-1.832363
H	-2.304309	0.781436	-1.833613
H	0.026763	1.665019	-2.529990

Z-TS12

$G_{\text{DCE}} = -999.319948$ Hartree

C	-3.960695	-1.009358	-0.627425
C	-2.640688	-1.581994	-1.190428
C	-2.375132	-1.856960	0.990749
C	-3.761476	-1.176689	0.909608
H	-4.112153	0.027698	-0.934384
H	-4.802089	-1.601166	-0.996041
H	-3.772230	-0.224983	1.446393
H	-4.525728	-1.819978	1.351952
C	-2.373661	-2.760471	-0.251735
H	-1.422705	-3.265123	-0.429605
H	-3.196503	-3.477035	-0.257236
H	-2.578426	-1.727699	-2.267950
H	-2.093944	-2.295163	1.946987
N	-1.345331	-0.894693	0.560557
N	-1.606840	-0.611319	-0.734578
C	-0.852720	0.181821	-1.473644
H	-0.958264	-0.143066	1.151888
C	0.837325	-1.637209	0.160087
H	0.630005	-2.633826	0.523030
C	1.095982	-0.918872	-0.934934
C	1.863797	-0.571192	0.313556
H	1.336500	-1.087905	-1.975369
C	3.325104	-1.014805	0.371704
H	3.588952	-1.281502	1.410111

H	3.979573	-0.175819	0.074100
C	4.825052	-2.581060	-0.492532
H	4.859873	-3.430689	-1.175271
H	5.519404	-1.805220	-0.842904
H	5.136903	-2.907609	0.508801
C	1.649193	0.666756	1.188576
H	1.630381	1.594675	0.601023
H	2.497841	0.737357	1.886430
C	0.389523	1.569601	2.954565
H	-0.573081	1.464816	3.458604
H	1.196223	1.439530	3.685663
H	0.463494	2.568622	2.507710
O	3.495878	-2.108016	-0.482879
O	0.460120	0.563487	1.959624
C	-0.410578	1.533760	-1.073222
C	-1.065254	2.234559	-0.057189
C	0.603686	2.162855	-1.804479
C	-0.685074	3.538162	0.246943
H	-1.891528	1.776065	0.482161
C	0.984680	3.461439	-1.494632
H	1.102401	1.625441	-2.606882
C	0.347005	4.149226	-0.460868
H	-1.205615	4.080663	1.029950
H	1.776297	3.941349	-2.060412
H	0.641876	5.165567	-0.221262
H	-0.986663	0.015918	-2.541500

Z-TS12_I

$G_{\text{DCE}} = -999.315425$ Hartree

C	-3.335125	1.337141	-0.935447
C	-3.095591	-0.174772	-1.157098
C	-3.124805	0.014701	1.049287
C	-3.506003	1.438802	0.608616
H	-2.497588	1.929752	-1.313421
H	-4.234695	1.646866	-1.471681
H	-2.878308	2.200869	1.069143
H	-4.542489	1.645410	0.887581
C	-3.872259	-0.825693	-0.001597
H	-3.699946	-1.901042	0.079773
H	-4.941424	-0.608244	-0.031641
H	-3.239219	-0.560849	-2.164642
H	-3.258997	-0.230684	2.101316

N	-1.711119	-0.186258	0.632626
N	-1.731967	-0.513313	-0.679554
C	-0.642739	-0.693048	-1.409057
C	-0.197962	1.681969	0.262932
C	0.367751	1.203269	-0.849354
C	1.228741	1.289417	0.386890
C	1.701322	0.120191	1.254024
H	2.422200	0.519272	1.984591
H	2.222160	-0.648978	0.667372
C	1.095294	-1.385292	2.952809
H	0.218691	-1.838173	3.419751
H	1.712047	-2.167665	2.493770
H	1.682591	-0.862930	3.717246
C	2.260241	2.416683	0.423691
H	3.252250	2.017800	0.145020
H	2.343331	2.809110	1.452171
C	2.771747	4.497967	-0.501805
H	2.376933	5.228825	-1.208025
H	2.873276	4.966295	0.486415
H	3.763034	4.165864	-0.838826
O	0.631402	-0.468236	1.977134
O	1.860516	3.420810	-0.463368
H	-0.959261	-0.576814	1.218951
H	0.478077	1.511341	-1.880600
H	-0.878631	2.431919	0.635164
C	0.463420	-1.611639	-1.057051
C	1.649000	-1.550371	-1.798292
C	0.301884	-2.609077	-0.093330
C	2.674472	-2.453278	-1.552383
H	1.769238	-0.784554	-2.560219
C	1.330709	-3.514793	0.148613
H	-0.633680	-2.698381	0.453710
C	2.520868	-3.432570	-0.570111
H	3.591917	-2.398555	-2.128891
H	1.195444	-4.294573	0.891546
H	3.320040	-4.141452	-0.380172
H	-0.836535	-0.581666	-2.475037

Z-TS12_II

$G_{\text{DCE}} = -999.309207$ Hartree

C	2.437312	-2.881475	-0.095298
C	1.056933	-2.414528	0.416405

C	0.816029	-2.270426	-1.780816
C	2.280313	-2.741210	-1.639571
H	3.247666	-2.274614	0.314309
H	2.605117	-3.920001	0.201344
H	2.981519	-2.025723	-2.078265
H	2.420165	-3.695657	-2.152358
C	0.110925	-2.999529	-0.633689
H	-0.928322	-2.698688	-0.509538
H	0.200775	-4.084657	-0.708537
H	0.840371	-2.558778	1.471264
H	0.371653	-2.325151	-2.773488
N	0.705877	-0.884581	-1.261866
N	1.019755	-0.970741	0.072112
C	0.978006	0.078510	0.878063
H	1.232350	-0.166082	-1.756813
C	-1.206178	0.393573	-0.997360
C	-1.010305	0.980473	0.194137
C	-2.239805	0.141582	0.048195
C	-3.575344	0.849155	-0.194462
C	-4.554315	2.638517	-1.329742
H	-4.295129	3.454933	-2.004535
H	-5.304924	1.995172	-1.808565
H	-4.980756	3.052687	-0.406209
C	-2.486660	-1.132755	0.843704
C	-1.677134	-2.613484	2.444047
H	-0.806045	-2.807530	3.074038
H	-2.539529	-2.406446	3.090173
H	-1.896048	-3.506257	1.840021
O	-3.366457	1.924228	-1.063848
O	-1.377611	-1.501179	1.625704
H	-1.192584	0.599523	-2.056665
H	-0.790862	1.980741	0.536222
H	-3.348207	-0.950201	1.507239
H	-2.778956	-1.957978	0.171639
H	-4.302989	0.134848	-0.619696
H	-3.984167	1.196411	0.770457
C	1.718196	1.331825	0.596825
C	1.499244	2.448835	1.412017
C	2.719568	1.387175	-0.378274
C	2.230968	3.612549	1.221772
H	0.750669	2.399142	2.199212
C	3.452418	2.554571	-0.567900
H	2.980694	0.501820	-0.954729
C	3.201066	3.672609	0.221777

H	2.048691	4.472537	1.857540
H	4.231129	2.584417	-1.322995
H	3.771325	4.583249	0.071436
H	0.832085	-0.190660	1.921964

Z-TS12_III

$G_{\text{DCE}} = -999.295492$ Hartree

C	1.174103	-3.022822	-0.218839
C	-0.295545	-2.730762	0.135093
C	-0.230609	-2.373805	-2.052310
C	1.230028	-2.734859	-1.744825
H	1.862259	-2.423516	0.363473
H	1.370953	-4.076085	-0.000158
H	1.895159	-1.904685	-1.993977
H	1.535998	-3.611151	-2.320545
C	-1.016089	-3.299776	-1.104554
H	-2.093903	-3.122730	-1.105530
H	-0.800939	-4.357564	-1.269609
H	-0.632411	-3.038025	1.123673
H	-0.514969	-2.343977	-3.103009
N	-0.462397	-1.037554	-1.420354
N	-0.649958	-1.306078	-0.088381
C	-0.953285	-0.310137	0.746646
C	0.933676	0.833532	-0.936598
C	0.434332	1.222344	0.256974
C	1.899002	0.920714	0.198836
C	2.541617	-0.180059	1.037261
C	2.218025	-1.637749	2.837325
H	1.422933	-2.115071	3.412798
H	2.856081	-2.414105	2.391478
H	2.830246	-1.021387	3.507177
C	2.876002	2.093201	0.074394
C	3.193072	4.156882	-0.969224
H	2.697306	4.840452	-1.658927
H	3.362378	4.666358	-0.011328
H	4.163096	3.857167	-1.388112
O	1.599068	-0.841714	1.844713
O	2.343772	3.040496	-0.805196
H	3.041726	2.530568	1.074294
H	3.851187	1.722986	-0.288433
H	3.091099	-0.892909	0.400410
H	3.291247	0.300696	1.686248

H	-0.149046	2.068365	0.594599
H	0.929783	1.088044	-1.985505
H	-1.257796	-0.522378	-1.809351
C	-2.150053	0.550326	0.492004
C	-2.391212	1.288995	-0.674569
C	-3.117732	0.542636	1.503040
C	-3.597423	1.963103	-0.838948
H	-1.617698	1.407472	-1.428692
C	-4.319677	1.221898	1.336390
H	-2.933187	-0.008739	2.420916
C	-4.566041	1.925105	0.160660
H	-3.771217	2.535506	-1.744201
H	-5.061664	1.201516	2.127850
H	-5.502857	2.456561	0.030323
H	-0.795143	-0.580815	1.786611

13 (P-C-1)

$G_{\text{DCE}} = -999.413842$ Hartree

C	1.614301	3.069225	-0.869865
C	1.581562	1.533803	-0.861169
C	-0.326634	2.040295	-1.869214
C	0.239542	3.419962	-1.509949
H	1.726873	3.466393	0.139342
H	2.443176	3.431363	-1.483171
H	-0.424313	3.970797	-0.836533
H	0.343100	4.014581	-2.420378
C	0.914526	1.214011	-2.206894
H	0.713741	0.153174	-2.374560
H	1.453053	1.628391	-3.061723
H	2.525802	1.044612	-0.634127
H	-1.182280	2.020105	-2.544004
N	-0.717850	1.381761	-0.559625
N	0.556919	1.160869	0.155841
C	0.512312	-0.234935	0.718960
C	1.837134	-0.954647	0.596875
C	2.173240	-1.719464	-0.523822
C	2.773644	-0.802394	1.621072
C	3.423928	-2.322773	-0.614280
H	1.458910	-1.857751	-1.331356
C	4.026014	-1.403430	1.531206
H	2.517307	-0.209407	2.495525
C	4.352365	-2.165116	0.412313

H	3.672327	-2.920634	-1.485155
H	4.743366	-1.281619	2.336122
H	5.325829	-2.639277	0.341103
H	0.299000	-0.100465	1.784501
H	-1.276547	1.991714	0.049948
C	-1.418004	0.080514	-0.741845
H	-1.797160	-0.091343	-1.743073
C	-0.658445	-0.942835	0.040125
C	-2.061011	-0.572050	0.447259
H	-0.511584	-1.929737	-0.382186
C	-3.137686	-1.585082	0.082232
H	-4.102175	-1.064451	-0.038838
H	-3.248472	-2.306842	0.909156
C	-3.721252	-3.212708	-1.494450
H	-3.356354	-3.657386	-2.420093
H	-3.818036	-3.991870	-0.727991
H	-4.704957	-2.758735	-1.669969
C	-2.393477	0.131221	1.752996
H	-2.051928	-0.491880	2.594643
H	-3.487445	0.229505	1.838584
C	-1.981769	2.027431	3.080438
H	-1.477930	2.992975	3.039462
H	-3.048643	2.176391	3.285933
H	-1.540478	1.418059	3.878310
O	-2.775689	-2.235021	-1.103115
O	-1.795486	1.404867	1.820000

14 (S-R-1)

$G_{\text{DCE}} = -999.416233$ Hartree

C	1.356615	3.197732	-0.817134
C	1.628175	1.703949	-0.577271
C	0.006202	1.673797	-2.091391
C	0.249557	3.179183	-1.913250
H	1.050180	3.713942	0.097905
H	2.274300	3.676441	-1.166392
H	-0.662968	3.691904	-1.606196
H	0.603074	3.625450	-2.845640
C	1.415278	1.087393	-1.960590
H	1.453548	-0.002007	-1.977607
H	2.120314	1.493519	-2.689215
H	2.525695	1.442896	-0.019274
H	-0.588838	1.388391	-2.958258

N	-0.677085	1.219501	-0.852341
N	0.407358	1.172882	0.152459
C	0.469881	-0.239146	0.829114
C	1.795824	-0.942028	0.661195
C	2.039156	-1.854936	-0.368762
C	2.803445	-0.690953	1.597559
C	3.273538	-2.489258	-0.469021
H	1.260613	-2.086590	-1.091203
C	4.039730	-1.321327	1.496204
H	2.613535	-0.006608	2.422174
C	4.276289	-2.220635	0.459468
H	3.448416	-3.201747	-1.268426
H	4.810329	-1.122658	2.233705
H	5.236282	-2.720463	0.381759
H	0.319746	-0.006691	1.883977
C	-1.287373	-0.099034	-0.876066
H	-1.533566	-0.496859	-1.855059
C	-0.713228	-0.953867	0.223769
C	-2.124924	-0.425023	0.322202
H	-0.618827	-2.022948	0.072345
C	-3.205180	-1.473755	0.104745
H	-4.148573	-0.971340	-0.171061
H	-3.381288	-2.021212	1.045771
C	-3.766636	-3.343134	-1.185529
H	-3.358960	-3.979086	-1.971451
H	-3.971585	-3.950957	-0.294772
H	-4.704641	-2.890503	-1.532345
C	-2.618377	0.653744	1.272313
H	-3.249442	0.175226	2.037821
H	-3.251096	1.357883	0.710105
C	-2.096568	2.318019	2.833606
H	-1.246020	2.812170	3.305034
H	-2.711577	3.062253	2.312742
H	-2.701255	1.827418	3.605588
O	-2.798585	-2.350305	-0.909235
O	-1.580654	1.362310	1.921332
H	0.086168	1.805124	0.893406

TS15 (TS-R-1)

$G_{DCE} = -999.386397$ Hartree

C	0.875541	3.616867	-0.723399
C	1.389540	2.203094	-0.382094

C	-0.043921	1.800051	-2.017280
C	-0.115480	3.333615	-1.893106
H	0.393315	4.090596	0.135575
H	1.703945	4.257432	-1.035593
H	-1.132121	3.671574	-1.685633
H	0.216883	3.796911	-2.825306
C	1.440475	1.519036	-1.751326
H	1.693461	0.458259	-1.696664
H	2.094511	2.035897	-2.456216
H	2.272589	2.132922	0.253549
H	-0.512726	1.357679	-2.895385
N	-0.659439	1.269031	-0.773581
N	0.282899	1.428528	0.229047
C	0.488234	-0.749308	0.851454
C	1.855554	-1.197941	0.586745
C	2.211863	-1.891488	-0.581129
C	2.852436	-0.905910	1.528907
C	3.525154	-2.289660	-0.789442
H	1.459712	-2.119599	-1.331514
C	4.167279	-1.303917	1.319365
H	2.585198	-0.371365	2.437496
C	4.505289	-1.997849	0.159672
H	3.787930	-2.831393	-1.692109
H	4.926648	-1.079427	2.061219
H	5.530555	-2.312755	-0.005801
H	0.329991	-0.298802	1.826293
C	-1.439423	0.161553	-0.757179
H	-1.825002	-0.121544	-1.732926
C	-0.628739	-1.180531	0.128112
C	-1.998298	-0.600848	0.386469
H	-0.562882	-2.000405	-0.577219
C	-3.140333	-1.523875	-0.050108
H	-4.068594	-0.937306	-0.146347
H	-3.296213	-2.283524	0.733135
C	-3.803015	-3.042478	-1.703633
H	-3.458309	-3.459568	-2.649536
H	-3.933532	-3.850648	-0.973311
H	-4.764975	-2.536674	-1.855476
C	-2.366417	-0.017194	1.745150
H	-2.266601	-0.820816	2.491862
H	-3.426564	0.279311	1.712537
C	-2.009800	1.612706	3.382875
H	-1.371153	2.466607	3.609999
H	-3.054612	1.942150	3.334673

H	-1.904536	0.857416	4.170871
O	-2.812893	-2.128250	-1.269094
O	-1.590834	1.092878	2.129969
H	-0.146945	1.801595	1.076252

16 (P-R-1)

$G_{\text{DCE}} = -999.42425$ Hartree

C	3.118696	-2.649503	-0.152719
C	1.932190	-2.408284	-1.107828
C	3.172318	-0.604631	-1.441672
C	3.992184	-1.383566	-0.393142
H	2.784717	-2.735175	0.884409
H	3.651184	-3.567413	-0.412197
H	4.154299	-0.792747	0.511556
H	4.967529	-1.630601	-0.819339
C	2.587137	-1.720316	-2.309674
H	1.869430	-1.373806	-3.054907
H	3.371382	-2.319828	-2.774722
H	1.284003	-3.258639	-1.312756
H	3.645661	0.253759	-1.915746
N	1.115562	-1.280476	-0.608637
H	0.755066	-1.349353	0.345291
C	1.736284	0.994774	-0.220351
H	2.501429	1.729891	-0.458180
N	1.945205	-0.173360	-0.706608
C	0.550071	1.399782	0.623564
C	0.509105	2.939571	0.575175
H	1.392560	3.364074	1.085143
H	-0.392236	3.292816	1.097136
C	0.380042	4.700891	-0.966950
H	0.400562	4.879650	-2.041834
H	-0.565903	5.071430	-0.553201
H	1.212950	5.235231	-0.491473
C	0.812263	0.967159	2.072249
H	-0.063119	1.233635	2.683249
H	1.685296	1.502347	2.477026
C	1.159614	-0.912932	3.437305
H	1.357163	-1.983285	3.373184
H	1.983759	-0.419579	3.966289
H	0.226025	-0.747314	3.988876
O	0.500281	3.302804	-0.776722
O	1.049927	-0.422892	2.109683

C	-0.746959	0.869414	0.043584
C	-1.640881	0.118972	0.695309
H	-0.934763	1.196316	-0.976540
H	-1.411557	-0.237153	1.700065
C	-2.936443	-0.332701	0.163580
C	-3.602719	-1.376429	0.815867
C	-3.527133	0.237369	-0.971809
C	-4.815134	-1.859441	0.334919
H	-3.161616	-1.816216	1.707241
C	-4.738781	-0.241966	-1.451098
H	-3.048301	1.073865	-1.472246
C	-5.384288	-1.294809	-0.802533
H	-5.316822	-2.671915	0.850467
H	-5.188290	0.212130	-2.328369
H	-6.332836	-1.664686	-1.178044

E-17

$G_{\text{DCE}} = -769.576217$ Hartree

C	1.668013	0.326132	1.855882
H	1.544944	1.403465	2.073734
C	1.621882	-0.037667	0.379514
C	2.042280	-1.496804	0.207321
H	1.350178	-2.141364	0.768502
H	3.050977	-1.652965	0.625585
C	2.352709	-3.143427	-1.412233
H	2.318108	-3.294821	-2.492509
H	3.362663	-3.379937	-1.046084
H	1.638616	-3.825409	-0.928996
C	2.580496	0.874174	-0.390224
H	2.567677	0.591727	-1.453553
H	3.610787	0.740143	-0.017564
C	2.981052	3.114677	-0.908669
H	2.570689	4.112402	-0.745411
H	4.015238	3.083117	-0.536161
H	2.992321	2.899728	-1.986955
O	2.021490	-1.800345	-1.165186
O	2.161067	2.205444	-0.217919
C	0.200495	0.187206	-0.104434
C	-0.873029	-0.199632	0.591061
H	0.094935	0.695375	-1.060389
O	1.799081	-0.488497	2.738302
C	-2.280575	-0.046712	0.185732

C	-3.285200	-0.246610	1.139629
C	-2.661101	0.292027	-1.119758
C	-4.627915	-0.094679	0.809825
H	-3.004230	-0.517707	2.154319
C	-4.001012	0.444651	-1.450860
H	-1.902469	0.421997	-1.885687
C	-4.991052	0.254940	-0.487134
H	-5.390367	-0.249944	1.567036
H	-4.276396	0.705676	-2.468304
H	-6.037977	0.372637	-0.749153
H	-0.721058	-0.666585	1.566101

Cyclobutene

$G_{\text{DCE}} = -155.873588$ Hartree

C	-0.000268	0.667762	0.811996
C	0.000268	0.781527	-0.697683
C	-0.000268	-0.781527	-0.697683
C	0.000268	-0.667762	0.811996
H	-0.000739	1.418142	1.597034
H	0.891092	1.238150	-1.140914
H	-0.889445	1.239196	-1.142000
H	-0.891092	-1.238150	-1.140914
H	0.889445	-1.239196	-1.142000
H	0.000739	-1.418142	1.597034

TS-C-2

$G_{\text{DCE}} = -731.115233$ Hartree

C	-1.892909	-2.495445	-0.566769
C	-1.160846	-1.560210	0.415903
C	-3.089567	-0.510284	0.093631
C	-3.245769	-1.757680	-0.795676
H	-1.318415	-2.641073	-1.483377
H	-2.037920	-3.471961	-0.098540
H	-3.414431	-1.490586	-1.842521
H	-4.099185	-2.355975	-0.467617
C	-2.305447	-1.045403	1.298425
H	-2.004382	-0.268455	2.006110
H	-2.827835	-1.851014	1.816899
H	-0.268304	-1.964828	0.883519
H	-3.990823	0.070106	0.289600

N	-2.047026	0.372502	-0.495344
N	-0.855713	-0.329060	-0.350811
C	0.268994	0.384401	-0.473122
C	1.609659	-0.182931	-0.218870
C	1.967899	-0.757089	1.008138
C	2.563699	-0.082106	-1.236686
C	3.249840	-1.256962	1.194702
H	1.258873	-0.782761	1.831808
C	3.845790	-0.588355	-1.048078
H	2.297812	0.383828	-2.181945
C	4.187119	-1.180122	0.164384
H	3.524020	-1.695072	2.148618
H	4.577787	-0.513075	-1.845026
H	5.188422	-1.569997	0.314893
H	0.221811	1.106556	-1.290939
H	-2.214057	0.627613	-1.470851
C	-1.266653	2.336517	0.628903
H	-2.193445	2.229482	1.181946
C	0.035239	1.945477	0.889579
H	0.445355	1.449476	1.765153
C	0.610432	3.090459	0.055689
H	1.004962	3.902610	0.668685
H	1.348689	2.837424	-0.713948
C	-0.856605	3.363249	-0.398142
H	-1.229566	4.375467	-0.221107
H	-1.075459	3.097040	-1.440336

P-C-2

$G_{\text{DCE}} = -731.184243$ Hartree

C	-1.381805	-2.656810	-0.651926
C	-0.561945	-1.601137	0.103410
C	-2.645204	-0.960949	0.511764
C	-2.839841	-2.164521	-0.418847
H	-1.106117	-2.687407	-1.706449
H	-1.222238	-3.647673	-0.220346
H	-3.359110	-1.890066	-1.342635
H	-3.456812	-2.911413	0.085848
C	-1.423522	-1.342831	1.347474
H	-1.058059	-0.547413	2.002766
H	-1.608913	-2.244184	1.935297
H	0.489010	-1.838865	0.252153
H	-3.534511	-0.571116	1.007213

N	-2.031306	0.147563	-0.336301
N	-0.684079	-0.347300	-0.692605
C	0.258074	0.794119	-0.448457
C	1.667862	0.319265	-0.183178
C	2.504619	0.095737	-1.278750
C	2.147607	0.057076	1.103236
C	3.800954	-0.375503	-1.096289
H	2.136451	0.294752	-2.282170
C	3.444734	-0.413145	1.287150
H	1.519479	0.216518	1.975619
C	4.273140	-0.628873	0.188595
H	4.442145	-0.540147	-1.956041
H	3.810031	-0.605364	2.290723
H	5.285391	-0.991278	0.334903
H	0.275636	1.339693	-1.400467
H	-2.561915	0.262830	-1.206412
C	-1.887411	1.481410	0.363203
H	-2.544129	1.490965	1.234168
C	-0.393075	1.711073	0.602092
H	-0.012374	1.557804	1.612389
C	-0.581588	3.167262	0.113679
H	-0.718957	3.862715	0.942739
H	0.184708	3.557835	-0.558286
C	-1.935404	2.746124	-0.517249
H	-2.790983	3.405565	-0.370521
H	-1.844223	2.514638	-1.583595

S-R-2

$G_{\text{DCE}} = -731.184958$ Hartree

C	-1.459491	-2.627152	-0.724395
C	-0.576409	-1.637046	0.047145
C	-2.624124	-0.918724	0.508675
C	-2.896849	-2.122622	-0.403477
H	-1.229452	-2.645239	-1.794495
H	-1.281236	-3.634604	-0.341714
H	-3.454658	-1.821004	-1.291528
H	-3.477961	-2.881067	0.125440
C	-1.390836	-1.362891	1.309336
H	-0.974982	-0.591967	1.963203
H	-1.553310	-2.278876	1.881424
H	0.481525	-1.877539	0.132304
H	-3.487248	-0.548323	1.060382

N	-2.095186	0.177202	-0.349904
N	-0.735414	-0.305893	-0.687538
C	0.280302	0.843202	-0.419332
C	1.671329	0.329402	-0.166980
C	2.103138	-0.060933	1.105585
C	2.549102	0.220436	-1.248685
C	3.390279	-0.556064	1.286098
H	1.442420	0.018879	1.964671
C	3.838286	-0.271572	-1.067178
H	2.229133	0.538312	-2.238614
C	4.258719	-0.661716	0.201018
H	3.718394	-0.852448	2.276848
H	4.513908	-0.341461	-1.913113
H	5.264365	-1.042020	0.346937
H	0.274729	1.383705	-1.371859
C	-1.900621	1.459317	0.350358
H	-2.550368	1.497901	1.227368
C	-0.405122	1.705169	0.636506
H	-0.022985	1.527636	1.643218
C	-0.599983	3.171377	0.181448
C	-1.930718	2.752171	-0.493735
H	-0.724323	-0.496132	-1.693363
H	0.182830	3.601927	-0.446716
H	-0.765598	3.827697	1.037286
H	-1.822017	2.532593	-1.559635
H	-2.790979	3.408738	-0.360278

TS-R-2

$G_{\text{DCE}} = -731.146878$ Hartree

C	-1.892494	-2.685345	-0.738290
C	-0.650291	-1.777195	-0.627994
C	-1.853876	-1.144327	1.118102
C	-2.728781	-2.256184	0.506733
H	-2.425181	-2.533545	-1.681252
H	-1.599765	-3.736963	-0.690930
H	-3.724243	-1.889429	0.251350
H	-2.837642	-3.075377	1.221574
C	-0.439049	-1.685528	0.886893
H	0.358350	-1.003598	1.181591
H	-0.290373	-2.666029	1.343218
H	0.212697	-2.035354	-1.242631
H	-2.129461	-0.799264	2.114242

N	-1.903086	-0.026682	0.147537
N	-1.057295	-0.374593	-0.912816
C	0.511999	1.459077	-0.501718
C	1.719035	0.695855	-0.220040
C	2.321507	0.670669	1.049252
C	2.319943	-0.022970	-1.268322
C	3.477807	-0.067712	1.262973
H	1.902558	1.248163	1.867529
C	3.475256	-0.760662	-1.053109
H	1.868001	0.006073	-2.257641
C	4.053817	-0.786691	0.215861
H	3.940720	-0.072343	2.244227
H	3.931984	-1.306848	-1.871791
H	4.961999	-1.355844	0.386351
H	0.337073	1.667689	-1.556455
C	-1.952398	1.291479	0.457709
H	-2.362608	1.468081	1.452705
C	-0.279778	2.148841	0.431025
H	0.088522	2.195332	1.453915
H	-1.536682	-0.276151	-1.809844
C	-2.300512	2.365334	-0.564618
C	-1.170060	3.287519	-0.093632
H	-0.710606	3.915932	-0.858515
H	-1.493496	3.924168	0.732556
H	-3.326407	2.736963	-0.507530
H	-2.115527	2.004318	-1.580647

P-R-2

$G_{\text{DCE}} = -731.190629$ Hartree

C	0.039037	-0.541974	0.345795
C	-0.713124	-0.661523	-1.011699
H	0.110447	-1.530925	0.810101
H	-0.767985	0.320404	-1.497424
C	1.408955	0.032322	0.142737
C	2.529626	-0.653705	0.387776
H	1.451994	1.049922	-0.242702
H	2.433626	-1.677843	0.752205
C	3.912916	-0.187019	0.214977
C	4.951769	-1.116908	0.336217
C	4.235177	1.147941	-0.065207
C	6.277612	-0.732054	0.167410
H	4.714753	-2.153644	0.561684

C	5.557940	1.533611	-0.232591
H	3.450500	1.895156	-0.139020
C	6.583551	0.594638	-0.119369
H	7.070108	-1.467128	0.262509
H	5.793463	2.571302	-0.445925
H	7.616715	0.900280	-0.248438
C	-2.088261	-1.187200	-0.822810
H	-2.312982	-2.249956	-0.869875
C	-4.497628	-0.824229	-0.278238
C	-5.208712	0.398058	-0.869507
C	-4.702796	-0.640473	1.238233
H	-4.691102	-1.810529	-0.697259
C	-4.378666	1.380104	-0.036973
H	-6.268227	0.411387	-0.609846
H	-5.073971	0.513570	-1.946250
H	-5.684316	-1.035229	1.510366
H	-3.951889	-1.180681	1.819302
C	-4.628008	0.906789	1.406956
H	-4.510992	2.441550	-0.238967
H	-5.563866	1.318202	1.791511
H	-3.828535	1.221390	2.083110
N	-3.015021	0.968750	-0.466686
H	-2.272372	1.246153	0.175779
N	-3.083195	-0.429208	-0.536362
H	-0.156739	-1.337458	-1.664437
H	-0.547460	0.087013	1.032663

Cyclopentene

$G_{\text{DCE}} = -195.188392$ Hartree

C	-0.000101	-1.218559	-0.150691
C	-1.228647	-0.320306	0.114155
C	-0.665773	1.072111	-0.051216
C	0.665935	1.072003	-0.051164
C	1.228583	-0.320498	0.114138
H	-0.000050	-1.520456	-1.202764
H	-1.618799	-0.453598	1.132581
H	-2.056992	-0.533433	-0.569672
H	-1.290559	1.957761	-0.114198
H	1.290937	1.957517	-0.114034
H	1.618824	-0.453906	1.132509
H	2.056853	-0.533689	-0.569771
H	-0.000189	-2.128704	0.454015

TS-C-3

$G_{\text{DCE}} = -770.429103$ Hartree

C	-1.501651	-2.855503	-0.707148
C	-0.866860	-1.913191	0.335072
C	-2.917264	-1.090728	0.126690
C	-2.939153	-2.275198	-0.857774
H	-0.935143	-2.858443	-1.639890
H	-1.515854	-3.875187	-0.314476
H	-3.164126	-1.951082	-1.877508
H	-3.705083	-2.997780	-0.565507
C	-2.044114	-1.619170	1.272173
H	-1.824325	-0.876068	2.042680
H	-2.451518	-2.524799	1.724716
H	0.080542	-2.237554	0.754789
H	-3.878003	-0.642921	0.380367
N	-2.005081	-0.041816	-0.404240
N	-0.736175	-0.600845	-0.343921
C	0.298196	0.245049	-0.450648
C	1.691027	-0.185791	-0.208395
C	2.102273	-0.741466	1.010561
C	2.631852	0.023751	-1.221947
C	3.426978	-1.114553	1.194454
H	1.393767	-0.853076	1.827900
C	3.957270	-0.356878	-1.037096
H	2.321698	0.474479	-2.161203
C	4.353530	-0.929510	0.167996
H	3.742439	-1.537670	2.142331
H	4.679841	-0.200711	-1.830863
H	5.388545	-1.219806	0.316072
H	0.174372	0.975985	-1.247821
H	-2.234289	0.277508	-1.347943
C	-1.493605	1.869222	0.888179
H	-2.163908	1.407050	1.604994
C	-0.115332	1.768291	0.928857
H	0.394282	1.291736	1.761433
C	0.497363	2.954319	0.193515
H	0.764098	3.731097	0.918652
H	1.412207	2.701835	-0.355414
C	-1.934879	3.024425	0.029872
H	-2.267684	3.831378	0.697385
C	-0.650352	3.426725	-0.722000

H	-0.604830	4.495976	-0.934497
H	-0.606599	2.912867	-1.689994
H	-2.783302	2.795049	-0.623240

P-C-3

$G_{\text{DCE}} = -770.490876$ Hartree

C	-0.922252	-3.074171	-0.271279
C	-0.311674	-1.832562	0.392827
C	-2.484602	-1.411269	0.540606
C	-2.440427	-2.722437	-0.259406
H	-0.529086	-3.217960	-1.278012
H	-0.715716	-3.970728	0.317872
H	-2.863357	-2.605374	-1.262034
H	-3.039268	-3.476332	0.255990
C	-1.318628	-1.549758	1.517766
H	-1.116563	-0.659816	2.116440
H	-1.455627	-2.406296	2.180838
H	0.742039	-1.895529	0.656645
H	-3.458900	-1.089326	0.908439
N	-1.920569	-0.326509	-0.365921
N	-0.521939	-0.729585	-0.594463
C	0.263586	0.528926	-0.499589
C	1.728409	0.259608	-0.248612
C	2.416188	-0.569165	-1.143839
C	2.415925	0.825538	0.823738
C	3.764793	-0.841746	-0.955227
H	1.885234	-1.000476	-1.989364
C	3.773258	0.559793	1.005574
H	1.912105	1.492159	1.517145
C	4.446585	-0.276389	0.122864
H	4.288069	-1.487154	-1.653037
H	4.301063	1.011585	1.838914
H	5.501920	-0.482788	0.266970
H	0.175640	0.986956	-1.496275
H	-2.400160	-0.338708	-1.272454
C	-1.949259	1.082253	0.214624
H	-2.561962	1.041131	1.118559
C	-0.478484	1.441253	0.486587
H	-0.195927	1.202672	1.514862
C	-0.352689	2.949949	0.170406
H	0.038392	3.513949	1.019104
H	0.346977	3.096737	-0.659347

C	-2.451394	2.144969	-0.763096
C	-1.774051	3.410372	-0.220249
H	-2.313591	3.760948	0.665669
H	-1.774915	4.224971	-0.946503
H	-3.540984	2.213478	-0.806261
H	-2.079546	1.927573	-1.773636

S-R-3

$G_{\text{DCE}} = -770.490703$ Hartree

C	-0.973601	-3.042950	-0.587975
C	-0.272764	-1.910287	0.175296
C	-2.419733	-1.435314	0.482121
C	-2.480409	-2.698254	-0.391427
H	-0.668136	-3.091736	-1.638122
H	-0.706621	-3.999127	-0.132372
H	-3.000298	-2.498055	-1.329923
H	-3.009084	-3.499694	0.128563
C	-1.196015	-1.694989	1.372414
H	-0.922586	-0.861865	2.022808
H	-1.281676	-2.606477	1.968014
H	0.800492	-2.001214	0.331614
H	-3.356018	-1.158401	0.965144
N	-1.977187	-0.314156	-0.388936
N	-0.562451	-0.654100	-0.651412
C	0.275985	0.623180	-0.446483
C	1.729415	0.326097	-0.197940
C	2.235271	0.102798	1.086945
C	2.592898	0.254219	-1.294491
C	3.583016	-0.192651	1.265302
H	1.587157	0.160727	1.956960
C	3.940838	-0.041172	-1.115853
H	2.211849	0.446487	-2.295358
C	4.436098	-0.265512	0.165695
H	3.970019	-0.357682	2.265416
H	4.602845	-0.085387	-1.974142
H	5.487985	-0.488902	0.310543
H	0.179318	1.125959	-1.415359
C	-1.979752	1.022355	0.257157
H	-2.584169	0.962884	1.168696
C	-0.521578	1.421218	0.579243
H	-0.236010	1.142741	1.595601
C	-0.430928	2.950932	0.357626

H	-0.051469	3.464913	1.242240
H	0.264341	3.174310	-0.459099
C	-2.491239	2.149055	-0.644576
C	-1.865610	3.391341	-0.006783
H	-2.415646	3.655824	0.902774
H	-1.883525	4.263811	-0.662589
H	-3.581349	2.179531	-0.704059
H	-2.108863	1.998990	-1.662223
H	-0.492436	-0.910239	-1.640311

TS-R-3

$G_{\text{DCE}} = -770.437058$ Hartree

C	0.688275	3.317165	-0.724526
C	-0.210059	2.064180	-0.819287
C	0.733029	1.821734	1.169364
C	1.323423	3.167634	0.692823
H	1.434698	3.344745	-1.523476
H	0.084589	4.224178	-0.806353
H	2.414399	3.146335	0.675625
H	1.006408	3.969608	1.364222
C	-0.697349	1.904008	0.624618
H	-1.302554	1.017193	0.803427
H	-1.215677	2.797069	0.979413
H	-0.959960	2.052044	-1.610408
H	0.888067	1.559370	2.215590
N	1.336973	0.809447	0.277920
N	0.661983	0.862721	-0.938906
C	-0.110534	-1.519889	-0.620026
C	-1.484908	-1.187926	-0.281676
C	-2.020414	-1.409063	0.998317
C	-2.312395	-0.633468	-1.274340
C	-3.333172	-1.052128	1.282220
H	-1.421594	-1.882006	1.770092
C	-3.620995	-0.274619	-0.988981
H	-1.906534	-0.476416	-2.271246
C	-4.131941	-0.477778	0.294443
H	-3.740020	-1.233501	2.271588
H	-4.248584	0.155109	-1.762839
H	-5.157847	-0.204172	0.518978
H	0.094958	-1.637530	-1.683157
C	2.013142	-0.313637	0.588312
H	2.238929	-0.354300	1.655917

C	0.896759	-1.895685	0.277658
H	0.579847	-2.043053	1.309850
H	1.316639	0.933505	-1.720294
C	3.174614	-0.778661	-0.274920
H	4.052521	-0.173252	-0.024802
H	2.947128	-0.629598	-1.337661
C	1.972204	-2.859625	-0.227990
H	1.852112	-3.835781	0.249116
H	1.834225	-3.012367	-1.304021
C	3.358215	-2.257640	0.018516
H	3.665304	-2.394361	1.062045
H	4.122894	-2.715600	-0.611862

P-R-3

$G_{\text{DCE}} = -770.475949$ Hartree

C	-0.296780	3.764216	-0.319589
C	-0.541683	2.497808	-1.160914
C	-0.432862	1.677978	0.897462
C	-0.213292	3.186664	1.125511
H	0.615270	4.287013	-0.621176
H	-1.126989	4.465999	-0.427867
H	0.736738	3.392497	1.624345
H	-1.014711	3.566034	1.763942
C	-1.440223	1.650898	-0.254513
H	-1.644226	0.650691	-0.640419
H	-2.367594	2.160211	0.013260
H	-0.866131	2.645830	-2.189751
H	-0.613426	1.051735	1.769354
N	0.784800	1.210479	0.174034
N	0.685916	1.654859	-1.154405
C	0.531991	-2.089152	-0.586211
C	-0.879666	-1.887927	-0.224321
C	-1.288743	-1.630589	1.092387
C	-1.850700	-1.894002	-1.234290
C	-2.625289	-1.385888	1.387485
H	-0.555821	-1.621196	1.896552
C	-3.190228	-1.654955	-0.940374
H	-1.549228	-2.096337	-2.258918
C	-3.580872	-1.393490	0.370874
H	-2.925657	-1.195284	2.413547
H	-3.928905	-1.675015	-1.735473
H	-4.624164	-1.204985	0.602499

H	0.758007	-1.980982	-1.648551
C	1.754736	0.499314	0.620620
H	1.671489	0.199362	1.663222
C	1.542698	-2.357341	0.250870
H	1.345394	-2.526223	1.310620
H	1.530199	2.172438	-1.402580
C	2.977261	0.185998	-0.174585
H	3.653366	1.049163	-0.076347
H	2.699081	0.113239	-1.234263
C	2.979733	-2.365497	-0.176148
H	3.506472	-3.235521	0.229168
H	3.039300	-2.428159	-1.268899
C	3.697883	-1.086794	0.291707
H	3.784684	-1.076920	1.385514
H	4.718065	-1.074409	-0.101010

Norbornene

$G_{\text{DCE}} = -272.545627$ Hartree

C	-1.180844	-0.776511	-0.521319
C	0.084269	-1.124973	0.324461
C	0.085498	1.124378	0.325722
C	-1.179769	0.778312	-0.520692
H	-1.124290	-1.200725	-1.526625
H	-2.081259	-1.171354	-0.040171
H	-1.123367	1.203472	-1.525732
H	-2.079433	1.173704	-0.038803
C	0.030960	-0.000967	1.376298
H	0.897632	-0.002005	2.042212
H	-0.895365	-0.000907	1.962069
C	1.274970	-0.668487	-0.500919
H	1.915796	-1.325241	-1.079508
C	1.275707	0.668127	-0.500156
H	1.916897	1.324876	-1.078351
H	0.113206	-2.152412	0.690991
H	0.115439	2.151322	0.693552

TS-C-4

$G_{\text{DCE}} = -847.78786$ Hartree

C	-1.681996	3.184899	-0.464249
C	-1.241558	2.062824	0.498302

C	0.654871	3.153895	0.130882
C	-0.349076	3.945454	-0.729702
H	-2.138400	2.779261	-1.368807
H	-2.419175	3.820069	0.032989
H	-0.062768	3.948871	-1.784849
H	-0.398477	4.985484	-0.398616
C	-0.182351	2.764441	1.355640
H	0.335120	2.101388	2.052502
H	-0.584065	3.631087	1.883024
H	-2.039886	1.511063	0.984539
H	1.626206	3.615868	0.303743
N	0.846266	1.805428	-0.464013
N	-0.377851	1.167472	-0.311001
C	-0.441262	-0.142676	-0.559937
C	-1.638858	-0.945121	-0.239131
C	-2.178563	-1.004351	1.052822
C	-2.209782	-1.711820	-1.259880
C	-3.295898	-1.789004	1.305982
H	-1.704771	-0.462658	1.868141
C	-3.332977	-2.492366	-1.004623
H	-1.779918	-1.688571	-2.257705
C	-3.878519	-2.527470	0.275540
H	-3.706018	-1.836253	2.309113
H	-3.776473	-3.076611	-1.803654
H	-4.750038	-3.141502	0.476835
H	0.099609	-0.453417	-1.449336
H	1.147643	1.814413	-1.439810
C	2.117296	0.056595	0.665650
H	2.195128	0.779624	1.470989
C	1.174853	-0.951012	0.579443
H	0.525178	-1.212461	1.410045
C	1.790237	-2.011249	-0.332962
C	3.290006	-0.324993	-0.198401
C	2.598935	-1.134088	-1.308327
H	1.085732	-2.725708	-0.765510
H	3.306284	-1.713958	-1.907212
H	1.999188	-0.519210	-1.987610
H	3.964364	0.479248	-0.493848
C	2.947705	-2.647829	0.487623
C	3.974670	-1.485698	0.600290
H	3.371220	-3.497930	-0.053423
H	2.605358	-3.008090	1.460280
H	4.923404	-1.740028	0.120188
H	4.190242	-1.202863	1.633317

P-C-4

$G_{\text{DCE}} = -847.858518$ Hartree

C	-0.763594	3.294068	-0.693242
C	-0.988873	1.930745	-0.020753
C	1.036150	2.482469	0.694261
C	0.682974	3.647312	-0.238959
H	-0.863726	3.220017	-1.776626
H	-1.485971	4.026661	-0.325501
H	1.390439	3.738009	-1.069439
H	0.726416	4.583055	0.322923
C	-0.300270	2.117941	1.337963
H	-0.273470	1.218076	1.958377
H	-0.705679	2.950509	1.916698
H	-2.012994	1.565340	-0.026030
H	1.921101	2.599076	1.320610
N	1.226661	1.257250	-0.193097
N	-0.104216	0.971391	-0.736569
C	-0.324322	-0.508764	-0.656089
C	-1.739649	-0.864881	-0.253425
C	-2.140456	-0.970922	1.081835
C	-2.690672	-1.041767	-1.260840
C	-3.466083	-1.247783	1.400925
H	-1.421862	-0.845622	1.887694
C	-4.017781	-1.318572	-0.944017
H	-2.387492	-0.963559	-2.302074
C	-4.407270	-1.421364	0.388221
H	-3.763150	-1.334129	2.441092
H	-4.744543	-1.459833	-1.737175
H	-5.439751	-1.642684	0.638049
H	-0.181276	-0.871961	-1.680002
H	1.836881	1.493108	-0.983670
C	1.793179	0.038966	0.516891
H	1.876455	0.304054	1.573262
C	0.801630	-1.107672	0.216723
H	0.398935	-1.539989	1.134740
C	1.686143	-2.121611	-0.544361
C	3.113194	-0.421649	-0.110352
C	2.609759	-1.188832	-1.348194
H	3.412732	-1.718518	-1.867086
H	2.079495	-0.568139	-2.082699
H	1.104287	-2.845851	-1.118447

H	3.836770	0.383396	-0.270953
C	2.670445	-2.744300	0.461359
C	3.638416	-1.567048	0.781715
H	3.207023	-3.578031	0.002454
H	2.163090	-3.129236	1.350032
H	4.666305	-1.808621	0.502462
H	3.645356	-1.293635	1.841001

S-R-4

$G_{\text{DCE}} = -847.858378$ Hartree

C	-0.786549	3.300024	-0.640156
C	-1.005966	1.943965	0.045013
C	1.071821	2.453302	0.640363
C	0.678461	3.646893	-0.242080
H	-0.948875	3.254341	-1.721951
H	-1.503389	4.020512	-0.239980
H	1.347883	3.732905	-1.100012
H	0.729166	4.578312	0.325638
C	-0.240916	2.099230	1.356098
H	-0.191492	1.189234	1.960233
H	-0.645593	2.916098	1.957422
H	-2.019220	1.547950	0.058533
H	1.964440	2.597007	1.248534
N	1.283523	1.279929	-0.247304
N	-0.084796	0.976021	-0.706965
C	-0.317433	-0.553255	-0.630422
C	-1.734458	-0.888301	-0.241722
C	-2.140445	-0.986666	1.092955
C	-2.680360	-1.061990	-1.256129
C	-3.471244	-1.246862	1.403621
H	-1.423609	-0.867102	1.900234
C	-4.011481	-1.324065	-0.945787
H	-2.371844	-1.005134	-2.297842
C	-4.408101	-1.414461	0.385627
H	-3.775602	-1.326145	2.442060
H	-4.734624	-1.466223	-1.741886
H	-5.444061	-1.624353	0.630680
H	-0.158378	-0.876927	-1.663778
C	1.813565	0.089915	0.464777
H	1.932137	0.330614	1.527920
C	0.825511	-1.087388	0.236372
H	0.441282	-1.488412	1.176385

C	1.696146	-2.126904	-0.508428
C	3.125516	-0.410379	-0.157751
C	2.606200	-1.218544	-1.356230
H	3.393568	-1.771903	-1.874937
H	2.075951	-0.601700	-2.091896
H	1.107834	-2.877937	-1.041866
H	3.829304	0.395756	-0.373206
C	2.695726	-2.707858	0.507880
C	3.669246	-1.519055	0.764622
H	3.222035	-3.560618	0.072121
H	2.201220	-3.059274	1.417989
H	4.691902	-1.777639	0.480807
H	3.692497	-1.209262	1.814012
H	-0.115040	1.232641	-1.697076

TS-R-4

$G_{\text{DCE}} = -847.802111$ Hartree

C	0.433407	3.498193	0.700836
C	1.047665	2.102383	0.957054
C	0.364336	1.949402	-1.144895
C	0.001531	3.410610	-0.796660
H	-0.404814	3.703090	1.373087
H	1.183132	4.276163	0.863371
H	-1.060491	3.610506	-0.950649
H	0.574966	4.098067	-1.423890
C	1.690901	1.780814	-0.395014
H	2.130388	0.788018	-0.461119
H	2.418951	2.539996	-0.687870
H	1.660333	1.991851	1.851316
H	0.309837	1.660699	-2.194345
N	-0.551068	1.131446	-0.323622
N	-0.052254	1.097268	0.970696
C	0.041599	-1.420348	0.750329
C	1.418071	-1.484193	0.305376
C	1.766148	-1.642799	-1.048010
C	2.445492	-1.348900	1.257063
C	3.100131	-1.651513	-1.434355
H	0.996645	-1.765440	-1.803844
C	3.776756	-1.356026	0.869549
H	2.183469	-1.228912	2.305558
C	4.106351	-1.503673	-0.479131
H	3.358762	-1.780594	-2.480190

H	4.559603	-1.250742	1.613228
H	5.147785	-1.513115	-0.784371
H	-0.114733	-1.438341	1.827677
C	-1.530599	0.269339	-0.673006
H	-1.622417	0.233306	-1.760506
C	-1.081189	-1.511460	-0.086738
H	-0.901317	-1.949855	-1.068497
H	-0.781669	1.330888	1.648957
C	-2.896725	0.304985	0.043539
C	-2.420152	-1.856758	0.569329
C	-2.815714	-0.568353	1.300472
H	-2.082323	-0.249124	2.047252
H	-3.788986	-0.648950	1.793449
C	-3.887963	-0.500178	-0.818562
C	-3.517581	-1.978187	-0.504223
H	-3.813781	-0.253581	-1.881456
H	-4.910456	-0.274767	-0.506118
H	-3.166760	-2.523448	-1.385132
H	-4.377806	-2.523458	-0.109045
H	-3.191833	1.347744	0.199870
H	-2.338021	-2.741024	1.206029

P-R-4

$G_{\text{DCE}} = -847.840491$ Hartree

C	-0.804554	2.908500	1.334039
C	0.324831	3.501700	0.471134
C	-0.600518	2.028737	-0.907794
C	-1.445308	1.865544	0.369329
H	-0.419141	2.456580	2.252526
H	-1.515250	3.685983	1.624401
H	-1.417277	0.838672	0.742246
H	-2.486051	2.103025	0.135828
C	-0.294778	3.529772	-0.930097
H	0.405306	3.831733	-1.711148
H	-1.206282	4.127591	-0.976722
H	0.789370	4.419078	0.829348
H	-0.963343	1.533160	-1.807405
N	0.751593	1.512223	-0.553076
N	1.379216	2.474515	0.252257
C	0.028993	-2.070731	0.506126
C	-1.393774	-1.824559	0.210837
C	-1.856054	-1.587603	-1.092593

C	-2.303381	-1.712695	1.270532
C	-3.186931	-1.258165	-1.326125
H	-1.173982	-1.670569	-1.936228
C	-3.635823	-1.386194	1.038237
H	-1.959145	-1.892590	2.286166
C	-4.080747	-1.153138	-0.260889
H	-3.530180	-1.087026	-2.341931
H	-4.327655	-1.316218	1.871579
H	-5.119124	-0.897387	-0.445338
H	0.323941	-1.844454	1.530945
C	1.287827	0.406728	-0.918247
H	0.684869	-0.186939	-1.598935
C	0.960838	-2.472613	-0.366713
H	0.650868	-2.761977	-1.373100
H	1.720726	2.038855	1.109658
C	2.639709	-0.034856	-0.458522
C	2.453506	-2.431463	-0.155615
C	3.038281	-1.370736	-1.115735
H	2.679763	-1.461403	-2.146825
H	4.128948	-1.451376	-1.137402
C	2.671859	-0.333644	1.082893
C	2.879590	-1.862650	1.202540
H	1.731843	-0.035993	1.562781
H	3.479935	0.221417	1.565368
H	2.336567	-2.295206	2.046268
H	3.940198	-2.078556	1.358072
H	3.333475	0.780011	-0.706776
H	2.894557	-3.415179	-0.347672

***E*-Cyclooctene**

$G_{\text{DCE}} = -312.998263$ Hartree

C	-0.413966	-0.522065	-1.358397
H	-1.490184	-0.336794	-1.334889
C	0.413966	0.522065	-1.358397
H	1.490184	0.336794	-1.334889
C	0.034981	-1.871510	-0.901221
H	-0.510280	-2.704358	-1.358222
H	1.102540	-2.008137	-1.112700
C	-0.034981	1.871510	-0.901221
H	-1.102540	2.008137	-1.112700
H	0.510280	2.704358	-1.358222
C	0.183001	1.877834	0.635533

H	1.260794	1.924503	0.841500
H	-0.248046	2.798155	1.048278
C	-0.413966	0.660993	1.376189
H	-0.560669	0.965017	2.418884
H	-1.420918	0.465721	0.984525
C	-0.183001	-1.877834	0.635533
H	0.248046	-2.798155	1.048278
H	-1.260794	-1.924503	0.841500
C	0.413966	-0.660993	1.376189
H	0.560669	-0.965017	2.418884
H	1.420918	-0.465721	0.984525

TS-C-5

$G_{\text{DCE}} = -888.249681$ Hartree

C	-2.850966	2.638240	-0.074758
C	-1.865073	1.679968	0.624784
C	-0.526074	3.273558	-0.143885
C	-1.911044	3.755590	-0.617358
H	-3.415326	2.127984	-0.857384
H	-3.561981	3.026777	0.658463
H	-1.955238	3.859020	-1.705082
H	-2.143496	4.731635	-0.184467
C	-0.835449	2.647336	1.220607
H	0.022582	2.153366	1.680211
H	-1.287321	3.356889	1.915769
H	-2.308905	0.918772	1.258874
H	0.290413	3.993230	-0.199692
N	-0.157408	2.045717	-0.896288
N	-1.061656	1.078247	-0.465197
C	-0.814505	-0.190286	-0.789658
C	-1.611467	-1.303204	-0.233898
C	-1.714953	-1.526842	1.145222
C	-2.232390	-2.185149	-1.124283
C	-2.462129	-2.595332	1.623622
H	-1.184906	-0.883536	1.843229
C	-2.986551	-3.249683	-0.641581
H	-2.131240	-2.031433	-2.195399
C	-3.105049	-3.452393	0.730750
H	-2.534163	-2.768035	2.692256
H	-3.473605	-3.924494	-1.337456
H	-3.686893	-4.287749	1.106490
H	-0.453468	-0.325424	-1.808594

H	-0.202811	2.161453	-1.910220
C	1.198920	-0.557454	-0.149978
H	1.019436	-0.733979	0.913506
C	1.830653	0.621785	-0.470360
H	2.153681	0.760904	-1.504818
C	1.502433	-1.795595	-0.960914
H	0.688220	-2.528001	-0.908277
H	1.635192	-1.517672	-2.015923
C	2.522800	1.461841	0.545771
H	2.049249	1.336842	1.526979
H	2.524357	2.526919	0.290751
C	3.984965	0.949244	0.642036
H	4.521646	1.223046	-0.274594
H	4.468793	1.495692	1.458455
C	4.118852	-0.564796	0.880253
H	5.097289	-0.730076	1.341060
H	3.386015	-0.878699	1.636224
C	2.807176	-2.432602	-0.440779
H	3.049197	-3.278445	-1.093607
H	2.625731	-2.857745	0.554556
C	4.013794	-1.479214	-0.373539
H	4.915575	-2.097295	-0.416845
H	4.041767	-0.867775	-1.286405

P-C-5

$G_{\text{DCE}} = -888.312673$ Hartree

C	-1.865303	3.227600	0.194469
C	-1.456835	1.783628	0.517504
C	0.505378	2.812464	0.453301
C	-0.480602	3.928016	0.071507
H	-2.450019	3.275229	-0.724670
H	-2.457471	3.653581	1.007852
H	-0.284582	4.328845	-0.928401
H	-0.369040	4.756207	0.774946
C	-0.274845	1.989746	1.474590
H	0.223377	1.075873	1.801865
H	-0.540059	2.590940	2.346997
H	-2.259350	1.121077	0.834329
H	1.522675	3.124727	0.677403
N	0.513694	1.844930	-0.728342
N	-0.837453	1.258636	-0.733228
C	-0.633368	-0.206168	-0.900613

C	-1.806192	-0.995630	-0.368796
C	-1.744726	-1.746471	0.805872
C	-3.008974	-0.938379	-1.080770
C	-2.872098	-2.427124	1.262879
H	-0.819338	-1.822778	1.369753
C	-4.135502	-1.608742	-0.619835
H	-3.056642	-0.360623	-2.000890
C	-4.067843	-2.355432	0.555381
H	-2.812380	-3.016629	2.171998
H	-5.062896	-1.557396	-1.180861
H	-4.943775	-2.886908	0.912936
H	-0.594965	-0.366198	-1.988662
H	0.610865	2.391424	-1.589023
C	0.763419	-0.541810	-0.361184
H	0.745786	-0.614803	0.732158
C	1.560159	0.698896	-0.765156
H	1.809677	0.615419	-1.829973
C	1.262521	-1.875490	-0.958660
H	0.376152	-2.409000	-1.321788
H	1.880756	-1.682863	-1.846244
C	2.817203	1.057828	0.010676
H	2.579681	1.202342	1.071493
H	3.195223	2.014233	-0.371867
C	3.929180	0.004984	-0.116127
H	3.981057	-0.352789	-1.152905
H	4.872521	0.529531	0.057837
C	3.841402	-1.190282	0.859646
H	4.816635	-1.295397	1.343582
H	3.136399	-0.964318	1.672802
C	1.998838	-2.814294	0.004153
H	1.901918	-3.832339	-0.387218
H	1.475269	-2.814839	0.970906
C	3.484907	-2.542952	0.233524
H	3.862327	-3.335793	0.888103
H	4.026190	-2.654041	-0.715630

S-R-5

$G_{\text{DCE}} = -888.31142$ Hartree

C	-1.826729	3.303675	-0.020491
C	-1.578561	1.839572	0.366638
C	0.452146	2.719823	0.504584
C	-0.404304	3.927887	0.088354

H	-2.272862	3.402488	-1.015366
H	-2.529056	3.745796	0.689696
H	-0.049307	4.351744	-0.852012
H	-0.367143	4.705874	0.854332
C	-0.494003	1.949316	1.434905
H	-0.107800	0.994734	1.795458
H	-0.839475	2.545355	2.282593
H	-2.451768	1.216646	0.550802
H	1.441141	2.972716	0.876070
N	0.564616	1.853328	-0.700134
N	-0.776522	1.254146	-0.795232
C	-0.610137	-0.276072	-0.897686
C	-1.794601	-1.023162	-0.346332
C	-1.846337	-1.468966	0.977867
C	-2.887751	-1.253172	-1.187343
C	-2.979632	-2.123488	1.451556
H	-1.003972	-1.321431	1.647373
C	-4.021705	-1.904002	-0.712643
H	-2.846606	-0.932749	-2.226464
C	-4.068642	-2.338037	0.609856
H	-3.008489	-2.472444	2.478516
H	-4.860916	-2.082191	-1.376820
H	-4.948848	-2.852293	0.981709
H	-0.556937	-0.446966	-1.979991
C	0.780344	-0.546236	-0.326841
H	0.740735	-0.609701	0.766589
C	1.545000	0.722404	-0.734588
H	1.825723	0.615281	-1.792016
C	1.295720	-1.885017	-0.897524
H	0.419127	-2.458089	-1.223571
H	1.884610	-1.692136	-1.805075
C	2.807722	1.062104	0.047280
H	2.575839	1.149080	1.116798
H	3.140121	2.050344	-0.292134
C	3.959558	0.063614	-0.133513
H	3.994539	-0.277301	-1.176851
H	4.885740	0.624527	0.019246
C	3.963461	-1.146723	0.825701
H	4.975202	-1.248616	1.229332
H	3.323304	-0.938306	1.695257
C	2.081467	-2.779744	0.069152
H	1.973501	-3.812337	-0.279237
H	1.600191	-2.745750	1.057159
C	3.575506	-2.497672	0.218125

H	3.990676	-3.289678	0.850972
H	4.064058	-2.607634	-0.759483
H	-1.199129	1.584099	-1.667666

TS-R-5

$G_{\text{DCE}} = -888.249527$ Hartree

C	-2.492899	3.024354	-0.791951
C	-2.464790	1.484279	-0.919252
C	-1.288337	1.837907	0.929668
C	-1.704080	3.272988	0.531327
H	-2.035160	3.513650	-1.656550
H	-3.523926	3.379455	-0.722152
H	-0.837499	3.924193	0.398752
H	-2.341039	3.705524	1.307249
C	-2.541460	1.040980	0.545084
H	-2.461640	-0.033158	0.697442
H	-3.433100	1.431760	1.039443
H	-3.165997	1.036187	-1.622302
H	-0.869106	1.700834	1.924704
N	-0.342485	1.415352	-0.123213
N	-1.074659	1.065076	-1.251078
C	0.097835	-1.157368	-1.174356
C	-0.951597	-1.760401	-0.373584
C	-0.828228	-1.948434	1.013759
C	-2.147622	-2.151355	-1.003126
C	-1.876794	-2.490954	1.747955
H	0.092129	-1.689037	1.528127
C	-3.192714	-2.691425	-0.270069
H	-2.248901	-2.013423	-2.077048
C	-3.060654	-2.858299	1.110594
H	-1.767331	-2.638108	2.817473
H	-4.109325	-2.988482	-0.769053
H	-3.875686	-3.287063	1.684916
H	-0.023465	-1.223328	-2.254324
C	1.301327	-0.657557	-0.662075
H	1.520744	-0.987835	0.351445
C	0.981426	1.167863	-0.144720
H	1.464978	1.530801	-1.056527
C	2.527760	-0.635060	-1.575729
H	2.240615	-1.027509	-2.556965
H	2.885899	0.388390	-1.755911
C	1.749010	1.460881	1.126154

H	1.362128	0.834602	1.940571
H	1.521236	2.500327	1.397525
C	3.275788	1.311008	1.020170
H	3.610471	1.723166	0.059748
H	3.696869	1.977291	1.777765
C	3.881350	-0.100351	1.232792
H	4.641199	-0.011418	2.014544
H	3.132413	-0.788841	1.647274
C	3.683913	-1.466544	-1.002143
H	4.322028	-1.796674	-1.828438
H	3.276683	-2.379943	-0.549395
C	4.568797	-0.732455	0.009823
H	5.316940	-1.447306	0.368306
H	5.131822	0.053004	-0.511928
H	-0.712167	1.549594	-2.076599

P-R-5

$G_{\text{DCE}} = -888.298003$ Hartree

C	-7.759419	1.327323	0.920500
C	-7.122330	1.414453	-0.478399
C	-6.894172	-0.740608	0.009306
C	-7.590071	-0.182628	1.266192
H	-7.261677	1.985497	1.637525
H	-8.811373	1.618816	0.883122
H	-7.004664	-0.361990	2.170712
H	-8.552335	-0.685531	1.386109
C	-7.521729	0.082681	-1.121545
H	-7.067786	-0.085739	-2.099547
H	-8.602520	-0.058094	-1.169064
H	-7.309018	2.321129	-1.051131
H	-6.825563	-1.822707	-0.090910
N	-5.528173	-0.141717	0.010021
N	-5.653557	1.199718	-0.370180
C	5.420017	-0.785476	0.172238
C	6.714247	-0.082344	0.169945
C	7.176986	0.648732	-0.932506
C	7.522369	-0.146460	1.310878
C	8.397578	1.309690	-0.883528
H	6.586446	0.684031	-1.843273
C	8.745270	0.514534	1.362142
H	7.181378	-0.719775	2.169433
C	9.186056	1.248228	0.264890

H	8.741965	1.867588	-1.748866
H	9.355024	0.453526	2.258176
H	10.141705	1.761555	0.298582
H	5.288792	-1.510636	0.976778
C	4.413621	-0.608789	-0.687797
H	4.502419	0.131482	-1.483504
C	-4.407816	-0.715404	0.255462
H	-4.467352	-1.772210	0.508739
C	3.110398	-1.349167	-0.622046
H	2.942045	-1.892428	-1.562895
H	3.153837	-2.102471	0.174321
C	-3.103587	-0.004342	0.191398
H	-2.952237	0.534735	1.140208
H	-3.165471	0.760531	-0.595318
C	-1.929486	-0.959748	-0.051252
H	-1.904307	-1.715212	0.744369
H	-2.085480	-1.494636	-0.995898
C	-0.595925	-0.216375	-0.095785
H	-0.629916	0.546550	-0.885079
H	-0.447048	0.320324	0.851031
C	1.922471	-0.410846	-0.377975
H	1.895547	0.354878	-1.165051
H	2.077011	0.122260	0.568626
C	0.586901	-1.150844	-0.342483
H	0.438879	-1.684160	-1.291363
H	0.615483	-1.917743	0.443524
H	-5.189960	1.798760	0.313945

Z-2-butene

$G_{\text{DCE}} = -157.097257$ Hartree

C	-0.666943	0.667143	-0.000003
C	0.666923	0.667152	-0.000004
H	-1.169223	1.633885	-0.000001
H	1.169177	1.633907	0.000018
C	-1.580411	-0.524067	0.000000
H	-1.037862	-1.471461	0.000093
H	-2.233599	-0.510436	0.879835
H	-2.233519	-0.510543	-0.879898
C	1.580425	-0.524053	0.000000
H	2.233419	-0.510604	0.879987
H	1.037902	-1.471460	-0.000257
H	2.233743	-0.510334	-0.879737

TS-C-6

$G_{\text{DCE}} = -732.336381$ Hartree

C	-1.736419	-2.620991	-0.545339
C	-1.017423	-1.646716	0.408695
C	-3.009612	-0.701134	0.163340
C	-3.134201	-1.956214	-0.720925
H	-1.191038	-2.737069	-1.483584
H	-1.812300	-3.603156	-0.072341
H	-3.357164	-1.699255	-1.760030
H	-3.941463	-2.598306	-0.360212
C	-2.152905	-1.196038	1.335700
H	-1.866175	-0.408964	2.037667
H	-2.613990	-2.029311	1.868503
H	-0.087303	-2.003671	0.840370
H	-3.931571	-0.167244	0.393418
N	-2.037794	0.233073	-0.466230
N	-0.807907	-0.403287	-0.371571
C	0.275536	0.374060	-0.524739
C	1.638278	-0.136242	-0.259625
C	2.020527	-0.621295	0.998087
C	2.584626	-0.064268	-1.286687
C	3.320867	-1.061781	1.209142
H	1.312011	-0.625481	1.822838
C	3.884180	-0.512961	-1.074382
H	2.299731	0.337427	-2.255528
C	4.251218	-1.014839	0.171253
H	3.613955	-1.429786	2.186707
H	4.610482	-0.461387	-1.878497
H	5.267043	-1.356880	0.340226
H	0.193966	1.057872	-1.371433
H	-2.260852	0.483214	-1.432337
C	-1.369109	2.227731	0.601881
H	-2.047543	1.872137	1.372129
C	-0.010195	2.002335	0.753627
H	0.291503	1.510616	1.677750
C	1.021818	2.934918	0.153721
H	1.069758	3.862084	0.733285
H	2.015922	2.480963	0.166204
H	0.783943	3.208930	-0.879408
C	-1.934693	3.184625	-0.401019
H	-3.009588	3.044077	-0.531815

H	-1.769418	4.217335	-0.068197
H	-1.444971	3.090212	-1.377472

P-C-6

$G_{\text{DCE}} = -732.399476$ Hartree

C	-1.344542	-2.737354	-0.333601
C	-0.560305	-1.595164	0.328642
C	-2.659210	-0.917012	0.570261
C	-2.809459	-2.213594	-0.240731
H	-1.015729	-2.897557	-1.360747
H	-1.217789	-3.668418	0.223903
H	-3.267814	-2.036747	-1.218879
H	-3.463751	-2.900126	0.301218
C	-1.483406	-1.217391	1.497273
H	-1.154105	-0.374991	2.107554
H	-1.702786	-2.066882	2.147454
H	0.486153	-1.796799	0.548417
H	-3.571161	-0.482657	0.980611
N	-2.005046	0.095467	-0.358556
N	-0.666951	-0.449825	-0.624842
C	0.257633	0.712374	-0.523668
C	1.677155	0.265637	-0.265021
C	2.304687	0.412047	0.973407
C	2.367981	-0.353414	-1.311621
C	3.605227	-0.053153	1.159918
H	1.799322	0.899972	1.802075
C	3.661210	-0.825613	-1.122691
H	1.883721	-0.464956	-2.278858
C	4.282883	-0.674770	0.115870
H	4.087655	0.075383	2.123322
H	4.186958	-1.304044	-1.942467
H	5.295405	-1.035834	0.263484
H	0.233846	1.183525	-1.517564
H	-2.509882	0.115654	-1.251173
C	-1.887808	1.533578	0.176207
H	-2.482222	1.563541	1.093337
C	-0.383978	1.690318	0.466594
H	-0.200796	1.339732	1.486460
C	0.152460	3.112234	0.338450
H	-0.359863	3.797434	1.019646
H	1.216907	3.124428	0.586556
H	0.044393	3.492043	-0.681718

C	-2.468374	2.481331	-0.861653
H	-3.513339	2.236232	-1.076770
H	-2.445701	3.504616	-0.481259
H	-1.898364	2.456621	-1.796635

S-R-6

$G_{\text{DCE}} = -732.398608$ Hartree

C	-1.495752	-2.673288	-0.572216
C	-0.569064	-1.666479	0.125577
C	-2.587974	-0.888413	0.621660
C	-2.914386	-2.134396	-0.216906
H	-1.309562	-2.736183	-1.649217
H	-1.316729	-3.668068	-0.158303
H	-3.504553	-1.870832	-1.095741
H	-3.479948	-2.858235	0.373946
C	-1.341373	-1.335085	1.400824
H	-0.889401	-0.571740	2.034988
H	-1.514491	-2.236544	1.993082
H	0.488320	-1.917666	0.185754
H	-3.422745	-0.471373	1.183842
N	-2.075073	0.139668	-0.321853
N	-0.736866	-0.368942	-0.669339
C	0.273009	0.781450	-0.484444
C	1.669682	0.280969	-0.234709
C	2.172340	0.087510	1.055680
C	2.476213	-0.022646	-1.335626
C	3.461545	-0.405150	1.236613
H	1.572214	0.329158	1.928280
C	3.762290	-0.520796	-1.154381
H	2.101231	0.145996	-2.343183
C	4.255444	-0.712622	0.133907
H	3.848706	-0.542936	2.240725
H	4.380467	-0.748960	-2.016209
H	5.260713	-1.094248	0.279021
H	0.248173	1.294198	-1.453411
C	-1.902075	1.526118	0.206321
H	-2.502491	1.603984	1.118858
C	-0.404565	1.675660	0.546768
H	-0.237545	1.265716	1.546285
C	0.153233	3.094921	0.520532
H	0.072119	3.542955	-0.474015
H	-0.382596	3.732984	1.228178

H	1.209223	3.088800	0.804418
C	-2.424278	2.517953	-0.826166
H	-3.457273	2.272132	-1.080722
H	-2.397354	3.538384	-0.435711
H	-1.836031	2.487028	-1.749826
H	-0.752602	-0.613879	-1.663296

TS-R-6

$G_{\text{DCE}} = -732.334354$ Hartree

C	2.014987	-2.753052	0.479201
C	0.723321	-1.909931	0.488964
C	1.899099	-0.952967	-1.127489
C	2.835846	-2.091083	-0.670611
H	2.530909	-2.717053	1.442927
H	1.788450	-3.800464	0.265586
H	3.803592	-1.707469	-0.343099
H	3.004862	-2.784981	-1.497761
C	0.519775	-1.611485	-1.000217
H	-0.317862	-0.947569	-1.207411
H	0.440397	-2.521799	-1.597889
H	-0.126952	-2.313649	1.039682
H	2.160295	-0.448899	-2.058331
N	1.864434	0.003562	-0.006167
N	1.039164	-0.546214	0.995697
C	-0.683119	1.601403	0.392653
C	-1.768165	0.657706	0.210950
C	-2.360685	0.456239	-1.048738
C	-2.302509	-0.010854	1.328028
C	-3.436020	-0.412500	-1.188570
H	-2.002403	1.010110	-1.911852
C	-3.368593	-0.883878	1.184269
H	-1.854408	0.151132	2.305160
C	-3.935808	-1.087689	-0.076708
H	-3.895655	-0.550547	-2.161500
H	-3.769319	-1.399825	2.050583
H	-4.778538	-1.762619	-0.187020
H	-0.613765	2.051758	1.384589
C	1.929680	1.348043	-0.069017
H	2.479914	1.686587	-0.947962
C	0.191369	2.079710	-0.584502
H	0.075710	1.628614	-1.573036
H	1.554515	-0.587586	1.877687

C	2.287752	2.047878	1.223592
H	3.274068	1.692529	1.539749
H	2.349892	3.126957	1.093233
H	1.570313	1.823346	2.016062
C	0.504417	3.572040	-0.627017
H	1.482596	3.782646	-1.069933
H	-0.251120	4.067717	-1.242640
H	0.461245	4.022149	0.367737

P-R-6

$G_{\text{DCE}} = -383.626682$ Hartree

C	-1.800069	-0.394969	-1.007063
C	-1.168321	-1.095641	0.209194
C	-0.538255	1.014446	0.502666
C	-1.349853	1.082958	-0.805761
H	-1.450042	-0.820511	-1.951357
H	-2.887666	-0.494045	-0.985815
H	-0.758436	1.478375	-1.634788
H	-2.199493	1.752665	-0.653528
C	-1.292308	-0.044052	1.316004
H	-0.797675	-0.326169	2.247130
H	-2.324890	0.254351	1.503760
H	-1.514386	-2.102683	0.435902
H	-0.260336	1.955670	0.975023
N	0.312504	-1.112553	0.056787
H	0.640142	-1.492421	-0.832186
C	1.892827	0.651527	0.058593
H	2.030820	1.719366	0.205663
N	0.687190	0.229670	0.171213
C	3.022133	-0.259399	-0.253545
H	3.964281	0.182070	0.071874
H	2.872657	-1.226607	0.237904
H	3.090241	-0.429106	-1.336101

***E*-1-phenylpropene**

$G_{\text{DCE}} = -348.763145$ Hartree

C	-2.377024	0.359940	0.107243
C	-1.383453	-0.503710	-0.117060
H	-2.144080	1.392079	0.367397
H	-1.640395	-1.539356	-0.343644

C	0.060340	-0.212903	-0.066259
C	0.966582	-1.277589	0.000504
C	0.573123	1.091301	-0.087151
C	2.337778	-1.052285	0.065693
H	0.585089	-2.295740	0.008218
C	1.941725	1.319063	-0.020737
H	-0.105441	1.934897	-0.173349
C	2.831487	0.248650	0.058672
H	3.020775	-1.894704	0.120526
H	2.318115	2.337522	-0.040550
H	3.900882	0.429153	0.106489
C	-3.831461	0.006719	0.039955
H	-4.329530	0.199324	0.996984
H	-4.349369	0.609874	-0.714758
H	-3.970637	-1.048166	-0.212474
