Supporting Information for:

A Theoretical Study of Cyclohexyne Addition to Carbonyl-C_α Bonds: Allowed and Forbidden Electrocyclic and Non-Pericyclic Ring Openings of Strained Cyclobutenes

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Contents:

1, B3LYP/6-31G(d), E = -233.3325677 hartrees

C	0.720981	1.054656	0.281800
C	1.590784	-0.198668	-0.116054
C	0.609664	-1.302080	-0.021454
C	-0.610361	-1.302055	0.021390
C	-1.590840	-0.197987	0.116121
C	-0.720495	1.054736	-0.281791
H	1.983616	-0.104099	-1.136653
H	2.454606	-0.286254	0.553204
H	0.676966	1.099150	1.377518
H	1.235862	1.964373	-0.054564
H	-2.454913	-0.285210	-0.552859
H	-1.983392	-0.103481	1.136921
H	-0.676319	1.098797	-1.377534
H	-1.234821	1.965113	0.053889

2a, B3LYP/6-31G(d), E = -269.9536876 hartrees

C	1.380452	-0.735070	-0.196311
C	1.403457	0.787226	0.117948
C	-0.036316	1.182684	-0.046752
C	-0.919135	0.108806	-0.007218
C	-0.047099	-1.181722	0.152049
H	2.170276	-1.293782	0.333134
H	2.114744	1.311515	-0.551929
H	1.822425	0.946792	1.142037
H	-0.362837	2.221741	-0.074726
H	-0.424239	-1.994229	-0.486340
H	-0.117469	-1.545380	1.192390
H	1.553594	-0.877686	-1.272711
O	-2.180581	0.032436	-0.050019

3a, B3LYP/6-31G(d), E = -503.3590815 hartrees

C	-2.912598	0.692926	0.517703
C	-1.445983	1.136823	0.638143
C	-0.490378	-0.036250	0.425819
C	-0.754723	-1.225009	-0.150897
C	-2.198033	-1.464404	-0.581703
C	-3.102118	-0.213688	-0.702841
H	-1.243661	1.947662	-0.084169
H	-1.285924	1.600358	1.629695
H	-3.193416	0.128150	1.421162

H	-3.582042	1.566966	0.473344
H	-2.224672	-2.007619	-1.543755
H	-2.666608	-2.166804	0.134791
H	-2.820060	0.349238	-1.606675
H	-4.165418	-0.487039	-0.824068
C	2.934653	-1.020717	0.078856
C	1.827090	-0.949102	1.166800
C	0.976608	0.306021	0.859189
C	1.613608	0.912001	-0.377634
C	2.335321	-0.227751	-1.093314
H	3.184088	-2.055753	-0.191268
H	2.250987	-0.935396	2.179869
H	1.151640	-1.806699	1.046905
H	0.966493	1.042395	1.675459
H	3.040368	0.127782	-1.851939
H	1.546467	-0.845010	-1.551606
H	3.863621	-0.539836	0.421535
O	1.559681	2.077066	-0.751250

4a (TS), B3LYP/6-31G(d), E = -503.3550423 hartrees

C	2.959308	-0.591143	0.581909
C	1.590487	-1.278837	0.478438
C	0.475050	-0.270509	0.169884
C	0.604982	0.998712	-0.291898
C	2.038494	1.473927	-0.533608
C	3.146591	0.394156	-0.576331
H	1.640299	-2.069887	-0.295331
H	1.384314	-1.820066	1.420777
H	3.009594	-0.032580	1.530161
H	3.771280	-1.335808	0.611703
H	2.084669	2.055382	-1.472369
H	2.300648	2.211650	0.249984
H	3.075713	-0.160978	-1.525204
H	4.157210	0.839234	-0.549585
C	-2.252707	1.145787	0.958360
C	-1.698776	-0.159880	1.581127
C	-0.940158	-0.841250	0.417001
C	-1.812033	-0.507426	-0.791578
C	-2.600314	0.778407	-0.495670
H	-1.430887	1.866569	0.922059
H	-2.527872	-0.799037	1.930908
H	-1.044177	0.038475	2.438556
H	-0.899021	-1.933305	0.534288
H	-3.669209	0.568487	-0.653448

H	-2.287541	1.549799	-1.205867
H	-3.103923	1.557601	1.519097
O	-1.940829	-1.173401	-1.805191

Negative Nuclear Hessian Mode 1 Eigenvalue = -49.07 cm^{-1}

5a, B3LYP/6-31G(d), E = -503.3659704 hartrees

C	-2.665063	0.519469	0.828857
C	-1.494982	1.462738	0.466118
C	-0.349610	0.653148	-0.069707
C	-0.422717	-0.623520	-0.468915
C	-1.659769	-1.482287	-0.426319
C	-2.893845	-0.568736	-0.240463
H	-1.815503	2.201052	-0.287033
H	-1.201715	2.053699	1.348408
H	-2.439016	0.025790	1.786290
H	-3.594994	1.088717	0.984355
H	-1.776205	-2.077657	-1.346744
H	-1.614928	-2.220173	0.395023
H	-3.111353	-0.075129	-1.199077
H	-3.783040	-1.165206	0.015189
C	2.063825	-0.748880	1.290774
C	2.107464	0.709487	0.809346
C	1.163513	0.877106	-0.454110
C	1.013727	-0.788874	-0.912183
C	1.934947	-1.599010	0.000441
H	3.111686	0.962764	0.439606
H	1.865419	1.425920	1.609663
H	2.925707	-1.692012	-0.472371
H	1.598072	-2.626491	0.227498
H	1.171319	-0.951430	-1.985873
O	1.470743	1.817547	-1.284007
H	2.936892	-1.042964	1.894636
H	1.176771	-0.911103	1.919445

6a (TS), B3LYP/6-31G(d), E = -503.286575 hartrees

C	-0.348090	-0.617430	-0.535745
C	0.992980	-0.857321	-1.097204
H	1.210283	-0.548503	-2.114916
C	-0.365633	0.655450	-0.091650
C	2.003845	-1.621930	-0.295112
H	2.986087	-1.576628	-0.792192
C	1.045005	1.170710	-0.187552

C	2.086610	-0.892559	1.077013
H	1.200358	-1.167009	1.667190
C	2.082464	0.624673	0.837109
H	1.968054	1.157485	1.800185
H	3.055451	0.941077	0.435113
H	1.807534	-2.702907	-0.111415
H	2.962944	-1.203658	1.671456
O	1.299883	2.283979	-0.724293
C	-1.523316	-1.560461	-0.359295
H	-1.203796	-2.515678	0.089323
H	-1.947734	-1.832109	-1.342207
C	-1.594179	1.424140	0.329747
H	-1.532274	1.705314	1.396261
H	-1.657440	2.373956	-0.221739
C	-2.852960	0.564072	0.092484
H	-3.716903	0.980306	0.632802
H	-3.110722	0.587044	-0.977130
C	-2.618979	-0.902121	0.506195
H	-2.307607	-0.923047	1.561573
H	-3.559774	-1.470821	0.444107

Negative Nuclear Hessian Mode 1 Eigenvalue = -340.00 cm^{-1}

6a' (TS), B3LYP/6-31G(d), E = -503.3583425 hartrees

C	-0.374317	-0.687354	-0.502014
C	0.924029	-1.198571	-0.993923
H	0.866743	-1.855482	-1.875567
C	-0.287879	0.574169	-0.039672
C	1.890598	-1.715077	0.053314
H	2.851160	-1.943072	-0.442848
C	1.092686	1.145371	-0.347703
C	2.144172	-0.659398	1.153260
H	1.297236	-0.664144	1.854249
C	2.267782	0.746734	0.556410
H	2.353877	1.491539	1.371633
H	3.178430	0.846914	-0.049156
H	1.619166	-2.666489	0.585641
H	3.036230	-0.911029	1.750076
O	1.206950	2.123956	-1.103598
C	-1.701692	-1.436344	-0.499418
H	-1.543145	-2.479066	-0.183824
H	-2.083956	-1.501304	-1.533508
C	-1.395457	1.372081	0.597445
H	-1.301081	1.428558	1.699626
H	-1.341823	2.412399	0.241630

C	-2.762439	0.761643	0.236622
H	-3.561920	1.208394	0.847815
H	-2.992298	1.001617	-0.811809
C	-2.755575	-0.767046	0.404275
H	-2.525858	-1.001696	1.455145
H	-3.759822	-1.176032	0.208113

Negative Nuclear Hessian Mode 1 Eigenvalue = -200.66 cm^{-1}

7a, B3LYP/6-31G(d), E = -503.3834818 hartrees

C	-0.208171	-0.745495	-0.529769
C	0.993045	-1.162920	-1.125091
H	1.423555	-0.377135	-1.754512
C	-0.403967	0.640809	-0.363247
C	2.071906	-1.714716	-0.215948
H	3.001490	-1.918780	-0.772169
C	0.736974	1.463706	-0.066868
C	2.306789	-0.592873	0.844008
H	1.570255	-0.734317	1.647693
C	2.140561	0.856149	0.307921
H	2.500265	1.543720	1.088061
H	2.823563	1.010381	-0.540913
H	1.808498	-2.652382	0.299260
H	3.300970	-0.679833	1.320419
O	0.662301	2.711624	0.046100
C	-1.218841	-1.718336	0.067021
H	-0.718042	-2.436849	0.737783
H	-1.662513	-2.333550	-0.733230
C	-1.778709	1.263046	-0.222911
H	-1.787371	1.935999	0.648877
H	-2.036302	1.913405	-1.077657
C	-2.864475	0.178575	-0.060645
H	-3.780346	0.613550	0.367593
H	-3.144884	-0.225325	-1.046245
C	-2.350981	-0.983244	0.804996
H	-1.976369	-0.579210	1.756917
H	-3.165965	-1.680870	1.052522

7a', B3LYP/6-31G(d), E = -503.428128 hartrees

C	-0.293994	-0.900931	-0.109863
C	0.704230	-1.837026	-0.039662
H	0.408265	-2.870638	-0.238777
C	-0.259365	0.546003	-0.002967

C	2.182783	-1.704656	0.223654
H	2.743601	-2.111324	-0.640892
C	0.881155	1.365038	-0.179210
C	2.712597	-0.294164	0.495563
H	2.390745	0.045523	1.489184
C	2.226951	0.718630	-0.556803
H	2.935065	1.548460	-0.660231
H	2.160823	0.211146	-1.532366
H	2.471741	-2.362046	1.066882
H	3.813649	-0.333121	0.523749
O	0.887144	2.622615	-0.042512
C	-1.673582	-1.504742	-0.432330
H	-1.678609	-2.575876	-0.188851
H	-1.841140	-1.431617	-1.520944
C	-1.514293	1.302089	0.413426
H	-1.584493	1.381666	1.518889
H	-1.413973	2.335047	0.062711
C	-2.829700	0.684808	-0.072605
H	-3.692824	1.198272	0.381299
H	-2.922473	0.808396	-1.163431
C	-2.854101	-0.809419	0.253949
H	-2.781526	-0.943638	1.344829
H	-3.802095	-1.274956	-0.060873

8a (TS), B3LYP/6-31G(d), E = -503.3579178 hartrees

C	-0.301184	-0.838199	-0.287885
C	0.808879	-1.766181	-0.675605
H	1.173697	-1.460814	-1.676732
C	-0.286871	0.524651	-0.093805
C	1.991473	-1.752848	0.286130
H	2.792557	-2.357271	-0.172411
C	0.934922	1.353139	-0.157244
C	2.625745	-0.370555	0.693663
H	2.245303	-0.046129	1.673953
C	2.310987	0.725710	-0.341216
H	3.028109	1.554247	-0.285751
H	2.363590	0.274130	-1.342697
H	1.748568	-2.274615	1.231593
H	3.721551	-0.448074	0.813035
O	0.864829	2.585169	-0.022609
C	-1.635854	-1.574503	-0.133363
H	-1.415394	-2.482108	0.443073
H	-1.892430	-1.956992	-1.135095
C	-1.541766	1.348903	0.196915

H	-1.555835	1.650704	1.258284
H	-1.475785	2.292863	-0.356645
C	-2.844957	0.618273	-0.134008
H	-3.709142	1.191640	0.234677
H	-2.958687	0.542594	-1.226511
C	-2.815180	-0.790296	0.460112
H	-2.696555	-0.710460	1.551965
H	-3.765349	-1.319632	0.287975

Negative Nuclear Hessian Mode 1 Eigenvalue = -707.79 cm^{-1}

2b, B3LYP/6-31G(d), LANL2DZ, E = -298.1588989 hartrees

C	2.783973	-0.730196	-0.210350
C	2.801881	0.798710	0.076325
C	1.343045	1.178631	-0.028202
C	0.503895	0.095763	0.030388
C	1.356449	-1.184179	0.153550
H	3.574928	-1.279937	0.335227
H	3.460427	1.329558	-0.632465
H	3.230220	1.000569	1.079339
H	0.997138	2.213216	-0.050806
H	0.975260	-1.986214	-0.497533
H	1.295033	-1.569004	1.187468
H	2.953939	-0.895458	-1.292298
O	-0.793981	0.027208	0.028711
K	-3.308976	0.000907	-0.025731

3b, B3LYP/6-31G(d), LANL2DZ, E = -531.559815 hartrees

C	-3.166242	-1.311583	-0.686546
C	-1.697982	-1.588351	-1.077165
C	-0.917356	-0.336728	-0.598711
C	-1.742504	0.155844	0.595403
C	-3.047783	-0.622184	0.683909
H	-3.780690	-2.219827	-0.655272
H	-1.569811	-1.769010	-2.151917
H	-1.343883	-2.483798	-0.548033
H	-1.065113	0.456505	-1.353326
H	-3.887897	0.022863	0.972782
H	-2.917292	-1.373122	1.483728
H	-3.626355	-0.622140	-1.409818
O	-1.426219	1.074685	1.346010
K	0.111373	2.944181	-0.120388
C	2.386375	-1.561191	1.092115

C	0.961793	-1.663204	0.532073
C	0.588874	-0.461809	-0.351997
C	1.456130	0.444185	-0.873007
C	2.948843	0.223984	-0.584135
C	3.354270	-1.153612	-0.021595
H	0.870541	-2.607573	-0.034263
H	0.242474	-1.761541	1.364711
H	2.415081	-0.798617	1.888101
H	2.685612	-2.513940	1.554737
H	3.534795	0.425038	-1.497602
H	3.284255	1.006358	0.125050
H	3.311445	-1.908552	-0.824400
H	4.393977	-1.141674	0.342735

4b (TS), B3LYP/6-31G(d), LANL2DZ, E = -531.5536695 hartrees

C	1.048925	-2.892555	-0.417735
C	0.747764	-2.358590	1.003287
C	0.666594	-0.819732	0.845099
C	1.767231	-0.575154	-0.170281
C	1.988566	-1.830693	-1.017073
H	0.123062	-2.954125	-1.004140
H	1.591261	-2.603318	1.667070
H	-0.148825	-2.803657	1.446108
H	0.926274	-0.295744	1.815504
H	3.049697	-2.108231	-0.918573
H	1.815595	-1.614269	-2.081327
H	1.495723	-3.894539	-0.403627
O	2.447750	0.440916	-0.293482
K	1.554672	2.935882	0.175512
C	-3.128001	-0.717793	-0.357441
C	-1.880856	-1.220986	0.383355
C	-0.699970	-0.240276	0.298888
C	-0.780209	1.055829	-0.087156
C	-2.167225	1.588388	-0.481445
C	-3.383143	0.754187	-0.037066
H	-2.142163	-1.405504	1.442944
H	-1.617776	-2.210149	-0.018201
H	-2.972768	-0.823580	-1.443930
H	-3.996134	-1.343961	-0.100878
H	-2.287882	2.620552	-0.110769
H	-2.196770	1.695411	-1.583656
H	-3.530186	0.865371	1.050382
H	-4.307953	1.110913	-0.518369

Negative Nuclear Hessian Mode 1 Eigenvalue = -24.27 cm^{-1}

5b, B3LYP/6-31G(d), LANL2DZ, E = -531.5750267 hartrees

C	-3.250824	-1.339699	-0.117915
C	-2.663133	-0.368704	-1.171530
C	-1.309411	0.081467	-0.702678
C	-0.613644	-0.446708	0.313808
C	-1.024566	-1.635204	1.132387
C	-2.202623	-2.340903	0.416915
H	-2.587063	-0.871911	-2.152192
H	-3.346982	0.481815	-1.327413
H	-3.639617	-0.750995	0.728090
H	-4.106010	-1.886251	-0.541364
H	-0.184747	-2.336652	1.270108
H	-1.326653	-1.326985	2.149310
H	-1.805361	-2.924365	-0.428964
H	-2.686116	-3.058312	1.095981
C	-0.664934	2.600490	0.903968
C	-0.692046	2.606398	-0.643197
C	-0.301822	1.172230	-1.035345
C	0.578792	0.544570	0.195009
C	0.526516	1.693038	1.257824
H	0.064689	3.312249	-1.021056
H	-1.664146	2.932215	-1.044250
H	0.188735	1.094928	-2.026359
H	1.467621	2.256153	1.147380
H	0.489482	1.316257	2.291487
O	1.808134	0.024764	-0.016873
K	4.029293	-1.032379	-0.311526
H	-0.582054	3.609777	1.327902
H	-1.597245	2.167321	1.289844

6b (TS), B3LYP/6-31G(d), LANL2DZ, E = -531.5480663 hartrees

C	-3.317224	-1.287285	0.285508
C	-3.006860	-0.037096	-0.567270
C	-1.522378	0.249237	-0.526215
C	-0.628844	-0.556788	0.115031
C	-0.869322	-2.002149	0.482765
C	-2.290577	-2.408824	0.027983
H	-3.338689	-0.210822	-1.606276
H	-3.594213	0.829189	-0.214667
H	-3.290945	-1.018400	1.353779
H	-4.334611	-1.648497	0.075419

H	-0.122357	-2.678406	0.031218
H	-0.773306	-2.145315	1.574813
H	-2.277351	-2.630861	-1.051258
H	-2.599517	-3.333864	0.536298
C	0.361621	2.866306	0.498448
C	-0.821427	2.770832	-0.510285
C	-0.758010	1.371550	-1.057425
C	0.568447	0.286839	0.349949
C	0.413357	1.532112	1.271547
H	0.281312	3.743500	1.179102
H	-0.736315	3.571847	-1.265338
H	-1.768702	2.934461	0.030263
H	0.006640	1.165256	-1.815789
H	1.265003	1.531377	1.971451
H	-0.504737	1.440203	1.870943
H	1.308455	2.981797	-0.071248
O	1.771828	-0.145523	0.156733
K	4.080632	-1.056615	-0.319621

Negative Nuclear Hessian Mode 1 Eigenvalue = -326.20 cm^{-1}

6b' (TS), B3LYP/6-31G(d), LANL2DZ, E = -531.5482811 hartrees

C	-3.353202	0.069304	-0.668162
C	-2.095952	0.135912	-1.561091
C	-0.824934	0.146739	-0.735243
C	-0.811606	-0.187005	0.562689
C	-2.006033	-0.564485	1.401763
C	-3.188370	-0.937447	0.483955
H	-2.080205	-0.722407	-2.257374
H	-2.133600	1.031763	-2.202497
H	-3.539904	1.067395	-0.240614
H	-4.238452	-0.185481	-1.269635
H	-1.755539	-1.412083	2.060927
H	-2.296537	0.261579	2.076388
H	-3.010070	-1.939099	0.061212
H	-4.117503	-1.000703	1.068841
C	1.702238	2.157296	0.419611
C	0.861613	2.059239	-0.872453
C	0.536288	0.593630	-1.176596
C	0.618391	-0.071702	1.071055
C	1.065103	1.321539	1.547375
H	1.846661	3.199554	0.748258
H	1.430129	2.527728	-1.692963
H	-0.047752	2.679222	-0.738074
H	0.777493	0.322763	-2.227278

H	1.775784	1.195960	2.377575
H	0.181027	1.855442	1.935619
H	2.702641	1.745662	0.211858
O	1.255764	-1.099652	1.449078
K	2.602026	-1.587801	-0.754856

Negative Nuclear Hessian Mode 1 Eigenvalue = -295.79 cm^{-1}

7b, B3LYP/6-31G(d), LANL2DZ, E = -531.561508 hartrees

C	1.390289	0.578624	-0.517313
C	2.039046	-0.458144	-1.159887
H	1.366027	-1.075599	-1.767212
C	0.000173	0.327576	-0.259532
C	3.044973	-1.329087	-0.460389
H	3.589178	-0.783376	0.325063
C	-0.272174	-0.957083	0.270590
C	2.118076	-2.413779	0.172085
H	1.771512	-3.081814	-0.643619
C	0.874544	-1.840460	0.912680
H	0.336989	-2.694060	1.349168
H	1.247662	-1.248875	1.767408
H	3.794967	-1.819464	-1.104044
H	2.685411	-3.055082	0.884773
O	-1.462272	-1.368284	0.528285
C	-1.006044	1.458073	-0.167018
H	-1.715703	1.497840	-1.018466
H	-1.631630	1.329539	0.736120
C	2.047093	1.800823	0.109070
H	2.561085	2.389070	-0.669160
H	2.834964	1.511123	0.826521
C	-0.265274	2.814146	-0.081534
H	0.037180	3.137062	-1.090800
H	-0.942421	3.589424	0.305968
C	0.994789	2.697456	0.794283
H	1.420913	3.691022	0.995598
H	0.713134	2.269614	1.769612
K	-3.798107	-0.567317	-0.240601

7b', B3LYP/6-31G(d), LANL2DZ, E = -531.6138037 hartrees

C	-0.473471	-0.278215	0.016767
C	0.625919	0.574161	0.157115
C	0.597753	2.091579	0.419249
C	-1.898847	0.090324	-0.040927

C	-0.701198	2.902688	0.470195
C	-2.429444	1.290753	-0.387290
C	-1.651255	2.543053	-0.687662
H	1.241213	2.518988	-0.368034
H	-1.230939	2.738725	1.429380
H	1.160238	2.247911	1.355196
H	-0.431121	3.978960	0.436195
H	-3.515834	1.393854	-0.346755
H	-2.350960	3.369424	-0.877644
H	-1.048390	2.429373	-1.608527
O	1.849553	0.135211	0.106389
C	-0.124724	-1.749655	-0.236623
C	-2.903894	-0.996799	0.353639
C	-1.149611	-2.767855	0.280254
H	0.000616	-1.928484	-1.323820
H	0.857258	-1.957727	0.203714
C	-2.559607	-2.392852	-0.177254
H	-3.911071	-0.699138	0.030829
H	-2.936265	-1.063161	1.456185
H	-0.879270	-3.778477	-0.062734
H	-1.129366	-2.789539	1.382555
H	-3.300689	-3.125443	0.176809
H	-2.604629	-2.396612	-1.278890
K	4.278582	-0.519128	-0.129492

8b (TS), B3LYP/6-31G(d), LANL2DZ, E = -531.5362916 hartrees

C	1.768817	0.470085	-0.265289
C	1.794981	1.930620	-0.624138
H	1.320880	2.023507	-1.630409
C	0.688345	-0.378829	-0.103437
C	0.985354	2.821277	0.333843
H	0.991337	3.838516	-0.092969
C	-0.706046	0.062255	-0.190325
C	-0.504197	2.453282	0.646962
H	-0.587745	1.958349	1.636144
C	-1.090048	1.509585	-0.423244
H	-2.189200	1.549139	-0.427718
H	-0.727870	1.829806	-1.411927
H	1.505071	2.919317	1.304197
H	-1.138059	3.364115	0.703661
O	-1.634028	-0.768197	-0.029071
C	3.170757	-0.115395	-0.101907
H	3.742012	0.610354	0.495274
H	3.639791	-0.063347	-1.101617

C	0.835426	-1.878466	0.168040
H	0.593934	-2.091529	1.224460
H	0.075204	-2.418159	-0.412201
C	2.226792	-2.430586	-0.151824
H	2.312692	-3.465774	0.210120
H	2.370943	-2.461186	-1.244068
C	3.293693	-1.532039	0.471117
H	3.147345	-1.505241	1.563110
H	4.305262	-1.928242	0.297871
K	-4.266980	-0.814988	0.029466

Negative Nuclear Hessian Mode 1 Eigenvalue = -537.34 cm^{-1}

5c, B3LYP/6-31G(d), E = -503.9767088 hartrees

C	-2.839198	0.838231	0.402702
C	-1.747451	1.519757	-0.458781
C	-0.533905	0.646079	-0.449953
C	-0.477839	-0.614667	-0.002293
C	-1.620041	-1.429057	0.512782
C	-2.930311	-0.684331	0.157506
H	-2.105107	1.666655	-1.490069
H	-1.526924	2.525768	-0.073686
H	-2.611236	1.013745	1.463384
H	-3.813673	1.303647	0.210664
H	-1.620823	-2.437336	0.077944
H	-1.538857	-1.569548	1.602546
H	-3.157009	-0.859358	-0.903162
H	-3.767225	-1.101445	0.730732
C	2.848584	0.595534	0.709263
C	1.889753	1.612527	0.046222
C	0.947175	0.735937	-0.807196
C	1.021088	-0.744682	-0.217886
C	1.965561	-0.634581	1.009076
H	3.354004	0.992585	1.597074
H	2.426851	2.366325	-0.540019
H	1.323185	2.148072	0.819091
H	1.165656	0.782166	-1.881106
H	2.537209	-1.557975	1.156538
H	1.385613	-0.464153	1.924097
H	3.636554	0.318345	-0.006603
O	1.357223	-1.801533	-1.103761
H	2.313511	-1.759716	-1.266000

6c (TS), B3LYP/6-31G(d), E = -503.929501 hartrees

C	2.623917	-0.896048	0.669199
C	1.481120	-1.676826	-0.016013
C	0.396094	-0.713757	-0.428278
C	0.484771	0.648998	-0.190078
C	1.778298	1.410822	-0.050283
C	2.950573	0.402045	-0.094774
H	1.873797	-2.201383	-0.900136
H	1.094037	-2.466107	0.646919
H	2.329385	-0.641965	1.697502
H	3.516893	-1.528649	0.743963
H	1.900006	2.165554	-0.839850
H	1.793700	1.966080	0.899904
H	3.173099	0.147895	-1.140739
H	3.855706	0.867632	0.313612
C	-2.831215	-0.581940	0.389324
C	-1.995099	-1.713777	-0.289919
C	-0.857279	1.091139	-0.012256
C	-1.848309	0.453693	0.982377
H	-3.513876	-0.973725	1.157928
H	-2.637284	-2.299551	-0.961397
H	-1.595697	-2.388129	0.478319
H	-2.415381	1.258643	1.479182
H	-1.263589	-0.037222	1.769365
H	-3.451858	-0.094644	-0.375385
O	-1.143250	2.384453	-0.388049
H	-1.983601	2.663433	0.009144
C	-0.904153	-0.948067	-0.965428
H	-1.201650	-0.371192	-1.837163

Negative Nuclear Hessian Mode 1 Eigenvalue = -257.87 cm^{-1}

6c' (TS), B3LYP/6-31G(d), E = -503.8983781 hartrees

C	2.898580	0.537290	-0.268719
C	2.005504	1.104899	0.858301
C	0.573967	0.699636	0.578591
C	0.273241	-0.566104	0.077035
C	1.179810	-1.257290	-0.925357
C	2.641337	-0.960684	-0.521567
H	2.339411	0.694623	1.823123
H	2.112040	2.195224	0.914863
H	2.700995	1.096817	-1.194440
H	3.957350	0.695954	-0.026184
H	1.020294	-2.343116	-0.940142
H	1.017912	-0.904587	-1.958649

H	2.874379	-1.521822	0.393776
H	3.321289	-1.327795	-1.301312
C	-2.726770	0.641836	-0.617775
C	-1.536750	1.623257	-0.627271
C	-1.099121	-0.879912	0.385321
C	-2.190942	-0.815595	-0.645492
H	-3.395711	0.815522	-1.472671
H	-1.937655	2.644598	-0.671858
H	-0.991573	1.463482	-1.571648
H	-3.000753	-1.543639	-0.489409
H	-1.750081	-1.003458	-1.634645
H	-3.319405	0.793582	0.295817
O	-1.366208	-1.593884	1.504302
H	-2.322867	-1.570884	1.688313
C	-0.545883	1.556865	0.533477
H	-0.533796	2.461384	1.151389

Negative Nuclear Hessian Mode 1 Eigenvalue = -346.44 cm^{-1}

7c, B3LYP/6-31G(d), E = -503.9404706 hartrees

C	0.199116	-0.848806	-0.455547
C	-1.005595	-1.140481	-1.017531
H	-1.324045	-0.429917	-1.783405
C	0.498974	0.579400	-0.452887
C	-2.175194	-1.651958	-0.240367
H	-1.875660	-2.230679	0.641136
C	-0.563173	1.310289	-0.002623
C	-2.813307	-0.286040	0.183864
H	-3.308612	0.144689	-0.695627
C	-1.810034	0.764502	0.753651
H	-2.424568	1.637517	1.022029
H	-1.428599	0.372137	1.708778
H	-2.916683	-2.238286	-0.799440
H	-3.597254	-0.443475	0.940579
O	-0.405646	2.675361	0.070705
H	-1.110256	3.055814	0.615697
C	1.916391	1.088014	-0.563075
H	2.145729	1.462343	-1.571111
H	2.059611	1.937378	0.117232
C	1.070453	-1.730813	0.423010
H	1.403620	-2.599480	-0.161850
H	0.510098	-2.144736	1.275832
C	2.885652	-0.065901	-0.201716
H	3.065099	-0.690770	-1.087831
H	3.858349	0.346838	0.091448

C	2.310455	-0.952659	0.917867
H	3.068518	-1.657510	1.280292
H	2.037393	-0.318023	1.772733

7c', B3LYP/6-31G(d), E = -504.0000276 hartrees

C	0.216144	0.518211	-0.054948
C	-0.962786	1.185826	0.065902
C	-2.362081	0.721874	0.404159
C	0.374065	-0.956789	0.017546
C	-2.681427	-0.775104	0.452341
C	-0.567785	-1.858576	-0.321439
C	-1.992505	-1.550878	-0.687683
H	-3.007378	1.198881	-0.346151
H	-2.372682	-1.208023	1.410588
H	-2.641747	1.195199	1.356735
H	-3.772481	-0.884588	0.396415
H	-0.310826	-2.912686	-0.221784
H	-2.528437	-2.484834	-0.890419
H	-2.045010	-0.951284	-1.610110
O	-1.054708	2.550955	-0.103945
C	1.481999	1.311937	-0.404203
C	1.716543	-1.477557	0.514810
C	2.782917	0.752090	0.192811
H	1.595602	1.349752	-1.499860
H	1.407621	2.355565	-0.067080
C	2.918471	-0.743263	-0.088020
H	1.782989	-2.554147	0.321904
H	1.760717	-1.352378	1.608947
H	3.635167	1.311396	-0.213165
H	2.784346	0.914440	1.279870
H	3.852732	-1.133726	0.335004
H	2.958962	-0.918286	-1.172652
H	-0.203245	2.900450	-0.404341

5d, B3LYP/6-31G(d), E = -1005.2029163 hartrees

C	4.384521	-0.594867	-1.353653
C	3.407801	0.598953	-1.236737
C	2.397082	0.304485	-0.170421
C	2.483649	-0.674034	0.739187
C	3.602592	-1.673371	0.846688
C	4.804616	-1.152977	0.022995
H	3.951989	1.522826	-0.983664

H	2.933833	0.794107	-2.211527
H	3.894900	-1.399721	-1.922546
H	5.280352	-0.310841	-1.926476
H	3.910079	-1.830650	1.892878
H	3.296667	-2.668350	0.477490
H	5.293923	-0.348317	0.590897
H	5.554988	-1.946759	-0.108884
C	-0.640858	-0.936637	-0.051715
C	-0.181015	0.518955	-0.437519
C	1.093048	0.952548	0.422638
C	1.222121	-0.321268	1.503349
C	-0.001129	-1.227326	1.350381
H	0.090314	0.541133	-1.503171
H	-0.727333	-0.980486	2.135943
H	0.226139	-2.301132	1.462052
H	1.383535	0.024673	2.532043
O	1.188205	2.198939	0.811357
C	-1.470821	1.375265	-0.363047
C	-2.225761	-0.870739	0.005046
H	-2.498077	-0.642560	1.045190
C	-2.564438	0.395869	-0.797722
H	-2.481414	0.222135	-1.879855
H	-3.556754	0.808794	-0.587675
C	-0.129961	-1.939976	-1.104530
H	0.956035	-1.848752	-1.198242
H	-0.353229	-2.982696	-0.841692
H	-0.565323	-1.743530	-2.094014
C	-3.019227	-2.138316	-0.385603
H	-2.659469	-2.493588	-1.362056
C	-4.524818	-1.853924	-0.534203
H	-4.729601	-1.138997	-1.337825
H	-5.077207	-2.777069	-0.757912
H	-4.938531	-1.436939	0.394052
C	-2.820820	-3.270803	0.637111
H	-1.764452	-3.512409	0.784900
H	-3.228554	-2.978999	1.614503
H	-3.339089	-4.186632	0.321136
O	-1.799564	1.831011	0.952362
O	-1.478138	2.532092	-1.179716
C	-1.008813	3.609455	-0.362038
H	0.082930	3.658683	-0.392860
H	-1.483119	4.529880	-0.727704
C	-1.442225	3.208086	1.061904
H	-0.601323	3.311999	1.749905
H	-2.329504	3.761593	1.410431

6d (TS), B3LYP/6-31G(d), E = -1005.1835777 hartrees

C	4.539483	-0.377804	-1.111213
C	3.704700	0.842420	-0.672287
C	2.449659	0.361695	0.023567
C	2.348104	-0.809279	0.719267
C	3.278294	-1.982490	0.434335
C	4.656138	-1.438542	0.001412
H	4.309836	1.480530	-0.004979
H	3.462425	1.473042	-1.539547
H	4.059049	-0.842813	-1.985862
H	5.543865	-0.065322	-1.436614
H	3.391824	-2.620385	1.322319
H	2.894163	-2.641806	-0.365472
H	5.145931	-0.980132	0.874121
H	5.310302	-2.259500	-0.331170
C	-0.632038	-0.969286	-0.055216
C	-0.139140	0.499671	-0.428904
C	1.199023	1.132812	0.096545
C	1.222742	-0.714928	1.616569
C	-0.025390	-1.469086	1.327262
H	-0.007503	0.494093	-1.524596
H	-0.766517	-1.312987	2.123035
H	0.110890	-2.567938	1.243240
H	1.253743	-0.085898	2.499860
O	1.229147	2.390814	0.183818
C	-1.401065	1.394335	-0.268998
C	-2.214153	-0.855876	0.022357
H	-2.462182	-0.689438	1.080917
C	-2.538825	0.461805	-0.690499
H	-2.513137	0.350515	-1.783244
H	-3.504701	0.896360	-0.412631
C	-0.168461	-1.913873	-1.184416
H	0.917719	-1.843705	-1.289426
H	-0.417390	-2.963627	-0.983888
H	-0.611474	-1.642592	-2.152753
C	-3.058108	-2.069040	-0.437380
H	-2.724923	-2.367200	-1.441977
C	-4.554209	-1.719708	-0.541706
H	-4.744609	-0.945471	-1.292111
H	-5.143554	-2.605049	-0.816950
H	-4.938820	-1.352137	0.419507
C	-2.893588	-3.278689	0.498892
H	-1.848110	-3.579762	0.607817
H	-3.268705	-3.038903	1.503154
H	-3.462593	-4.143091	0.129491

O	-1.657967	1.825485	1.065739
O	-1.421332	2.565247	-1.075614
C	-1.225354	3.713735	-0.262150
H	-0.247903	4.157201	-0.465338
H	-2.025708	4.433994	-0.492283
C	-1.298223	3.195574	1.189551
H	-0.328071	3.294424	1.681308
H	-2.080186	3.694533	1.780610

Negative Nuclear Hessian Mode 1 Eigenvalue = -321.04 cm^{-1}

6d' (TS), B3LYP/6-31G(d), E = -1005.1824398 hartrees

C	4.362771	-0.622717	-1.367883
C	3.222975	0.415607	-1.392438
C	2.320670	0.228683	-0.203684
C	2.501642	-0.640220	0.818115
C	3.818375	-1.379308	0.991045
C	4.908655	-0.819252	0.056563
H	3.651236	1.435138	-1.378930
H	2.685302	0.347356	-2.355685
H	3.983006	-1.588888	-1.733575
H	5.170876	-0.321987	-2.051729
H	4.142290	-1.314692	2.042127
H	3.677612	-2.456790	0.796279
H	5.250976	0.153037	0.440386
H	5.787526	-1.481569	0.042216
C	-0.605987	-0.928761	-0.060924
C	-0.234365	0.554592	-0.456062
C	1.098492	1.081449	0.093094
C	1.351474	-0.715562	1.704440
C	0.042751	-1.355956	1.303784
H	-0.086939	0.559765	-1.550265
H	-0.674019	-1.129237	2.107178
H	0.069219	-2.475919	1.271979
H	1.572317	-0.888921	2.766850
O	1.233184	2.270520	0.440357
C	-1.526369	1.384705	-0.269076
C	-2.198044	-0.909060	0.044956
H	-2.438024	-0.760776	1.106963
C	-2.617781	0.390267	-0.662284
H	-2.608761	0.276994	-1.755349
H	-3.602411	0.764351	-0.363276
C	-0.108039	-1.860199	-1.186447
H	.972408	-1.730957	-1.306731
H	-0.291598	-2.917889	-0.960921

H	-0.584211	-1.630515	-2.150494
C	-2.978546	-2.166942	-0.408475
H	-2.628467	-2.454467	-1.410169
C	-4.491371	-1.899639	-0.518758
H	-4.724229	-1.144181	-1.276616
H	-5.029175	-2.818982	-0.787806
H	-4.899118	-1.547166	0.438549
C	-2.752661	-3.358914	0.537110
H	-1.690576	-3.585672	0.666239
H	-3.160443	-3.138655	1.533199
H	-3.257069	-4.260568	0.163077
O	-1.768239	1.810217	1.069363
O	-1.607103	2.557716	-1.068829
C	-1.237719	3.673929	-0.264240
H	-0.194155	3.946944	-0.441627
H	-1.900943	4.508819	-0.527870
C	-1.426737	3.186062	1.189330
H	-0.500834	3.299391	1.757817
H	-2.255654	3.695831	1.702060

Negative Nuclear Hessian Mode 1 Eigenvalue = -279.17 cm^{-1}

7d, B3LYP/6-31G(d), E = -1005.202502 hartrees

C	.616442	-0.701588	-0.758901
C	3.844661	0.577923	-0.377055
C	2.424961	0.246192	0.027959
C	2.117419	-0.944187	0.729452
C	2.926500	-2.195587	0.418225
C	4.416391	-1.827349	0.272229
H	4.395216	1.079263	0.442025
H	3.831270	1.290278	-1.210390
H	4.256627	-1.058508	-1.736407
H	5.690927	-0.488410	-0.877692
H	2.795644	-2.952907	1.203901
H	2.599888	-2.659796	-0.528955
H	4.800126	-1.493051	1.248686
H	5.004730	-2.714104	-0.011338
C	-0.802440	-0.946847	-0.183134
C	-0.169412	0.501304	-0.560100
C	1.343556	1.021912	-0.475932
C	0.988133	-0.905051	1.528280
C	-0.200990	-1.696869	1.094468
H	-0.295664	0.551931	-1.651936
H	-0.978089	-1.782229	1.868335
H	0.074613	-2.723078	0.808353

H	0.699192	0.104935	1.826879
O	1.514350	2.110065	-1.089792
C	-1.252052	1.520525	-0.096002
C	-2.338859	-0.632179	0.083876
H	-2.455015	-0.595278	1.176567
C	-2.564268	0.804818	-0.396531
H	-2.731232	0.856634	-1.480639
H	-3.397196	1.311763	0.101059
C	-0.556100	-1.834826	-1.422401
H	0.521899	-1.881202	-1.612457
H	-0.914258	-2.862763	-1.289072
H	-1.029387	-1.428563	-2.326396
C	-3.380250	-1.656726	-0.428629
H	-3.187438	-1.844236	-1.495214
C	-4.819115	-1.120027	-0.315184
H	-4.973869	-0.223517	-0.924145
H	-5.544549	-1.876898	-0.643336
H	-5.059427	-0.861182	0.725147
C	-3.293966	-3.000647	0.315958
H	-2.294264	-3.439669	0.270119
H	-3.541835	-2.867592	1.377657
H	-4.004558	-3.726824	-0.101962
O	-1.193311	1.834196	1.298690
O	-1.250116	2.779040	-0.754592
C	-0.582228	3.729193	0.066293
H	0.371277	4.007798	-0.387173
H	-1.234696	4.608836	0.171430
C	-0.372961	2.993467	1.409446
H	0.677783	2.716237	1.549137
H	-0.717644	3.565012	2.279475

7d', B3LYP/6-31G(d), E = -1005.2554561 hartrees

C	-4.870625	0.169077	0.265350
C	-3.611709	0.896832	-0.223524
C	-2.310928	0.120531	-0.023778
C	-2.355058	-1.321312	-0.147695
C	-3.668950	-2.020362	0.205980
C	-4.913523	-1.263622	-0.270601
H	-3.762858	1.139729	-1.294180
H	-3.513217	1.866991	0.273730
H	-4.873850	0.131429	1.366303
H	-5.773562	0.724028	-0.034259
H	-3.663726	-3.042292	-0.197475
H	-3.741550	-2.117378	1.302957

H	-4.932332	-1.240792	-1.371207
H	-5.827283	-1.786003	0.053886
C	0.807823	-0.964069	0.274607
C	0.236736	0.473011	0.614131
C	-1.177936	0.950625	0.153861
C	-1.330261	-2.120445	-0.552072
C	0.018894	-1.588715	-0.911900
H	0.192952	0.546642	1.711181
H	-0.080130	-0.787711	-1.665179
H	0.621722	-2.383187	-1.370412
H	-1.466576	-3.202536	-0.544206
O	-1.286871	2.218137	0.131143
C	1.384502	1.466934	0.241236
C	2.314024	-0.722358	-0.156014
H	2.310175	-0.589380	-1.249059
C	2.654842	0.642619	0.447088
H	2.849697	0.562322	1.525733
H	3.506527	1.147464	-0.018648
C	0.700446	-1.842460	1.536428
H	-0.340867	-1.877099	1.868053
H	1.020200	-2.877818	1.363545
H	1.305579	-1.434326	2.357580
C	3.359584	-1.822661	0.159761
H	3.314196	-2.041749	1.236394
C	4.791459	-1.338701	-0.142429
H	5.078825	-0.485003	0.479214
H	5.519153	-2.141928	0.035850
H	4.887778	-1.031744	-1.192912
C	3.118588	-3.140004	-0.598506
H	2.150784	-3.588514	-0.361612
H	3.149313	-2.974933	-1.683810
H	3.897797	-3.874909	-0.353462
O	1.357312	1.896094	-1.119477
O	1.463316	2.643932	1.030543
C	1.014091	3.760822	0.275438
H	0.031340	4.083145	0.624608
H	1.750640	4.568963	0.401679
C	0.935608	3.253677	-1.179994
H	-0.088857	3.315360	-1.553335
H	1.622422	3.789423	-1.852826

8d (TS), B3LYP/6-31G(d), E = -1005.1988025 hartrees

C	4.456976	-0.817198	-1.012767
C	3.658821	0.497535	-0.903622

C	2.322751	0.261123	-0.232408
C	2.172398	-0.703070	0.796942
C	3.022495	-1.965268	0.747700
C	4.456807	-1.606903	0.309048
H	4.272463	1.226096	-0.339641
H	3.501299	0.943025	-1.893156
H	4.004700	-1.447544	-1.794172
H	5.492949	-0.617953	-1.330531
H	3.036580	-2.459891	1.728765
H	2.625415	-2.702720	0.028363
H	4.929945	-0.995125	1.092729
H	5.066169	-2.518734	0.208781
C	-0.750499	-0.996382	0.223247
C	-0.334085	0.386332	-0.436102
C	1.147823	0.886204	-0.752718
C	1.150409	-0.446794	1.701495
C	-0.121885	-1.239330	1.666812
H	-0.735399	0.318063	-1.460616
H	-0.824169	-0.895832	2.440150
H	0.001724	-2.324756	1.808374
H	0.909597	0.611512	1.774708
O	1.185600	1.796759	-1.625856
C	-1.296112	1.429969	0.196321
C	-2.334552	-0.874446	0.374292
H	-2.602898	-1.327505	1.339502
C	-2.596575	0.656532	0.466008
H	-3.309932	0.999456	-0.285086
H	-2.989603	0.956795	1.442276
C	-0.249097	-2.107856	-0.718795
H	0.806063	-1.935174	-0.938809
H	-0.336345	-3.107731	-0.277168
H	-0.782170	-2.105805	-1.677429
C	-3.247041	-1.597981	-0.665412
H	-2.867295	-1.398789	-1.678409
C	-4.711878	-1.113220	-0.618908
H	-4.834133	-0.076299	-0.942715
H	-5.338981	-1.734297	-1.272306
H	-5.117057	-1.193891	0.399318
C	-3.276987	-3.122522	-0.442498
H	-2.287868	-3.579306	-0.474390
H	-3.715827	-3.349853	0.539282
H	-3.899334	-3.615309	-1.201594
O	-0.844422	2.042412	1.404505
O	-1.595499	2.534475	-0.662361
C	-0.741529	3.620667	-0.324603
H	0.027013	3.747055	-1.090351

H	-1.359792	4.526230	-0.240994
C	-0.117054	3.207696	1.029520
H	0.950132	2.984576	0.922593
H	-0.255782	3.954006	1.820911

Negative Nuclear Hessian Mode 1 Eigenvalue = -61.15 cm^{-1}

5e, B3LYP/6-31G(d), LANL2DZ, E = -1033.3973828 hartrees

C	-3.517329	-2.572405	1.476398
C	-3.021750	-1.105575	1.520201
C	-2.132060	-0.866212	0.335754
C	-2.011814	-1.666594	-0.731230
C	-2.745252	-2.958692	-0.948970
C	-3.921925	-3.023367	0.055775
H	-3.880723	-0.411147	1.508463
H	-2.496435	-0.911943	2.470367
H	-2.709203	-3.228491	1.837487
H	-4.364335	-2.709807	2.164615
H	-3.123069	-3.046300	-1.980975
H	-2.072424	-3.822854	-0.803131
H	-4.731290	-2.369464	-0.306284
H	-4.333358	-4.042549	0.092912
C	1.090311	-1.098438	-0.044019
C	0.260764	0.100282	0.555088
C	-1.133205	0.210794	-0.178010
C	-0.967768	-0.822314	-1.445278
C	0.476587	-1.344636	-1.463716
H	0.083699	-0.077885	1.660655
H	1.052824	-0.781588	-2.211770
H	0.547850	-2.406096	-1.749628
H	-1.284400	-0.394835	-2.418673
O	-1.643943	1.447319	-0.351931
C	1.232193	1.293424	0.543379
C	2.588171	-0.573078	-0.110014
H	2.736327	-0.161959	-1.119181
C	2.589477	0.638057	0.839170
H	2.617982	0.325613	1.894154
H	3.420935	1.333856	0.669310
C	0.945986	-2.346679	0.848382
H	-0.110575	-2.600177	0.972412
H	1.449016	-3.222586	0.422897
H	1.364187	-2.172935	1.848253
C	3.730539	-1.591249	0.107197
H	3.539441	-2.148325	1.035638
C	5.094124	-0.894254	0.267794

H	5.131894	-0.261665	1.161074
H	5.898664	-1.636014	0.351140
H	5.317439	-0.260566	-0.601578
C	3.816163	-2.599693	-1.052746
H	2.872134	-3.128697	-1.216694
H	4.072725	-2.085646	-1.989191
H	4.594030	-3.350511	-0.863565
O	1.289165	1.962383	-0.721902
O	0.912296	2.309970	1.511361
C	0.885699	3.583590	0.859288
H	-0.159260	3.887550	0.669052
H	1.374669	4.331875	1.501036
C	1.630979	3.321395	-0.447035
H	1.293057	3.942583	-1.288824
H	2.722288	3.439101	-0.318463
K	-2.874925	3.584629	-0.674537

6e (TS), B3LYP/6-31G(d), LANL2DZ, E = -1033.367 hartrees

C	4.443893	-0.961863	-0.937124
C	3.679031	0.281443	-0.432153
C	2.401325	-0.169034	0.243532
C	2.220570	-1.380516	0.837084
C	3.103961	-2.577807	0.534729
C	4.507164	-2.081001	0.121595
H	4.322332	0.853676	0.260785
H	3.471904	0.961890	-1.276670
H	3.935783	-1.353247	-1.833539
H	5.461981	-0.683748	-1.248219
H	3.184102	-3.243777	1.407018
H	2.682973	-3.193668	-0.280675
H	5.026381	-1.695595	1.014040
H	5.111874	-2.918378	-0.257469
C	-0.734040	-1.243251	-0.080989
C	-0.164272	0.229689	-0.205395
C	1.183976	0.633780	0.481324
C	1.047429	-1.259915	1.687063
C	-0.245045	-1.889608	1.285272
H	-0.013934	0.412615	-1.297178
H	-1.012522	-1.730401	2.055260
H	-0.176582	-2.982466	1.131829
H	1.066035	-0.564645	2.531384
O	1.304802	1.877478	0.807300
C	-1.377832	1.127080	0.118278
C	-2.317265	-1.078638	-0.095499

H	-2.645233	-1.133422	0.952624
C	-2.547117	0.378004	-0.529283
H	-2.481397	0.491355	-1.621885
H	-3.512845	0.786069	-0.205626
C	-0.209823	-2.070576	-1.271391
H	0.882732	-2.047238	-1.284641
H	-0.519353	-3.119947	-1.218112
H	-0.561466	-1.666070	-2.229432
C	-3.159898	-2.128859	-0.858753
H	-2.745942	-2.249333	-1.870362
C	-4.624366	-1.678780	-1.017908
H	-4.714467	-0.768863	-1.620855
H	-5.216395	-2.462296	-1.507689
H	-5.083927	-1.480107	-0.039979
C	-3.135831	-3.499654	-0.158884
H	-2.120198	-3.878430	-0.009519
H	-3.610304	-3.432779	0.829751
H	-3.690592	-4.245633	-0.742148
O	-1.577509	1.258257	1.523063
O	-1.299303	2.476316	-0.397962
C	-1.563226	3.394977	0.675239
H	-0.614403	3.814878	1.048210
H	-2.214259	4.201219	0.306244
C	-2.223538	2.514932	1.732093
H	-2.029457	2.837004	2.764745
H	-3.313041	2.433290	1.568495
K	1.157669	3.364169	-1.345189

Negative Nuclear Hessian Mode 1 Eigenvalue = -394.97 cm^{-1}

6e' (TS), B3LYP/6-31G(d), LANL2DZ, E = -1033.3772659 hartrees

C	4.373567	-0.990636	-1.499353
C	3.244031	0.034874	-1.719614
C	2.332441	0.078271	-0.518016
C	2.535618	-0.532079	0.666743
C	3.841827	-1.238856	0.971644
C	4.931464	-0.911726	-0.068646
H	3.677671	1.035996	-1.901928
H	2.687501	-0.211529	-2.640311
H	3.980091	-2.005360	-1.671713
H	5.176005	-0.832287	-2.234735
H	4.183656	-0.964986	1.983980
H	3.669969	-2.329860	1.007205
H	5.310996	0.107259	0.110905
H	5.787545	-1.592528	0.046411

C	-0.527894	-1.227781	-0.149808
C	-0.238553	0.173236	-0.834730
C	1.055056	0.887209	-0.477002
C	1.361325	-0.464372	1.571571
C	0.227706	-1.434287	1.222154
H	-0.111366	-0.013512	-1.964871
H	-0.511910	-1.382602	2.034861
H	0.562827	-2.494978	1.219693
H	1.634731	-0.612485	2.638988
O	1.116209	2.138272	-0.417911
C	-1.549014	0.977977	-0.772063
C	-2.105747	-1.206409	0.069448
H	-2.271515	-0.829912	1.090186
C	-2.622885	-0.107024	-0.872699
H	-2.673042	-0.458589	-1.914438
H	-3.610722	0.282895	-0.597673
C	-0.100122	-2.342463	-1.128800
H	0.972184	-2.252782	-1.338286
H	-0.271304	-3.342465	-0.717505
H	-0.633049	-2.272755	-2.086439
C	-2.870523	-2.548408	-0.030649
H	-2.622360	-3.019976	-0.992561
C	-4.395814	-2.335440	-0.011922
H	-4.744017	-1.755028	-0.872693
H	-4.917420	-3.300650	-0.029527
H	-4.709314	-1.807008	0.899057
C	-2.490570	-3.525970	1.095613
H	-1.417639	-3.737130	1.123908
H	-2.771126	-3.113274	2.074287
H	-3.019667	-4.479862	0.974774
O	-1.686477	1.710444	0.457681
O	-1.679015	1.944920	-1.821502
C	-1.942146	3.231408	-1.248342
H	-1.012654	3.822017	-1.202242
H	-2.686170	3.753919	-1.867430
C	-2.449819	2.884418	0.146251
H	-2.235057	3.649328	0.907224
H	-3.530641	2.658422	0.144251
K	0.444231	2.354684	2.187358

Negative Nuclear Hessian Mode 1 Eigenvalue = -200.87 cm^{-1}

7e, B3LYP/6-31G(d), LANL2DZ, E = -1033.3856305 hartrees

C	4.718930	-0.682442	-0.504161
C	3.893056	0.398019	0.228827

C	2.456596	-0.053148	0.410436
C	2.167364	-1.424800	0.715126
C	3.011813	-2.490394	0.031923
C	4.499297	-2.084855	0.091580
H	4.373558	0.596700	1.205104
H	3.927200	1.344776	-0.326433
H	4.419981	-0.702402	-1.565232
H	5.789619	-0.426180	-0.481433
H	2.862026	-3.474139	0.500201
H	2.730766	-2.596075	-1.031387
H	4.834254	-2.090245	1.141861
H	5.115282	-2.824573	-0.441906
C	-0.720781	-1.295803	-0.304565
C	-0.113830	0.217931	-0.248508
C	1.372481	0.734232	-0.012652
C	1.002588	-1.646769	1.399740
C	-0.109466	-2.367693	0.713589
H	-0.267565	0.570484	-1.292016
H	-0.897528	-2.728256	1.389414
H	0.254796	-3.235712	0.145868
H	0.642551	-0.814401	2.006241
O	1.519763	1.953297	-0.406752
C	-1.209515	1.030879	0.493632
C	-2.263442	-1.091857	0.029649
H	-2.382758	-1.371754	1.086451
C	-2.513197	0.419877	-0.019344
H	-2.683555	0.775651	-1.046965
H	-3.366367	0.738357	0.592556
C	-0.456111	-1.797621	-1.740786
H	0.623439	-1.794718	-1.932561
H	-0.813415	-2.820494	-1.898830
H	-0.927524	-1.156531	-2.496657
C	-3.286831	-1.942542	-0.762431
H	-3.083768	-1.820402	-1.836672
C	-4.732185	-1.469824	-0.516331
H	-4.896179	-0.442646	-0.858743
H	-5.442626	-2.115043	-1.048412
H	-4.983776	-1.511728	0.552291
C	-3.190984	-3.440436	-0.420729
H	-2.190787	-3.849448	-0.590131
H	-3.442223	-3.610132	0.634941
H	-3.897912	-4.021432	-1.026524
O	-1.079163	0.898216	1.910884
O	-1.228182	2.451477	0.238338
C	-0.970794	3.141546	1.470189
H	0.109434	3.337126	1.575740

H	-1.529425	4.088772	1.464698
C	-1.462124	2.141586	2.505616
H	-0.967580	2.223323	3.483727
H	-2.557879	2.198385	2.635272
K	0.125864	3.543868	-1.886580

7e', B3LYP/6-31G(d), LANL2DZ, E = -1033.4359093 hartrees

C	-4.867921	-0.328597	-0.059392
C	-3.620692	0.370109	-0.618533
C	-2.285002	-0.292587	-0.258358
C	-2.279589	-1.756519	-0.184535
C	-3.579389	-2.442623	0.241521
C	-4.839167	-1.824807	-0.375249
H	-3.734504	0.419787	-1.719645
H	-3.598070	1.413052	-0.284979
H	-4.908085	-0.198288	1.035125
H	-5.774874	0.142507	-0.468722
H	-3.519881	-3.515015	0.008694
H	-3.677651	-2.365895	1.339572
H	-4.831399	-1.971207	-1.467879
H	-5.737366	-2.330777	0.010088
C	0.840305	-1.223029	0.313523
C	0.241109	0.239551	0.357738
C	-1.203210	0.591034	-0.113644
C	-1.218595	-2.560004	-0.438785
C	0.143668	-2.058118	-0.798280
H	0.261709	0.553630	1.427821
H	0.091291	-1.409928	-1.691542
H	0.787755	-2.905669	-1.065367
H	-1.336932	-3.636703	-0.302507
O	-1.369479	1.872183	-0.226346
C	1.344686	1.127380	-0.281938
C	2.370789	-1.039621	-0.079658
H	2.433420	-1.202537	-1.166868
C	2.646038	0.450222	0.146288
H	2.823236	0.668305	1.210731
H	3.499231	0.837664	-0.423450
C	0.656379	-1.867421	1.701245
H	-0.399262	-1.840492	1.987775
H	0.973759	-2.915530	1.724914
H	1.225144	-1.324385	2.466777
C	3.416137	-1.985494	0.564678
H	3.284281	-1.960431	1.656196
C	4.853920	-1.514332	0.271315

H	5.063318	-0.529446	0.701416
H	5.581534	-2.221232	0.689450
H	5.035786	-1.453618	-0.810510
C	3.273584	-3.445619	0.098109
H	2.293812	-3.871794	0.331489
H	3.417603	-3.520121	-0.988330
H	4.033067	-4.077472	0.576003
O	1.216280	1.148439	-1.701313
O	1.372260	2.510622	0.134682
C	1.293385	3.343812	-1.032425
H	0.255950	3.682605	-1.180818
H	1.962458	4.206411	-0.898584
C	1.728015	2.404780	-2.152034
H	1.275793	2.632415	-3.127507
H	2.827784	2.371980	-2.251976
K	-0.676216	3.418080	1.748260

8e (TS), B3LYP/6-31G(d), LANL2DZ, E = -1033.3837072 hartrees

C	4.750402	-0.690281	-0.504733
C	3.899506	0.433484	0.127039
C	2.472648	-0.028477	0.352502
C	2.208234	-1.376000	0.762979
C	3.080058	-2.479635	0.183701
C	4.558079	-2.038873	0.211982
H	4.375993	0.732827	1.079546
H	3.913484	1.325620	-0.513297
H	4.458046	-0.810232	-1.560909
H	5.815186	-0.409802	-0.501320
H	2.947477	-3.418803	0.740172
H	2.807344	-2.689095	-0.866076
H	4.888610	-1.944958	1.259535
H	5.191968	-2.809244	-0.252692
C	-0.657930	-1.362131	-0.286763
C	-0.103649	0.169332	-0.305537
C	1.371896	0.723784	-0.097934
C	1.044846	-1.558456	1.465366
C	-0.066225	-2.333797	0.837885
H	-0.259150	0.463428	-1.366268
H	-0.862143	-2.618364	1.540246
H	0.291445	-3.257563	0.361061
H	0.679155	-0.664098	1.971703
O	1.502609	1.918197	-0.561176
C	-1.233327	0.972176	0.384518
C	-2.223380	-1.189555	-0.047972

H	-2.397729	-1.435421	1.009178
C	-2.505738	0.313675	-0.166333
H	-2.630047	0.626340	-1.214010
H	-3.400541	0.620883	0.388290
C	-0.294384	-1.949311	-1.667160
H	0.792854	-1.917852	-1.800680
H	-0.608135	-2.992564	-1.775683
H	-0.742789	-1.376558	-2.488828
C	-3.178004	-2.096222	-0.863083
H	-2.911829	-2.017627	-1.927403
C	-4.645684	-1.649046	-0.727314
H	-4.810921	-0.642643	-1.126353
H	-5.307286	-2.335168	-1.271039
H	-4.962004	-1.649474	0.324799
C	-3.070865	-3.574057	-0.445348
H	-2.051185	-3.962594	-0.522138
H	-3.393968	-3.701929	0.596717
H	-3.717252	-4.202094	-1.071514
O	-1.172855	0.866778	1.812223
O	-1.216663	2.379305	0.130367
C	-1.982363	2.978322	1.183990
H	-1.629743	4.011014	1.319158
H	-3.055152	2.990603	0.928088
C	-1.693932	2.070604	2.392493
H	-0.927078	2.492839	3.060723
H	-2.602846	1.857596	2.977448
K	0.359074	4.021446	-1.425865

Negative Nuclear Hessian Mode 1 Eigenvalue = -53.76 cm^{-1}

5f, B3LYP/6-31G(d), LANL2DZ, E = -961.5806195 hartrees

C	-3.489309	-2.445158	1.646687
C	-2.959316	-0.989895	1.647966
C	-2.103006	-0.790339	0.431060
C	-2.035854	-1.613357	-0.623675
C	-2.806378	-2.891308	-0.794187
C	-3.951154	-2.910168	0.248299
H	-3.803173	-0.276941	1.653612
H	-2.398399	-0.792185	2.576770
H	-2.684649	-3.113860	1.992037
H	-4.315798	-2.551355	2.364774
H	-3.219485	-2.988295	-1.811869
H	-2.149950	-3.768846	-0.653814
H	-4.755919	-2.242625	-0.099223
H	-4.385667	-3.918084	0.316672

C	1.115056	-1.115814	-0.079019
C	0.331618	0.091970	0.569800
C	-1.079035	0.241860	-0.128202
C	-0.995629	-0.807035	-1.386295
C	0.431936	-1.365312	-1.464459
H	0.161719	-0.148312	1.634824
H	0.986172	-0.829409	-2.248757
H	0.461082	-2.431904	-1.739328
H	-1.343683	-0.379308	-2.349320
O	-1.543740	1.498667	-0.318885
C	1.311359	1.300042	0.588462
C	2.604874	-0.603039	-0.206891
H	2.708364	-0.165589	-1.212152
C	2.660716	0.570308	0.788744
H	2.730568	0.187148	1.819251
H	3.524094	1.227971	0.627641
C	1.000311	-2.362571	0.821293
H	-0.052683	-2.602903	0.996756
H	1.471108	-3.246699	0.375022
H	1.467601	-2.193544	1.800173
C	3.747653	-1.637914	-0.082879
H	3.605864	-2.212870	0.843666
C	5.127402	-0.960801	0.010155
H	5.226214	-0.347692	0.912175
H	5.926439	-1.713104	0.029654
H	5.306679	-0.310908	-0.857608
C	3.752169	-2.624103	-1.264726
H	2.795853	-3.144447	-1.376397
H	3.950546	-2.093823	-2.206416
H	4.535861	-3.382714	-1.141413
C	1.628557	3.638550	1.251316
H	1.258907	4.512988	1.802249
H	2.720676	3.612694	1.373670
C	1.259080	3.663767	-0.241965
H	0.215450	3.991526	-0.343902
H	1.878842	4.351704	-0.830784
K	-3.226657	3.222647	-1.054224
C	1.378085	2.189801	-0.706676
H	0.571034	1.941273	-1.396464
H	2.332530	2.034138	-1.226405
C	1.008978	2.315064	1.719311
H	1.380953	1.974883	2.694914
H	-0.079424	2.434173	1.796625

6f (TS), B3LYP/6-31G(d), LANL2DZ, E = -961.550989 hartrees

C	-3.868153	-1.604280	1.678826
C	-3.272633	-0.192790	1.484813
C	-2.145190	-0.271447	0.474265
C	-2.039426	-1.209212	-0.504793
C	-2.807752	-2.517502	-0.468566
C	-4.109903	-2.328650	0.339776
H	-4.078155	0.494437	1.158343
H	-2.918680	0.206150	2.448780
H	-3.170831	-2.203089	2.283561
H	-4.806265	-1.546748	2.247909
H	-3.043049	-2.870172	-1.484020
H	-2.202751	-3.315025	-0.001252
H	-4.821547	-1.736703	-0.260184
H	-4.589395	-3.301411	0.523414
C	1.030162	-1.081037	-0.035137
C	0.442155	0.231328	0.632619
C	-1.014567	0.678695	0.292623
C	-1.026843	-0.734763	-1.443661
C	0.344564	-1.329969	-1.445218
H	0.422914	0.023732	1.720764
H	0.961013	-0.875990	-2.233870
H	0.353094	-2.418957	-1.635341
H	-1.198492	0.189341	-2.006364
O	-1.268045	1.943868	0.299773
C	1.540230	1.328258	0.485134
C	2.581332	-0.788016	-0.191305
H	2.742656	-0.489629	-1.238088
C	2.811281	0.470477	0.663881
H	2.920319	0.195490	1.724664
H	3.720389	1.017283	0.381227
C	0.750499	-2.278777	0.897615
H	-0.323005	-2.370006	1.082181
H	1.095513	-3.227675	0.472126
H	1.240626	-2.152492	1.871549
C	3.581231	-1.943899	0.062371
H	3.346364	-2.411860	1.029112
C	5.033327	-1.437508	0.146645
H	5.185210	-0.756591	0.990630
H	5.727545	-2.278861	0.268511
H	5.319403	-0.903883	-0.770286
C	3.496673	-3.025125	-1.030375
H	2.487282	-3.433615	-1.140284
H	3.790123	-2.608739	-2.003887
H	4.174892	-3.859580	-0.809977
C	1.492879	3.814203	0.775929

H	0.464767	4.144969	0.586764
H	2.007067	4.615238	1.321649
C	2.163096	3.462961	-0.562014
H	1.973613	4.203162	-1.350258
H	3.253423	3.399407	-0.432915
K	-3.353950	1.968927	-1.374553
C	1.582930	2.075694	-0.884554
H	0.566521	2.191083	-1.270086
H	2.170865	1.541501	-1.639773
C	1.467137	2.476861	1.547278
H	2.331750	2.413709	2.222865
H	0.568052	2.391964	2.163966

Negative Nuclear Hessian Mode 1 Eigenvalue = -466.27 cm^{-1}

6f' (TS), B3LYP/6-31G(d), LANL2DZ, E = -961.5565304 hartrees

C	3.872408	-1.544937	-1.802227
C	2.881083	-0.370844	-1.932357
C	2.126969	-0.172860	-0.639926
C	2.359519	-0.808197	0.525887
C	3.572686	-1.698248	0.713570
C	4.583925	-1.535899	-0.438751
H	3.426310	0.553157	-2.200788
H	2.191514	-0.554614	-2.774081
H	3.322891	-2.494289	-1.906876
H	4.607174	-1.512155	-2.620000
H	4.053727	-1.477801	1.681859
H	3.247660	-2.752040	0.782907
H	5.120679	-0.580225	-0.320702
H	5.342243	-2.331388	-0.397634
C	-0.792928	-1.143435	-0.021362
C	-0.438675	0.221431	-0.745589
C	0.952693	0.778912	-0.486867
C	1.288300	-0.559677	1.522566
C	-0.010773	-1.348518	1.328904
H	-0.400809	-0.024206	-1.827703
H	-0.678119	-1.080693	2.162298
H	0.132162	-2.447139	1.431574
H	1.629487	-0.687402	2.574315
O	1.168050	2.019997	-0.468225
C	-1.658488	1.173076	-0.604761
C	-2.357687	-1.019725	0.232867
H	-2.479597	-0.672826	1.269755
C	-2.806766	0.143501	-0.669478
H	-2.930979	-0.201401	-1.708176

H	-3.766136	0.576812	-0.358874
C	-0.457517	-2.299111	-0.991181
H	0.608861	-2.279107	-1.239385
H	-0.673611	-3.280893	-0.555824
H	-1.018821	-2.217074	-1.931283
C	-3.219915	-2.300980	0.117070
H	-3.008625	-2.782134	-0.848725
C	-4.726875	-1.982523	0.141907
H	-5.035836	-1.371330	-0.712546
H	-5.315048	-2.908801	0.117767
H	-5.001125	-1.441386	1.058065
C	-2.908729	-3.311018	1.235934
H	-1.849805	-3.583909	1.270468
H	-3.171832	-2.890128	2.216178
H	-3.491581	-4.231691	1.104335
C	-1.845112	3.628306	-1.042103
H	-0.833333	4.031943	-0.911768
H	-2.427806	4.363064	-1.611144
C	-2.442801	3.308899	0.336404
H	-2.292082	4.108812	1.072732
H	-3.527075	3.147887	0.248106
K	2.351200	2.234992	1.907700
C	-1.737969	1.996754	0.720445
H	-0.728491	2.221644	1.077052
H	-2.258606	1.457034	1.519576
C	-1.767579	2.252360	-1.735409
H	-2.679858	2.076423	-2.321760
H	-0.925345	2.197431	-2.433479

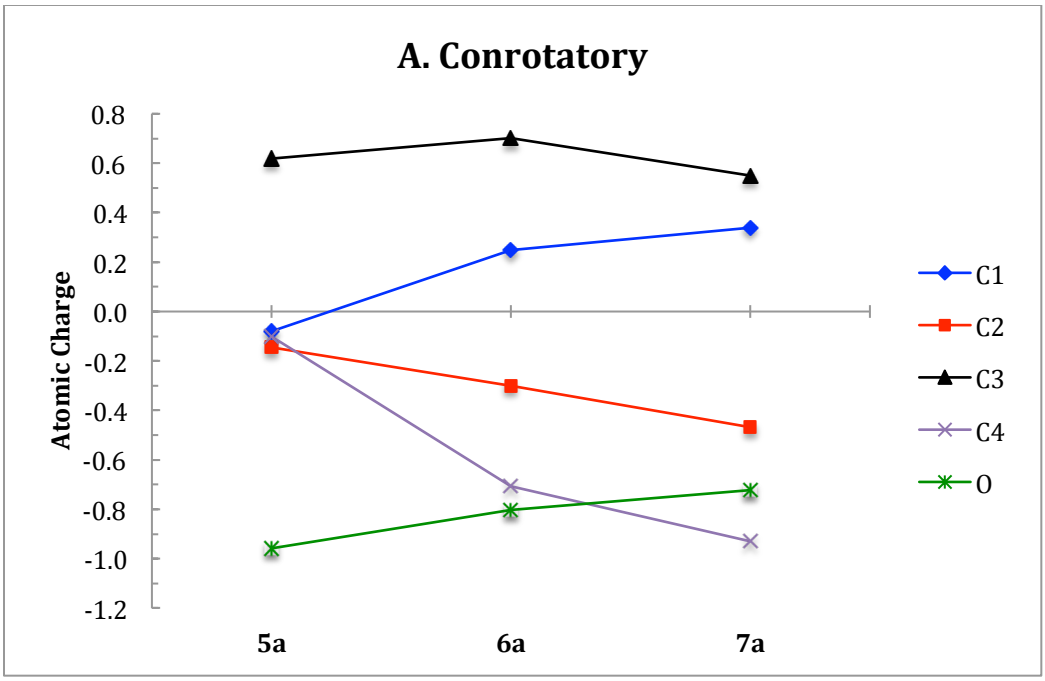
Negative Nuclear Hessian Mode 1 Eigenvalue = -221.36 cm^{-1}

Table S1. Summary of computed Gibbs free energies, ΔG, for the model alkoxide, potassium alkoxide, and alcohol systems.

	Gas Phase				THF		
	a			c	a		b
	B3LYP/6-31G(d)	B3LYP/6-311++G(d,p)	M06-2X	B3LYP/6-31G(d)	B3LYP/6-31G(d)	B3LYP/6-311++G(d,p)	B3LYP/6-31G(d)
1 + 2	0.0	0.0	0.0	-	0.0	-	0.0
3	-29.8	-22.2	-32.4	-	-19.8	-	-25.5
4	-27.1	-19.7	-26.6	-	-16.4	-	-21.5
5	-33.4	-26.9	-38.0	0.0	-26.8	0.0	-32.9
6	-30.6	-22.1	-31.8	28.9	-22.0	14.3	-18.2
6’	-29.7	-21.5	-29.1	47.8	-21.2	16.0	-17.5
7	-43.9	-35.2	-37.0	22.3	-33.9	2.7	-25.6
7’	-71.3	-61.0	-71.3	-14.1	-61.0	-23.0	-57.5
8	-29.4	-23.3	-33.1	-	-	-	-11.5

Table S2. Summary of computed Gibbs free energies, ΔG, for the more complex alkoxide and potassium alkoxide guanacastepene precursors.

	Gas Phase		THF	
	d		e	f
	B3LYP/6-31G(d)	M06-2X	B3LYP/6-31G(d)	B3LYP/6-31G(d)
5	0.0	0.0	0.0	0.0
6	10.9	13.4	18.8	17.5
6’	11.0	15.1	10.7	13.8
7	0.8	1.8	9.1	-
7’	-32.1	-30.5	-22.2	-
8	3.7	5.0	10.5	-



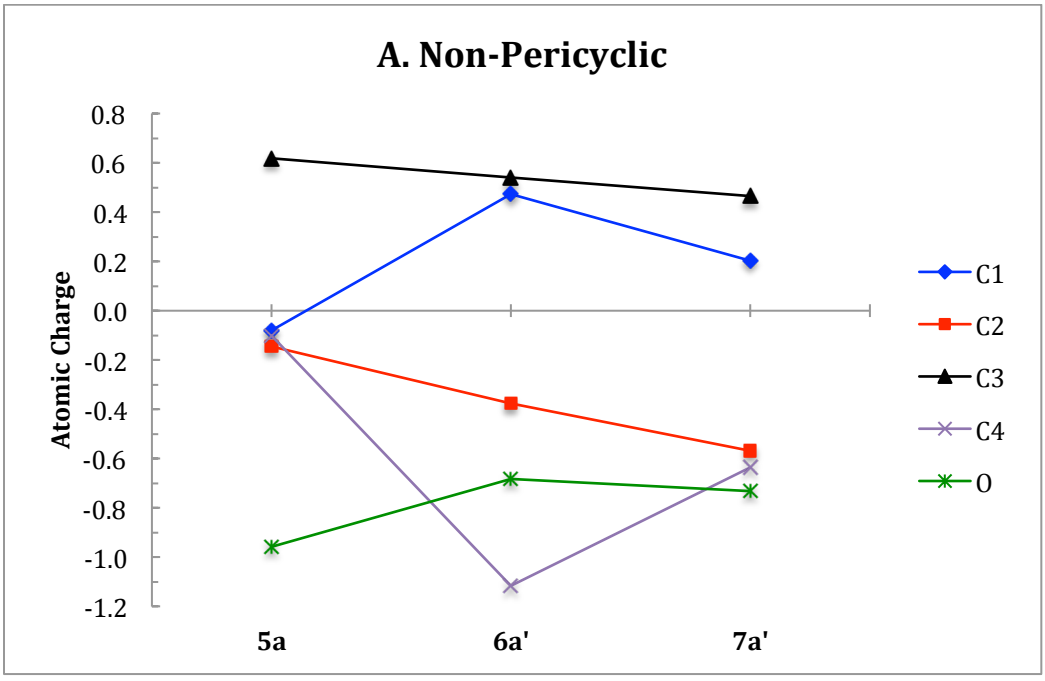
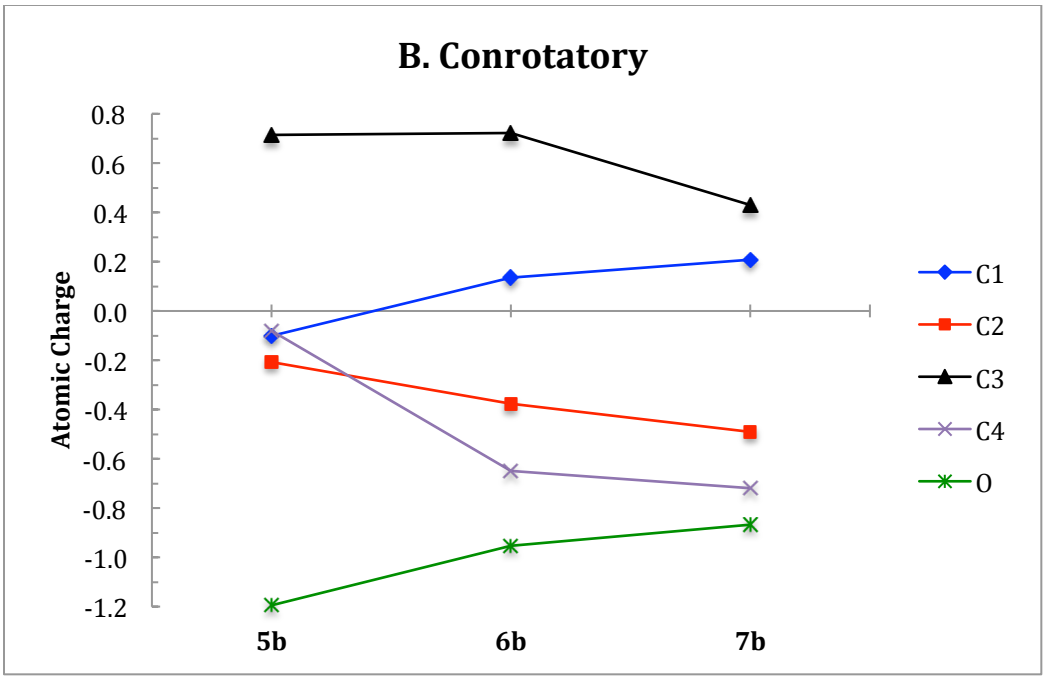


Figure S1. Atomic charges on the four carbons and the oxygen substituent in the cyclobutene ring of **5a** throughout the two ring opening pathways.



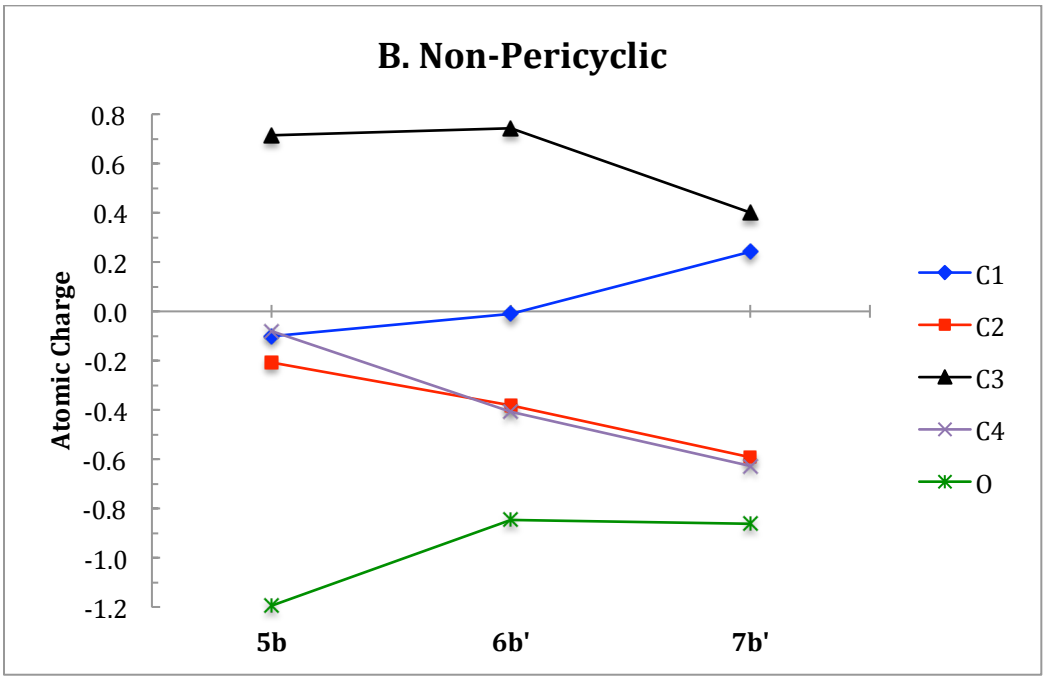
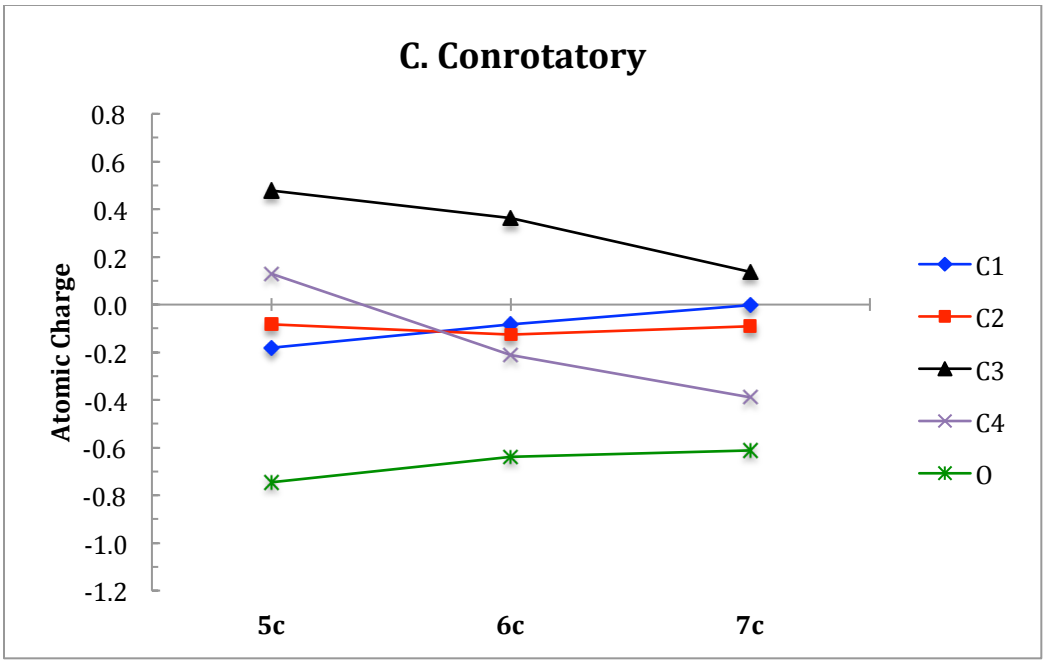


Figure S2. Atomic charges on the four carbons and the oxygen substituent in the cyclobutene ring of **5b** throughout the two ring opening pathways.



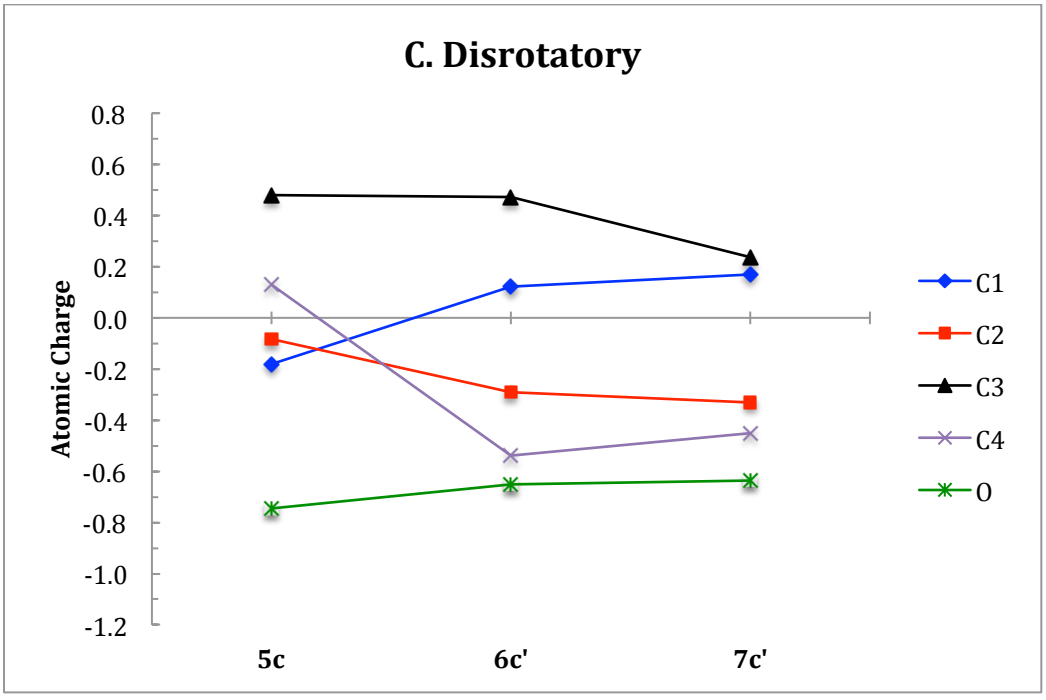
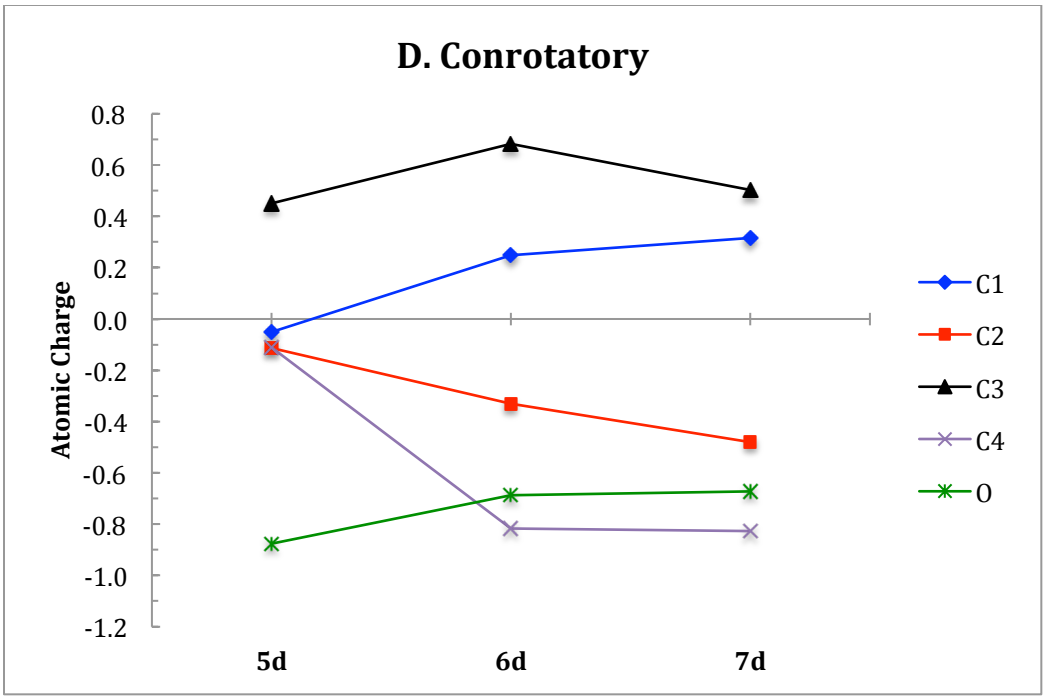


Figure S3. Atomic charges on the four carbons and the oxygen substituent in the cyclobutene ring of **5c** throughout the two ring opening pathways.



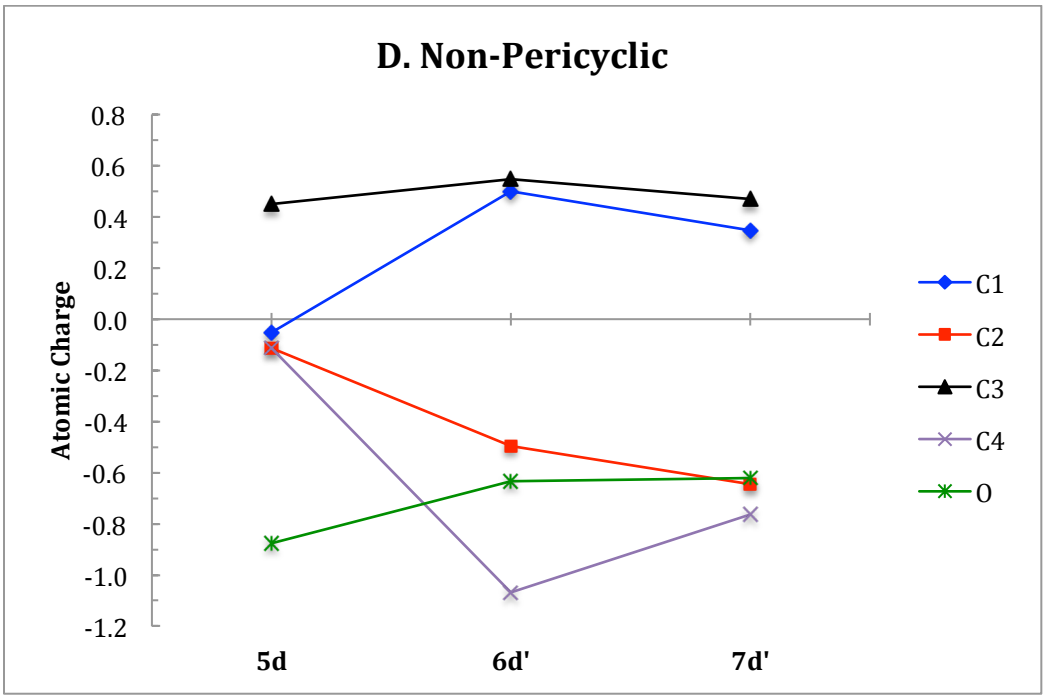
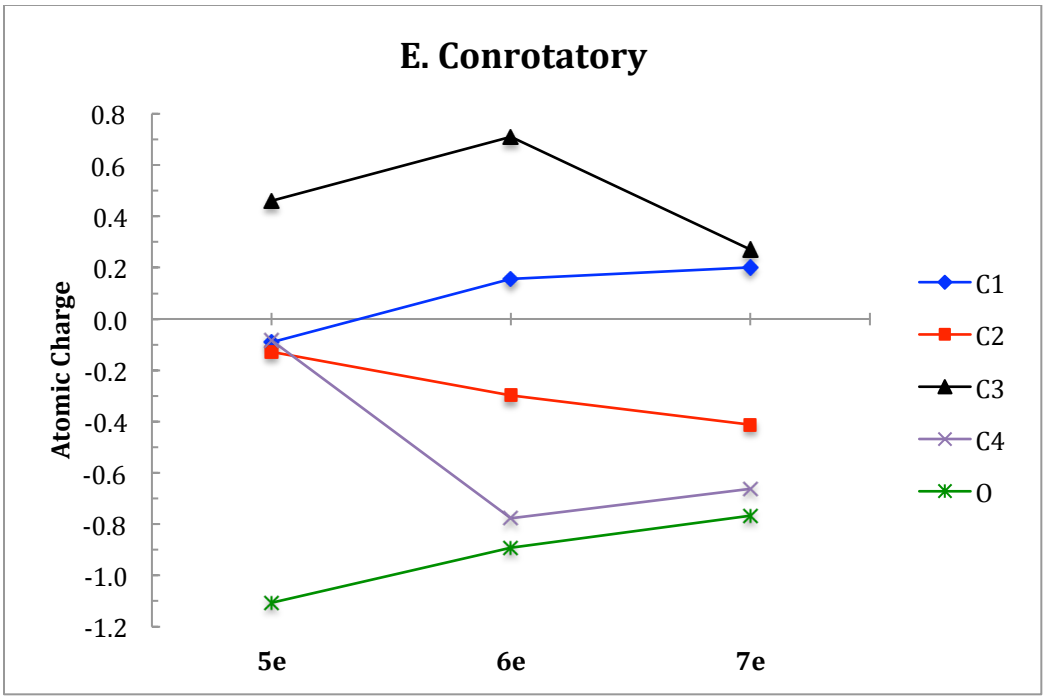


Figure S4. Atomic charges on the four carbons and the oxygen substituent in the cyclobutene ring of **5d** throughout the two ring opening pathways.



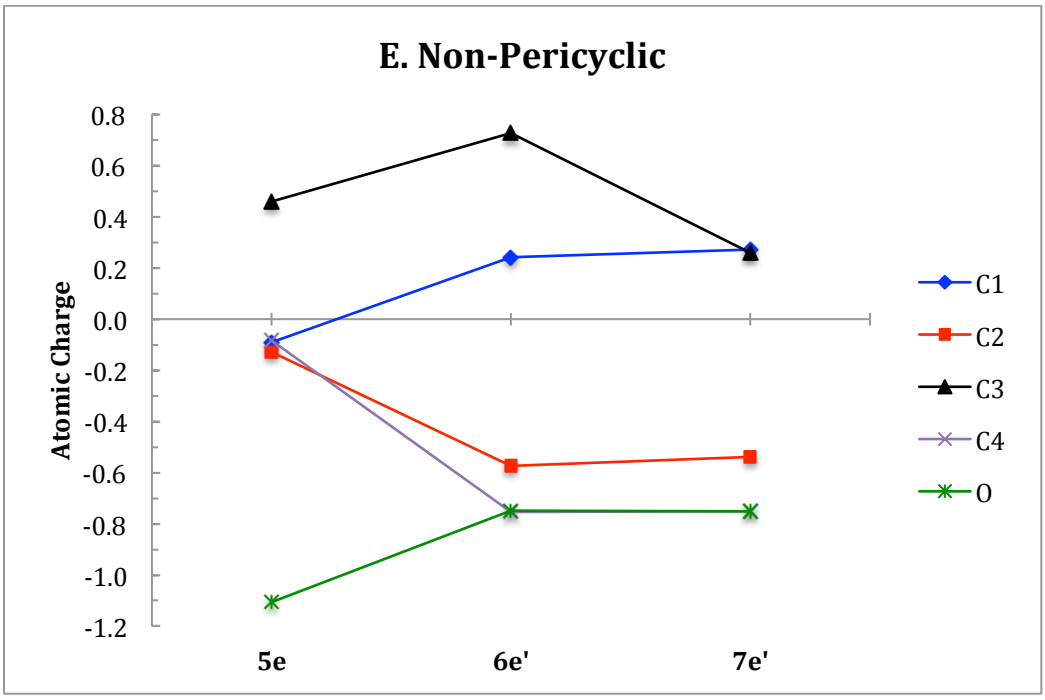


Figure S5. Atomic charges on the four carbons and the oxygen substituent in the cyclobutene ring of **5e** throughout the two ring opening pathways.

Table S3. Atomic charges on the four carbons and the oxygen substituent in the cyclobutene ring of **5a-e** throughout the two ring opening pathways.

	5a	**6a**	**6a'**	**7a**	**7a'**
C1	-0.080	0.248	0.474	0.339	0.202
C2	-0.146	-0.301	-0.375	-0.468	-0.569
C3	0.618	0.702	0.541	0.55	0.464
C4	-0.101	-0.707	-1.116	-0.93	-0.636
O	-0.959	-0.804	-0.683	-0.722	-0.732

	5b	**6b**	**6b'**	**7b**	**7b'**
C1	-0.102	0.136	-0.009	0.209	0.241
C2	-0.208	-0.375	-0.381	-0.491	-0.593
C3	0.715	0.722	0.744	0.430	0.401
C4	-0.081	-0.649	-0.407	-0.719	-0.627
O	-1.195	-0.952	-0.845	-0.866	-0.861

	5c	**6c**	**6c'**	**7c**	**7c'**
C1	-0.181	-0.083	0.121	-0.002	0.169
C2	-0.084	-0.127	-0.291	-0.090	-0.332
C3	0.479	0.362	0.473	0.137	0.237
C4	0.130	-0.211	-0.539	-0.389	-0.452
O	-0.745	-0.638	-0.652	-0.612	-0.637

	5d	**6d**	**6d'**	**7d**	**7d'**
C1	-0.052	0.249	0.501	0.317	0.346
C2	-0.113	-0.331	-0.495	-0.480	-0.645
C3	0.450	0.682	0.548	0.504	0.470
C4	-0.112	-0.817	-1.068	-0.827	-0.763
O	-0.876	-0.688	-0.634	-0.671	-0.621

	5e	**6e**	**6e'**	**7e**	**7e'**
C1	-0.091	0.157	0.242	0.200	0.272
C2	-0.128	-0.299	-0.574	-0.412	-0.538
C3	0.460	0.711	0.727	0.270	0.259
C4	-0.083	-0.778	-0.754	-0.661	-0.751
O	-1.107	-0.893	-0.749	-0.767	-0.752