

ELECTRONIC SUPPLEMENTARY INFORMATION

Claisen rearrangements of benzyl vinyl ethers: theoretical investigation of mechanism, substituent effects, and regioselectivity

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Boat Transition States

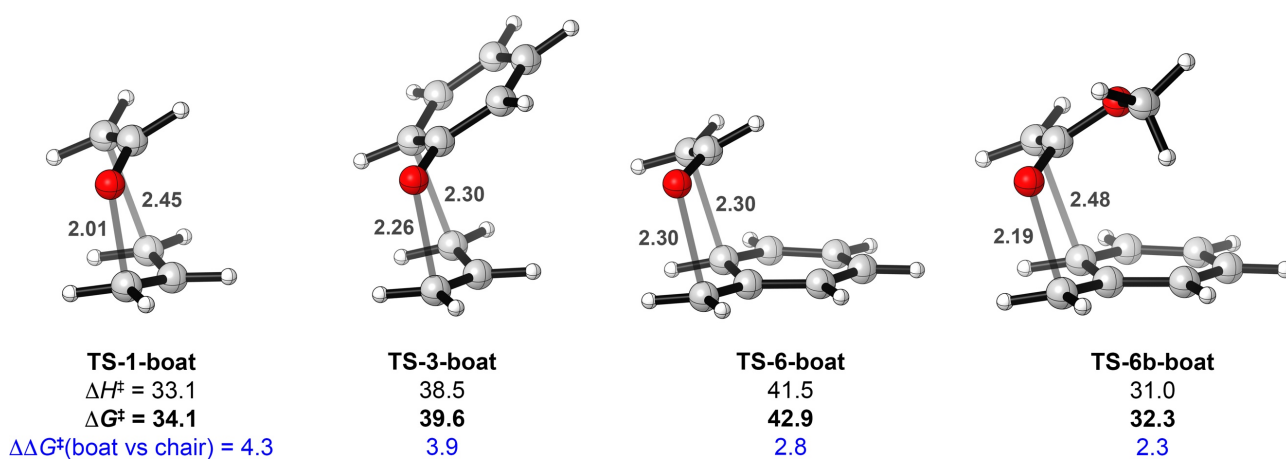


Figure S1. Boat transition states for Claisen rearrangements of **1**, **3**, **6**, and **6b**, calculated with CBS-QB3. Distances in Å. ΔH^\ddagger and ΔG^\ddagger in kcal mol⁻¹.

Tandem [3,3]-Rearrangement/Alder–Ene Reaction

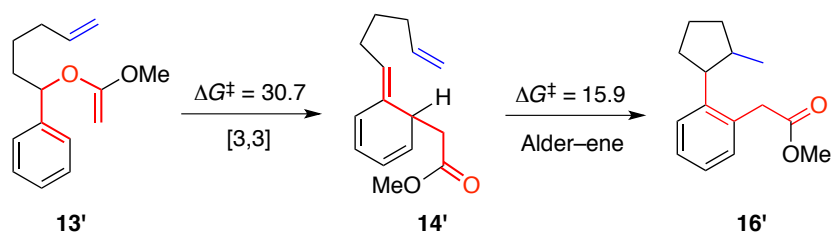


Figure S2. Calculated barriers for the [3,3]-rearrangement of **13'** and the Alder–ene reaction of the resulting isotoluene **14'** leading to **16'**, calculated with SCS-MP2/cc-pVTZ//B3LYP/6-31G(d). ΔG^\ddagger in kcal mol⁻¹.

Computational Methods

Quantum chemical calculations were performed in Gaussian 09.¹

Our initial calculations (Table 1 of the paper) compared the performance of various theoretical methods for calculating the activation enthalpies of the Claisen rearrangements of **1**, **3**, and **6**. Most of the data reported in Table 1 employ geometries which were optimised with B3LYP/6-31G(d). For each of these species, harmonic vibrational frequency calculations were performed at the same level of theory to determine the nature of the stationary point (minimum or first-order saddle point) and to obtain unscaled thermochemical quantities. The identities of selected transition states were also confirmed by intrinsic reaction coordinate (IRC) analysis.² Subsequently, single-point energies were calculated with several methods, viz. M06-2X/cc-pVTZ, ω B97X-D/cc-pVTZ, and SCS-MP2/cc-pVTZ, using the B3LYP/6-31G(d) optimised geometries. Enthalpies were calculated by adding the thermochemical corrections derived from the B3LYP/6-31G(d) frequency calculations to the relevant single-point electronic potential energies. These results were then compared against enthalpies calculated with CBS-QB3.

Figure 1 of the paper reports CBS-QB3 transition states, activation free energies, and reaction free energies for the Claisen rearrangements of **1**, **3**, **6**, and **6b**. Table 2 of the paper compares the Claisen rearrangements of these four substrates versus C–O bond homolysis; this analysis is based on CBS-QB3 calculations. In contrast, the analysis of substituent effects in Table 3 of the paper utilises Gibbs free energies derived from SCS-MP2/cc-pVTZ single-point energy calculations on B3LYP/6-31G(d) optimised geometries. In this case, free energies were calculated by adding the thermochemical quantities derived from the B3LYP frequencies to the SCS-MP2 single-point electronic energies. All Gibbs free energies are reported at a standard state of 298.15 K and 1 mol L⁻¹.

The computational data listed below are divided into two sections. The first section contains data obtained from CBS-QB3 calculations, which are relevant to Figure 1, Table 1, and Table 2 of the paper. The second section contains the results of B3LYP/6-31G(d) geometry optimisations and single-point energy calculations with various theoretical methods, as relevant to Tables 1 and 3 of the paper.

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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 and D. J. Fox, Gaussian 09, Revision E.01, Gaussian, Inc., Wallingford CT, 2013.
 - 2 (a) C. Gonzalez and H. B. Schlegel, *J. Chem. Phys.*, 1989, **90**, 2154. (b) C. Gonzalez and H. B. Schlegel, *J. Phys. Chem.*, 1990, **94**, 5523.

Optimised Geometries and Energies

1. CBS-QB3 calculations relevant to Figure 1, Table 1, and Table 2, and Figure S1

The optimised Cartesian coordinates of species computed with CBS-QB3 are given below. Underneath each set of coordinates are listed the following energies (in Hartree):

E: CBS-QB3 electronic potential energy plus zero-point energy

H: CBS-QB3 enthalpy at 298.15 K

G: CBS-QB3 Gibbs free energy at 298.15 K and 1 mol L⁻¹

For certain species, single-point calculations were also performed with B3LYP/6-311G(2d,d,p) in implicit solvent (xylene-mixture or *N,N*-dimethylformamide) as modelled with the SMD solvent model. The energies listed as E_{gas}, E_{xylenes}, and E_{DMF} for these species refer to the B3LYP/6-311G(2d,d,p) potential energy in the gas phase, with free energy of solvation in xylenes included, and with free energy of solvation in DMF included, respectively.

1

C	-2.529062	0.359491	0.000389
H	-3.584909	0.126034	0.000730
H	-2.250542	1.404032	0.000379
C	-1.650604	-0.643890	-0.000004
H	-1.966258	-1.681425	-0.000020
O	-0.296274	-0.581852	-0.000457
C	0.300972	0.707154	-0.000195
H	-0.032483	1.270949	0.883501
H	-0.032384	1.271301	-0.883700
C	1.794362	0.587962	-0.000120
H	2.314850	1.543130	-0.000429
C	2.480703	-0.548172	0.000307
H	1.979396	-1.507827	0.000565
H	3.564298	-0.546649	0.000367

0 imaginary frequencies
E = -270.021146
H = -270.013364
G = -270.048743

TS-1

O	0.558353	-1.345569	-0.247022
C	1.307671	-0.442259	0.267895
C	1.475589	0.808376	-0.291089
H	1.221298	0.973678	-1.329168
C	-1.291196	-0.923425	0.178945
C	-1.385774	0.381727	-0.309833
H	-1.737037	-1.744363	-0.366303
H	-1.165818	-1.093143	1.241141
H	-1.700661	0.519770	-1.339710
C	-0.726300	1.412445	0.324696
H	1.696168	-0.603865	1.287054
H	2.132876	1.530200	0.182425
H	-0.697369	2.407220	-0.104027
H	-0.496227	1.353874	1.381080

1 imaginary frequency
E = -269.975018
H = -269.967969
G = -270.001184

TS-1-boat (4.3 kcal mol⁻¹ higher in energy than the chair TS TS-1)

H	0.905013	2.286970	0.554937
C	0.923631	1.399240	-0.065517
C	1.415573	0.204437	0.412786

H	1.636705	0.120080	1.473112
C	1.253746	-0.969197	-0.316289
O	-0.716641	-1.326916	-0.096153
C	-1.347800	-0.323840	0.378865
C	-1.470034	0.891679	-0.263790
H	0.825489	1.563019	-1.130007
H	1.144159	-0.927756	-1.391445
H	1.574941	-1.919385	0.087644
H	-1.690595	-0.379218	1.425265
H	-1.289774	0.958579	-1.327978
H	-2.023507	1.699121	0.201365

1 imaginary frequency
E = -269.967850
H = -269.960590
G = -269.994386

2

C	-0.598339	0.776936	-0.112620
C	-2.040083	0.332802	-0.182603
H	-2.757304	1.131673	-0.477825
O	-2.429560	-0.782327	0.053411
C	0.386190	-0.336791	0.264290
C	1.798199	0.161354	0.387642
C	2.821602	-0.245330	-0.357446
H	-0.552184	1.612741	0.600361
H	0.060856	-0.777444	1.213444
H	0.330849	-1.137305	-0.478137
H	1.971672	0.918137	1.152295
H	3.820496	0.152872	-0.219461
H	2.697672	-0.998247	-1.130302
H	-0.340986	1.222360	-1.083242

0 imaginary frequencies
E = -270.049267
H = -270.041229
G = -270.077771

3

C	-1.374756	0.648662	0.000000
C	0.000000	0.397391	0.000000
C	0.901697	1.469014	0.000000
C	0.431166	2.773914	0.000000
C	-0.941323	3.034352	0.000000
C	-1.832459	1.968272	0.000000
O	0.562602	-0.846942	0.000000
C	-0.285071	-1.984643	0.000000
C	0.536021	-3.238682	0.000000
C	1.861948	-3.297199	0.000000
H	1.962682	1.250380	0.000000
H	1.139818	3.594694	0.000000
H	-1.306089	4.054559	0.000000
H	-2.900993	2.153486	0.000000
H	-2.090829	-0.161683	0.000000
H	-0.939022	-1.971442	0.884586
H	-0.939022	-1.971442	-0.884586
H	-0.053842	-4.152626	0.000000
H	2.379182	-4.249376	0.000000
H	2.463972	-2.397491	0.000000

0 imaginary frequencies
E = -423.393629
H = -423.383548
G = -423.425558

TS-3

C	2.538127	-0.515730	-0.486804
C	2.287854	0.825597	-0.304350
C	1.087337	1.397666	-0.723101
H	2.904372	1.375841	0.400224
H	0.891678	2.447500	-0.544823
H	0.521535	0.951054	-1.531740
O	1.061950	-1.278081	0.901597
H	2.021844	-1.081516	-1.250316
H	3.408266	-0.987569	-0.050393
C	-0.029092	-0.731140	0.548590
C	-0.308270	0.652046	0.865439
C	-0.984877	-1.404388	-0.292753
H	0.294857	1.107517	1.639782
C	-2.163864	-0.803102	-0.646438
H	-0.757053	-2.423469	-0.585117
H	-2.888917	-1.346636	-1.243794
C	-2.468361	0.522247	-0.230031
C	-1.569942	1.222472	0.532793
H	-3.420526	0.963073	-0.502039
H	-1.805124	2.224845	0.875368

1 imaginary frequency

E = -423.338564

H = -423.329067

G = -423.368683

TS-3-boat (3.9 kcal mol⁻¹ higher in energy than the chair TS TS-3)

H	0.524623	2.123718	1.095045
C	1.206444	1.579466	0.454482
C	1.957792	0.518626	0.961866
H	1.712442	0.146298	1.952287
C	2.738044	-0.259502	0.144686
O	1.042387	-1.330690	-0.890985
C	-0.036189	-0.771509	-0.536421
C	-0.342715	0.585769	-0.932607
H	1.557416	2.112403	-0.419582
H	3.020097	0.074162	-0.844237
H	3.228574	-1.149999	0.513224
C	-0.962305	-1.397542	0.373415
H	0.223315	0.982080	-1.765481
C	-1.592059	1.172056	-0.591584
C	-2.136701	-0.784200	0.720296
H	-0.712858	-2.391719	0.726695
H	-2.838751	-1.294246	1.372383
C	-2.465329	0.511614	0.234764
H	-1.843941	2.151565	-0.985094
H	-3.411907	0.962582	0.509273

1 imaginary frequency

E = -423.331945

H = -423.322246

G = -423.362463

4

C	1.129330	1.026320	0.067916
O	1.043126	2.241161	0.006385
C	2.394939	0.321534	-0.165009
H	3.262467	0.942382	-0.356001
C	2.453100	-1.026659	-0.191245
H	3.399003	-1.518923	-0.396498
C	1.281366	-1.860588	0.025433
H	1.391997	-2.936842	-0.044291
C	0.089210	-1.310883	0.299671
H	-0.786316	-1.933449	0.454503
C	-0.102799	0.171399	0.420124

H	-0.272028	0.384017	1.489464
C	-1.361625	0.683963	-0.335701
H	-1.306246	1.776425	-0.311144
H	-1.303823	0.376378	-1.384267
C	-2.649821	0.218001	0.275042
H	-2.828467	0.541182	1.300362
C	-3.564667	-0.533404	-0.331862
H	-4.484731	-0.821602	0.163997
H	-3.431060	-0.876967	-1.353422

0 imaginary frequencies
E = -423.379211
H = -423.368904
G = -423.411541

6

C	2.317571	-1.292703	0.142465
C	0.946619	-1.063676	0.217504
C	0.439318	0.232961	0.098134
C	1.326978	1.292475	-0.099787
C	2.700121	1.065184	-0.165932
C	3.199063	-0.229206	-0.045348
C	-1.038884	0.502947	0.226367
O	-1.771063	-0.568267	-0.368896
C	-3.123961	-0.508042	-0.303331
C	-3.889600	0.441028	0.236882
H	0.943464	2.302321	-0.207581
H	3.377286	1.897613	-0.321534
H	4.266626	-0.409349	-0.102898
H	2.698888	-2.303990	0.230896
H	0.260271	-1.890222	0.353991
H	-1.326109	0.584872	1.284024
H	-1.300419	1.448739	-0.262852
H	-3.549505	-1.385264	-0.778437
H	-4.964190	0.325749	0.199639
H	-3.501155	1.329861	0.714197

0 imaginary frequencies
E = -423.395787
H = -423.385709
G = -423.428299
E_{gas} = -424.278323
E_{xylenes} = -424.287826
E_{DMF} = -424.288598

TS-6

C	1.492451	-1.182471	0.670746
C	0.234108	-0.543282	0.905425
C	0.058763	0.828465	0.498807
C	1.029108	1.375880	-0.404210
C	2.171645	0.692460	-0.709356
C	2.423408	-0.588189	-0.133396
C	-1.110342	1.499964	0.801924
O	-2.425621	0.400608	-0.567316
C	-2.216743	-0.815943	-0.320285
C	-1.034669	-1.476370	-0.676380
H	-2.907853	-1.354891	0.355497
H	-0.930810	-2.535845	-0.468627
H	-0.421341	-1.066099	-1.468294
H	-0.379443	-0.915239	1.715629
H	0.853065	2.364990	-0.813009
H	2.910772	1.133271	-1.368495
H	3.367081	-1.083758	-0.332850
H	1.681295	-2.154953	1.110855
H	-1.754854	1.177317	1.606460
H	-1.299317	2.487262	0.401708

1 imaginary frequency
E = -423.334190
H = -423.324628
G = -423.364331
E_{gas} = -424.212413
E_{xylenes} = -424.222870
E_{DMF} = -424.224800

TS-6-boat (2.8 kcal mol⁻¹ higher in energy than the chair TS **TS-6**)

C	1.097513	-1.491897	0.926109
C	-0.063086	-0.842635	0.568829
C	-0.294622	0.517671	0.988032
H	0.240417	0.867903	1.859991
H	1.732980	-1.118830	1.714928
H	1.328073	-2.473917	0.534351
C	-0.958432	-1.391130	-0.410274
H	-0.740944	-2.373359	-0.816005
C	-2.078447	-0.713165	-0.798538
H	-2.758248	-1.152526	-1.519726
C	-2.384818	0.560909	-0.236153
H	-3.309517	1.055178	-0.512231
C	-1.525256	1.153326	0.647036
H	-1.756195	2.121491	1.076657
O	2.517705	-0.286042	-0.415155
C	1.811054	0.603333	-0.945887
H	1.467854	0.472312	-1.989210
C	1.266616	1.682499	-0.232856
H	1.746945	1.983892	0.689329
H	0.683863	2.432732	-0.754629

1 imaginary frequency
E = -423.329282
H = -423.319503
G = -423.359875

7

C	-1.093534	0.966968	-0.182517
C	-1.223623	2.275359	-0.456656
H	-2.143024	2.807558	-0.238684
H	-0.422200	2.846851	-0.912492
C	-2.199129	0.189426	0.365623
H	-3.074848	0.728259	0.713083
C	-2.172761	-1.158525	0.377493
H	-3.022211	-1.716895	0.755646
C	-1.038363	-1.894000	-0.168529
H	-1.113183	-2.972691	-0.255975
C	0.069214	-1.256678	-0.571095
H	0.915594	-1.795007	-0.980017
C	0.230337	0.236929	-0.401636
H	0.719845	0.641537	-1.292746
C	1.184034	0.516658	0.789498
C	2.624933	0.134810	0.554009
H	0.837217	0.009921	1.699016
H	1.175919	1.588699	1.033547
O	3.068035	-0.315776	-0.472591
H	3.295966	0.322289	1.422213

0 imaginary frequencies
E = -423.375707
H = -423.365449
G = -423.407542

6b

C	3.951307	-0.647483	-0.048186
C	2.879623	-1.502961	0.196252
C	1.578883	-1.006351	0.249559

C	1.337338	0.354385	0.052604
C	2.414919	1.206841	-0.202107
C	3.715135	0.711350	-0.247361
C	-0.053103	0.933913	0.152911
O	-1.012209	-0.090183	-0.090943
C	-2.320527	0.228115	0.015332
C	-2.835454	1.436994	0.288833
H	2.237199	2.264965	-0.369484
H	4.541627	1.384249	-0.447106
H	4.962448	-1.036520	-0.089199
H	3.054632	-2.562726	0.345348
H	0.743763	-1.670595	0.430504
H	-0.220641	1.352954	1.154199
H	-0.181019	1.744836	-0.573896
O	-3.004934	-0.912749	-0.210304
H	-3.900444	1.589248	0.354410
H	-2.201104	2.293564	0.447587
C	-4.424464	-0.846417	-0.177935
H	-4.772465	-1.854425	-0.395237
H	-4.783988	-0.538404	0.809407
H	-4.804795	-0.153999	-0.935957

0 imaginary frequencies
E = -537.762357
H = -537.749773
G = -537.799117
E_{gas} = -538.837257
E_{xylenes} = -538.847931
E_{DMF} = -538.850147

TS-6b

C	-3.058132	-0.882531	-0.015368
C	-1.953506	-1.366960	-0.669286
C	-0.809547	-0.545114	-0.839914
C	-0.876898	0.841124	-0.487121
C	-2.015861	1.284494	0.254470
C	-3.077764	0.449579	0.478163
C	0.224876	1.664610	-0.696382
O	1.515719	0.932359	0.823307
C	1.569742	-0.313087	0.649702
C	0.561054	-1.196846	1.016724
O	2.571192	-0.860560	-0.123530
H	0.687324	-2.259542	0.861010
H	-0.180127	-0.856928	1.722886
H	-0.014043	-0.878679	-1.494245
H	-2.037446	2.309456	0.608827
H	-3.949260	0.807623	1.014216
H	-3.926195	-1.516314	0.128484
H	-1.934619	-2.385768	-1.038714
H	0.965743	1.412422	-1.441410
H	0.219367	2.689576	-0.350857
C	3.689291	-0.012653	-0.392219
H	4.408231	-0.635447	-0.923060
H	3.414025	0.843105	-1.013113
H	4.132178	0.360411	0.535151

1 imaginary frequency
E = -537.716945
H = -537.704587
G = -537.751416
E_{gas} = -538.788900
E_{xylenes} = -538.799259
E_{DMF} = -538.801338

TS-6b-boat (2.3 kcal mol⁻¹ higher in energy than the chair TS **TS-6b**)

C	2.234095	-0.823248	-0.757017
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C	1.240935	-1.166001	0.191840
C	0.762612	-0.173777	1.107868
C	1.180694	1.180825	0.903908
C	2.104185	1.495600	-0.054822
C	2.649226	0.479359	-0.884074
C	-0.215609	-0.501736	2.036591
O	-1.958438	-0.735710	0.733833
C	-1.579875	-0.602853	-0.456320
C	-0.812966	-1.541106	-1.146660
H	1.072304	-2.206969	0.427048
H	-0.412448	-1.529616	2.299770
H	-0.635673	0.254206	2.686862
H	0.773519	1.951822	1.549446
H	2.433580	2.520601	-0.180126
H	3.403518	0.739324	-1.618337
H	2.654770	-1.597296	-1.388466
O	-1.788669	0.576745	-1.124427
H	-0.817081	-2.556652	-0.782387
H	-0.524554	-1.357086	-2.172148
C	-2.531938	1.574966	-0.425999
H	-2.733806	2.355743	-1.158286
H	-3.469080	1.172544	-0.035149
H	-1.956340	1.992918	0.404634

l imaginary frequency
E = -537.712842
H = -537.700336
G = -537.747716

7b

C	0.653707	0.234516	0.571067
C	1.917396	0.955054	0.103105
C	2.897651	0.170436	-0.638814
C	2.860846	-1.177223	-0.645414
C	1.840678	-1.905505	0.099582
C	0.832077	-1.260873	0.701316
C	2.103360	2.263557	0.341818
C	-0.506529	0.530659	-0.415185
C	-1.863677	0.109882	0.108757
O	-2.109407	-0.242486	1.236412
H	2.969017	2.789140	-0.046190
H	1.403319	2.842324	0.934780
H	3.696619	0.704398	-1.143322
H	3.621557	-1.740856	-1.174576
H	1.921016	-2.985212	0.168510
H	0.073232	-1.795476	1.260092
H	0.348736	0.638051	1.540843
H	-0.333174	0.050086	-1.381410
H	-0.553118	1.607601	-0.612119
O	-2.799329	0.208206	-0.858280
C	-4.143579	-0.124652	-0.464702
H	-4.749910	0.012687	-1.357096
H	-4.196254	-1.158279	-0.119522
H	-4.482732	0.534669	0.335772

0 imaginary frequencies
E = -537.770952
H = -537.758125
G = -537.807117

Allyl radical

C	0.000000	0.000000	0.441876
H	0.000000	0.000000	1.530002
C	0.000000	1.226812	-0.195739
C	0.000000	-1.226812	-0.195739
H	0.000000	-1.295503	-1.278179

H	0.000000	-2.154477	0.361982
H	0.000000	1.295503	-1.278179
H	0.000000	2.154477	0.361982

0 imaginary frequencies
E = -117.009498
H = -117.004710
G = -117.030974

Oxallyl radical

O	-1.192068	0.112498	0.000000
C	0.000000	0.427886	0.000000
C	1.055850	-0.526692	0.000000
H	0.295057	1.494343	0.000000
H	2.095076	-0.219216	0.000000
H	0.811309	-1.582269	0.000000

0 imaginary frequencies
E = -152.932831
H = -152.928347
G = -152.954732

Phenoxy radical

O	0.000000	0.000000	2.300007
C	0.000000	0.000000	1.048569
C	0.000000	1.237783	0.288993
C	0.000000	1.223477	-1.085674
C	0.000000	0.000000	-1.782221
C	0.000000	-1.223477	-1.085674
C	0.000000	-1.237783	0.288993
H	0.000000	2.160865	0.856591
H	0.000000	2.153987	-1.642493
H	0.000000	0.000000	-2.866167
H	0.000000	-2.153987	-1.642493
H	0.000000	-2.160865	0.856591

0 imaginary frequencies
E = -306.302693
H = -306.296424
G = -306.328585

Benzyl radical

C	0.000000	0.000000	2.397425
C	0.000000	0.000000	0.993604
C	0.000000	1.216281	0.251231
C	0.000000	1.209620	-1.131356
C	0.000000	0.000000	-1.835757
C	0.000000	-1.209620	-1.131356
C	0.000000	-1.216281	0.251231
H	0.000000	2.157318	0.790869
H	0.000000	2.148846	-1.673502
H	0.000000	0.000000	-2.919394
H	0.000000	-2.148846	-1.673502
H	0.000000	-2.157318	0.790869
H	0.000000	-0.926813	2.957263
H	0.000000	0.926813	2.957263

0 imaginary frequencies
E = -270.378058
H = -270.371372
G = -270.404095

2-Methoxy oxallyl radical

C	0.983619	1.600895	0.000000
C	0.000000	0.540425	0.000000
O	-1.204437	0.709093	0.000000
O	0.582293	-0.687945	0.000000

H	2.041572	1.379175	0.000000
H	0.632153	2.622440	0.000000
C	-0.327889	-1.797087	0.000000
H	0.296399	-2.687970	0.000000
H	-0.963676	-1.774114	0.887338
H	-0.963676	-1.774114	-0.887338

0 imaginary frequencies
E = -267.321602
H = -267.314787
G = -267.348004

2. B3LYP/6-31G(d) and single-point energy calculations relevant to Table 1, Table 3, and Figure S2

The Cartesian coordinates of species optimised with B3LYP/6-31G(d) are given below. For these species, single-point energy calculations were also performed with SCS-MP2/cc-pVTZ and in certain cases with M06-2X/cc-pVTZ and ω B97X-D/cc-pVTZ using the B3LYP/6-31G(d) geometries. As appropriate, underneath each set of coordinates below are listed the following energies (in Hartree):

E: B3LYP/6-31G(d) electronic potential energy (excluding zero-point energy)

H: B3LYP/6-31G(d) enthalpy at 298.15 K

G: B3LYP/6-31G(d) Gibbs free energy at 298.15 K and 1 mol L⁻¹

E_{M06-2X}: M06-2X/cc-pVTZ single-point electronic potential energy

E _{ω B97X-D}: ω B97X-D/cc-pVTZ single-point electronic potential energy

E_{SCS-MP2}: SCS-MP2/cc-pVTZ single-point electronic potential energy

1

C	2.529520	0.360958	-0.000175
H	3.588642	0.130909	-0.000337
H	2.248754	1.407495	-0.000099
C	1.650609	-0.646067	-0.000074
H	1.966873	-1.685718	-0.000138
O	0.294161	-0.585953	0.000126
C	-0.296973	0.705123	0.000107
H	0.043308	1.269326	-0.883784
H	0.043306	1.269365	0.883972
C	-1.793032	0.591589	0.000107
H	-2.310059	1.551149	0.000255
C	-2.485603	-0.545403	-0.000066
H	-1.989536	-1.510311	-0.000202
H	-3.571700	-0.541789	-0.000063

0 imaginary frequencies

E = -270.507232

H = -270.380517

G = -270.415804

E_{M06-2X} = -270.487256

E _{ω B97X-D} = -270.515450

E_{SCS-MP2} = -269.947112

TS-1

O	0.511360	-1.358147	-0.252509
C	1.291480	-0.471808	0.261666
C	1.465903	0.784780	-0.289625
H	1.224960	0.954436	-1.332617
C	-1.285061	-0.900738	0.182352
C	-1.374829	0.412085	-0.301796
H	-1.765741	-1.712702	-0.352650
H	-1.172829	-1.069549	1.249193
H	-1.692562	0.555931	-1.332768
C	-0.669360	1.425173	0.322008
H	1.677419	-0.646237	1.281446
H	2.145381	1.493089	0.179226
H	-0.630138	2.424689	-0.102309
H	-0.446174	1.368570	1.382923

1 imaginary frequency

E = -270.461128

H = -270.337139

G = -270.370093

E_{M06-2X} = -270.432782

E _{ω B97X-D} = -270.461642

E_{SCS-MP2} = -269.896937

2

C	-0.599118	0.782919	-0.114936
C	-2.041232	0.334248	-0.182848
H	-2.763817	1.130076	-0.476397
O	-2.427313	-0.789063	0.054928
C	0.383604	-0.334285	0.263221
C	1.797651	0.162752	0.388462
C	2.824661	-0.249120	-0.355550
H	-0.550493	1.620629	0.599457
H	0.052472	-0.776650	1.212552
H	0.327172	-1.135064	-0.482519
H	1.969525	0.924623	1.151648
H	3.827022	0.147832	-0.218912
H	2.702961	-1.006400	-1.127729
H	-0.339733	1.228377	-1.087623

0 imaginary frequencies

E = -270.535753

H = -270.409432

G = -270.445801

E_{M06-2X} = -270.510505

E_{ωB97X-D} = -270.544038

E_{SCS-MP2} = -269.977694

3

C	-1.377434	0.645699	0.000000
C	0.000000	0.396467	0.000000
C	0.903381	1.469665	0.000000
C	0.430891	2.776878	0.000000
C	-0.944318	3.036271	0.000000
C	-1.836638	1.967189	0.000000
O	0.565475	-0.848253	0.000000
C	-0.284600	-1.982929	0.000000
C	0.536363	-3.239665	0.000000
C	1.866301	-3.298202	0.000000
H	1.966777	1.250891	0.000000
H	1.140892	3.599853	0.000000
H	-1.310946	4.058583	0.000000
H	-2.907899	2.151659	0.000000
H	-2.093327	-0.168124	0.000000
H	-0.942639	-1.965613	0.884634
H	-0.942639	-1.965613	-0.884634
H	-0.055933	-4.154663	0.000000
H	2.386832	-4.251399	0.000000
H	2.471412	-2.397792	0.000000

0 imaginary frequencies

E = -424.164459

H = -423.987768

G = -424.029582

E_{M06-2X} = -424.133257

E_{ωB97X-D} = -424.164729

E_{SCS-MP2} = -423.252721

TS-3

C	2.511397	-0.518980	-0.485286
C	2.275949	0.831485	-0.316291
C	1.060611	1.399158	-0.714062
H	2.898756	1.382514	0.386064
H	0.873058	2.455785	-0.548910
H	0.495091	0.957886	-1.529526
O	1.085129	-1.270558	0.894344
H	1.998549	-1.081314	-1.257452
H	3.391110	-0.992530	-0.063361
C	-0.017966	-0.728711	0.548644

C	-0.290607	0.662083	0.850561
C	-0.976116	-1.412433	-0.281536
H	0.306918	1.118394	1.632393
C	-2.161931	-0.814991	-0.633068
H	-0.746713	-2.434308	-0.571181
H	-2.891340	-1.365843	-1.222868
C	-2.467472	0.514691	-0.223612
C	-1.564272	1.224496	0.529269
H	-3.425220	0.951263	-0.493245
H	-1.798794	2.231837	0.865625

1 imaginary frequency

E = -424.106008

H = -423.932138

G = -423.971424

$E_{M06-2X} = -424.066235$

$E_{\omega B97X-D} = -424.099489$

$E_{SCS-MP2} = -423.193201$

4

C	1.139453	1.022170	0.072565
O	1.070984	2.245760	0.030710
C	2.386919	0.302292	-0.207367
H	3.257576	0.911434	-0.431450
C	2.429099	-1.050646	-0.220180
H	3.363868	-1.557692	-0.451398
C	1.255859	-1.869224	0.048688
H	1.355185	-2.949962	-0.006244
C	0.075086	-1.300761	0.351534
H	-0.805058	-1.911174	0.541039
C	-0.101331	0.187079	0.444975
H	-0.285834	0.428566	1.507221
C	-1.348476	0.693229	-0.341310
H	-1.288119	1.788305	-0.331119
H	-1.273966	0.369468	-1.386418
C	-2.648330	0.234842	0.255101
H	-2.846485	0.575280	1.273626
C	-3.549691	-0.535604	-0.356628
H	-4.479791	-0.823024	0.126361
H	-3.396764	-0.897543	-1.371570

0 imaginary frequencies

E = -424.147018

H = -423.971061

G = -424.013499

$E_{M06-2X} = -424.112023$

$E_{\omega B97X-D} = -424.149498$

$E_{SCS-MP2} = -423.238974$

6

C	2.328668	-1.290717	0.152713
C	0.955124	-1.068620	0.241471
C	0.436856	0.226239	0.113784
C	1.316859	1.291194	-0.103506
C	2.693490	1.071758	-0.182404
C	3.202678	-0.220785	-0.055513
C	-1.043229	0.483387	0.257137
O	-1.768768	-0.544287	-0.417833
C	-3.123816	-0.490099	-0.342815
C	-3.889617	0.420861	0.266087
H	0.923703	2.299467	-0.214760
H	3.364807	1.909350	-0.352542
H	4.273243	-0.395177	-0.122738
H	2.718358	-2.300948	0.247325
H	0.274423	-1.900315	0.395700
H	-1.340579	0.486816	1.317479

H	-1.310392	1.463856	-0.161045
H	-3.549660	-1.335109	-0.877394
H	-4.967044	0.309403	0.226733
H	-3.498781	1.277644	0.802183

0 imaginary frequencies

E = -424.166402

H = -423.989231

G = -424.031439

E_{M06-2X} = -424.135169

E_{ωB97X-D} = -424.166977

E_{SCS-MP2} = -423.255753

TS-6

C	1.494958	-1.189339	0.656173
C	0.224447	-0.562481	0.886375
C	0.048166	0.818907	0.501928
C	1.024348	1.387909	-0.381890
C	2.176556	0.714456	-0.690122
C	2.430178	-0.576653	-0.134031
C	-1.139601	1.472230	0.794333
O	-2.412315	0.410734	-0.565690
C	-2.209528	-0.816215	-0.328747
C	-1.018533	-1.470498	-0.674915
H	-2.904275	-1.355006	0.345652
H	-0.918543	-2.535819	-0.480926
H	-0.406952	-1.062786	-1.472573
H	-0.382304	-0.941483	1.702499
H	0.846778	2.385896	-0.775083
H	2.921375	1.172991	-1.334669
H	3.380264	-1.064762	-0.335408
H	1.685266	-2.169860	1.083852
H	-1.777019	1.146806	1.607139
H	-1.332016	2.468253	0.410402

1 imaginary frequency

E = -424.099661

H = -423.926118

G = -423.965477

E_{M06-2X} = -424.059736

E_{ωB97X-D} = -424.093189

E_{SCS-MP2} = -423.189097

7

C	-1.092032	0.968165	-0.186704
C	-1.206762	2.285316	-0.441698
H	-2.125352	2.825885	-0.228527
H	-0.393008	2.860546	-0.876439
C	-2.213304	0.196376	0.339516
H	-3.095540	0.743368	0.664708
C	-2.192444	-1.154975	0.363409
H	-3.054119	-1.708507	0.727815
C	-1.046183	-1.899393	-0.147140
H	-1.119397	-2.982182	-0.214370
C	0.070720	-1.266451	-0.543281
H	0.926794	-1.813112	-0.926425
C	0.231900	0.231235	-0.400064
H	0.720394	0.622015	-1.301290
C	1.192472	0.531885	0.782224
C	2.631141	0.135534	0.546782
H	0.844723	0.045042	1.704959
H	1.188320	1.611239	1.004291
O	3.068078	-0.337865	-0.480171
H	3.309515	0.332478	1.408382

0 imaginary frequencies

E = -424.139729

H = -423.964320
 G = -424.006281
 $E_{M06-2X} = -424.107197$
 $E_{\omega B97X-D} = -424.143258$
 $E_{SCS-MP2} = -423.235622$

6a

C	4.230544	0.274227	0.062234
C	3.339676	1.315659	-0.210028
C	1.971335	1.064041	-0.298602
C	1.474888	-0.231619	-0.107264
C	2.371497	-1.267234	0.173659
C	3.743279	-1.018826	0.253260
C	-0.000337	-0.518004	-0.247128
O	-0.741275	0.508259	0.402979
C	-2.107468	0.438841	0.320046
C	-2.828373	-0.519060	-0.283615
H	1.995001	-2.275148	0.334610
H	4.427758	-1.833796	0.473538
H	5.297196	0.471456	0.129017
H	3.712514	2.326298	-0.355137
H	1.276920	1.873507	-0.502436
H	-0.292143	-0.551683	-1.310115
H	-0.246836	-1.497459	0.189828
H	-2.553032	1.285502	0.827536
O	-4.193685	-0.584390	-0.364288
H	-2.386090	-1.370469	-0.785696
C	-4.923091	0.461559	0.249653
H	-5.978967	0.239391	0.083327
H	-4.724754	0.507668	1.330235
H	-4.679587	1.436280	-0.197527

0 imaginary frequencies

E = -538.680043
 H = -538.466914
 G = -538.515505
 $E_{SCS-MP2} = -537.567905$

TS-6a

C	1.044018	-2.279799	0.053417
C	0.277778	-1.569041	0.938999
C	0.390650	-0.140066	1.010477
C	1.493911	0.510627	0.339657
C	2.215738	-0.264930	-0.634891
C	1.999879	-1.608929	-0.772405
C	1.722439	1.861231	0.506724
O	-0.148308	2.461663	-0.653373
C	-1.100977	1.850236	-0.115401
C	-1.306279	0.458939	-0.298335
H	-1.729360	2.329737	0.661052
O	-2.419290	-0.101302	0.258218
H	-0.880039	-0.030649	-1.171064
H	-0.039504	0.352339	1.877126
H	2.973734	0.234929	-1.233142
H	2.580635	-2.183536	-1.489098
H	0.940860	-3.359468	-0.019902
H	-0.445205	-2.070474	1.576229
H	1.298701	2.412460	1.336783
H	2.471385	2.378296	-0.083714
C	-2.955285	-1.220953	-0.439819
H	-3.798740	-1.581055	0.153080
H	-3.311436	-0.929185	-1.436990
H	-2.211489	-2.020177	-0.539660

1 imaginary frequency

E = -538.619825

H = -538.411089
G = -538.457717
E_{SCS-MP2} = -537.510329

Int-6a

C	-2.378998	0.470044	-0.140658
C	-1.080714	1.028469	-0.508475
C	0.090902	0.061099	-0.714853
C	-0.305503	-1.394209	-0.729915
C	-1.547933	-1.812309	-0.441919
C	-2.604751	-0.861725	-0.113040
C	-0.928113	2.356857	-0.676374
C	1.268837	0.288697	0.295236
C	2.601404	-0.180328	-0.292334
O	2.888331	-0.120261	-1.466352
H	0.557989	0.294793	-1.682301
H	0.012781	2.798304	-0.995168
H	-1.753727	3.044118	-0.512156
O	1.169231	-0.361568	1.539872
H	1.364210	1.381568	0.442743
H	3.310056	-0.567646	0.469757
H	-3.179260	1.172216	0.082594
H	-3.590076	-1.244143	0.140648
H	-1.788322	-2.872324	-0.455167
H	0.477177	-2.109247	-0.972180
C	0.237951	0.200211	2.451513
H	0.391980	-0.312205	3.404681
H	0.415926	1.277851	2.587752
H	-0.797721	0.050507	2.125546

0 imaginary frequencies

E = -538.650269
H = -538.439614
G = -538.487886
E_{SCS-MP2} = -537.549146

6b

C	3.956231	-0.631864	-0.082799
C	2.907347	-1.479534	0.280226
C	1.604320	-0.989681	0.368520
C	1.334488	0.354363	0.085425
C	2.387758	1.196253	-0.287222
C	3.693243	0.709075	-0.365786
C	-0.058664	0.919039	0.229837
O	-1.009338	-0.080488	-0.129164
C	-2.320764	0.219461	0.021566
C	-2.840614	1.395653	0.413270
H	2.186220	2.239719	-0.520742
H	4.501214	1.374698	-0.657916
H	4.970824	-1.015453	-0.150018
H	3.103826	-2.526622	0.495628
H	0.786598	-1.649040	0.641256
H	-0.247562	1.232858	1.267763
H	-0.185571	1.803242	-0.409658
O	-3.003393	-0.902502	-0.304255
H	-3.907808	1.534911	0.507961
H	-2.210299	2.242519	0.641955
C	-4.420268	-0.836269	-0.260466
H	-4.774474	-1.820343	-0.571570
H	-4.776687	-0.620465	0.754788
H	-4.802890	-0.071072	-0.947522

0 imaginary frequencies

E = -538.693926

H = -538.481246

G = -538.529843

E_{SCS-MP2} = -537.584557

TS-6b

C	-3.061555	-0.874065	-0.014856
C	-1.951293	-1.373755	-0.652022
C	-0.793252	-0.560484	-0.814668
C	-0.862887	0.835704	-0.486693
C	-2.009956	1.296220	0.233621
C	-3.081090	0.468121	0.458735
C	0.255579	1.646824	-0.682809
O	1.504666	0.937752	0.820231
C	1.563695	-0.315705	0.651481
C	0.538943	-1.193181	0.998769
O	2.568795	-0.865681	-0.116142
H	0.663564	-2.260579	0.854214
H	-0.197443	-0.856209	1.715064
H	-0.005479	-0.898338	-1.480713
H	-2.031329	2.329594	0.571231
H	-3.960039	0.840224	0.977768
H	-3.937014	-1.502269	0.128165
H	-1.933859	-2.399170	-1.010603
H	0.994434	1.391524	-1.432845
H	0.249742	2.680846	-0.355954
C	3.677149	-0.010745	-0.390760
H	4.406235	-0.632834	-0.914222
H	3.395593	0.837239	-1.023611
H	4.115915	0.379801	0.533999

1 imaginary frequency

E = -538.644212

H = -538.434958

G = -538.481216

E_{SCS-MP2} = -537.531684

Int-6b

C	2.918553	0.155046	-0.613956
C	1.924516	0.950583	0.099188
C	0.653032	0.239110	0.567678
C	0.812849	-1.260429	0.687820
C	1.827178	-1.916202	0.099558
C	2.873262	-1.195868	-0.618671
C	2.103194	2.268662	0.308338
C	-0.508720	0.555267	-0.412995
C	-1.866971	0.127370	0.109609
O	-2.117801	-0.199995	1.250675
H	0.352602	0.641256	1.542549
H	1.391197	2.863277	0.875412
H	2.974252	2.790940	-0.078986
H	-0.335046	0.090270	-1.389333
H	-0.549801	1.638532	-0.591710
H	3.733580	0.684604	-1.102445
H	3.644593	-1.767017	-1.129124
H	1.892365	-2.999949	0.160452
H	0.033481	-1.790939	1.226713
O	-2.798338	0.188321	-0.867517
C	-4.136581	-0.150509	-0.466482
H	-4.745634	-0.047639	-1.365034
H	-4.176806	-1.176088	-0.090032
H	-4.487542	0.527965	0.315741

0 imaginary frequencies

E = -538.697667

H = -538.485567
G = -538.534231
E_{SCS-MP2} = -537.593851

6c

C	3.474006	-0.322330	0.006773
C	2.636149	-1.356625	0.424551
C	1.250016	-1.232209	0.307251
C	0.690019	-0.067224	-0.225788
C	1.535688	0.967613	-0.646753
C	2.919268	0.841605	-0.530440
C	-0.811422	0.096077	-0.425174
O	-1.469426	-0.914547	0.326759
C	-2.780307	-1.185393	0.037130
C	-3.630185	-0.477687	-0.709012
H	1.100823	1.874149	-1.057871
H	3.564356	1.652502	-0.858521
H	4.552451	-0.421677	0.097832
H	3.060138	-2.265048	0.844610
H	0.598303	-2.035345	0.631792
O	-1.272774	1.391314	-0.124191
H	-1.075311	-0.034302	-1.482938
H	-3.068233	-2.113932	0.522844
H	-4.634540	-0.859000	-0.856658
H	-3.375918	0.474940	-1.156279
C	-1.170703	1.775030	1.246805
H	-1.516292	2.809969	1.293370
H	-1.807319	1.149971	1.882727
H	-0.136023	1.720485	1.606486

0 imaginary frequencies

E = -538.691430
H = -538.478913
G = -538.526921
E_{SCS-MP2} = -537.583822

TS-6c

C	-3.040526	-0.136509	0.319722
C	-2.139195	0.440337	1.176698
C	-0.732574	0.266718	0.971764
C	-0.303024	-0.728223	0.024729
C	-1.263401	-1.255667	-0.892519
C	-2.595800	-0.964204	-0.754235
C	1.047659	-1.022785	-0.132042
O	1.465755	0.887008	-1.328751
C	1.122073	1.773318	-0.495288
C	-0.215651	2.095879	-0.222772
H	1.888551	2.212495	0.174704
H	-0.443923	2.906213	0.465563
H	-0.969336	1.856753	-0.965479
H	-0.057128	0.529717	1.775917
H	-0.922783	-1.917414	-1.685364
H	-3.322578	-1.390352	-1.439819
H	-4.106359	0.026398	0.458386
H	-2.478251	1.071415	1.993602
O	1.915513	-0.760190	0.850166
H	1.397283	-1.653508	-0.947030
C	3.296829	-0.824784	0.473998
H	3.871405	-0.616301	1.377261
H	3.545399	-1.826793	0.101532
H	3.489235	-0.077639	-0.300927

1 imaginary frequency
E = -538.632498
H = -538.423150
G = -538.468629
E_{SCS-MP2} = -537.520227

Int-6c

C	0.116346	-2.262529	0.390463
C	-0.449263	-0.961147	0.079650
C	0.485904	0.194477	-0.271451
C	1.873617	-0.276232	-0.650451
C	2.303035	-1.526113	-0.406193
C	1.423648	-2.533923	0.175397
C	-1.787192	-0.786369	0.126392
C	0.567070	1.201662	0.907451
C	1.207962	2.526207	0.569913
O	1.596043	2.861285	-0.528909
H	0.057067	0.753063	-1.114041
O	-2.361818	0.422607	-0.133667
H	-2.470307	-1.591686	0.397656
H	1.106584	0.765302	1.760733
H	-0.443454	1.427870	1.279542
H	1.292207	3.228495	1.431828
H	-0.551673	-3.031398	0.774427
H	1.824404	-3.519235	0.396905
H	3.321200	-1.812891	-0.659767
H	2.528734	0.466942	-1.094598
C	-3.765814	0.395113	-0.358215
H	-4.294789	-0.053956	0.493726
H	-4.083740	1.433024	-0.472952
H	-4.011901	-0.163542	-1.270583

0 imaginary frequencies

E = -538.663839
H = -538.452542
G = -538.501733
E_{SCS-MP2} = -537.559199

6d

C	2.708633	-1.474404	-0.000536
C	1.604808	-2.321147	-0.000410
C	0.315842	-1.777669	0.000019
C	0.118954	-0.399091	0.000274
C	1.245688	0.447024	0.000132
C	2.536541	-0.086349	-0.000280
C	-1.251081	0.234424	0.000539
O	-2.245911	-0.782776	0.001430
C	-3.541248	-0.377286	-0.000031
C	-4.025049	0.868748	-0.001278
O	0.960469	1.787791	0.000486
H	3.404867	0.562536	-0.000341
H	3.715331	-1.883879	-0.000853
H	1.738619	-3.399034	-0.000631
H	-0.553969	-2.424804	0.000103
H	-1.378938	0.879392	0.882118
H	-1.379784	0.878534	-0.881525
H	-4.192748	-1.247152	-0.000108
H	-5.099475	1.011816	-0.002478
H	-3.404768	1.756995	-0.001255
C	2.039575	2.708147	-0.000057
H	1.586765	3.701458	-0.000025
H	2.666174	2.594944	0.894398
H	2.665482	2.594690	-0.894966

0 imaginary frequencies

E = -538.689837

H = -538.477311
G = -538.525194
E_{SCS-MP2} = -537.579339

TS-6d

C	2.355029	0.853161	0.531095
C	1.128491	1.399507	0.278318
C	0.071537	0.588290	-0.277302
C	0.411644	-0.731292	-0.798821
C	1.700512	-1.261665	-0.449058
C	2.641414	-0.505345	0.191005
C	-0.539649	-1.496948	-1.429890
O	-1.708691	-1.983897	0.483602
C	-1.840443	-0.874116	1.057342
C	-0.767947	-0.166393	1.638168
H	-2.805773	-0.334291	0.973020
H	-0.978235	0.740281	2.200975
H	0.128131	-0.708999	1.920027
O	-1.013123	1.156697	-0.891860
H	1.922174	-2.282707	-0.748652
H	3.618471	-0.920086	0.420624
H	3.127177	1.459987	0.996815
H	0.923591	2.430127	0.545165
H	-1.459312	-1.068522	-1.800802
H	-0.315080	-2.517040	-1.721478
C	-1.439974	2.443645	-0.472238
H	-2.383860	2.627731	-0.988619
H	-1.606548	2.476084	0.611812
H	-0.719889	3.221969	-0.754544

1 imaginary frequency

E = -538.617389
H = -538.409031
G = -538.454236
E_{SCS-MP2} = -537.508770

Int-6d

C	2.131308	-0.812225	-0.752545
C	1.213987	0.318155	-0.812957
C	-0.080727	0.258465	0.022558
C	-0.037272	-0.812363	1.094178
C	0.892000	-1.781852	1.116639
C	1.981385	-1.807876	0.148948
C	1.465520	1.387633	-1.591140
C	-1.266711	-0.044762	-0.936265
C	-2.618238	-0.119261	-0.251705
O	-3.434596	-0.989763	-0.464978
O	-0.410994	1.538605	0.583176
H	0.804357	2.248269	-1.603979
H	2.351014	1.430980	-2.219718
H	-1.092595	-0.976454	-1.481345
H	-1.303546	0.779733	-1.663933
H	-2.833251	0.705216	0.459118
H	2.979326	-0.804416	-1.433731
H	2.695854	-2.625413	0.188263
H	0.846913	-2.565878	1.868640
H	-0.850350	-0.793220	1.816578
C	0.489864	2.028991	1.568559
H	0.067800	2.973212	1.921401
H	0.584574	1.335438	2.414930
H	1.487930	2.212368	1.150579

0 imaginary frequencies

E = -538.654995

H = -538.444670

G = -538.492629

E_{SCS-MP2} = -537.555524

6e

C	2.535781	1.157266	-0.101755
C	2.007884	-0.138278	0.013403
C	0.626737	-0.324552	0.118252
C	-0.231554	0.783939	0.095672
C	0.294238	2.070078	-0.028545
C	1.678657	2.249485	-0.120779
C	-1.719374	0.591392	0.263335
O	-2.131032	-0.582310	-0.437869
C	-3.443718	-0.920457	-0.352792
C	-4.428203	-0.286148	0.291683
H	-0.370353	2.929801	-0.056691
H	2.089046	3.251028	-0.218336
H	3.611945	1.275346	-0.180104
O	2.925543	-1.149702	0.016001
H	0.197264	-1.315459	0.197680
H	-1.982012	0.476986	1.326708
H	-2.267883	1.463565	-0.117957
H	-3.619164	-1.834437	-0.914129
H	-5.429560	-0.699307	0.254103
H	-4.289734	0.628996	0.855054
C	2.454269	-2.483748	0.119872
H	3.342938	-3.117326	0.097260
H	1.914538	-2.649695	1.061718
H	1.798586	-2.747258	-0.720434

0 imaginary frequencies

E = -538.689481

H = -538.476987

G = -538.525247

E_{SCS-MP2} = -537.578533

TS-6e

C	1.635197	1.135983	-0.443673
C	1.313013	-0.015610	0.233470
C	-0.040367	-0.247137	0.663310
C	-0.987503	0.832700	0.607496
C	-0.637161	1.985465	-0.170798
C	0.630079	2.125568	-0.668632
C	-2.278834	0.622766	1.080092
O	-2.962774	-0.703325	-0.393222
C	-2.099080	-1.632207	-0.460067
C	-0.825745	-1.438424	-1.006688
H	-2.272201	-2.565656	0.109451
H	-0.126391	-2.269377	-1.055583
H	-0.677076	-0.629485	-1.714227
H	-0.173931	-1.030340	1.401630
H	-1.383129	2.760078	-0.325282
H	0.899297	3.016617	-1.229257
H	2.641193	1.313975	-0.806228
O	2.165698	-1.039114	0.525274
H	-2.482917	-0.120898	1.840420
H	-3.042644	1.380615	0.943933
C	3.519370	-0.908880	0.118176
H	4.024132	-1.815480	0.456273
H	3.603502	-0.829247	-0.973699
H	3.992953	-0.032630	0.580033

1 imaginary frequency

E = -538.624464

H = -538.415432
G = -538.460628
E_{SCS-MP2} = -537.515542

Int-6e

C	0.101632	2.349294	0.238447
C	0.902594	1.275574	-0.342519
C	0.324762	-0.140190	-0.261089
C	-1.185272	-0.157335	-0.148844
C	-1.894290	0.914536	0.264638
C	-1.207790	2.172962	0.522535
C	2.109630	1.508830	-0.890824
C	0.914207	-0.911396	0.951309
C	2.275603	-1.525500	0.712756
O	2.821585	-1.633734	-0.363298
H	0.605671	-0.702592	-1.158084
H	2.696806	0.718653	-1.345974
H	2.536381	2.509040	-0.889987
H	0.256103	-1.751844	1.223034
H	0.964511	-0.271889	1.842612
H	2.759103	-1.932605	1.630141
H	0.575050	3.317383	0.381720
H	-1.795017	2.997338	0.919278
H	-2.969753	0.872206	0.394295
O	-1.679612	-1.390235	-0.442868
C	-3.082030	-1.587329	-0.322536
H	-3.267475	-2.624962	-0.604884
H	-3.418459	-1.418203	0.708581
H	-3.632987	-0.917445	-0.994636

0 imaginary frequencies

E = -538.667314
H = -538.456064
G = -538.503612
E_{SCS-MP2} = -537.563690

6f

C	2.270659	0.260487	-0.031789
C	1.418210	1.360626	-0.221772
C	0.052560	1.165719	-0.361374
C	-0.504964	-0.122651	-0.310962
C	0.352399	-1.204581	-0.116097
C	1.733393	-1.029609	0.019387
C	-1.988202	-0.319442	-0.464974
O	-2.656057	0.282431	0.652632
C	-4.012304	0.230158	0.654576
C	-4.829328	-0.330787	-0.243475
H	-0.056680	-2.211189	-0.066934
H	2.368537	-1.895498	0.167184
O	3.597388	0.556229	0.089688
H	1.855001	2.353740	-0.258519
H	-0.598826	2.024252	-0.503770
H	-2.360946	0.150004	-1.387187
H	-2.239563	-1.387875	-0.509808
H	-4.392790	0.734031	1.539584
H	-5.900020	-0.277686	-0.082808
H	-4.486187	-0.844071	-1.134028
C	4.507407	-0.513534	0.288818
H	5.495993	-0.056430	0.360869
H	4.291805	-1.059511	1.216851
H	4.494059	-1.217366	-0.554023

0 imaginary frequencies

E = -538.689274

H = -538.476727

G = -538.525427

E_{SCS-MP2} = -537.578295

TS-6f

C	1.726423	0.305549	-0.071518
C	1.014821	-0.578673	0.705762
C	-0.388036	-0.369782	0.903552
C	-0.985108	0.889682	0.527344
C	-0.213657	1.742384	-0.334225
C	1.089539	1.464887	-0.625770
C	-2.314712	1.150654	0.805275
O	-3.220527	-0.236390	-0.595743
C	-2.649464	-1.341446	-0.363367
C	-1.313583	-1.599972	-0.696185
H	-3.154583	-2.077967	0.294194
H	-0.895674	-2.585418	-0.504638
H	-0.840577	-1.013928	-1.476854
H	-0.861142	-0.932278	1.701386
H	-0.681181	2.639973	-0.730872
H	1.687726	2.118654	-1.252537
O	3.048429	0.204541	-0.375083
H	1.477906	-1.459791	1.133677
H	-2.840988	0.627947	1.593857
H	-2.792842	2.048477	0.428954
C	3.764261	-0.915953	0.123843
H	4.786303	-0.806759	-0.242515
H	3.768682	-0.930264	1.221426
H	3.340247	-1.857844	-0.247727

1 imaginary frequency

E = -538.625186

H = -538.416285

G = -538.461702

E_{SCS-MP2} = -537.513107

Int-6f

C	-0.023788	2.286649	0.339863
C	1.095661	1.560429	-0.251005
C	0.949648	0.045087	-0.395974
C	-0.486835	-0.435662	-0.412117
C	-1.485098	0.346460	0.043216
C	-1.237481	1.717719	0.484389
C	2.222943	2.197264	-0.618962
C	1.726906	-0.658802	0.748294
C	1.920746	-2.145228	0.563403
O	1.569065	-2.785213	-0.404615
H	1.431370	-0.266127	-1.331243
H	3.047530	1.676291	-1.099203
H	2.350431	3.264334	-0.455933
H	1.232147	-0.493542	1.716593
H	2.731260	-0.217345	0.855591
H	2.453809	-2.647028	1.403700
H	0.133296	3.326173	0.618298
H	-2.082090	2.266076	0.890807
O	-2.805965	0.006883	0.140394
H	-0.648580	-1.453534	-0.743101
C	-3.168970	-1.300656	-0.271115
H	-4.246349	-1.380720	-0.114834
H	-2.937726	-1.462953	-1.332215
H	-2.652287	-2.064545	0.325363

0 imaginary frequencies

E = -538.664972

H = -538.454069
G = -538.501881
E_{SCS-MP2} = -537.561506

6g

Identical to 6e

TS-6g

C	-1.287152	1.649680	0.124123
C	-0.023324	1.998239	0.503684
C	0.959846	0.986899	0.767084
C	0.528079	-0.382310	0.876655
C	-0.784946	-0.718343	0.400858
C	-1.666047	0.270503	0.035803
C	1.452274	-1.362242	1.210877
O	2.571129	-1.362552	-0.617251
C	2.894756	-0.154581	-0.820303
C	1.969609	0.825126	-1.201954
H	3.897898	0.193057	-0.503293
H	2.310646	1.839700	-1.394046
H	1.048019	0.520709	-1.686585
H	1.860942	1.281406	1.294168
H	-1.066811	-1.764890	0.374636
O	-2.943968	0.075491	-0.400670
H	-2.040545	2.395592	-0.110392
H	0.258925	3.045023	0.572115
H	2.359898	-1.115627	1.747140
H	1.178986	-2.411696	1.196407
C	-3.407998	-1.260742	-0.513435
H	-4.430579	-1.193584	-0.888866
H	-2.796029	-1.838372	-1.218708
H	-3.409220	-1.768193	0.460446

1 imaginary frequency

E = -538.623341
H = -538.414462
G = -538.459817
E_{SCS-MP2} = -537.513972

Int-6g

C	-1.344881	0.852453	0.016265
C	-0.009447	1.343272	-0.298856
C	1.116414	0.314756	-0.427869
C	0.623464	-1.078054	-0.744788
C	-0.653179	-1.437595	-0.554499
C	-1.648458	-0.465200	-0.106359
C	0.251373	2.659085	-0.427278
C	1.947631	0.279032	0.882409
C	3.261508	-0.459151	0.783191
O	3.704023	-0.970215	-0.223351
H	1.803651	0.632256	-1.221448
H	1.240860	3.023465	-0.690957
H	-0.520123	3.409421	-0.275900
H	1.364408	-0.158738	1.705713
H	2.177546	1.306882	1.204940
H	3.843540	-0.492365	1.732729
H	-2.099072	1.585144	0.282667
O	-2.863334	-1.034806	0.122235
H	-1.002047	-2.450243	-0.735346
H	1.364780	-1.796708	-1.079560
C	-3.923725	-0.187117	0.536675
H	-4.147966	0.570639	-0.225280
H	-4.791596	-0.834108	0.675368
H	-3.683690	0.315639	1.482656

0 imaginary frequencies

E = -538.666574
H = -538.455645
G = -538.503444
E_{SCS-MP2} = -537.562557

6h

Identical to **6d**

TS-6h

C	-0.784883	2.336904	-0.130465
C	0.471961	2.259978	0.405333
C	1.006507	0.978346	0.757033
C	0.136913	-0.172287	0.798099
C	-1.153261	-0.047126	0.154302
C	-1.597641	1.176967	-0.294344
C	0.625798	-1.397581	1.213083
O	1.901525	-1.815229	-0.474414
C	2.622255	-0.782892	-0.601556
C	2.127052	0.441549	-1.069726
H	3.636442	-0.777658	-0.153778
H	2.805518	1.282354	-1.191872
H	1.228113	0.449862	-1.676568
H	1.884991	0.952739	1.393441
O	-1.867769	-1.200052	0.090807
H	-2.579089	1.283739	-0.740969
H	-1.191605	3.298202	-0.434335
H	1.085879	3.147400	0.525281
H	1.499912	-1.455220	1.849216
H	0.019079	-2.290204	1.140452
C	-3.154235	-1.166422	-0.508788
H	-3.531672	-2.189215	-0.463336
H	-3.833199	-0.500578	0.039488
H	-3.097210	-0.843782	-1.555990

l imaginary frequency

E = -538.624193
H = -538.415074
G = -538.460304
E_{SCS-MP2} = -537.512411

Int-6h

C	1.495559	0.033078	-0.035296
C	0.379854	-0.822062	-0.472658
C	-1.014662	-0.197556	-0.472077
C	-1.003431	1.305751	-0.623872
C	0.102540	2.017509	-0.352877
C	1.359916	1.383246	0.022267
C	0.571864	-2.105829	-0.818774
C	-1.755497	-0.578839	0.838321
C	-3.241122	-0.305134	0.824397
O	-3.868642	0.110956	-0.125635
H	-1.593360	-0.637219	-1.293221
H	-0.252110	-2.718475	-1.176055
H	1.547491	-2.573402	-0.755943
H	-1.315422	-0.061991	1.703399
H	-1.630840	-1.654030	1.046102
H	-3.761286	-0.541456	1.781178
O	2.638892	-0.658075	0.233057
H	2.192612	2.018071	0.302389
H	0.086590	3.103231	-0.414705
H	-1.938488	1.783845	-0.896081
C	3.800342	0.083342	0.568915
H	3.652373	0.661730	1.490480
H	4.592597	-0.651155	0.724597
H	4.085680	0.766764	-0.241584

0 imaginary frequencies

E = -538.664010

H = -538.452912

G = -538.500680

E_{SCS-MP2} = -537.560770

6i

C	4.045940	0.000019	0.189658
C	3.357922	1.208775	0.066003
C	1.985315	1.207181	-0.181571
C	1.287789	0.000118	-0.307858
C	1.985307	-1.206995	-0.182014
C	3.357913	-1.208688	0.065574
C	-0.195649	0.000150	-0.552413
O	-0.871880	-0.000611	0.726188
C	-2.209284	-0.000470	0.727192
C	-3.041493	0.000151	-0.338593
H	1.450252	-2.148863	-0.278592
H	3.889945	-2.151393	0.158834
H	5.115888	-0.000019	0.379229
H	3.889964	2.151442	0.159594
H	1.450255	2.149082	-0.277798
H	-0.509384	0.890835	-1.110923
H	-0.509247	-0.889977	-1.111895
H	-2.594242	-0.000977	1.743088
C	-4.451427	0.000184	-0.151617
H	-2.681329	0.000624	-1.361248
N	-5.608722	0.000226	-0.016568

0 imaginary frequencies

E = -516.413836

H = -516.235762

G = -516.283609

E_{SCS-MP2} = -515.328597

TS-6i

C	1.646122	-1.945485	-0.115382
C	0.614810	-1.628050	0.726084
C	0.261026	-0.254808	0.935373
C	1.157643	0.781479	0.461239
C	2.179943	0.396062	-0.480631
C	2.414048	-0.920339	-0.757467
C	0.948264	2.095741	0.798312
O	-0.990784	2.330936	-0.595061
C	-1.705171	1.374050	-0.251237
C	-1.373595	0.014553	-0.554365
H	-2.568295	1.530576	0.425453
C	-2.297283	-1.025042	-0.242011
H	-0.700754	-0.164504	-1.387309
H	-0.384895	-0.019323	1.774929
H	2.784313	1.176520	-0.935151
H	3.205916	-1.202515	-1.445306
H	1.895669	-2.986704	-0.300493
H	0.021660	-2.402950	1.200609
H	0.258853	2.384185	1.581966
H	1.552611	2.888319	0.369352
N	-3.030521	-1.882866	0.050991

1 imaginary frequency

E = -516.347369

H = -516.173451

G = -516.218145

E_{SCS-MP2} = -515.262407

Int-6i

C	0.060278	0.559442	-0.548588
C	-1.206543	1.100785	0.118393
C	-2.327188	0.181545	0.281947
C	-2.365156	-1.008859	-0.355481
C	-1.283397	-1.422925	-1.242447
C	-0.164624	-0.690983	-1.367165
C	-1.269337	2.373703	0.552434
C	1.174939	0.310723	0.526591
C	2.578353	0.154118	-0.091125
O	2.843777	0.476764	-1.223088
H	-2.142635	2.749247	1.078591
H	-0.459012	3.080687	0.390232
H	-3.159094	0.507069	0.901688
H	-3.223833	-1.664293	-0.240151
H	-1.405682	-2.337819	-1.816410
H	0.637966	-0.993185	-2.033542
H	0.488551	1.334477	-1.194535
C	0.910460	-0.810840	1.433973
H	1.236146	1.216864	1.153099
H	3.349352	-0.246973	0.598271
N	0.754474	-1.705778	2.156611

0 imaginary frequencies

E = -516.370415

H = -516.194770

G = -516.241388

E_{SCS-MP2} = -515.299257

6j

C	-3.710910	0.610336	-0.173522
C	-2.789651	1.306495	0.614194
C	-1.501160	0.806352	0.789618
C	-1.115912	-0.391118	0.172323
C	-2.040118	-1.077841	-0.620305
C	-3.335060	-0.583065	-0.789572
C	0.272109	-0.937845	0.377706
O	1.221517	0.037355	-0.085709
C	2.536167	-0.269181	0.065187
C	3.079675	-1.391164	0.566199
H	-1.746253	-2.003791	-1.109385
H	-4.044774	-1.126547	-1.407250
H	-4.716598	0.999584	-0.307181
H	-3.077235	2.238474	1.093118
H	-0.783264	1.350358	1.397641
H	0.471790	-1.137277	1.440567
H	0.412134	-1.875487	-0.175672
C	3.376311	0.807515	-0.400495
H	4.157011	-1.482778	0.621000
H	2.484314	-2.222305	0.921725
N	4.063147	1.668289	-0.770984

0 imaginary frequencies

E = -516.404050

H = -516.226784

G = -516.274242

E_{SCS-MP2} = -515.321853

TS-6j

C	-2.742660	-1.124964	0.058957
C	-1.578911	-1.534885	-0.532303
C	-0.506223	-0.598866	-0.738285
C	-0.774967	0.814334	-0.566876
C	-1.979691	1.181261	0.119540
C	-2.931082	0.244129	0.423251
C	0.211715	1.745693	-0.854017

O	1.515911	1.280539	0.785657
C	1.693670	0.028368	0.711007
C	0.683089	-0.908013	1.000857
C	2.886732	-0.463440	0.010293
H	0.909488	-1.969647	0.957542
H	-0.094824	-0.603930	1.692348
H	0.274065	-0.881633	-1.438829
H	-2.139119	2.228790	0.361927
H	-3.852980	0.541974	0.914551
H	-3.541636	-1.837858	0.244534
H	-1.433165	-2.573221	-0.815954
H	1.023180	1.518910	-1.535057
H	0.064302	2.795150	-0.622450
N	3.841910	-0.823507	-0.548345

l imaginary frequency
E = -516.343878
H = -516.169769
G = -516.213819
E_{SCS-MP2} = -515.263364

Int-6j

C	0.495754	0.144563	0.639236
C	1.669274	1.003084	0.161217
C	2.650658	0.367752	-0.712140
C	2.706994	-0.975523	-0.852090
C	1.793562	-1.846899	-0.120349
C	0.786140	-1.340953	0.610432
C	1.766345	2.301436	0.502948
C	-0.742522	0.446713	-0.248980
C	-2.041307	-0.098060	0.299362
O	-2.183310	-0.657592	1.365518
H	2.559206	2.932502	0.110255
H	1.065052	2.771068	1.188333
H	3.375863	1.008491	-1.208475
H	3.468528	-1.428416	-1.481401
H	1.954832	-2.921110	-0.165046
H	0.109697	-1.985614	1.163203
H	0.228069	0.438166	1.661356
H	-0.599484	0.059509	-1.267048
H	-0.868883	1.534736	-0.362696
C	-3.222735	0.123772	-0.571490
N	-4.142768	0.299442	-1.258785

0 imaginary frequencies
E = -516.374286
H = -516.198413
G = -516.245381
E_{SCS-MP2} = -515.299373

6k

C	3.440354	-0.168020	0.164270
C	2.656239	0.563327	1.060957
C	1.273241	0.612681	0.901817
C	0.664845	-0.077235	-0.153685
C	1.450090	-0.809512	-1.047106
C	2.836728	-0.853420	-0.889947
C	-0.843002	-0.044912	-0.319361
O	-1.432659	-0.614897	0.849684
C	-2.745322	-0.999669	0.784201
C	-3.611545	-0.846783	-0.218377
H	0.979532	-1.348067	-1.866214
H	3.441387	-1.423921	-1.589299
H	4.519326	-0.201484	0.287899
H	3.123856	1.098948	1.882321
H	0.661660	1.182595	1.595393

C	-1.331447	1.339714	-0.530089
H	-1.130558	-0.638001	-1.198153
H	-3.012822	-1.486275	1.717247
H	-4.618360	-1.229604	-0.098092
H	-3.386972	-0.336419	-1.147683
N	-1.693839	2.429197	-0.699568

0 imaginary frequencies
E = -516.396564
H = -516.219604
G = -516.266778
E_{SCS-MP2} = -515.317992

TS-6k

C	-2.852349	0.000847	0.496918
C	-1.825666	0.365960	1.333592
C	-0.476117	0.085883	0.973980
C	-0.208616	-0.746071	-0.164675
C	-1.294631	-1.049071	-1.042285
C	-2.578782	-0.688693	-0.717592
C	1.106040	-1.091856	-0.512906
O	1.651503	0.851119	-1.333091
C	1.402819	1.689052	-0.413990
C	0.097163	2.077274	-0.095678
H	2.216110	2.002868	0.262577
H	-0.080515	2.808255	0.688535
H	-0.695479	1.919714	-0.818504
H	0.300668	0.207135	1.720805
H	-1.089828	-1.599537	-1.956573
H	-3.399475	-0.952252	-1.378684
H	-3.881128	0.230732	0.759925
H	-2.026224	0.892595	2.262028
C	2.158692	-1.114607	0.442760
H	1.290195	-1.623661	-1.440281
N	2.997477	-1.123873	1.252022

1 imaginary frequency
E = -516.343445
H = -516.169541
G = -516.213418
E_{SCS-MP2} = -515.263781

Int-6k

C	-1.853131	1.399277	0.354384
C	-0.460822	1.138546	0.049945
C	-0.046949	-0.293757	-0.271757
C	-1.204573	-1.196132	-0.624587
C	-2.482644	-0.847738	-0.396321
C	-2.808712	0.460913	0.147650
C	0.441438	2.160304	0.083344
C	0.733989	-0.899868	0.931332
C	1.457999	-2.189644	0.616507
O	1.456768	-2.746481	-0.459392
H	0.658731	-0.284359	-1.112891
C	1.816067	2.008342	-0.237020
H	0.120016	3.160766	0.361723
H	0.064028	-1.076903	1.784978
H	1.492530	-0.188952	1.289022
H	2.033102	-2.610711	1.471054
H	-2.119329	2.390581	0.712784
H	-3.848986	0.694418	0.358983
H	-3.293432	-1.534102	-0.624722
H	-0.944650	-2.167995	-1.030563
N	2.946840	1.878237	-0.493728

0 imaginary frequencies
E = -516.389174

H = -516.212884
G = -516.259076
E_{SCS-MP2} = -515.310734

6l

C	-3.045727	-0.980339	-0.000488
C	-2.050853	-1.959023	-0.000102
C	-0.701043	-1.600651	0.000280
C	-0.320140	-0.258892	0.000302
C	-1.331241	0.727274	-0.000036
C	-2.687380	0.364426	-0.000383
C	1.130959	0.164636	0.000443
O	1.959697	-0.986140	0.000856
C	3.305007	-0.773905	-0.000297
C	3.958890	0.390422	-0.000736
C	-0.972921	2.116179	0.000102
H	-3.444383	1.142118	-0.000563
H	-4.094593	-1.261301	-0.000766
H	-2.324413	-3.010533	-0.000116
H	0.070281	-2.361447	0.000658
H	1.349849	0.783117	-0.882817
H	1.349552	0.783577	0.883436
H	3.820452	-1.729952	-0.000822
H	5.042635	0.380120	-0.001746
H	3.471936	1.358457	-0.000111
N	-0.661743	3.237743	0.000213

0 imaginary frequencies

E = -516.410029
H = -516.232538
G = -516.279084
E_{SCS-MP2} = -515.328105

TS-6l

C	2.487828	0.679729	0.484086
C	1.317891	1.372058	0.366281
C	0.136199	0.721056	-0.158381
C	0.287896	-0.577732	-0.809461
C	1.525164	-1.271715	-0.590333
C	2.584491	-0.673807	0.033748
C	-0.788108	-1.200452	-1.410084
O	-1.820639	-1.718654	0.474344
C	-1.928215	-0.628884	1.097064
C	-0.817038	0.005987	1.692131
H	-2.869176	-0.053998	1.030366
H	-0.962139	0.925006	2.254131
H	0.049200	-0.594500	1.948543
C	-0.919626	1.595566	-0.611520
H	1.609970	-2.286607	-0.969320
H	3.518696	-1.212754	0.160902
H	3.360741	1.163199	0.913577
H	1.236240	2.403379	0.693611
H	-1.669744	-0.651634	-1.715542
H	-0.692290	-2.212284	-1.787197
N	-1.762181	2.305513	-0.983574

1 imaginary frequency

E = -516.336451
H = -516.162935
G = -516.206515
E_{SCS-MP2} = -515.259172

Int-6l

C	0.108872	0.206635	-0.104365
C	-1.236427	0.860708	0.295754
C	-2.381112	-0.034951	0.422506

C	-2.380268	-1.277702	-0.106524
C	-1.227043	-1.771464	-0.848132
C	-0.079099	-1.079254	-0.906954
C	-1.333115	2.170888	0.581723
C	0.858382	-0.132870	1.229092
C	2.231918	-0.754959	1.094809
O	2.771268	-1.063580	0.056730
H	-2.267668	2.590147	0.944186
H	-0.506621	2.860401	0.441879
H	-3.269389	0.361511	0.908273
H	-3.262753	-1.906659	-0.030120
H	-1.313823	-2.717506	-1.376165
H	0.783728	-1.434712	-1.456458
C	0.923846	1.164104	-0.877307
H	0.231242	-0.818865	1.815535
H	0.954035	0.778012	1.837758
H	2.743044	-0.918126	2.070268
N	1.546048	1.943948	-1.470373

0 imaginary frequencies

E = -516.369560

H = -516.194281

G = -516.240102

E_{SCS-MP2} = -515.300161

6m

C	-2.406359	1.227297	0.022775
C	-1.286817	2.052056	0.091983
C	-0.004529	1.503444	0.140927
C	0.177718	0.115283	0.113301
C	-0.940668	-0.715221	0.034848
C	-2.232044	-0.165560	-0.004997
C	1.555531	-0.497062	0.213880
O	2.507483	0.395287	-0.351230
C	3.813579	0.015904	-0.301785
C	4.332169	-1.109588	0.196827
H	-0.822801	-1.794685	0.000655
C	-3.372760	-1.031992	-0.083856
H	-3.406822	1.645639	-0.014537
H	-1.413276	3.130642	0.108508
H	0.865729	2.149156	0.187383
H	1.817488	-0.686153	1.266795
H	1.588648	-1.463296	-0.308968
H	4.430817	0.789255	-0.750057
H	5.405430	-1.254137	0.154984
H	3.742878	-1.901058	0.644705
N	-4.297554	-1.735003	-0.146150

0 imaginary frequencies

E = -516.409625

H = -516.232100

G = -516.278925

E_{SCS-MP2} = -515.327126

TS-6m

C	1.709666	1.299635	-0.474736
C	1.492398	0.084542	0.142153
C	0.162760	-0.275837	0.588910
C	-0.838331	0.763595	0.647156
C	-0.579633	1.978020	-0.058906
C	0.653408	2.238952	-0.606106
C	-2.107124	0.464816	1.139917
O	-2.755482	-0.773788	-0.363753
C	-1.861489	-1.667000	-0.501077
C	-0.609177	-1.390961	-1.067604
H	-1.985162	-2.631257	0.025512

H	0.110381	-2.197445	-1.188854
H	-0.521752	-0.558741	-1.758551
H	0.095990	-1.091402	1.300582
H	-1.374172	2.716988	-0.124428
H	0.842100	3.181550	-1.110437
H	2.699813	1.542683	-0.847822
C	2.556051	-0.857818	0.297817
H	-2.250949	-0.319048	1.873345
H	-2.904348	1.197102	1.073259
N	3.408684	-1.639685	0.431753

1 imaginary frequency

E = -516.344185

H = -516.170014

G = -516.213719

E_{SCS-MP2} = -515.261376

Int-6m

C	-0.504236	2.288826	0.179024
C	0.483465	1.357409	-0.354407
C	0.180121	-0.139833	-0.247284
C	-1.317105	-0.416568	-0.134031
C	-2.197416	0.540631	0.245574
C	-1.768132	1.905951	0.474869
C	1.629500	1.813424	-0.894563
C	0.902026	-0.776080	0.970679
C	2.360431	-1.109290	0.737314
O	2.926483	-1.066544	-0.332777
H	0.568404	-0.644269	-1.138493
H	2.365904	1.144731	-1.326131
H	1.851126	2.877750	-0.910275
H	0.421512	-1.728623	1.246716
H	0.819161	-0.139174	1.861713
H	2.902680	-1.448513	1.647907
H	-0.206514	3.329490	0.284985
H	-2.495840	2.626065	0.836520
H	-3.247877	0.291530	0.364681
C	-1.753041	-1.755293	-0.366489
N	-2.069157	-2.861672	-0.552790

0 imaginary frequencies

E = -516.385410

H = -516.209270

G = -516.255583

E_{SCS-MP2} = -515.308913

6n

C	2.449617	-0.025686	0.006568
C	1.603985	-1.142087	0.104826
C	0.222786	-0.971280	0.125119
C	-0.336534	0.308575	0.042065
C	0.511944	1.418763	-0.062062
C	1.893006	1.261817	-0.076447
C	-1.830494	0.525308	0.102323
O	-2.502198	-0.685890	-0.209658
C	-3.862137	-0.668364	-0.160453
C	-4.667804	0.355931	0.132723
H	0.088855	2.417900	-0.135799
H	2.545250	2.125213	-0.158522
C	3.873062	-0.197256	-0.013392
H	2.034300	-2.136604	0.165234
H	-0.431134	-1.832712	0.196247
H	-2.127225	0.858330	1.109582
H	-2.133521	1.314052	-0.601693
H	-4.244791	-1.654486	-0.407304
H	-5.739694	0.196308	0.126298

H -4.316542 1.351096 0.378596
 N 5.028216 -0.335188 -0.029000
 0 imaginary frequencies
 E = -516.409918
 H = -516.232436
 G = -516.279630
 E_{SCS-MP2} = -515.327100

TS-6n

C 1.843391 0.065546 0.063436
 C 1.012999 -0.709388 0.842946
 C -0.374073 -0.376162 0.960078
 C -0.827910 0.911072 0.487160
 C 0.052315 1.646064 -0.374362
 C 1.341717 1.245761 -0.585929
 C -2.151579 1.284887 0.667251
 O -3.023136 -0.097914 -0.698529
 C -2.579461 -1.236715 -0.369812
 C -1.252423 -1.627158 -0.608758
 H -3.187097 -1.880015 0.294980
 H -0.933805 -2.632152 -0.342724
 H -0.695589 -1.134079 -1.398461
 H -0.929158 -0.848321 1.763751
 H -0.315993 2.558021 -0.836574
 H 2.010891 1.823674 -1.214450
 C 3.222759 -0.292300 -0.094778
 H 1.397371 -1.595117 1.338196
 H -2.752977 0.861389 1.462090
 H -2.536718 2.190304 0.211247
 N 4.343106 -0.575720 -0.230459
 1 imaginary frequency
 E = -516.342373
 H = -516.168416
 G = -516.212302
 E_{SCS-MP2} = -515.261193

Int-6n

C -0.621891 2.090915 0.364634
 C 0.651872 1.670625 -0.210633
 C 0.878129 0.170392 -0.393558
 C -0.400558 -0.623712 -0.485956
 C -1.577783 -0.122561 -0.049175
 C -1.676196 1.254322 0.452442
 C 1.602288 2.566285 -0.534040
 C 1.736063 -0.385124 0.778215
 C 2.292242 -1.771307 0.542550
 O 2.133784 -2.418607 -0.469721
 H 1.458073 -0.003361 -1.308042
 H 2.535781 2.269871 -1.005611
 H 1.469118 3.627457 -0.341692
 H 1.167296 -0.390118 1.719112
 H 2.591231 0.284939 0.957633
 H 2.900034 -2.175116 1.382698
 H -0.719398 3.126861 0.679990
 H -2.628725 1.588713 0.850414
 C -2.767684 -0.924644 -0.079978
 H -0.328952 -1.639042 -0.860538
 N -3.744804 -1.556069 -0.089029
 0 imaginary frequencies
 E = -516.383070
 H = -516.207253
 G = -516.253773
 E_{SCS-MP2} = -515.307343

6o

Identical to **6m**

TS-6o

C	1.547896	1.373922	-0.229999
C	0.320461	1.826993	-0.616693
C	-0.777756	0.911646	-0.785157
C	-0.497367	-0.507090	-0.808579
C	0.773635	-0.942195	-0.330349
C	1.774048	-0.034526	-0.047792
C	-1.528444	-1.413592	-1.041387
O	-2.601739	-1.134885	0.708325
C	-2.799619	0.114707	0.807977
C	-1.769749	1.016252	1.117552
H	-3.754973	0.535787	0.442020
H	-2.004465	2.072361	1.229093
H	-0.907985	0.654895	1.668515
H	-1.631062	1.264453	-1.355455
H	0.963307	-2.006332	-0.225730
C	3.060076	-0.489319	0.389947
H	2.373155	2.060680	-0.071177
H	0.149878	2.889109	-0.765685
H	-2.396205	-1.133853	-1.625869
H	-1.356546	-2.479020	-0.934377
N	4.108532	-0.845683	0.748422

1 imaginary frequency

E = -516.342941

H = -516.168867

G = -516.212618

E_{SCS-MP2} = -515.259796

Int-6o

C	-1.407998	1.035633	0.093969
C	-0.040628	1.413520	-0.220515
C	0.988471	0.297656	-0.401449
C	0.365221	-1.038919	-0.735480
C	-0.934355	-1.297619	-0.530838
C	-1.838576	-0.248290	-0.042869
C	0.302132	2.713461	-0.317284
C	1.849773	0.159042	0.882931
C	3.100254	-0.673451	0.710369
O	3.463546	-1.173366	-0.332193
H	1.678806	0.572544	-1.208204
H	1.305590	3.023011	-0.597751
H	-0.416954	3.505310	-0.126378
H	1.261524	-0.263309	1.710465
H	2.168621	1.154421	1.230678
H	3.708223	-0.791145	1.635328
H	-2.101992	1.814574	0.396878
C	-3.199174	-0.587269	0.245035
H	-1.354117	-2.278112	-0.732917
H	1.036063	-1.809352	-1.101592
N	-4.300693	-0.883370	0.478260

0 imaginary frequencies

E = -516.384103

H = -516.208252

G = -516.254809

E_{SCS-MP2} = -515.307959

6p

Identical to **6l**

TS-6p

C	-0.778415	2.424445	-0.167450
C	0.431106	2.226801	0.442969
C	0.863651	0.900265	0.781530
C	-0.082782	-0.187491	0.728574
C	-1.316721	0.057163	0.013229
C	-1.647313	1.326094	-0.416378
C	0.308889	-1.456643	1.129311
O	1.649378	-1.864176	-0.452724
C	2.453278	-0.886864	-0.490399
C	2.074023	0.381305	-0.955836
H	3.423487	-0.967358	0.036402
H	2.814028	1.176868	-1.003335
H	1.236232	0.457948	-1.640650
H	1.684755	0.809727	1.484812
C	-2.240127	-1.017728	-0.198859
H	-2.595467	1.490308	-0.918016
H	-1.094027	3.422545	-0.456743
H	1.093786	3.063888	0.643298
H	1.116514	-1.584513	1.838908
H	-0.339589	-2.312792	0.983882
N	-2.989753	-1.892470	-0.363845

l imaginary frequency

E = -516.341769

H = -516.167756

G = -516.211501

E_{SCS-MP2} = -515.261404

Int-6p

C	1.630174	0.277959	0.032805
C	0.620943	-0.670414	-0.476381
C	-0.828908	-0.189340	-0.471326
C	-0.966223	1.313154	-0.541560
C	0.046921	2.134391	-0.211401
C	1.346649	1.604892	0.154978
C	0.946663	-1.905748	-0.891017
C	-1.558039	-0.714093	0.796811
C	-3.062873	-0.576431	0.755320
O	-3.694499	-0.125564	-0.175862
H	-1.350467	-0.628402	-1.330091
H	0.197282	-2.576401	-1.303100
H	1.963336	-2.281920	-0.832233
H	-1.187441	-0.214163	1.703456
H	-1.331922	-1.782268	0.940398
H	-3.585715	-0.947762	1.665096
C	2.944005	-0.198523	0.342210
H	2.118005	2.287296	0.498911
H	-0.086777	3.212537	-0.215037
H	-1.943420	1.701499	-0.810185
N	4.006749	-0.602998	0.592434

0 imaginary frequencies

E = -516.383908

H = -516.207955

G = -516.254331

E_{SCS-MP2} = -515.308435

6q

C	-1.962333	-0.902077	-0.784114
C	-0.617824	-0.652251	-1.029007
C	0.010593	0.510059	-0.567434
C	-0.765264	1.417271	0.159320
C	-2.114137	1.189316	0.412872
C	-2.754203	0.022380	-0.062600
C	1.469445	0.755485	-0.823451

O	2.243284	-0.035847	0.094835
C	3.588666	0.034118	-0.008033
O	4.085016	-0.810328	0.928700
C	5.495722	-0.908778	1.032447
N	-4.108173	-0.202784	0.157079
C	-4.670207	-1.508098	-0.145790
C	4.301352	0.788000	-0.864778
C	-4.829545	0.653910	1.082523
H	-0.306270	2.325896	0.543596
H	-2.666573	1.924125	0.985922
H	-2.396741	-1.821174	-1.158417
H	-0.040144	-1.386284	-1.586503
H	1.748512	0.473534	-1.847786
H	1.719510	1.815346	-0.683875
H	5.381679	0.769705	-0.866329
H	3.817993	1.438555	-1.578925
H	5.687154	-1.624086	1.834235
H	5.939329	-1.275595	0.097877
H	5.944781	0.059719	1.287377
H	-5.876307	0.344654	1.113122
H	-4.427481	0.613803	2.107934
H	-4.805091	1.698608	0.750480
H	-5.739429	-1.495818	0.075196
H	-4.557066	-1.747182	-1.209883
H	-4.206630	-2.320930	0.436414

0 imaginary frequencies
E = -672.661200
H = -672.370658
G = -672.429780
E_{SCS-MP2} = -671.268901

TS-6q

C	0.445157	1.148421	-0.605583
C	-0.586924	1.902345	0.040339
C	-1.824585	1.375002	0.279261
C	-2.146600	0.023704	-0.104743
C	-1.138297	-0.749791	-0.686100
C	0.167713	-0.242113	-0.841913
N	-3.419371	-0.468619	0.104131
C	1.699088	1.684404	-0.846929
O	2.827125	0.809616	0.808997
C	2.565736	-0.421119	0.725882
O	3.414681	-1.264502	0.025781
C	4.689056	-0.718418	-0.298806
C	1.365371	-1.006778	1.118697
H	1.228414	-2.079623	1.046617
H	0.714500	-0.446230	1.775201
H	0.876591	-0.817032	-1.428226
H	-0.380416	2.932574	0.320376
H	-2.578229	1.995466	0.749060
H	-1.329098	-1.772096	-0.987835
H	2.396439	1.194135	-1.514194
H	1.919538	2.715780	-0.595156
H	5.253276	-1.534404	-0.756740
H	4.613510	0.116326	-1.004284
H	5.211110	-0.361864	0.596334
C	-3.745209	-1.812388	-0.342277
C	-4.495676	0.413473	0.530239
H	-5.419927	-0.162528	0.598401
H	-4.299569	0.841885	1.521212
H	-4.662376	1.241374	-0.174045
H	-4.768705	-2.052132	-0.049428
H	-3.662969	-1.921640	-1.434629
H	-3.079913	-2.551021	0.121782

1 imaginary frequency

E = -672.614629
 H = -672.327679
 G = -672.385262
 E_{SCS-MP2} = -671.215799

Int-6q

C	0.572104	-0.166942	0.654700
C	1.800715	-0.248694	0.095831
C	2.377063	0.940576	-0.547746
C	1.755882	2.137241	-0.520233
C	0.472593	2.330009	0.142135
C	-0.286327	1.076377	0.573644
N	2.639978	-1.386969	0.175427
C	-0.025006	3.563399	0.350861
C	-1.461724	0.827225	-0.410779
C	-2.431858	-0.234012	0.071072
O	-3.226571	-0.654686	-0.939312
C	-4.222477	-1.624906	-0.576813
O	-2.528549	-0.645996	1.208227
H	-0.742810	1.257379	1.554758
H	-0.956367	3.724806	0.887908
H	0.492352	4.451067	-0.003957
H	-1.088156	0.550421	-1.402100
H	-2.034072	1.756314	-0.543056
H	2.241926	3.013458	-0.943927
H	3.368953	0.862267	-0.981921
H	0.114339	-1.018722	1.143081
H	-4.761236	-1.849412	-1.497933
H	-3.752257	-2.527223	-0.176779
H	-4.902442	-1.217293	0.176265
C	2.200018	-2.452986	1.058711
C	3.150580	-1.904120	-1.092360
H	3.983414	-2.588100	-0.895915
H	2.380647	-2.452547	-1.664545
H	3.521376	-1.093974	-1.723318
H	3.006086	-3.187860	1.154386
H	1.980532	-2.044699	2.049284
H	1.299462	-2.980655	0.694323

0 imaginary frequencies

E = -672.664551
 H = -672.374828
 G = -672.433053
 E_{SCS-MP2} = -671.279906

6r

C	2.924030	1.177899	-0.000102
C	3.271337	-0.184301	-0.000010
C	2.260331	-1.157455	0.000164
C	0.921184	-0.774993	0.000233
C	0.571719	0.578936	0.000132
C	1.584950	1.547733	-0.000027
C	-0.869727	1.034545	0.000129
O	-1.722713	-0.096899	0.000015
C	-3.061610	0.121631	0.000038
O	-3.638480	-1.099733	0.000044
C	-5.058399	-1.148409	-0.000227
C	-3.680311	1.314008	-0.000024
H	1.324371	2.603842	-0.000088
H	3.704541	1.931819	-0.000221
C	4.650901	-0.574983	-0.000103
H	2.528897	-2.209019	0.000240
H	0.139363	-1.525189	0.000372
H	-1.073321	1.654528	0.885952
H	-1.073229	1.654653	-0.885631

H	-4.758227	1.386449	-0.000041
H	-3.124262	2.240154	-0.000087
H	-5.319372	-2.207630	-0.000313
H	-5.470938	-0.665947	0.894519
H	-5.470598	-0.665865	-0.895083
N	5.770841	-0.890343	-0.000188

0 imaginary frequencies
E = -630.937713
H = -630.724693
G = -630.778416
E_{SCS-MP2} = -629.656092

TS-6r

C	-2.320277	1.196673	0.416549
C	-2.551785	-0.114628	-0.111382
C	-1.537734	-0.802240	-0.751758
C	-0.243401	-0.224793	-0.855713
C	-0.049868	1.146838	-0.478144
C	-1.102892	1.797962	0.237852
C	1.215388	1.723222	-0.611627
O	2.231238	0.723130	0.869428
C	2.057354	-0.511969	0.644901
O	2.951030	-1.211318	-0.129008
C	4.215621	-0.582912	-0.347770
C	0.873253	-1.186408	0.943557
H	0.792400	-2.252065	0.759915
H	0.205762	-0.739898	1.667630
H	0.474615	-0.689461	-1.523592
H	-0.933131	2.802902	0.615232
H	-3.126366	1.707732	0.932108
C	-3.849321	-0.709244	0.022734
H	-1.720079	-1.794963	-1.150051
H	1.905230	1.360245	-1.363963
H	1.405143	2.723814	-0.239331
H	4.821370	-1.320584	-0.877230
H	4.122849	0.322561	-0.955703
H	4.693292	-0.317409	0.601098
N	-4.905320	-1.184625	0.136476

1 imaginary frequency
E = -630.887276
H = -630.677602
G = -630.728262
E_{SCS-MP2} = -629.604567

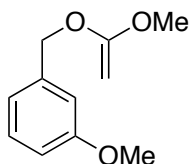
Int-6r

C	2.726879	0.133748	-0.684615
C	2.362642	1.430537	-0.617554
C	1.188273	1.866605	0.131158
C	0.188625	0.793691	0.563204
C	0.784171	-0.589755	0.633562
C	1.946654	-0.895366	0.014842
C	0.978392	3.167513	0.402462
C	-1.023657	0.777380	-0.409854
C	-2.185527	-0.055002	0.102421
O	-3.140519	-0.173730	-0.840633
C	-4.308821	-0.918699	-0.449955
O	-2.271992	-0.535352	1.213497
H	-0.213320	1.044479	1.551835
H	0.132067	3.502283	0.996812
H	1.654560	3.937452	0.040642
H	-0.729505	0.415785	-1.401228
H	-1.383157	1.804795	-0.553199
H	2.976223	2.194813	-1.088231
H	3.621115	-0.173406	-1.217060

C	2.453169	-2.238154	0.039076
H	0.210970	-1.349776	1.153600
H	-4.961688	-0.914317	-1.322834
H	-4.036307	-1.941372	-0.177268
H	-4.800261	-0.441428	0.401792
N	2.880655	-3.320234	0.040536

0 imaginary frequencies
E = -630.941439
H = -630.728914
G = -630.782037
E_{SCS-MP2} = -629.665882

6e' (2-OMe derivative of 6e)



C	-2.980603	-1.898441	-0.295454
C	-3.497436	-0.611538	-0.216404
C	-2.632282	0.471270	0.002207
C	-1.259136	0.252792	0.149794
C	-0.747390	-1.048631	0.065836
C	-1.606992	-2.124201	-0.161702
O	-3.226613	1.699507	0.057086
C	-2.401762	2.835677	0.263332
C	0.725904	-1.305576	0.281148
O	1.472978	-0.175570	-0.162762
C	2.811911	-0.191286	0.034408
C	3.541944	-1.198578	0.543388
H	-1.210129	-3.133509	-0.237539
H	-3.651199	-2.734920	-0.473529
H	-4.559355	-0.415771	-0.326749
H	-0.571392	1.073446	0.308943
H	0.940114	-1.476306	1.347071
H	1.044315	-2.202434	-0.267156
O	3.268050	1.011338	-0.387154
H	4.611876	-1.111604	0.665581
H	3.085089	-2.130981	0.841419
H	-3.073675	3.696055	0.265110
H	-1.876017	2.783947	1.225982
H	-1.664416	2.951154	-0.541735
C	4.668252	1.234046	-0.321427
H	4.829689	2.237038	-0.719753
H	5.030174	1.186118	0.713448
H	5.215148	0.502360	-0.929206

0 imaginary frequencies
E = -653.217159
H = -652.969152
G = -653.023677
E_{SCS-MP2} = -651.907531

TS-6e' (2-OMe derivative of TS-6e, leading from 6e' to 1,2,3-trisubstituted product)

C	-2.128409	1.958823	0.455680
C	-2.626309	0.635354	0.286722
C	-1.812341	-0.336741	-0.254564
C	-0.464099	-0.025471	-0.613032
C	-0.022722	1.332697	-0.581482
C	-0.865729	2.303142	0.047787
O	-2.160063	-1.638363	-0.468956
C	-3.476299	-2.039004	-0.123056
C	1.296891	1.619987	-0.948969

O	2.330068	0.821529	0.612972
C	1.944386	-0.384188	0.714452
C	0.721368	-0.756541	1.261288
O	2.624473	-1.384328	0.053103
H	0.446584	-1.803040	1.329902
H	0.218517	-0.048015	1.904992
H	0.066748	-0.754201	-1.216476
H	-0.502088	3.320432	0.163600
H	-2.779987	2.704990	0.902181
H	-3.643898	0.412309	0.586768
H	1.815734	0.984321	-1.656494
H	1.683665	2.628173	-0.849014
H	-3.545161	-3.098063	-0.377633
H	-3.666525	-1.908869	0.950657
H	-4.229385	-1.477309	-0.691683
C	3.928844	-1.045172	-0.413461
H	4.347205	-1.970267	-0.815676
H	3.900015	-0.283123	-1.199129
H	4.559263	-0.675357	0.402865

l imaginary frequency
E = -653.168015
H = -652.923312
G = -652.975473
E_{SCS-MP2} = -651.857585

6g'

Identical to 6e'

TS-6g' (2-OMe derivative of TS-6g', leading from 6e' to 1,2,4-trisubstituted product)

C	-2.429289	0.220410	0.035714
C	-2.111349	1.608218	0.146246
C	-0.862018	2.006884	0.541868
C	0.148386	1.042310	0.819451
C	-0.206652	-0.342874	0.859964
C	-1.498818	-0.734070	0.378222
C	0.776688	-1.287225	1.161228
O	-3.698109	-0.029127	-0.402794
C	-4.097651	-1.383441	-0.536849
O	1.907868	-1.229760	-0.588058
C	2.213878	-0.013220	-0.760956
C	1.328753	0.948446	-1.237866
O	3.400256	0.481768	-0.257095
H	1.659125	1.970240	-1.387400
H	0.443305	0.612629	-1.759473
H	1.065793	1.362360	1.301744
H	-1.728258	-1.792432	0.325011
H	-2.891102	2.325997	-0.089878
H	-0.626395	3.064398	0.619708
H	1.642338	-1.005207	1.747842
H	0.556152	-2.348087	1.119351
H	-5.125244	-1.359411	-0.903933
H	-3.464883	-1.918965	-1.257075
H	-4.067258	-1.908349	0.427416
C	4.366306	-0.495774	0.122208
H	5.260883	0.065833	0.400022
H	4.031076	-1.097413	0.973516
H	4.594947	-1.172619	-0.708661

l imaginary frequency
E = -653.167325
H = -652.922735
G = -652.974948
E_{SCS-MP2} = -651.856052

13'

C	0.778069	3.538702	1.113815
C	0.427575	4.232826	-0.044034
C	-0.223481	3.561157	-1.082049
C	-0.514408	2.202755	-0.966474
C	-0.164322	1.497548	0.192935
C	0.478331	2.179525	1.231427
C	-0.443976	0.011367	0.307180
O	-1.779959	-0.197510	-0.190549
C	-2.491378	-1.273023	0.219090
O	-3.680557	-1.193186	-0.424536
C	-4.629050	-2.218409	-0.175037
C	-2.119174	-2.228753	1.089121
H	0.742867	1.646283	2.141869
H	1.276789	4.053936	1.930536
H	0.654076	5.291761	-0.136043
H	-0.507847	4.098062	-1.983325
H	-1.035720	1.686020	-1.766565
H	-0.411941	-0.271791	1.366756
C	0.544630	-0.855001	-0.496676
H	-2.788963	-3.032099	1.359144
H	-1.142445	-2.227723	1.550391
H	-5.497989	-1.975899	-0.789006
H	-4.235934	-3.201745	-0.462742
H	-4.920627	-2.241723	0.882587
H	0.165147	-1.883820	-0.506199
H	0.538520	-0.502326	-1.536255
C	1.975281	-0.839850	0.054701
C	2.932767	-1.725746	-0.766169
H	2.357171	0.189140	0.071390
H	1.977377	-1.186988	1.097615
C	4.346196	-1.688740	-0.252108
H	2.567687	-2.761341	-0.771935
H	2.915125	-1.381366	-1.811789
C	5.029941	-2.740766	0.199504
H	4.823120	-0.706539	-0.249014
H	6.049477	-2.648806	0.564662
H	4.596234	-3.739007	0.217247

0 imaginary frequencies

E = -734.027506

H = -733.689784

G = -733.753911

E_{SCS-MP2} = -732.473186

TS-13' ([3,3]-sigmatropic rearrangement)

C	3.021807	-2.462587	0.456584
C	4.055333	-1.697657	-0.149960
C	3.756849	-0.530147	-0.811690
C	2.414938	-0.063067	-0.866297
C	1.350719	-0.899349	-0.392032
C	1.709364	-2.072469	0.344061
C	0.025868	-0.455423	-0.526318
O	0.060031	1.127244	0.906603
C	1.060279	1.853800	0.640353
O	0.917199	2.972012	-0.156951
C	-0.419806	3.408447	-0.385558
C	2.376874	1.500411	0.920962
H	3.187286	2.180895	0.685563
H	2.553688	0.720947	1.648755
H	2.173086	0.753980	-1.538539
H	0.926526	-2.682671	0.784148
H	3.273800	-3.375287	0.989696
H	5.083452	-2.045224	-0.090452
H	4.542721	0.060601	-1.274096

H	-0.162774	0.286366	-1.297741
C	-1.180352	-1.184803	-0.009601
H	-0.333212	4.350385	-0.931639
H	-0.990700	2.690185	-0.983683
H	-0.952284	3.573558	0.557723
C	-2.485891	-0.395043	-0.168554
H	-1.268914	-2.147865	-0.539530
H	-1.025879	-1.429736	1.048739
C	-3.712008	-1.159390	0.363074
H	-2.380173	0.558717	0.359923
H	-2.646442	-0.155783	-1.229160
C	-4.984793	-0.364610	0.254225
H	-3.822898	-2.110486	-0.175469
H	-3.532376	-1.415734	1.418825
C	-6.057165	-0.718402	-0.454982
H	-4.999400	0.580526	0.800560
H	-6.946851	-0.095692	-0.499225
H	-6.088595	-1.649997	-1.017212

1 imaginary frequency
E = -733.982719
H = -733.648285
G = -733.711131
E_{SCS-MP2} = -732.422272

14'

C	1.791826	2.825965	-0.074224
C	1.876510	1.795871	0.781683
C	0.753077	0.788449	0.922262
C	-0.142088	0.703797	-0.323787
C	-0.243190	1.938728	-1.100512
C	0.655317	2.942206	-0.978276
C	1.239165	-0.568775	1.492895
C	-0.846944	-0.411502	-0.621130
C	-1.871220	-0.598244	-1.706792
C	-3.156586	-1.307870	-1.231502
C	-4.007318	-0.524890	-0.208449
C	-3.476912	-0.524486	1.201553
C	-3.325120	0.549634	1.978509
H	-3.545372	1.552443	1.617813
H	-2.976847	0.469208	3.005052
H	-3.242148	-1.508923	1.612421
H	0.098089	1.195354	1.718452
H	-0.670313	-1.309233	-0.034403
H	-1.031846	2.020571	-1.842003
H	0.567666	3.830178	-1.599302
H	2.574446	3.579763	-0.113924
H	2.725469	1.695386	1.453153
C	2.018580	-1.440012	0.525768
H	0.395231	-1.162524	1.848739
H	1.879817	-0.358479	2.358346
H	-1.431733	-1.216033	-2.505975
H	-2.143885	0.353214	-2.177081
H	-5.007559	-0.985169	-0.191661
H	-4.150690	0.508311	-0.552502
H	-2.896079	-2.289470	-0.809833
H	-3.776244	-1.511821	-2.114328
O	3.173624	-0.849650	0.147849
O	1.673102	-2.535999	0.137373
C	3.962344	-1.586200	-0.800246
H	4.829506	-0.959059	-1.009165
H	4.273643	-2.545758	-0.378436
H	3.390405	-1.768789	-1.713654

0 imaginary frequencies
E = -734.023145
H = -733.685523

G = -733.750864
E_{SCS-MP2} = -732.474391

TS-14' (Alder-ene reaction)

C	0.918913	2.974805	-0.049785
C	1.207598	1.917689	0.755857
C	0.474393	0.657147	0.661434
C	-0.364909	0.448172	-0.541119
C	-0.657572	1.622322	-1.319608
C	-0.049444	2.826157	-1.091236
C	1.186284	-0.560025	1.286643
C	-1.037683	-0.759581	-0.694100
C	-2.183112	-1.011228	-1.640131
C	-3.465725	-1.348750	-0.841940
C	-3.567486	-0.429051	0.381529
C	-2.391305	-0.623459	1.302778
C	-1.834764	0.340935	2.137916
H	-2.256321	1.346920	2.140981
H	-1.395790	0.026762	3.084386
H	-2.183011	-1.665434	1.548400
H	-0.536707	0.728872	1.488156
H	-0.581156	-1.651253	-0.278919
H	-1.336688	1.534937	-2.161416
H	-0.272158	3.672320	-1.736533
H	1.434559	3.923238	0.075780
H	1.963535	2.007764	1.532249
C	2.164493	-1.233429	0.342330
H	0.465897	-1.318945	1.597774
H	1.728762	-0.222807	2.176824
H	-1.946434	-1.837548	-2.323518
H	-2.383730	-0.136135	-2.265433
H	-4.497323	-0.653293	0.928522
H	-3.633935	0.622753	0.071545
H	-3.418960	-2.390788	-0.495549
H	-4.354848	-1.270395	-1.480210
O	3.263872	-0.472607	0.147418
O	1.995286	-2.311470	-0.187989
C	4.222643	-1.001674	-0.782183
H	5.023630	-0.263231	-0.828584
H	4.606478	-1.964353	-0.433564
H	3.766991	-1.136945	-1.766630

1 imaginary frequency

E = -733.996869
H = -733.663937
G = -733.722349
E_{SCS-MP2} = -732.448694