Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Cycloreversion of the CO_2 Trimer: a Paradigmatic Pseudopericyclic [2+2+2] Cycloaddition Reaction

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1 Gaussian reference

See References section at the end of this document (cite 1)

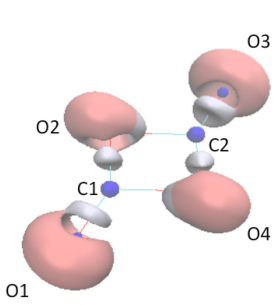
2 ELF analysis

ELF fluctuation analysis:

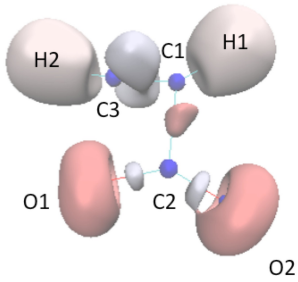
The fluctuation analysis follows the procedure outlined in Ref. 34 and 35, which consists in balancing the contributions to the fluctuations in the atomic pair (A,B) from A to B, against those occurring from B to A. The importance of interactions between pairs of basins in each member of the basin pair can be calculated from the contribution analysis (CA):

$$CA(\Omega_i|\Omega_j) = \frac{V(\Omega_i, \Omega_j)}{\sum_{k \neq j} V(\Omega_j, \Omega_k)} \cdot 100 = \frac{-V(\Omega_i, \Omega_j)}{\sigma^2(\Omega_j)} \cdot 100 \qquad (1)$$

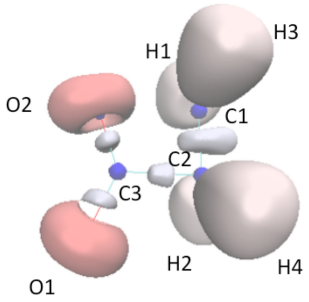
These numbers are included in Tables S1-S3 and the labels of the atoms in these tables correspond to the following structures:



TS1a



TS1b



TS1c

Table S1. ELF analysis of the TS1a species. Basin volume [Vol(Ω_i)], populations [N(Ω_i)] and variance of the basin populations [$\sigma^2(\Omega_i)$] are fiven in the first columns. The percentage of the contribution to the variance of a each basin from other basins is given in parenthesis, while boldfaced numbers refer to the contributing basins.

i	basin(Ω_i)	Vol(Ω_i)	N(Ω_i)	$\sigma^2(\Omega_i)$	Contributions Analysis greater than 5%. **Basin** (% contribution)
1	C(C1)	0.83	2.09	0.25	**7** (20.0) **8** (20.0) **9** (4.0) **10** (4.0) **11** (28.0) **12** (8.0) **13** (8.0) **14** (8.0)
2	C(O1)	0.26	2.12	0.34	**7** (15.2) **8** (15.2) **12** (39.4) **14** (30.3)
3	C(O2)	0.26	2.11	0.33	**11** (18.8) **13** (65.6) **15** (15.6)
4	C(C2)	0.82	2.08	0.25	**10** (8.3) **13** (4.2) **15** (4.2) **16** (29.2) **17** (8.3) **18** (20.8) **19** (16.7) **20** (8.3)
5	C(O3)	0.26	2.11	0.34	**17** (40.6) **18** (15.6) **19** (12.5) **20** (31.2)
6	C(O4)	0.26	2.11	0.33	**9** (15.6) **10** (65.6) **16** (18.8)
7	V(C1,O1)	14.58	1.41	0.93	**1** (5.4) **2** (5.4) **8** (21.5) **9** (4.3) **11** (7.5) **12** (28.0) **13** (3.2) **14** (22.6)
8	V(C1,O1)	14.54	1.41	0.93	**1** (5.5) **2** (5.5) **7** (22.0) **9** (3.3) **11** (7.7) **12** (27.5) **13** (3.3) **14** (23.1)
9	V(C1,O4)	7.81	1.23	0.82	**6** (6.2) **7** (4.9) **8** (3.7) **10** (51.9) **11** (7.4) **13** (3.7) **16** (14.8)
10	V(O4)	104.19	4.53	1.54	**6** (13.7) **9** (27.5) **16** (38.6)
11	V(C1,O2)	16.63	2.08	1.18	**1** (6.0) **3** (5.1) **7** (6.0) **8** (6.0) **9** (5.1) **12** (3.4) **13** (50.4) **14** (3.4) **15** (10.3)
12	V(O1)	72.34	2.78	1.27	**2** (10.3) **7** (20.6) **8** (19.8) **11** (3.2) **14** (38.9)
13	V(O2)	104.14	4.53	1.55	**3** (13.7) **11** (38.6) **15** (27.5)
14	V(O1)	60.7	2.22	1.14	**2** (8.9) **7** (18.7) **8** (18.7) **11** (3.6) **12** (43.7)
15	V(O2,C2)	7.78	1.23	0.82	**3** (6.2) **10** (3.7) **11** (14.8) **13** (51.9) **16** (7.4) **18** (4.9) **19** (3.7)
16	V(C2,O4)	16.66	2.08	1.18	**4** (6.0) **6** (5.1) **9** (10.3) **10** (50.4) **15** (5.1) **17** (3.4) **18** (6.0) **19** (6.0) **20** (3.4)
17	V(O3)	72.37	2.8	1.28	**5** (10.3) **16** (3.2) **18** (20.6) **19** (19.8) **20** (38.9)
18	V(C2,O3)	14.71	1.45	0.94	**4** (5.4) **5** (5.4) **10** (3.2) **15** (4.3) **16** (7.5) **17** (28.0) **19** (21.5) **20** (22.6)
19	V(C2,O3)	14.48	1.38	0.91	**4** (4.5) **5** (4.5) **10** (3.4) **15** (3.4) **16** (7.9) **17** (28.1) **18** (22.5) **20** (23.6)
20	V(O3)	60.69	2.22	1.14	**5** (8.9) **16** (3.6) **17** (43.8) **18** (18.8) **19** (18.8)

Table S2. ELF analysis of the TS1b species. Basin volume [Vol(Ω_i)], populations [N(Ω_i)] and variance of the basin populations [$\sigma^2(\Omega_i)$] are fiven in the first columns. The percentage of the contribution to the variance of a each basin from other basins is given in parenthesis, while boldfaced numbers refer to the contributing basins.

i	basin (Ω_i)	Vol (Ω_i)	N(Ω_i)	σ^2 (Ω_i)	Contributions Analysis greater than 5%. **Basin** (% contribution)
1	C(C1)	0.81	2.08	0.25	**6** (34.8) **7** (4.3) **8** (26.1) **9** (30.4) **10** (4.3)
2	C(O1)	0.26	2.12	0.34	**11** (48.4) **12** (19.4) **13** (32.3)
3	C(C2)	0.84	2.09	0.25	**10** (12.5) **11** (8.3) **12** (29.2) **13** (4.2) **14** (33.3) **15** (4.2) **16** (8.3)
4	C(O2)	0.26	2.11	0.34	**14** (25) **15** (34.4) **16** (40.6)
5	C(C3)	0.8	2.09	0.26	**6** (3.8) **7** (30.8) **8** (23.1) **9** (23.1) **10** (19.2)
6	V(H1,C1)	85.05	2.25	0.65	**1** (12.5) **7** (6.3) **8** (28.1) **9** (28.1) **10** (6.3) **11** (3.1) **13** (9.4)
7	V(H2,C3)	91.65	2.19	0.69	**5** (11.6) **6** (5.8) **8** (24.6) **9** (24.6) **10** (23.2)
8	V(C1,C3)	58.6	2.02	1.05	**1** (5.8) **5** (5.8) **6** (17.5) **7** (16.5) **9** (29.1) **10** (16.5)
9	V(C1,C3)	58.6	1.98	1.04	**1** (6.7) **5** (5.8) **6** (17.3) **7** (16.3) **8** (28.8) **10** (16.3)
10	V(C3)	24.68	1.65	1.00	**3** (3) **5** (5.1) **6** (4.0) **7** (16.2) **8** (17.2) **9** (17.2) **11** (4.0) **12** (9.1) **13** (4.0) **14** (11) **15** (3.0) **16**(5.1)
11	V(O1)	100.4	3.37	1.37	**2** (11) **12** (32.4) **13** (40.4) **14** (3.7)
12	V(O1,C2)	16.9	2.07	1.19	**2** (5.1) **3** (5.9) **10** (7.6) **11** (37.3) **13** (23.7) **14** (10.2)
13	V(O1)	31.86	2.26	1.16	**2** (8.6) **6** (5.2) **10** (3.4) **11** (47.4) **12** (24.1)
14	V(C2,O2)	21.75	2.45	1.33	**3** (6) **4** (6.0) **10** (8.3) **11** (3.8) **12** (9.0) **15** (28.6) **16** (34.6)
15	V(O2)	64.7	2.33	1.16	**4** (9.5) **14** (32.8) **16** (44.8)
16	V(O2)	78.01	2.94	1.30	**4** (10) **10** (3.8) **14** (35.4) **15** (40.0)

Table S3. ELF analysis of the TS1c species. Basin volume [Vol(Ω_i)], populations [N(Ω_i)] and variance of the basin populations [$\sigma^2(\Omega_i)$] are fiven in the first columns. The percentage of the contribution to the variance of a each basin from other basins is given in parenthesis, while boldfaced numbers refer to the contributing basins.

i	basin(Ω_i)	Vol(Ω_i)	N(Ω_i)	$\sigma^2(\Omega_i)$	Contributions Analysis greater than 5%. **Basin** (% contribution)
1	C(C1)	0.83	2.09	0.25	**6** (30.4) **8** (34.8) **10** (30.4) **11** (4.3)
2	C(C2)	0.81	2.1	0.26	**7** (29.2) **9** (29.2) **10** (29.2) **11** (12.5
3	C(C3)	0.84	2.09	0.25	**11** (12.5) **12** (29.2) **13** (4.2) **14** (8.3) **15** (33.3) **16** (4.2) **17** (8.3)
4	C(O1)	0.26	2.11	0.33	**15** (25.0) **16** (34.4) **17** (40.6)
5	C(O2)	0.26	2.11	0.33	**12** (19.4) **13** (35.5) **14** (45.2)
6	V(H1,C1)	74.75	2.06	0.6	**1** (12.1) **7** (3.4) **8** (32.8) **9** (3.4) **10** (31.0) **11** (3.4) **13** (6.9)
7	V(H2,C2)	79.71	2.09	0.68	**2** (10.4) **9** (28.4) **10** (26.9) **11** (19.4
8	V(H3,C1)	75.85	2.11	0.61	**1** (13.6) **6** (32.2) **7** (3.4) **9** (3.4) **10** (30.5) **11** (3.4) **13** (6.8)
9	V(H4,C2)	78.75	2.05	0.67	**2** (10.4) **7** (28.4) **10** (26.9) **11** (19.4
10	V(C1,C2)	35.77	2.33	1.15	**1** (6.1) **2** (6.1) **6** (15.7) **7** (15.7 **8** (15.7) **9** (15.7) **11** (15.7)
11	V(C2,C3)	18.72	1.43	0.92	**2** (3.4) **3** (3.4) **7** (14.6) **9** (14.6 **10** (20.2) **12** (10.1) **13** (4.5) **14** (3.4) **15** (11.2) **16** (3.4) **17** (5.6)
12	V(C3,O2)	18.44	2.09	1.2	**3** (5.8) **5** (5.0) **11** (7.5) **13** (26.7 **14** (35.0) **15** (10)
13	V(O2)	36.21	2.47	1.22	**5** (9.0) **6** (3.3) **8** (3.3) **11** (3.3) **12** (26.2) **14** (45.9)
14	V(O2)	95.91	3.16	1.32	**5** (10.6) **12** (31.8) **13** (42.4) **15** (3)
15	V(C3,O1)	20.07	2.39	1.3	**3** (6.2) **4** (6.2) **11** (7.8) **12** (9.3) **14** (3.1) **16** (28.7) **17** (34.9)
16	V(O1)	65.07	2.34	1.17	**4** (9.3) **15** (31.4) **17** (44.9)
17	V(O1)	77.42	2.97	1.31	**4** (9.8)" **11** (3.8)" **15** (34.1)" **16** (40.2)"

3 ACID representations

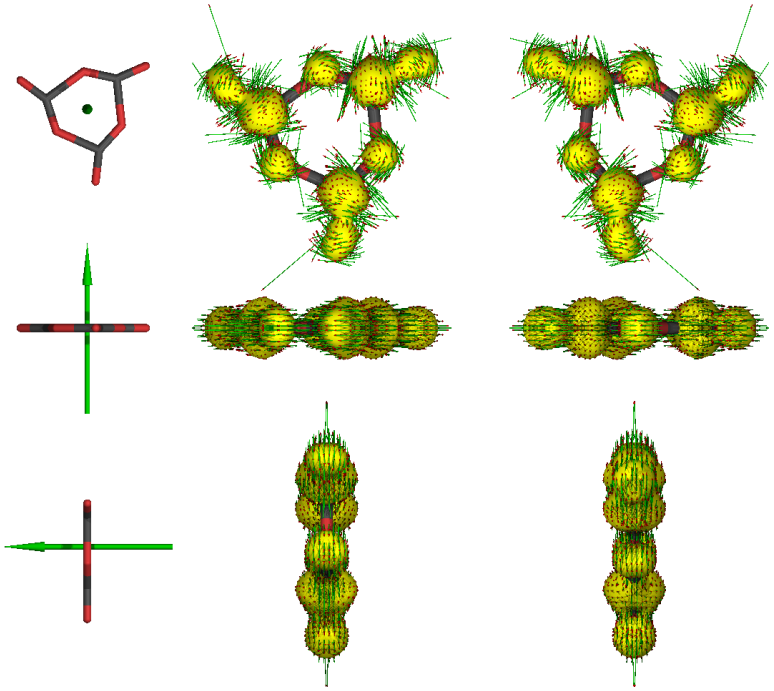


Figure S1: **Multiple view, surface and vectors of TS1a**

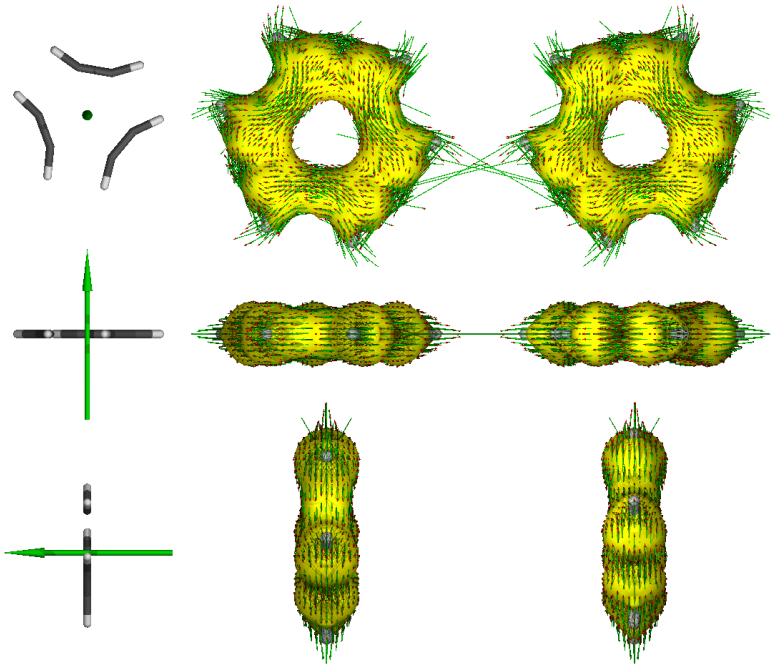


Figure S2: **Multiple view, surface and vectors of TS1b**

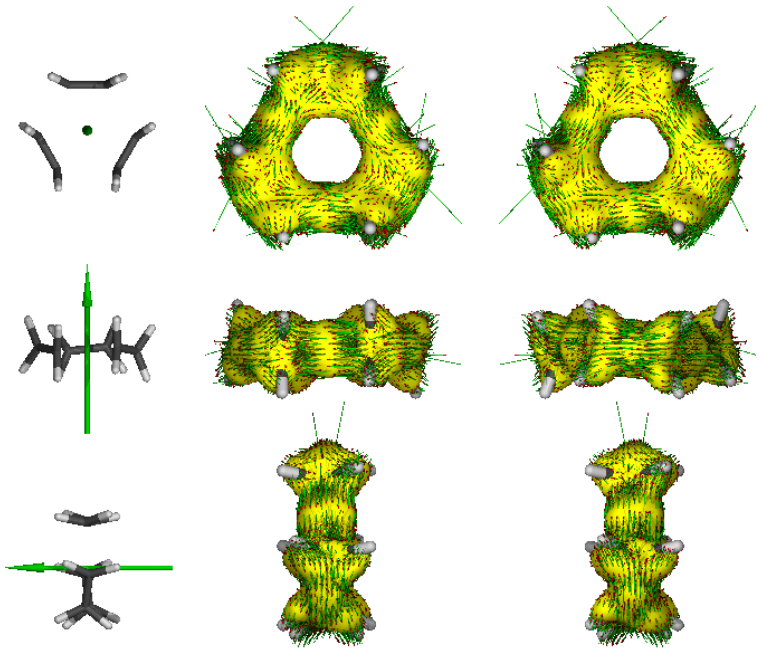


Figure S3: **Multiple view, surface and vectors of TS1c**

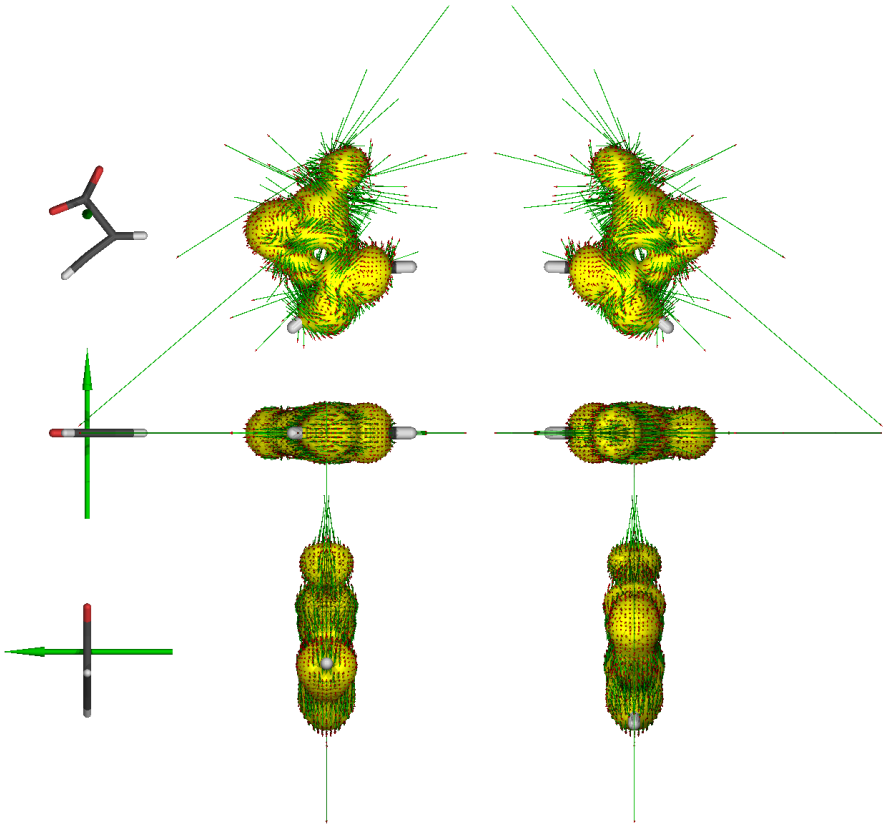


Figure S4: **Multiple view, surface and vectors of TS1f**

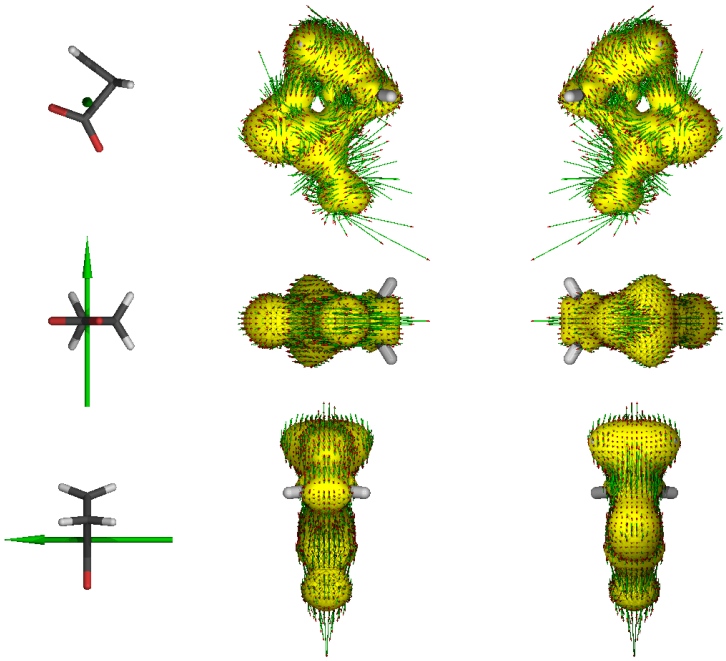


Figure S5: **Multiple view, surface and vectors of TS1g**

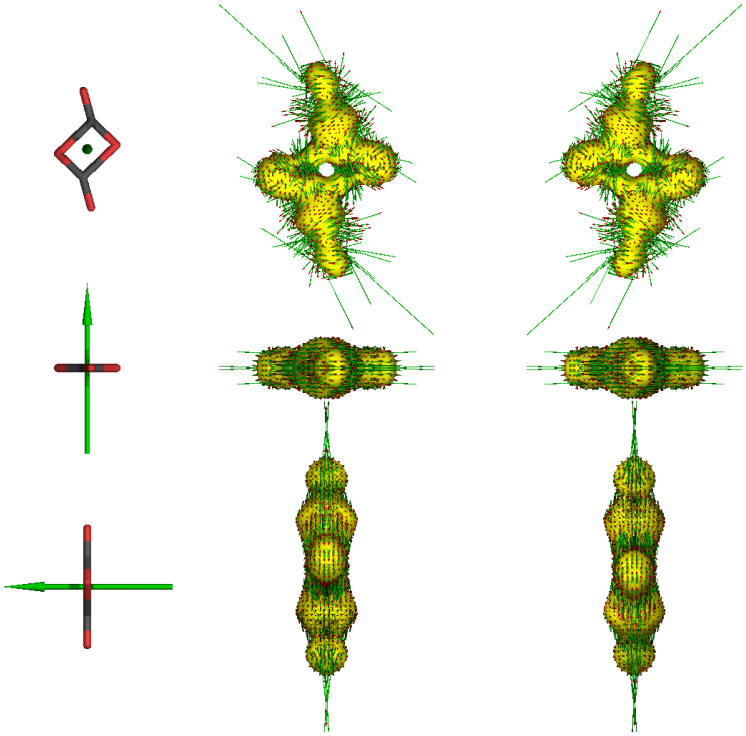


Figure S6: **Multiple view, surface and vectors of TS1h**

4 Geometric parameters

Bond distances between ring atoms along the reaction coordinate for the cycloreversion of 1,3,5-Trioxane-2,4,6-trione

Reaction Coordinate	d_{1-2}	d_{2-3}	d_{3-4}	d_{4-5}	d_{5-6}	d_{6-1}
-3.55072	1.354	1.358	1.354	1.358	1.354	1.358
-3.19733	1.351	1.382	1.351	1.382	1.351	1.382
-2.84258	1.343	1.413	1.343	1.413	1.343	1.413
-2.48740	1.330	1.447	1.330	1.447	1.330	1.447
-2.13211	1.317	1.482	1.317	1.483	1.317	1.483
-1.77679	1.302	1.519	1.302	1.519	1.302	1.519
-1.42144	1.287	1.555	1.287	1.556	1.287	1.556
-1.06610	1.272	1.593	1.272	1.594	1.272	1.594
-0.71075	1.257	1.630	1.257	1.631	1.257	1.631
-0.35543	1.242	1.668	1.242	1.668	1.242	1.669
0.00000	1.228	1.705	1.229	1.706	1.228	1.706
0.35542	1.216	1.742	1.216	1.743	1.216	1.743
0.71074	1.204	1.779	1.204	1.779	1.204	1.780
1.06608	1.194	1.816	1.194	1.816	1.194	1.817
1.42143	1.185	1.852	1.185	1.852	1.185	1.853
1.77679	1.177	1.889	1.177	1.888	1.177	1.890
2.13216	1.170	1.925	1.170	1.924	1.170	1.925
2.48753	1.165	1.961	1.165	1.960	1.165	1.961
2.84289	1.161	1.996	1.161	1.996	1.161	1.997
3.19825	1.158	2.032	1.158	2.032	1.158	2.033
3.55360	1.155	2.068	1.155	2.067	1.155	2.068
3.90892	1.154	2.103	1.154	2.103	1.154	2.104
4.26420	1.153	2.139	1.153	2.138	1.153	2.139
4.61943	1.153	2.174	1.153	2.174	1.153	2.175
4.97462	1.152	2.209	1.152	2.209	1.153	2.210

Reaction Coordinate	d_{1-2}	d_{2-3}	d_{3-4}	d_{4-5}	d_{5-6}	d_{6-1}
5.32978	1.153	2.244	1.153	2.244	1.153	2.244
5.68497	1.153	2.277	1.153	2.277	1.153	2.277
6.04021	1.153	2.309	1.153	2.309	1.153	2.310
6.39551	1.153	2.341	1.153	2.341	1.153	2.341
6.75085	1.154	2.371	1.154	2.371	1.154	2.371
7.10622	1.154	2.400	1.154	2.400	1.154	2.400
7.46161	1.154	2.429	1.154	2.430	1.154	2.430
7.81700	1.155	2.458	1.155	2.458	1.155	2.458
8.17238	1.155	2.487	1.155	2.487	1.155	2.487
8.52775	1.155	2.516	1.155	2.516	1.155	2.516
8.88312	1.155	2.544	1.155	2.544	1.155	2.544
9.23850	1.155	2.571	1.155	2.572	1.155	2.571
9.59388	1.155	2.599	1.155	2.600	1.155	2.599
9.94927	1.155	2.627	1.155	2.627	1.155	2.627
10.30466	1.155	2.655	1.155	2.655	1.155	2.655
10.66005	1.155	2.682	1.155	2.682	1.155	2.682
11.01542	1.156	2.709	1.156	2.708	1.156	2.709
11.37077	1.156	2.736	1.156	2.734	1.156	2.736
11.72613	1.155	2.761	1.155	2.760	1.155	2.762
12.08152	1.155	2.786	1.155	2.786	1.155	2.788
12.43691	1.155	2.812	1.155	2.813	1.155	2.815
12.79228	1.155	2.839	1.155	2.839	1.155	2.841
13.14754	1.155	2.867	1.155	2.863	1.155	2.866

Bond distances between ring atoms along the reaction coordinate for the cycloreversion of Benzene

Reaction Coordinate	d_{1-2}	d_{2-3}	d_{3-4}	d_{4-5}	d_{5-6}	d_{6-1}
-7.57465	1.394	1.404	1.394	1.404	1.394	1.404
-7.34529	1.395	1.427	1.395	1.427	1.395	1.427
-7.11576	1.393	1.452	1.393	1.451	1.393	1.452
-6.88620	1.391	1.477	1.391	1.477	1.391	1.477
-6.65664	1.388	1.503	1.388	1.502	1.388	1.502
-6.42708	1.385	1.528	1.385	1.527	1.385	1.528
-6.19752	1.382	1.554	1.382	1.553	1.382	1.553
-5.96796	1.378	1.580	1.378	1.578	1.378	1.579
-5.73841	1.375	1.606	1.375	1.604	1.375	1.605
-5.50885	1.372	1.631	1.372	1.630	1.372	1.630
-5.27930	1.368	1.657	1.368	1.655	1.368	1.656
-5.04974	1.365	1.683	1.365	1.681	1.365	1.682
-4.82019	1.361	1.709	1.361	1.707	1.361	1.708
-4.59064	1.357	1.735	1.357	1.732	1.357	1.734
-4.36110	1.353	1.761	1.353	1.758	1.353	1.760
-4.13155	1.349	1.787	1.349	1.784	1.349	1.786
-3.90201	1.344	1.813	1.344	1.810	1.344	1.812
-3.67248	1.339	1.839	1.339	1.837	1.339	1.838
-3.44294	1.333	1.865	1.334	1.863	1.334	1.864
-3.21341	1.328	1.892	1.328	1.889	1.328	1.890
-2.98388	1.321	1.918	1.321	1.915	1.321	1.916
-2.75435	1.314	1.944	1.315	1.941	1.315	1.943
-2.52482	1.307	1.970	1.307	1.967	1.307	1.969
-2.29529	1.299	1.997	1.299	1.994	1.300	1.995
-2.06576	1.291	2.023	1.291	2.020	1.291	2.021
-1.83622	1.283	2.049	1.283	2.046	1.283	2.047
-1.60668	1.274	2.074	1.274	2.071	1.274	2.073
-1.37713	1.265	2.100	1.265	2.097	1.265	2.098
-1.14759	1.256	2.126	1.256	2.123	1.256	2.124
-0.91805	1.248	2.151	1.248	2.148	1.248	2.150
-0.68853	1.240	2.177	1.240	2.174	1.240	2.175
-0.45901	1.234	2.202	1.234	2.200	1.234	2.201
-0.22951	1.227	2.228	1.227	2.225	1.227	2.226
0.00000	1.222	2.253	1.222	2.251	1.222	2.252
0.22953	1.217	2.279	1.217	2.276	1.217	2.277
0.45904	1.213	2.304	1.213	2.301	1.213	2.303
0.68857	1.209	2.329	1.209	2.327	1.209	2.328
0.91811	1.205	2.355	1.205	2.352	1.205	2.354
1.14764	1.202	2.380	1.202	2.378	1.202	2.379
1.37717	1.200	2.405	1.200	2.403	1.200	2.404
1.60670	1.198	2.430	1.198	2.429	1.198	2.430
1.83623	1.197	2.456	1.197	2.454	1.197	2.455

Reaction Coordinate	d_{1-2}	d_{2-3}	d_{3-4}	d_{4-5}	d_{5-6}	d_{6-1}
2.06577	1.196	2.481	1.196	2.479	1.196	2.480
2.29531	1.195	2.506	1.195	2.504	1.195	2.505
2.52485	1.194	2.531	1.194	2.530	1.194	2.530
2.75440	1.194	2.556	1.194	2.555	1.194	2.555
2.98396	1.194	2.580	1.194	2.580	1.194	2.579
3.21351	1.193	2.605	1.193	2.604	1.193	2.604
3.44307	1.193	2.630	1.193	2.629	1.193	2.629
3.67263	1.193	2.655	1.193	2.654	1.193	2.654
3.90219	1.193	2.679	1.193	2.678	1.193	2.679
4.13175	1.193	2.704	1.193	2.703	1.193	2.703
4.36131	1.193	2.729	1.193	2.727	1.193	2.728
4.59087	1.193	2.753	1.193	2.752	1.193	2.753
4.82043	1.193	2.778	1.194	2.777	1.193	2.777
5.04999	1.194	2.802	1.194	2.801	1.194	2.801
5.27955	1.194	2.826	1.194	2.826	1.194	2.826
5.50911	1.194	2.850	1.194	2.851	1.194	2.850
5.73867	1.194	2.875	1.194	2.876	1.194	2.874
5.96823	1.194	2.899	1.194	2.900	1.194	2.899
6.19779	1.194	2.924	1.194	2.924	1.194	2.923
6.42735	1.194	2.948	1.194	2.948	1.194	2.947
6.65691	1.194	2.972	1.194	2.972	1.194	2.972
6.88647	1.194	2.996	1.194	2.996	1.194	2.997
7.11604	1.194	3.020	1.194	3.020	1.194	3.021
7.34559	1.195	3.044	1.195	3.045	1.195	3.046
7.57501	1.195	3.067	1.195	3.069	1.195	3.070
7.80430	1.195	3.090	1.194	3.091	1.195	3.097
8.03371	1.195	3.113	1.194	3.112	1.195	3.124
8.26309	1.195	3.136	1.195	3.136	1.195	3.149
8.49257	1.195	3.160	1.195	3.161	1.195	3.173
8.72211	1.195	3.184	1.195	3.187	1.195	3.195
8.95167	1.195	3.208	1.195	3.212	1.195	3.218
9.18123	1.195	3.233	1.195	3.238	1.195	3.240
9.41079	1.195	3.257	1.195	3.263	1.195	3.263
9.64035	1.195	3.281	1.195	3.287	1.195	3.286
9.86991	1.195	3.306	1.195	3.311	1.195	3.309
10.09947	1.195	3.331	1.195	3.335	1.195	3.332
10.32903	1.195	3.356	1.195	3.359	1.195	3.355
10.55859	1.195	3.380	1.195	3.382	1.195	3.379
10.78814	1.195	3.405	1.195	3.406	1.195	3.403
11.01769	1.196	3.429	1.195	3.430	1.196	3.427
11.24723	1.196	3.452	1.196	3.454	1.196	3.452
11.47676	1.196	3.474	1.196	3.479	1.196	3.476

Reaction Coordinate	d_{1-2}	d_{2-3}	d_{3-4}	d_{4-5}	d_{5-6}	d_{6-1}
11.70629	1.196	3.495	1.196	3.503	1.196	3.502
11.93580	1.196	3.516	1.196	3.527	1.196	3.529
12.16530	1.196	3.536	1.196	3.550	1.196	3.557
12.39483	1.196	3.556	1.196	3.572	1.196	3.585
12.62433	1.196	3.575	1.196	3.596	1.196	3.613
12.85380	1.196	3.595	1.196	3.621	1.196	3.638
13.08328	1.196	3.617	1.196	3.647	1.196	3.662
13.31278	1.196	3.639	1.196	3.674	1.196	3.684
13.54230	1.196	3.661	1.196	3.701	1.196	3.705
13.77176	1.196	3.685	1.196	3.728	1.196	3.725
14.00116	1.196	3.711	1.196	3.753	1.196	3.746
14.23059	1.196	3.739	1.196	3.775	1.196	3.766
14.46008	1.196	3.768	1.196	3.795	1.196	3.787
14.68952	1.196	3.796	1.196	3.815	1.196	3.810
14.91896	1.196	3.821	1.196	3.837	1.196	3.835
15.14844	1.196	3.844	1.196	3.860	1.196	3.860
15.37787	1.196	3.866	1.196	3.883	1.196	3.886
15.60732	1.196	3.887	1.196	3.907	1.196	3.912
15.83679	1.196	3.908	1.196	3.931	1.196	3.938
16.06631	1.196	3.928	1.196	3.954	1.196	3.964
16.29585	1.196	3.948	1.196	3.977	1.196	3.990
16.52531	1.196	3.967	1.196	4.001	1.196	4.015
16.75462	1.196	3.986	1.196	4.028	1.196	4.039
16.98403	1.196	4.004	1.196	4.056	1.196	4.062
17.21328	1.196	4.025	1.196	4.084	1.196	4.085
17.44235	1.196	4.050	1.196	4.109	1.196	4.106
17.67150	1.196	4.079	1.196	4.130	1.196	4.124
17.90073	1.196	4.109	1.196	4.150	1.196	4.143
18.12959	1.196	4.134	1.196	4.174	1.196	4.166

Bond distances between ring atoms along the reaction coordinate for the cycloreversion of Cyclohexane

Reaction Coordinate	d_{1-2}	d_{2-3}	d_{3-4}	d_{4-5}	d_{5-6}	d_{6-1}
-7.53678	1.537	1.537	1.537	1.537	1.537	1.537
-7.28538	1.538	1.538	1.538	1.539	1.538	1.538
-7.03398	1.539	1.540	1.540	1.540	1.540	1.540
-6.78257	1.541	1.541	1.541	1.541	1.541	1.541
-6.53118	1.542	1.543	1.542	1.543	1.542	1.543
-6.27980	1.545	1.545	1.545	1.545	1.545	1.545
-6.02855	1.548	1.548	1.548	1.549	1.548	1.548
-5.77767	1.552	1.554	1.552	1.554	1.552	1.554
-5.52744	1.558	1.563	1.558	1.564	1.558	1.563
-5.27738	1.564	1.578	1.564	1.578	1.564	1.578
-5.02682	1.569	1.597	1.569	1.598	1.569	1.598
-4.77582	1.570	1.620	1.570	1.621	1.570	1.621
-4.52462	1.570	1.646	1.570	1.646	1.570	1.646
-4.27332	1.567	1.673	1.567	1.673	1.567	1.673
-4.02198	1.562	1.701	1.562	1.702	1.562	1.701
-3.77063	1.556	1.729	1.556	1.730	1.556	1.730
-3.51927	1.548	1.759	1.548	1.760	1.548	1.759
-3.26790	1.540	1.788	1.540	1.790	1.540	1.789
-3.01653	1.530	1.819	1.530	1.820	1.530	1.819
-2.76516	1.520	1.849	1.520	1.850	1.520	1.849
-2.51379	1.509	1.879	1.509	1.880	1.509	1.880
-2.26242	1.497	1.910	1.497	1.911	1.497	1.910
-2.01104	1.484	1.940	1.484	1.941	1.484	1.940
-1.75966	1.471	1.970	1.471	1.972	1.471	1.971
-1.50828	1.458	2.000	1.458	2.002	1.458	2.001
-1.25689	1.444	2.030	1.444	2.032	1.444	2.031
-1.00550	1.430	2.060	1.430	2.061	1.430	2.061
-0.75411	1.417	2.090	1.417	2.091	1.416	2.090
-0.50273	1.403	2.119	1.403	2.121	1.403	2.120
-0.25139	1.390	2.149	1.390	2.151	1.390	2.150
0.00000	1.379	2.179	1.379	2.180	1.379	2.180
0.25137	1.368	2.209	1.368	2.210	1.368	2.209
0.50272	1.358	2.238	1.358	2.240	1.358	2.239
0.75408	1.350	2.268	1.350	2.269	1.350	2.269
1.00545	1.343	2.298	1.343	2.299	1.343	2.299
1.25682	1.336	2.327	1.336	2.328	1.336	2.328
1.50819	1.331	2.356	1.331	2.358	1.331	2.357
1.75955	1.327	2.385	1.327	2.387	1.327	2.387
2.01091	1.324	2.414	1.324	2.415	1.324	2.415
2.26226	1.321	2.442	1.321	2.443	1.321	2.443
2.51363	1.320	2.470	1.320	2.471	1.320	2.471

Reaction Coordinate	d_{1-2}	d_{2-3}	d_{3-4}	d_{4-5}	d_{5-6}	d_{6-1}
2.76501	1.319	2.498	1.319	2.499	1.319	2.499
3.01640	1.319	2.525	1.319	2.526	1.319	2.526
3.26781	1.318	2.552	1.318	2.552	1.318	2.552
3.51922	1.318	2.578	1.318	2.579	1.318	2.579
3.77063	1.318	2.604	1.318	2.605	1.318	2.605
4.02205	1.319	2.631	1.319	2.631	1.319	2.632
4.27347	1.319	2.657	1.319	2.657	1.319	2.658
4.52488	1.319	2.682	1.319	2.683	1.319	2.684
4.77630	1.319	2.708	1.319	2.709	1.319	2.710
5.02772	1.319	2.734	1.319	2.735	1.320	2.735
5.27914	1.320	2.760	1.320	2.761	1.320	2.761
5.53056	1.320	2.785	1.320	2.787	1.320	2.786
5.78198	1.320	2.811	1.320	2.813	1.320	2.811
6.03340	1.321	2.836	1.321	2.839	1.321	2.836
6.28482	1.321	2.861	1.321	2.865	1.321	2.861
6.53624	1.321	2.887	1.321	2.891	1.321	2.887
6.78766	1.321	2.912	1.321	2.917	1.321	2.912
7.03908	1.322	2.938	1.322	2.942	1.322	2.937
7.29050	1.322	2.963	1.322	2.967	1.322	2.962
7.54192	1.322	2.989	1.322	2.992	1.322	2.988
7.79334	1.322	3.014	1.322	3.017	1.322	3.014
8.04476	1.322	3.039	1.322	3.042	1.322	3.040
8.29618	1.322	3.064	1.322	3.067	1.322	3.065
8.54760	1.323	3.089	1.323	3.093	1.323	3.091
8.79902	1.323	3.114	1.323	3.118	1.323	3.116
9.05044	1.323	3.140	1.323	3.143	1.323	3.141
9.30186	1.323	3.165	1.323	3.168	1.323	3.166
9.55328	1.323	3.191	1.323	3.193	1.323	3.191
9.80470	1.323	3.216	1.323	3.218	1.323	3.216
10.05612	1.323	3.241	1.323	3.243	1.323	3.241
10.30752	1.323	3.266	1.323	3.269	1.323	3.266
10.55890	1.323	3.290	1.323	3.295	1.323	3.291
10.81027	1.323	3.314	1.323	3.321	1.323	3.316
11.06160	1.323	3.338	1.323	3.347	1.323	3.341
11.31293	1.323	3.361	1.324	3.373	1.323	3.365
11.56426	1.323	3.384	1.324	3.399	1.324	3.389
11.81555	1.324	3.408	1.324	3.424	1.324	3.412
12.06671	1.324	3.431	1.324	3.447	1.324	3.433

5 Cartesian Coordinates

1a
SCF Energy: -565.731812151
Num. Imaginary Frequencies: 0

C	1.195443	0.690428	0.000000
O	2.211834	1.276953	0.000000
O	1.147095	-0.662371	0.000000
C	0.000295	-1.380361	0.000000
O	-0.000059	-2.553943	0.000000
O	-1.147167	-0.662303	0.000000
C	-1.195613	0.690044	0.000000
O	-2.211795	1.277055	0.000000
O	0.000000	1.324526	0.000000

1b
SCF Energy: -232.229923431
Num. Imaginary Frequencies: 0

C	1.203395	-0.694910	0.000000
C	1.203441	0.694823	0.000000
C	0.000000	-1.389606	0.000000
C	-1.203505	-0.694723	0.000000
C	-1.203447	0.694809	0.000000
C	0.000116	1.389611	0.000000
H	2.140475	1.235610	0.000000
H	2.140349	-1.235823	0.000000
H	-0.000152	-2.471507	0.000000
H	-2.140395	-1.235753	0.000000
H	-2.140281	1.235939	0.000000
H	0.000005	2.471510	0.000000

1c
SCF Energy: -235.843701188
Num. Imaginary Frequencies: 0

C	1.400868	-0.392296	-0.233037
C	1.040247	1.016985	0.232929
H	1.447269	-0.405213	-1.327045
C	-0.360707	1.409320	-0.232929
H	1.074669	1.050624	1.326943
H	1.776400	1.736807	-0.129228
C	-1.400864	0.392295	0.233072
H	-0.616065	2.406771	0.129120
H	-0.372687	1.455894	-1.326947
C	-1.040250	-1.016975	-0.232937
H	-1.447209	0.405213	1.327083
H	-2.392360	0.669894	-0.129008
C	0.360702	-1.409326	0.232907
H	-1.776394	-1.736818	0.129195
H	-1.074684	-1.050572	-1.326954
H	0.372667	-1.455957	1.326921
H	0.616065	-2.406761	-0.129189
H	2.392353	-0.669894	0.129086

TS1a
SCF Energy: -565.682058286
Num. Imaginary Frequencies: 1
Imaginary Frequency: -664.2393

C	-1.015741	1.162189	0.000001
O	-1.391451	-0.007392	0.000005
C	-0.499105	-1.460138	-0.000001
O	0.701852	-1.201315	-0.000001
C	1.514601	0.298306	0.000000
O	0.689761	1.208613	-0.000002
O	-1.266635	-2.327289	-0.000002
O	2.649191	0.066629	0.000001
O	-1.382535	2.260487	-0.000002

TS1b
SCF Energy: -231.912604802
Num. Imaginary Frequencies: 1
Imaginary Frequency: -654.1995

C	1.732436	0.323410	0.000000
C	1.526816	-0.881017	0.000000
C	-0.586986	-1.661934	0.000000
C	-1.526075	-0.880257	0.000000
C	-1.146214	1.338204	0.000000
C	0.000000	1.761484	0.000000
H	-0.152563	-2.633873	0.000000
H	-2.561407	-0.632144	0.000000
H	-2.205176	1.448374	0.000000
H	0.731844	2.534780	0.000000
H	2.357618	1.185240	0.000000
H	1.829818	-1.901720	0.000000

TS1c
SCF Energy: -235.651148834
Num. Imaginary Frequencies: 1
Imaginary Frequency: -746.4777

C	0.001737	1.784586	0.089207
C	1.264019	1.259903	-0.089380
C	1.545114	-0.893339	0.088687
C	0.459816	-1.724823	-0.087861
C	-1.547099	-0.891151	0.087624
C	-1.723634	0.464742	-0.088213
H	1.974159	-0.812967	1.076962
H	2.233422	-0.752347	-0.729755
H	0.270382	-2.118612	-1.075915
H	0.143283	-2.351523	0.730982
H	-1.767659	-1.557018	-0.731804
H	-1.693350	-1.303780	1.075334
H	-2.109014	1.051752	0.730583
H	-1.969091	0.826326	-1.076251
H	-0.281081	2.115721	1.077954
H	-0.465433	2.310587	-0.728429
H	1.698116	1.292449	-1.078178
H	1.966547	1.299901	0.728134

2a
SCF Energy: -188.599339699
Num. Imaginary Frequencies: 0

C	0.000000	0.000000	-0.000001
O	0.000000	0.000000	1.154563
O	0.000000	0.000000	-1.154562

2b
SCF Energy: -77.3295061188
Num. Imaginary Frequencies: 0

C	0.000027	0.597890	0.000000
C	0.000027	-0.597891	0.000000
H	0.000110	1.662965	0.000000
H	-0.000438	-1.662961	0.000000

2c
SCF Energy: -78.5748054591
Num. Imaginary Frequencies: 0

C	0.661786	0.000000	-0.000001
C	-0.661786	0.000000	-0.000002
H	1.228646	0.922316	0.000005
H	1.228648	-0.922315	0.000005
H	-1.228646	-0.922316	0.000004
H	-1.228647	0.922315	0.000003

1d
SCF Energy: -154.666800236
Num. Imaginary Frequencies: 0

C	0.783573	0.663569	0.000007
C	-0.783607	0.663545	-0.000005
C	-0.783573	-0.663569	-0.000007
H	-1.544248	-1.429150	-0.000014
H	1.544248	1.429150	0.000014
C	0.783607	-0.663545	0.000005
H	-1.544598	1.428813	-0.000010
H	1.544598	-1.428813	0.000010

1e
SCF Energy: -157.186477667
Num. Imaginary Frequencies: 0

C	-0.839507	-0.669065	0.141538
C	-0.669062	0.839501	-0.141582
C	0.839497	0.669064	0.141597
C	0.669073	-0.839498	-0.141554
H	-1.230089	1.543422	0.469928
H	-0.845526	1.061106	-1.193819
H	1.543437	1.230094	-0.469886
H	1.061057	0.845545	1.193843
H	-1.543401	-1.230073	-0.470019
H	-1.061145	-0.845581	1.193759
H	1.230067	-1.543422	0.469982
H	0.845590	-1.061105	-1.193783

2d
SCF Energy: -154.599597861
Num. Imaginary Frequencies: 0

C	1.314359	-0.901834	0.000000
C	0.000000	-0.881794	0.000000
C	-0.812919	0.341759	0.000000
C	-0.321973	1.561100	0.000000
H	-0.539442	-1.828747	0.000000
H	-1.894942	0.211519	0.000000
H	2.080867	-1.659497	0.000000
H	-0.723292	2.561337	0.000000

2e
SCF Energy: -157.084997003
Num. Imaginary Frequencies: 0

C	1.449328	-0.616011	0.167880
C	0.706598	0.589996	-0.287622
C	-0.706598	0.589997	0.287621
C	-1.449327	-0.616012	-0.167880
H	-2.326497	-0.964222	0.358209
H	-1.279635	-0.996619	-1.165896
H	-1.234008	1.508865	-0.001570
H	-0.652814	0.608064	1.380133
H	2.326494	-0.964225	-0.358210
H	1.279639	-0.996614	1.165899
H	1.234007	1.508866	0.001569
H	0.652814	0.608063	-1.380133

3d
SCF Energy: -154.603585907
Num. Imaginary Frequencies: 0

C	-1.824051	0.002884	-0.000015
C	-0.593074	0.449602	0.000051
C	0.593074	-0.449602	0.000016
C	1.824051	-0.002884	-0.000028
H	-0.387202	1.515308	-0.000036
H	0.387203	-1.515308	-0.000039
H	-2.308921	-0.960697	-0.000042
H	2.308921	0.960697	-0.000030

3e
SCF Energy: -157.083123675
Num. Imaginary Frequencies: 0

C	1.907404	0.144137	-0.016976
C	0.574807	-0.504775	-0.002490
C	-0.574805	0.504774	-0.002419
C	-1.907400	-0.144146	-0.017015
H	0.471502	-1.178473	-0.859257
H	-0.471496	1.178591	-0.859083
H	2.034810	1.136605	0.392554
H	-2.034885	-1.136444	0.392908
H	2.792234	-0.405955	-0.300163
H	-2.792192	0.405892	-0.300427
H	-0.463848	1.147469	0.883531
H	0.463845	-1.147626	0.883345

4d
SCF Energy: -77.3295061452
Num. Imaginary Frequencies: 0

C	0.000000	0.597961	0.000000
C	0.000000	-0.597961	0.000000
H	0.000282	1.662888	0.000000
H	-0.000282	-1.662888	0.000000

TS1d
SCF Energy: -154.593005241
Num. Imaginary Frequencies: 1
Imaginary Frequency: -484.5827

C	-1.202910	-0.644450	0.000043
C	-0.734034	0.589720	0.000021
C	0.734033	0.589721	-0.000032
C	1.202910	-0.644450	-0.000033
H	1.350114	1.484273	-0.000069
H	2.151713	-1.155895	-0.000061
H	-2.151712	-1.155895	0.000092
H	-1.350115	1.484272	0.000044

TS1e
SCF Energy: -157.084445139
Num. Imaginary Frequencies: 1
Imaginary Frequency: -206.7699

C	-0.716350	0.641487	0.261059
C	0.716350	0.641487	-0.261060
C	1.312042	-0.659478	0.169245
C	-1.312042	-0.659479	-0.169244
H	0.704321	0.703248	-1.351628
H	-1.221712	-0.947903	-1.207976
H	-0.704322	0.703250	1.351626
H	-2.077105	-1.152362	0.413891
H	-1.289618	1.504963	-0.097389
H	1.221720	-0.947896	1.207980
H	2.077097	-1.152367	-0.413894
H	1.289617	1.504964	0.097386

TS2d
SCF Energy: -154.593018896
Num. Imaginary Frequencies: 1
Imaginary Frequency: -182.0160

C	1.683145	-0.381390	-0.213597
C	-1.683146	-0.381389	0.213597
C	-0.695200	0.309922	-0.279518
C	0.695200	0.309922	0.279517
H	0.863897	0.955150	1.143249
H	-0.863897	0.955152	-1.143248
H	2.728991	-0.526345	0.001286
H	-2.728990	-0.526349	-0.001290

TS2e
SCF Energy: -157.077848425
Num. Imaginary Frequencies: 1
Imaginary Frequency: -140.0632

C	-1.810831	-0.182324	-0.314139
C	-0.629476	0.444899	0.330363
C	0.629474	-0.444919	0.330337
C	1.810834	0.182321	-0.314134
H	-0.390578	1.391650	-0.177367
H	0.390572	-1.391662	-0.177403
H	-1.677139	-0.874459	-1.133941
H	1.677130	0.874734	-1.133692
H	-2.804026	0.204553	-0.138142
H	2.804019	-0.204631	-0.138265
H	0.880894	-0.738103	1.352110
H	-0.880883	0.738059	1.352143

TS3d
SCF Energy: -154.587936493

Num. Imaginary Frequencies: 1
Imaginary Frequency: -1422.3715

C	-1.712771	-0.096957	0.324969
C	-0.767807	0.410950	-0.331222
C	0.767807	-0.410950	-0.331223
C	1.712771	0.096957	0.324969
H	-0.664489	1.272187	-0.971387
H	0.664488	-1.272186	-0.971388
H	-2.058522	-0.846310	1.008908
H	2.058522	0.846309	1.008909

TS3e
SCF Energy: -157.078645103
Num. Imaginary Frequencies: 1
Imaginary Frequency: -969.7223

C	1.909397	0.106976	0.000057
C	0.677643	-0.594715	-0.000050
C	-0.677643	0.594714	-0.000054
C	-1.909397	-0.106977	0.000045
H	2.326377	0.488363	-0.921568
H	2.326365	0.488103	0.921794
H	0.464345	-1.162004	0.898927
H	0.464413	-1.161868	-0.899130
H	-0.464352	1.162005	0.898925
H	-0.464405	1.161868	-0.899133
H	-2.326384	-0.488082	0.921782
H	-2.326363	-0.488378	-0.921581

1f
SCF Energy: -265.910864109
Num. Imaginary Frequencies: 0

C	1.337688	-0.077641	-0.000048
C	0.592487	1.025092	-0.000026
C	-0.560928	0.092659	0.000081
O	-1.735654	0.048337	-0.000067
O	0.320820	-1.043040	0.000058
H	2.374441	-0.371973	-0.000214
H	0.728752	2.088936	0.000248

1g
SCF Energy: -267.164799608
Num. Imaginary Frequencies: 0

C	-1.398712	-0.175994	0.000116
C	-0.498534	1.061095	-0.000047
C	0.614327	0.034140	0.000038
O	-0.214064	-1.037480	-0.000113
O	1.803858	0.013991	0.000061
H	-1.984567	-0.342314	-0.897545
H	-0.526098	1.678947	0.892380
H	-1.984205	-0.342246	0.898034
H	-0.525966	1.678082	-0.893094

1h
SCF Energy: -377.134136175
Num. Imaginary Frequencies: 0

C	-0.941596	-0.000041	-0.000919
O	-2.105205	0.000017	0.000069
O	-0.000046	-1.008848	0.000596
C	0.941636	0.000026	-0.000902
O	2.105211	-0.000033	0.000098
O	0.000010	1.008875	0.000604

TS1f
SCF Energy: -265.839963830
Num. Imaginary Frequencies: 1
Imaginary Frequency: -885.7987

C	-1.553685	0.015553	0.000035
O	0.110635	1.251001	-0.000036
C	0.559861	0.090957	-0.000018
O	1.619165	-0.443580	0.000041
H	-2.260954	0.819426	0.000160
C	-0.805172	-0.977880	-0.000039
H	-0.783468	-2.050573	-0.000072

TS1g
SCF Energy: -267.094644357
Num. Imaginary Frequencies: 1
Imaginary Frequency: -853.7411

C	1.566330	0.112197	0.000257
C	0.735905	-1.008556	-0.000232
C	-0.626255	0.108100	-0.000055
O	-1.688019	-0.433246	0.000184
O	-0.209818	1.279536	-0.000169
H	1.921599	0.552201	-0.919731
H	0.641854	-1.572620	0.917292
H	1.921215	0.551652	0.920664
H	0.642146	-1.571996	-0.918175

TS1h
SCF Energy: -377.109606372
Num. Imaginary Frequencies: 1
Imaginary Frequency: -707.2577

C	1.021267	-0.164612	0.000008
O	2.132173	0.139613	0.000014
O	0.160490	-1.069169	0.000005
C	-1.021269	0.164612	-0.000008
O	-2.132176	-0.139607	-0.000014
O	-0.160484	1.069163	-0.000005

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