Supplementary Information for

Density-Based Quantification of Steric Effect: Validation by Taft Steric Parameters from Acid-Catalyzed Hydrolysis of Esters

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(a) Reactant and transition state structures of 1-water mechanism for H, CH_3 and t-butyl groups.

1-Water Mechanism, Group H

Step 1, Reactant				Transition State			
O	-0.94853	-1.70087	0.92107	O	-0.78906	-1.39674	0.60502
O	0.94302	-0.66927	-0.86786	O	1.02554	-0.59981	-0.79026
C	1.94152	-1.73616	-0.84461	C	1.99271	-1.67467	-0.81140
H	2.90701	-1.30830	-0.58839	H	2.19162	-1.85534	-1.86323
H	1.62006	-2.47285	-0.11174	H	2.90049	-1.36426	-0.29787
H	1.93473	-2.13738	-1.85040	H	1.56982	-2.56563	-0.34621
C	0.70997	-0.03356	0.18827	C	0.47977	-0.30251	0.37020
H	-1.69089	-1.97995	0.37588	H	-0.45477	-2.24932	0.93685
O	1.43647	-0.21494	1.21881	O	1.24756	-0.50600	1.43370
H	1.16385	0.33098	1.97482	H	0.88297	-0.05698	2.21156
H	-1.20907	-1.89583	1.82671	H	-1.25774	-1.57244	-0.23045
H	-0.08204	0.70712	0.15965	H	-0.12285	0.59866	0.33667

Step 2, Reactant				Transition State			
O	0.16482	-1.75557	-0.13076	O	0.15104	-1.29957	-0.13977
O	1.08110	0.22647	-0.52160	O	0.66834	0.58807	-0.77228
C	1.06222	1.66357	-0.57118	C	1.26351	1.85982	-0.40429
H	0.10732	2.00889	-0.97376	H	0.50319	2.62796	-0.52150
H	1.22809	2.07835	0.42295	H	1.63290	1.81504	0.61611
H	1.87255	1.94829	-1.23634	H	2.07121	2.00654	-1.11357
C	0.01666	-0.28301	0.15079	C	-0.41202	0.03647	0.00765
H	1.00452	-2.10388	0.23556	H	1.03936	-0.59973	-0.61538
O	0.11202	-0.06180	1.48530	O	-0.39029	0.44768	1.27642
H	-0.76414	-0.09543	1.89518	H	-1.26707	0.71550	1.57991
H	-0.57703	-2.28083	0.23194	H	0.31037	-1.72207	0.72278

H	-0.95927	-0.04184	-0.27391	H	-1.35922	0.10680	-0.51744

1-Water Mechanism, Group CH3

Step 1, Reactant				Transition State			
O	-0.92699	-1.75202	0.89272	O	-0.71069	-1.36286	0.82656
O	0.94459	-0.62746	-0.87064	O	0.88472	-0.69072	-0.84012
C	1.88503	-1.73878	-0.80740	C	1.85222	-1.76025	-0.81346
H	2.86880	-1.35726	-0.54628	H	2.81401	-1.38172	-0.47201
H	1.51652	-2.44291	-0.06478	H	1.50720	-2.57000	-0.16977
H	1.87400	-2.16242	-1.80439	H	1.92360	-2.10531	-1.84083
C	0.72038	0.05304	0.17084	C	0.42357	-0.24510	0.32594
H	-1.65545	-2.05869	0.34399	H	-0.30871	-2.11552	1.29605
O	1.43777	-0.18976	1.20747	O	1.33072	-0.30044	1.31191
H	1.20599	0.36811	1.96690	H	1.03296	0.21413	2.07681
H	-1.14201	-2.04370	1.78393	H	-1.23579	-1.70928	0.08256
C	-0.27841	1.13827	0.11478	C	-0.40329	0.99381	0.18927
H	-0.90119	1.10170	1.00779	H	-0.80595	1.27892	1.16051
H	0.25839	2.09056	0.09382	H	0.25185	1.78090	-0.18544
H	-0.88369	1.03297	-0.78049	H	-1.21330	0.82270	-0.51804

Step 2, Reactant				Transition State			
O	0.11385	-1.75976	-0.14718	O	0.15835	-1.29681	-0.14316
O	0.99400	0.22780	-0.55228	O	0.65669	0.59971	-0.79267
C	1.06385	1.66240	-0.59627	C	1.26453	1.85152	-0.38767
H	0.25906	2.06264	-1.21433	H	0.50117	2.62500	-0.43312
H	1.01837	2.07675	0.41139	H	1.67689	1.76039	0.61313
H	2.02486	1.89311	-1.04798	H	2.04102	2.03794	-1.12246
C	-0.06802	-0.26412	0.15677	C	-0.44789	0.04074	-0.02242
C	-1.44324	0.08248	-0.34053	H	1.02720	-0.58148	-0.61905
H	-1.63832	1.12968	-0.10792	O	-0.39521	0.45435	1.25266
H	-1.49730	-0.07772	-1.41600	H	-1.26662	0.71132	1.58111
H	1.03384	-2.04069	0.03986	H	0.33526	-1.68682	0.73067
O	0.13870	-0.08663	1.49059	C	-1.75370	0.12702	-0.74489
H	-0.69628	-0.13984	1.97774	H	-2.50038	-0.46547	-0.21614
H	-0.48626	-2.31111	0.39314	H	-2.07001	1.16991	-0.78393
H	-2.18298	-0.53659	0.16990	H	-1.63152	-0.25575	-1.75579

1-Water Mechanism, Group tBu

Step 1, Reactant				Transition State			
O	-0.85721	-1.97227	1.08794	O	0.06425	-1.92132	0.00791
O	0.90003	-0.71017	-0.89992	O	0.83600	0.31704	-0.51214
C	1.90712	-1.76205	-0.89225	C	2.17825	0.34918	0.01865
H	2.88349	-1.31255	-0.72573	H	2.24029	1.07808	0.82466
H	1.65713	-2.47473	-0.10923	H	2.46690	-0.64141	0.37094
H	1.83945	-2.21198	-1.87639	H	2.80519	0.64950	-0.81566
C	0.71601	-0.01749	0.14712	C	-0.11530	-0.22484	0.22833
C	-0.28156	1.10204	0.10444	C	-1.52027	0.04134	-0.30894
H	-1.78654	-1.73896	0.98196	H	0.28756	-2.14451	-0.91132

O	1.48986	-0.24175	1.14587	O	0.10985	-0.11197	1.53914
H	1.28475	0.31949	1.91509	H	-0.66222	-0.38890	2.05560
H	-0.66924	-1.77789	2.01342	H	0.76548	-2.27982	0.57938
C	-0.86906	1.36695	1.49401	C	-1.81435	1.51822	0.00165
H	-0.10912	1.68488	2.21330	H	-1.05668	2.17465	-0.43055
H	-1.58327	2.18670	1.40323	H	-2.78243	1.77434	-0.43296
H	-1.39163	0.49083	1.88148	H	-1.86362	1.69281	1.07860
C	-1.38677	0.79403	-0.90654	C	-2.56400	-0.84204	0.38101
H	-1.95027	-0.09561	-0.61935	H	-3.55163	-0.52363	0.04197
H	-2.06931	1.64521	-0.92843	H	-2.43621	-1.89417	0.12672
H	-0.98219	0.65095	-1.90887	H	-2.55174	-0.73591	1.47005
C	0.53627	2.32876	-0.36311	C	-1.55872	-0.18880	-1.82269
H	-0.14472	3.18050	-0.41108	H	-1.27853	-1.21040	-2.09359
H	1.33877	2.55949	0.34046	H	-2.58171	-0.02505	-2.16701
H	0.96139	2.16005	-1.35418	H	-0.90502	0.50758	-2.34930

Step 2, Reactant				Transition State			
O	0.09545	-1.75152	-0.06878	O	0.06354	-1.27276	0.16985
O	0.94281	0.18962	-0.67239	O	0.68145	0.53001	-0.66709
C	1.27845	1.58801	-0.69136	C	1.33251	1.74150	-0.21280
H	0.68832	2.09892	-1.45215	H	0.60235	2.54815	-0.23046
H	1.12114	2.03807	0.28828	H	1.73761	1.59773	0.78595
H	2.33343	1.63289	-0.95116	H	2.12426	1.92492	-0.93364
C	-0.08129	-0.21114	0.14096	C	-0.52222	0.06273	0.02661
C	-1.52109	0.09212	-0.31464	C	-1.74600	0.06621	-0.88205
H	1.04102	-1.94119	-0.23314	H	0.98955	-0.62952	-0.31352
O	0.21886	0.04977	1.43426	O	-0.62696	0.63746	1.24049
H	-0.56866	0.01940	1.99750	H	-1.50969	1.00546	1.38925
H	-0.18770	-2.26951	0.71033	H	0.17944	-1.49469	1.11182
C	-1.88424	1.53725	0.06337	C	-2.90335	-0.61986	-0.14717
H	-1.24302	2.27148	-0.42329	H	-3.21515	-0.07090	0.74501
H	-2.90896	1.71800	-0.26759	H	-3.76038	-0.66865	-0.82139
H	-1.84785	1.69911	1.14314	H	-2.63474	-1.63850	0.14248
C	-2.50596	-0.85884	0.38065	C	-1.43719	-0.69431	-2.17473
H	-3.52012	-0.54730	0.12489	H	-2.32172	-0.65301	-2.81304
H	-2.37871	-1.89019	0.04585	H	-0.60500	-0.24324	-2.71735
H	-2.42086	-0.82931	1.47113	H	-1.20894	-1.74312	-1.97815
C	-1.61381	-0.08538	-1.83137	C	-2.09367	1.52263	-1.21436
H	-1.31244	-1.08954	-2.13636	H	-1.27368	2.00965	-1.74761
H	-2.65121	0.06702	-2.13624	H	-2.97361	1.52839	-1.86043
H	-0.99302	0.64395	-2.35558	H	-2.33101	2.10812	-0.32208

(b) Transition state structures of 2-water mechanism for H, CH_3 and t-butyl groups.

2-Water Mechanism, Group H

Step 1, Reactant				Transition State			
O	-1.06767	-1.80659	1.11062	O	-0.98577	0.53750	1.11252
O	0.76942	-0.77545	-0.85909	O	0.46517	-0.29192	-0.81905
C	1.85854	-1.74477	-0.95003	C	1.05394	-1.52991	-0.34518

H	2.80312	-1.21734	-0.83992	H	2.13701	-1.43129	-0.32064
H	1.72055	-2.48836	-0.16797	H	0.65750	-1.75608	0.64439
H	1.75541	-2.17852	-1.93788	H	0.74875	-2.28017	-1.06729
C	0.62690	-0.11922	0.20643	C	0.55916	0.74551	-0.06284
H	-1.65185	-1.53911	0.37789	H	-1.59221	-0.11042	0.67060
O	1.47260	-0.23418	1.14929	O	1.52070	0.77970	0.81000
H	1.24974	0.33010	1.91192	H	1.57460	1.65034	1.23690
H	-1.57370	-1.64280	1.91344	H	-0.68257	0.10964	1.92608
O	-2.28115	-0.79875	-1.18449	O	-2.48450	-1.19400	-0.26619
H	-1.57744	-0.92075	-1.83283	H	-1.88446	-1.79097	-0.72984
H	-3.06396	-1.18431	-1.59381	H	-3.08475	-1.77034	0.22129
H	-0.19914	0.58408	0.25405	H	0.14843	1.66153	-0.46839

Step 2, Reactant				Transition State			
O	-0.79300	-1.08364	-0.15136	O	0.06611	-1.26334	0.56423
O	0.54786	0.70061	-0.42888	O	0.91225	0.78848	0.36769
C	1.58368	1.54388	0.08215	C	0.76308	2.14661	-0.05094
H	1.43505	1.71804	1.15152	H	0.22730	2.19151	-1.00277
H	2.56528	1.09971	-0.08907	H	0.22825	2.72355	0.70501
H	1.50727	2.48562	-0.45630	H	1.76713	2.54602	-0.17450
C	0.41570	-0.48205	0.27623	C	-0.28878	0.08363	0.44084
H	-1.87613	-0.22137	-0.04213	H	1.83711	-0.86579	-0.20326
O	1.49197	-1.30785	-0.01690	O	-0.99850	0.54275	1.54854
H	1.57116	-1.98076	0.67223	H	-1.92711	0.29654	1.44754
H	-0.68813	-1.37975	-1.07113	H	0.32004	-1.42228	1.48611
O	-2.67122	0.49495	0.02892	O	2.68800	-1.21474	-0.57439
H	-2.28660	1.38816	0.00519	H	3.05148	-0.57301	-1.21277
H	-3.14019	0.39530	0.87483	H	2.52050	-2.05963	-1.03304
H	0.31112	-0.30848	1.35034	H	-0.86588	0.19029	-0.48121

Step 3, Reactant				Transition State			
O	-0.51870	-1.54953	-0.12794	O	0.36796	-1.41764	-0.31658
O	0.80835	0.23593	-0.53603	O	0.68342	0.84225	-1.11827
C	0.99830	1.66455	-0.54956	C	0.59815	2.24389	-0.78062
H	0.14800	2.12537	-1.05276	H	-0.45817	2.45751	-0.62595
H	1.09631	2.04206	0.46856	H	1.17247	2.44951	0.12142
H	1.91088	1.84748	-1.11136	H	0.97793	2.81815	-1.62275
C	-0.43089	-0.19162	0.05978	C	-0.09630	-0.25931	0.03602
H	1.87594	-0.40281	-0.09254	H	1.61351	0.57304	-1.20910
O	-0.43158	0.10316	1.41542	O	0.28436	0.18167	1.22576
H	-0.80671	0.98126	1.56094	H	-0.27259	0.91944	1.51879
H	0.09822	-1.99001	0.47567	H	1.23583	-1.64163	0.17231
O	2.76314	-0.94304	0.28598	O	2.57181	-1.94222	0.86374
H	3.27806	-1.31226	-0.45039	H	2.83863	-2.86513	0.76933
H	3.34372	-0.33807	0.77622	H	2.50517	-1.79090	1.81501
H	-1.23957	0.30272	-0.47789	H	-1.10250	-0.02187	-0.29564

2-Water Mechanism, Group CH3

Step 1, Reactant				Transition State			
O	-1.22606	-1.47049	1.15527	O	-0.95781	0.40036	1.14037
O	0.66784	-0.45544	-0.84495	O	0.37692	-0.37239	-0.81358
C	1.45430	-1.65490	-1.09546	C	1.05032	-1.54007	-0.29328
H	2.51005	-1.41590	-0.98967	H	2.12680	-1.38101	-0.30538
H	1.14607	-2.42254	-0.38803	H	0.69959	-1.74250	0.71906
H	1.21209	-1.93332	-2.11541	H	0.77470	-2.34854	-0.96362
C	0.73317	0.10603	0.29202	C	0.39351	0.71903	-0.09116
C	-0.08474	1.30756	0.53089	C	-0.19859	1.91657	-0.74743
H	-0.97579	1.27300	-0.09124	H	-1.16039	1.65678	-1.18539
H	-0.33378	1.38215	1.58836	H	-0.31324	2.71937	-0.02126
H	-1.58375	-1.51437	0.24930	H	-1.60026	-0.22136	0.69283
O	1.57167	-0.36135	1.14036	O	1.42942	0.83790	0.71709
H	1.55851	0.12348	1.98429	H	1.45771	1.71739	1.12516
H	-1.82667	-0.88657	1.63081	H	-0.58342	-0.08636	1.89017
O	-2.07758	-1.56933	-1.51015	O	-2.50092	-1.21531	-0.24000
H	-1.33683	-1.77334	-2.09281	H	-1.90306	-1.80251	-0.71957
H	-2.75294	-2.21951	-1.73462	H	-3.10371	-1.79969	0.23514
H	0.52507	2.17141	0.24658	H	0.49183	2.22710	-1.53462

Step 2, Reactant				Transition State			
O	-0.84176	-0.96675	-0.53580	O	0.06264	-1.24347	0.72386
O	0.47751	0.83509	-0.53701	O	0.87606	0.79419	0.42714
C	1.54610	1.63609	-0.02636	C	0.79855	2.14320	-0.03638
H	1.33040	1.96539	0.99197	H	0.61750	2.17376	-1.11260
H	2.49074	1.09029	-0.05336	H	0.01405	2.68753	0.49257
H	1.60993	2.50317	-0.68027	H	1.76326	2.59646	0.18226
C	0.38901	-0.45502	-0.01650	C	-0.33594	0.08580	0.49701
C	0.30971	-0.52617	1.49081	C	-1.14231	0.12229	-0.78154
H	1.24465	-0.17917	1.92905	H	-1.49023	1.13474	-0.98286
H	-0.51413	0.09516	1.84566	H	-0.52692	-0.22627	-1.61231
H	-1.90148	-0.14213	-0.27320	H	1.74837	-0.85941	-0.19960
O	1.44087	-1.19661	-0.55091	O	-1.03314	0.59200	1.60062
H	1.54689	-2.01056	-0.04084	H	-1.95294	0.30039	1.55129
H	-0.74969	-1.07691	-1.49691	H	0.39158	-1.30265	1.63345
O	-2.70859	0.55061	-0.07202	O	2.52529	-1.16203	-0.73916
H	-2.33509	1.39753	0.22532	H	2.71934	-0.48193	-1.41179
H	-3.27455	0.21027	0.64119	H	2.29791	-1.99698	-1.19035
H	0.13926	-1.56118	1.78954	H	-2.00588	-0.53499	-0.67228

Step 3, Reactant				Transition State			
O	-0.41545	-1.61748	-0.11671	O	-0.14664	-1.57442	-0.23510
O	0.78872	0.24068	-0.57865	O	0.85774	0.53180	-0.91089
C	1.00801	1.67301	-0.60990	C	0.98310	1.95410	-0.73954
H	0.37922	2.09990	-1.38685	H	0.13920	2.41737	-1.24519
H	0.79066	2.10618	0.36597	H	0.98707	2.21056	0.32185
H	2.05865	1.80593	-0.85732	H	1.91428	2.27586	-1.20380
C	-0.45533	-0.25818	0.07297	C	-0.45168	-0.34053	0.08683

C	-1.64254	0.34358	-0.62602	C	-1.67504	0.22390	-0.53925
H	-1.68572	1.41939	-0.45514	H	-1.74289	1.29367	-0.34553
H	-1.58097	0.14113	-1.69481	H	-1.67029	0.02227	-1.60789
H	1.69569	-0.29854	-0.18049	H	1.66453	0.08493	-0.57171
O	-0.36908	0.02045	1.42386	O	-0.11855	-0.00164	1.31882
H	-0.77054	0.87807	1.61828	H	-0.51678	0.84438	1.57662
H	0.21245	-2.01298	0.50691	H	0.68878	-1.83586	0.21289
O	2.71341	-0.92156	0.28767	O	2.45349	-1.22992	0.43721
H	3.24793	-1.30543	-0.42233	H	3.18997	-1.75147	0.09644
H	3.29731	-0.32670	0.77977	H	2.70409	-0.97929	1.33473
H	-2.53950	-0.11823	-0.21421	H	-2.52744	-0.27650	-0.07350

2-Water Mechanism, Group tBu

Step 1, Reactant				Transition State			
O	-0.94504	-1.82774	0.52576	O	0.78948	-0.46140	1.40655
O	1.09530	-0.42668	-0.92114	O	0.76419	0.74746	-0.76839
C	2.05293	-1.52252	-0.94906	C	1.79523	1.73889	-0.56493
H	3.01180	-1.16167	-0.58386	H	1.36167	2.73635	-0.59903
H	1.67099	-2.33317	-0.33237	H	2.28711	1.56078	0.39165
H	2.10908	-1.81002	-1.99304	H	2.49168	1.59487	-1.38552
C	0.79554	0.11048	0.18931	C	-0.13172	0.58435	0.16991
C	-0.13211	1.28899	0.18970	C	-1.27312	-0.34919	-0.19757
H	-1.79016	-1.83547	0.04008	H	1.52622	-0.92333	0.91417
O	1.41969	-0.30358	1.23112	O	-0.35111	1.65460	0.91138
H	1.15853	0.17159	2.03976	H	-1.09043	1.51624	1.52399
H	-1.19276	-1.78761	1.45573	H	1.20858	0.15225	2.02837
O	-3.30073	-1.89100	-1.00837	O	2.64268	-1.57656	-0.09820
H	-3.34633	-2.70127	-1.52853	H	2.47593	-1.14619	-0.94708
H	-4.11997	-1.88059	-0.50060	H	2.45638	-2.51038	-0.25659
C	-0.94272	1.36016	1.48772	C	-0.73074	-1.66322	-0.76349
H	-0.31146	1.45422	2.37588	H	-0.22251	-2.24930	0.00431
H	-1.56284	2.25684	1.44182	H	-1.57411	-2.24858	-1.13529
H	-1.59361	0.49201	1.59809	H	-0.04396	-1.49036	-1.59395
C	-1.06058	1.23401	-1.02334	C	-2.17671	-0.62265	1.00648
H	-1.69996	2.11813	-0.99940	H	-2.68354	0.27980	1.36133
H	-0.49860	1.24076	-1.95777	H	-2.95605	-1.31989	0.69357
H	-1.69343	0.34532	-0.99212	H	-1.62336	-1.07311	1.83133
C	0.80692	2.51385	0.08777	C	-2.07250	0.39605	-1.28301
H	0.18220	3.40857	0.06464	H	-1.47223	0.54607	-2.18199
H	1.47340	2.57356	0.95071	H	-2.94318	-0.20914	-1.54249
H	1.40228	2.47588	-0.82644	H	-2.42285	1.36572	-0.92193

Step 2, Reactant				Transition State			
O	1.05177	-0.47488	1.11656	O	0.00344	-1.17842	0.69291
O	0.64101	1.30939	-0.11976	O	0.90511	0.77032	0.24642
C	-0.12106	2.36208	-0.71562	C	0.99518	2.18032	0.03726
H	-0.40009	2.10061	-1.73771	H	0.93493	2.41372	-1.02703
H	-1.00950	2.59098	-0.12710	H	0.21492	2.70841	0.58530

H	0.53174	3.23351	-0.73337	H	1.96932	2.48436	0.41797
C	-0.03012	0.29996	0.57210	C	-0.34817	0.16366	0.45602
C	-0.90892	-0.65061	-0.28407	C	-1.31413	0.19290	-0.75852
H	2.15144	-0.55156	0.30917	H	1.70750	-0.92075	-0.26026
O	-0.70292	0.89685	1.63225	O	-0.87683	0.74048	1.61445
H	-1.38790	0.30656	1.97317	H	-1.80676	0.49423	1.70436
H	1.34241	-0.03135	1.93019	H	0.39518	-1.21959	1.57781
O	3.05259	-0.59841	-0.29449	O	2.45115	-1.30710	-0.79573
H	2.99896	0.08244	-0.98756	H	2.84430	-0.59330	-1.33272
H	3.10194	-1.46125	-0.73985	H	2.08438	-1.98245	-1.39760
C	-0.13739	-1.06027	-1.54164	C	-1.90599	1.59045	-0.98960
H	0.77645	-1.60572	-1.29332	H	-1.16866	2.30996	-1.34256
H	-0.76657	-1.72265	-2.14092	H	-2.67719	1.50887	-1.75948
H	0.12356	-0.19360	-2.15321	H	-2.37705	1.98493	-0.08619
C	-1.24583	-1.90783	0.53264	C	-0.55336	-0.25705	-2.00935
H	-1.77183	-1.67068	1.46263	H	-0.14821	-1.26517	-1.88923
H	-1.90854	-2.53978	-0.06252	H	-1.23764	-0.26655	-2.86115
H	-0.35285	-2.48287	0.77759	H	0.26847	0.42532	-2.24148
C	-2.23048	0.02027	-0.68936	C	-2.47869	-0.77454	-0.49719
H	-2.09042	0.84850	-1.38228	H	-3.06271	-0.49086	0.38410
H	-2.84592	-0.72843	-1.19332	H	-3.15563	-0.74328	-1.35390
H	-2.78962	0.38010	0.17762	H	-2.13395	-1.80081	-0.37047

Step 3, Reactant				Transition State			
O	-0.34372	-1.48561	0.19377	O	-0.11529	-0.89913	0.77809
O	0.81433	0.32563	-0.46949	O	0.82291	1.14131	-0.45154
C	1.25413	1.70537	-0.42130	C	1.75661	1.63429	0.51442
H	0.89742	2.21232	-1.31413	H	1.33657	2.53274	0.96175
H	0.89153	2.18300	0.48655	H	1.94511	0.88584	1.29001
H	2.34224	1.67189	-0.41389	H	2.69252	1.88170	0.01159
C	-0.46375	-0.12012	0.19128	C	-0.69678	0.22439	0.47122
C	-1.67508	0.30769	-0.66205	C	-1.68064	0.18676	-0.67566
H	1.65694	-0.36453	-0.25268	H	1.27992	0.41970	-0.94929
O	-0.44713	0.33949	1.48723	O	-0.83141	1.05468	1.46858
H	-0.89820	1.19109	1.56449	H	-1.31719	1.85717	1.21537
H	0.23447	-1.75503	0.92321	H	0.32657	-0.84912	1.64392
O	2.66937	-1.15229	0.00245	O	2.18959	-0.84546	-1.62074
H	2.95391	-1.62737	-0.79116	H	3.02694	-0.93172	-1.14892
H	3.43896	-0.65336	0.31087	H	1.71188	-1.66355	-1.43472
C	-1.99809	1.79938	-0.50402	C	-2.13588	1.59307	-1.06534
H	-2.83587	2.03029	-1.16524	H	-2.81693	1.50606	-1.91361
H	-2.32224	2.04872	0.51104	H	-2.69044	2.08432	-0.26033
H	-1.17152	2.45222	-0.78259	H	-1.29387	2.22024	-1.36072
C	-2.88710	-0.49784	-0.17175	C	-2.88038	-0.60995	-0.11706
H	-3.78084	-0.12151	-0.67372	H	-3.66506	-0.61042	-0.87563
H	-2.78309	-1.55836	-0.40255	H	-2.60028	-1.64240	0.09845
H	-3.02820	-0.38408	0.90601	H	-3.27599	-0.14853	0.79042
C	-1.40080	-0.00730	-2.13484	C	-1.09625	-0.54634	-1.88432

H	-2.32109	0.14408	-2.70319	H	-1.90776	-0.73258	-2.59041
H	-0.63267	0.65119	-2.54619	H	-0.34161	0.05620	-2.39211
H	-1.08395	-1.04385	-2.26827	H	-0.66293	-1.50821	-1.60357

(c) Transition state structures of 3-water mechanism for H, CH_3 and t-butyl groups.

3-Water Mechanism, Group H

Step 1, Reactant				Transition State			
O	-0.98829	-2.08400	0.87163	O	-1.50007	-2.54083	-0.08871
O	0.80600	-0.76854	-0.91472	O	0.27838	-0.71369	-0.60164
C	1.94320	-1.67197	-1.06642	C	1.52786	-1.41819	-0.83143
H	2.85871	-1.11172	-0.89131	H	2.26847	-1.07817	-0.11094
H	1.82891	-2.48704	-0.35474	H	1.35125	-2.48880	-0.74195
H	1.87873	-2.02199	-2.09013	H	1.81527	-1.15202	-1.84281
C	0.60363	-0.22695	0.20432	C	-0.34696	-0.93922	0.49036
H	-1.60141	-1.74604	0.19686	H	-2.06688	-2.14497	-0.78325
O	1.43647	-0.37885	1.15430	O	0.28832	-1.49173	1.46935
H	1.16666	0.10430	1.95708	H	-0.26240	-1.52938	2.27024
H	-1.50350	-2.14034	1.69512	H	-2.06008	-2.66438	0.70462
O	-2.33928	-0.75661	-1.20434	O	-2.72639	-1.03718	-2.01907
H	-1.63017	-0.58901	-1.83617	H	-1.96969	-0.53149	-2.33907
H	-3.05315	-1.13377	-1.73064	H	-3.10430	-1.44156	-2.80838
O	-2.44649	-2.29041	3.27353	O	-2.68585	-2.57006	2.39514
H	-2.21208	-1.64270	3.94757	H	-2.65732	-1.64629	2.67226
H	-2.33775	-3.14452	3.70679	H	-2.08068	-3.02341	2.99417
H	-0.26107	0.42288	0.29577	H	-1.24340	-0.35482	0.66266

Step 2, Reactant				Transition State			
O	0.84628	-0.11459	-0.64964	O	-0.66042	-0.12854	1.09116
O	-0.92485	0.39825	0.63864	O	0.95258	0.37770	-0.36121
C	-2.29677	0.79327	0.74279	C	2.33614	0.35338	-0.71410
H	-2.51630	1.58483	0.02157	H	2.95328	0.54463	0.16800
H	-2.95701	-0.05857	0.57414	H	2.60397	-0.60889	-1.15342
H	-2.43137	1.16897	1.75411	H	2.48657	1.14429	-1.44549
C	-0.57542	0.01668	-0.64095	C	0.61763	-0.49310	0.67955
H	1.32384	0.80176	-0.38001	H	-0.47822	1.61350	0.24691
O	-1.12993	-1.21723	-0.92419	O	0.65989	-1.79693	0.17725
H	-1.18131	-1.33343	-1.88186	H	0.68852	-2.41192	0.92138
H	1.15803	-0.92063	-0.02258	H	-1.30503	-0.48619	0.43537
O	1.94244	1.99259	-0.00930	O	-0.90096	2.50850	0.16177
H	1.32399	2.57302	0.45462	H	-1.86296	2.41189	0.29365
H	2.25826	2.49594	-0.77162	H	-0.73769	2.86363	-0.73185
O	1.55715	-2.01821	0.74942	O	-2.39017	-1.16115	-0.74360
H	1.98108	-1.74022	1.57234	H	-2.79398	-0.52241	-1.34264
H	0.78109	-2.53101	1.01387	H	-1.86458	-1.73639	-1.31242
H	-0.83598	0.77313	-1.38512	H	1.30021	-0.37035	1.52479

Step 3, Reactant				Transition State			
O	0.76350	0.51817	-1.15909	O	0.85048	0.73749	-0.71735

O	-0.72192	-0.24944	0.36984	O	-0.98130	-0.38578	0.63995
C	-1.58093	-1.30664	0.86037	C	-1.92759	-1.45695	0.58673
H	-2.12701	-1.74623	0.02497	H	-2.45651	-1.45708	-0.36953
H	-0.95965	-2.04573	1.35978	H	-1.37308	-2.38768	0.70288
H	-2.26318	-0.84085	1.56685	H	-2.64287	-1.35840	1.40385
C	0.13342	-0.62004	-0.77571	C	0.29897	-0.40000	-0.87031
H	-1.29909	0.70269	0.14909	H	-1.44515	0.47230	0.48787
O	1.01881	-1.57600	-0.33210	O	0.99578	-1.46450	-0.57332
H	0.67407	-2.45885	-0.51977	H	0.53815	-2.27358	-0.85257
H	1.42465	0.76202	-0.46390	H	1.69315	0.70079	-0.09895
O	-1.93204	1.79047	-0.04085	O	-1.95161	2.02487	-0.02213
H	-2.77411	1.64215	-0.49485	H	-2.80383	2.05983	-0.47201
H	-1.41378	2.37732	-0.61062	H	-1.30230	2.26541	-0.69475
O	2.51814	1.05195	0.82181	O	2.86984	0.68069	0.75075
H	2.15568	1.65585	1.48081	H	2.70301	1.09191	1.60883
H	2.62233	0.21282	1.28687	H	3.11350	-0.23424	0.94428
H	-0.52674	-0.98225	-1.56395	H	-0.51790	-0.47982	-1.58155

3-Water Mechanism, Group CH3

Step 1, Reactant

				Transition State			
O	-0.84874	-2.30242	0.93353	O	-1.03548	-1.97541	0.20425
O	0.58314	-0.37447	-0.76457	O	0.85753	-0.59157	-0.70496
C	1.52169	-1.26948	-1.42574	C	1.91309	-1.57556	-0.80877
H	2.52870	-0.87430	-1.31327	H	2.74992	-1.28134	-0.17864
H	1.42818	-2.25771	-0.97919	H	1.52667	-2.55059	-0.51573
H	1.21151	-1.27203	-2.46503	H	2.19841	-1.57198	-1.85582
C	0.68098	-0.18301	0.48691	C	0.22240	-0.49346	0.42156
C	-0.29307	0.70955	1.13732	C	-0.74672	0.62847	0.53273
H	-1.25159	0.63729	0.62794	H	-1.31470	0.72126	-0.39038
H	-0.37976	0.46354	2.19420	H	-1.40988	0.46719	1.38167
H	-1.27338	-2.17377	0.06783	H	-1.72669	-1.71131	-0.44660
O	1.67751	-0.70864	1.09674	O	0.85084	-0.94880	1.47724
H	1.66766	-0.51981	2.05193	H	0.34575	-0.77368	2.28851
H	-1.47705	-1.94079	1.58241	H	-1.47008	-2.04787	1.08235
O	-1.99248	-1.77074	-1.59167	O	-2.78511	-1.14364	-1.68947
H	-1.35584	-1.34186	-2.17505	H	-3.50278	-1.74914	-1.90922
H	-2.35431	-2.49704	-2.11200	H	-3.21991	-0.31900	-1.44219
H	0.09365	1.72908	1.03741	H	-0.16179	1.53756	0.69633
O	-2.62175	-1.19219	2.83089	O	-1.91217	-1.93391	2.78613
H	-2.23646	-0.44392	3.30101	H	-2.11590	-1.02896	3.05042
H	-2.89261	-1.80491	3.52406	H	-1.22047	-2.22033	3.39447

Step 2, Reactant

				Transition State			
O	-0.90972	0.11244	0.61442	O	-0.60938	-0.24052	1.08893
O	0.67932	-0.13892	-0.93630	O	0.47675	0.44156	-0.71375
C	2.03804	-0.19746	-1.38148	C	1.64816	0.60176	-1.51439
H	2.53067	0.76707	-1.24589	H	2.41349	1.16343	-0.97513
H	2.58613	-0.97940	-0.85310	H	2.04057	-0.36973	-1.82045

H	1.99522	-0.43702	-2.44158	H	1.34176	1.16162	-2.39583
C	0.50889	-0.09870	0.44301	C	0.56063	-0.47098	0.35690
C	1.24459	1.01725	1.14543	C	1.75205	-0.24667	1.26080
H	2.31851	0.84341	1.08681	H	2.68184	-0.43948	0.72659
H	1.00070	1.97151	0.67618	H	1.74539	0.78063	1.62763
H	-1.21972	1.02578	0.17210	H	-0.71981	1.55299	0.29417
O	0.79025	-1.36098	0.94688	O	0.55192	-1.75177	-0.21819
H	0.93715	-1.30495	1.90070	H	0.83074	-2.39479	0.44649
H	-1.45251	-0.70660	0.20772	H	-1.36509	-0.58787	0.56091
O	-1.61217	2.24060	-0.42979	O	-1.18134	2.43461	0.29686
H	-0.89406	2.58435	-0.97850	H	-0.72384	3.03517	-0.32038
H	-1.78718	2.92481	0.23002	H	-1.15425	2.82214	1.19143
H	0.94337	1.03716	2.19338	H	1.68222	-0.93098	2.10760
O	-2.16206	-1.82182	-0.28453	O	-2.64790	-1.22345	-0.45180
H	-2.39870	-1.69947	-1.21367	H	-3.04791	-0.55210	-1.01689
H	-1.59367	-2.60380	-0.26125	H	-2.21066	-1.82902	-1.06252

Step 3, Reactant | Transition State

O	0.79749	0.18785	-1.15419	O	0.88000	0.49494	-0.94335
O	-0.53448	0.19242	0.66830	O	-0.67705	0.04380	0.87309
C	-1.40891	-0.42705	1.64265	C	-1.59690	-0.84394	1.51921
H	-2.35295	-0.70098	1.17354	H	-2.47998	-1.00296	0.89819
H	-0.89947	-1.29713	2.04977	H	-1.08153	-1.78977	1.68712
H	-1.56408	0.31496	2.42176	H	-1.88631	-0.41565	2.47896
C	0.08701	-0.68728	-0.39374	C	0.32317	-0.61551	-0.56824
C	-0.99465	-1.36314	-1.19197	C	-0.75845	-1.15558	-1.43756
H	-1.54609	-2.07179	-0.57309	H	-1.27463	-1.98039	-0.94791
H	-1.67769	-0.61312	-1.59231	H	-1.45718	-0.36016	-1.69250
H	-1.02536	1.05372	0.19220	H	-1.17740	0.82072	0.49871
O	0.93011	-1.54278	0.28193	O	1.12113	-1.45025	0.07946
H	0.48454	-2.38013	0.46734	H	0.70276	-2.31660	0.19916
H	1.56600	0.52345	-0.62586	H	1.69046	0.72110	-0.36810
O	-1.61543	2.10411	-0.37097	O	-1.97416	2.02858	-0.27102
H	-2.57359	2.07292	-0.23988	H	-2.90555	1.80811	-0.39442
H	-1.47465	2.07935	-1.32825	H	-1.60587	2.06204	-1.16298
H	-0.51991	-1.90032	-2.01297	H	-0.27823	-1.52482	-2.34715
O	2.87987	1.03493	0.31546	O	2.90838	1.08619	0.50015
H	2.62674	1.69169	0.97494	H	2.68112	1.73743	1.17571
H	3.19524	0.27993	0.82686	H	3.19891	0.30505	0.98801

3-Water Mechanism, Group tBu

Step 1, Reactant | Transition State

O	-0.70352	-2.21028	0.94046	O	-1.01055	-1.67091	0.09032
O	0.46078	-0.50805	-1.14808	O	1.05294	-0.56193	-0.71908
C	1.33289	-1.50935	-1.74566	C	1.98067	-1.66966	-0.70677
H	2.32312	-1.07726	-1.87408	H	2.79837	-1.45512	-0.02147
H	1.36130	-2.38058	-1.09423	H	1.45689	-2.57916	-0.41674
H	0.87331	-1.73814	-2.70121	H	2.34402	-1.74337	-1.72705

C	0.68751	-0.11585	0.03785	C	0.33654	-0.34560	0.34511
C	-0.17602	0.96088	0.62252	C	-0.42236	0.97129	0.35156
H	-0.05945	-2.34643	1.65554	H	-1.81936	-1.42179	-0.41596
O	1.73505	-0.57371	0.62040	O	0.84061	-0.83466	1.46063
H	1.83565	-0.23867	1.53011	H	0.31376	-0.58227	2.23659
H	-0.55074	-2.92151	0.29499	H	-1.32401	-1.92506	0.99140
O	1.13794	-2.27902	3.11713	O	-3.36120	-1.12364	-1.17662
H	2.03060	-2.31253	2.75335	H	-4.00587	-1.80118	-0.94028
H	1.06166	-1.39020	3.48510	H	-3.72594	-0.30057	-0.82885
O	-0.45761	-4.25355	-1.01141	O	-1.73369	-2.23625	2.63841
H	-0.34866	-3.91400	-1.90711	H	-1.78169	-1.41239	3.13847
H	-1.25587	-4.79257	-1.04877	H	-1.03722	-2.74653	3.06883
C	-0.30556	0.79433	2.13962	C	-1.57851	0.96750	1.35387
H	0.65967	0.84529	2.65279	H	-2.00167	1.97344	1.38162
H	-0.90869	1.62261	2.51484	H	-2.36729	0.27163	1.06274
H	-0.80141	-0.14306	2.39590	H	-1.25180	0.73194	2.37111
C	-1.55141	0.96628	-0.04391	C	0.62042	2.02324	0.78176
H	-1.47312	1.14302	-1.11713	H	1.48610	2.01612	0.11618
H	-2.07442	0.02396	0.12616	H	0.15126	3.00754	0.73028
H	-2.13656	1.77506	0.39689	H	0.95625	1.85195	1.80663
C	0.57667	2.27319	0.30085	C	-0.92751	1.30327	-1.05324
H	-0.01839	3.09953	0.69385	H	-1.57733	0.52189	-1.44959
H	1.55966	2.29100	0.77596	H	-1.50144	2.23054	-1.00035
H	0.69361	2.40353	-0.77666	H	-0.09900	1.45277	-1.74668

Step 2, Reactant				Transition State			
O	1.05354	0.35457	-0.66422	O	0.79809	-0.14471	-1.07839
O	0.31562	-0.25939	1.33179	O	0.56430	0.31820	1.05214
C	-0.41840	-1.01784	2.29971	C	0.05581	0.23231	2.38321
H	-1.24275	-0.42473	2.69705	H	-0.74217	0.96003	2.54087
H	-0.79211	-1.94843	1.87350	H	-0.30204	-0.77414	2.60107
H	0.28285	-1.24512	3.10104	H	0.89006	0.46702	3.04312
C	-0.00987	-0.39786	-0.01311	C	-0.03256	-0.42864	0.01324
C	-1.36640	0.19944	-0.46374	C	-1.48196	-0.00815	-0.35336
H	1.30623	1.23478	-0.13479	H	1.39628	1.50080	-0.23976
O	0.17258	-1.72148	-0.36882	O	0.08441	-1.77465	0.38477
H	-0.31607	-1.92649	-1.17703	H	-0.46866	-2.31894	-0.19059
H	1.92255	-0.24911	-0.73524	H	1.65610	-0.59939	-0.91510
O	1.71861	2.39525	0.58679	O	1.76151	2.42160	-0.34649
H	1.23981	2.41046	1.42699	H	1.09162	3.05140	-0.01804
H	1.44230	3.19583	0.12071	H	1.90452	2.59112	-1.29688
O	3.07111	-1.07004	-0.87348	O	3.16504	-1.40917	-0.51888
H	3.81717	-0.74923	-0.34936	H	3.80394	-0.81175	-0.11274
H	2.86519	-1.94940	-0.52833	H	2.93705	-2.03490	0.17924
C	-1.49310	1.63262	0.05967	C	-1.55503	1.52018	-0.43354
H	-0.74926	2.29555	-0.38866	H	-0.83152	1.91568	-1.15138
H	-2.48163	2.01502	-0.20465	H	-2.55410	1.81434	-0.76455
H	-1.39272	1.67053	1.14710	H	-1.37090	1.98284	0.53935

C	-1.43468	0.21314	-1.99834	C	-1.84394	-0.59993	-1.72442
H	-1.41250	-0.79365	-2.42712	H	-1.74526	-1.68982	-1.74346
H	-2.38304	0.66574	-2.29539	H	-2.88793	-0.36433	-1.94352
H	-0.62470	0.79700	-2.43619	H	-1.22423	-0.18455	-2.51925
C	-2.54025	-0.64073	0.06205	C	-2.50626	-0.52349	0.66726
H	-2.68154	-0.53356	1.13667	H	-2.37526	-0.09127	1.65822
H	-3.45146	-0.28797	-0.42619	H	-3.50390	-0.24593	0.31805
H	-2.42390	-1.70118	-0.17409	H	-2.47679	-1.61203	0.75577

Step 3, Reactant				Transition State			
O	0.69357	-0.77024	-1.02757	O	0.68914	-0.87293	-0.99190
O	0.70547	0.69635	0.66541	O	0.81885	0.82366	0.67420
C	0.38828	1.29382	1.94172	C	0.55439	1.48420	1.91802
H	-0.42023	2.01339	1.82592	H	-0.24497	2.21731	1.80368
H	0.11985	0.50091	2.63559	H	0.27078	0.72208	2.64324
H	1.29884	1.78618	2.27650	H	1.47083	1.97396	2.24872
C	-0.02714	-0.50444	0.09203	C	-0.05490	-0.65719	0.05686
C	-1.49450	-0.17901	-0.26125	C	-1.48781	-0.22427	-0.23422
H	1.02812	1.41915	-0.08461	H	0.97636	1.49600	-0.04756
O	0.14942	-1.50580	1.01931	O	0.18230	-1.48421	1.06974
H	-0.57596	-1.52184	1.65797	H	-0.48218	-1.39453	1.76983
H	1.60412	-1.05832	-0.76310	H	1.57044	-1.30249	-0.73517
O	1.49407	2.32992	-0.95564	O	1.31686	2.73721	-1.05034
H	0.81430	2.99601	-1.13127	H	0.67561	2.79945	-1.76888
H	1.66074	1.89619	-1.80487	H	2.17419	2.64774	-1.48402
O	3.14202	-1.56275	-0.27280	O	2.93500	-1.96200	-0.35201
H	3.72338	-0.82220	-0.06278	H	3.63593	-1.30498	-0.25897
H	3.04587	-2.04449	0.55761	H	2.85323	-2.36805	0.52019
C	-1.56368	1.14659	-1.02461	C	-2.09630	-1.38878	-1.04103
H	-1.30086	1.99524	-0.38678	H	-3.15712	-1.18125	-1.19397
H	-0.90020	1.14055	-1.89250	H	-1.61563	-1.48744	-2.01523
H	-2.58610	1.29461	-1.37860	H	-2.00453	-2.33473	-0.50180
C	-2.00659	-1.31637	-1.15811	C	-1.51446	1.05221	-1.07498
H	-1.86820	-2.28928	-0.68008	H	-1.22507	1.92361	-0.48278
H	-3.07503	-1.16995	-1.33050	H	-0.85687	0.97299	-1.94344
H	-1.49959	-1.32403	-2.12337	H	-2.53400	1.20913	-1.43295
C	-2.39458	-0.11145	0.97994	C	-2.30534	-0.03047	1.04504
H	-2.07909	0.63854	1.70446	H	-1.89025	0.73779	1.69710
H	-3.40065	0.15447	0.64908	H	-3.30939	0.28630	0.75633
H	-2.47646	-1.07978	1.48328	H	-2.41804	-0.96080	1.61001

(d) Transition state structures of 4-water mechanism for H, CH_3 and t-butyl groups.

4-Water Mechanism, Group H

Step 1, Reactant				Transition State			
O	-1.35701	-2.22529	1.14593	O	-1.11792	-1.98480	0.57107
O	0.67928	-0.74173	-1.04947	O	0.58784	-0.70825	-0.77477
C	1.63289	-1.76424	-1.41769	C	1.70237	-1.61533	-0.94019
H	2.64434	-1.38265	-1.28986	H	2.59474	-1.18423	-0.49064

H	1.47225	-2.64472	-0.79691	H	1.45971	-2.57304	-0.48148
H	1.43004	-1.98287	-2.46133	H	1.82437	-1.72154	-2.01336
C	0.70910	-0.32533	0.18981	C	0.16448	-0.50213	0.43306
H	-1.71680	-1.88860	0.30821	H	-1.79105	-1.79098	-0.11886
O	1.52544	-0.70342	1.01231	O	0.94550	-0.75172	1.42148
H	1.25410	-0.27804	2.44023	H	0.58208	-0.37015	2.29616
H	-1.48104	-1.51599	1.79183	H	-1.56590	-1.88731	1.44346
O	-2.09873	-1.45247	-1.47715	O	-2.78651	-1.21582	-1.44436
H	-2.76197	-0.78746	-1.69164	H	-2.56476	-1.63185	-2.28561
H	-1.24934	-1.03561	-1.67445	H	-3.72733	-1.38956	-1.32425
O	-1.49900	-0.33951	3.40217	O	-2.17583	-1.52524	3.02591
H	-1.98442	0.49622	3.39062	H	-1.48205	-0.95676	3.39963
H	-1.84342	-0.83617	4.15665	H	-2.21975	-2.29253	3.60733
O	0.96928	-0.01040	3.38657	O	0.00855	0.18088	3.59733
H	-0.06546	-0.14731	3.45824	H	-0.13526	1.13590	3.56990
H	1.41376	-0.59433	4.02108	H	0.59919	0.02288	4.34560
H	-0.07164	0.41050	0.39757	H	-0.61875	0.24394	0.51972

Step 2, Reactant				Transition State			
O	-0.69520	-1.33544	0.48303	O	-0.81594	-1.44138	0.73987
O	1.01411	-0.46884	-0.77094	O	0.51801	-0.39909	-0.72865
C	1.76859	-1.67032	-0.98970	C	1.39039	-1.45800	-1.15392
H	2.67419	-1.66828	-0.38329	H	2.39678	-1.30258	-0.76642
H	1.16729	-2.55257	-0.76629	H	1.01148	-2.43016	-0.83197
H	2.03232	-1.66451	-2.04451	H	1.40449	-1.41303	-2.24115
C	0.40991	-0.36921	0.45299	C	0.15464	-0.43330	0.62133
H	-1.38360	-1.11065	-0.26039	H	-1.20174	-1.10522	-1.20465
O	1.25161	-0.68631	1.48622	O	1.27043	-0.68565	1.41236
H	0.94808	-0.21989	2.29390	H	1.09782	-0.30846	2.29783
H	-1.16979	-1.33474	1.45161	H	-1.33012	-1.26394	1.55828
O	-2.30054	-0.71277	-1.34372	O	-1.87333	-1.27557	-1.91658
H	-2.09114	-1.16690	-2.17004	H	-1.42480	-1.28152	-2.78308
H	-3.22063	-0.93531	-1.15227	H	-2.29122	-2.14482	-1.76871
O	-1.71689	-1.25263	2.71150	O	-1.95315	-0.62342	3.06868
H	-1.14908	-0.63581	3.21888	H	-1.14130	-0.26254	3.46927
H	-1.67242	-2.10329	3.16678	H	-2.25664	-1.30602	3.67725
O	0.12521	0.55755	3.65599	O	0.53801	0.40908	3.84388
H	-0.08796	1.49304	3.55248	H	0.60392	1.36880	3.91805
H	0.56958	0.48436	4.50946	H	0.97654	0.06096	4.62968
H	-0.02024	0.62853	0.53861	H	-0.28083	0.54066	0.85652

Step 3, Reactant				Transition State			
O	-1.04702	0.69453	-1.13875	O	-1.46406	0.17888	0.52601
O	-0.30432	-0.73037	0.47194	O	0.56519	-0.50324	-0.79161
C	0.78204	-1.48146	1.06893	C	1.09525	-1.54823	0.03354
H	1.34967	-1.98227	0.28348	H	1.96552	-1.15359	0.55468
H	1.40401	-0.78608	1.62703	H	0.34184	-1.88393	0.75343
H	0.32252	-2.20477	1.73774	H	1.39511	-2.38350	-0.59914

C	0.10748	0.18391	-0.64477	C	-0.34603	0.77351	0.26591
H	-1.10025	-1.40181	0.12631	H	-0.15539	-0.89890	-1.35033
O	0.92375	1.13088	-0.10887	O	0.54993	1.02495	1.17881
H	1.86453	0.83053	-0.17141	H	0.56367	0.40229	1.96068
H	-1.39263	1.36898	-0.50083	H	-1.48555	-0.40320	1.37878
O	-2.06734	-2.24242	-0.24278	O	-1.42038	-1.63511	-2.12823
H	-1.70535	-3.07011	-0.58823	H	-1.25184	-2.56489	-2.32256
H	-2.58921	-1.85747	-0.96095	H	-2.18233	-1.63650	-1.53568
O	-1.90962	2.50845	0.65349	O	-1.63637	-1.25401	2.59426
H	-2.51493	2.12287	1.29786	H	-0.75977	-1.20505	3.01878
H	-1.13795	2.77546	1.16767	H	-1.76469	-2.18063	2.35664
O	3.39590	0.15757	-0.30782	O	0.93433	-0.57234	3.24589
H	3.53012	-0.50551	0.38013	H	1.23052	-0.10408	4.03665
H	4.10386	0.79987	-0.17895	H	1.65465	-1.16903	3.00432
H	0.59773	-0.45349	-1.38257	H	-0.37048	1.48511	-0.55057

4-Water Mechanism, Group CH3

Step 1, Reactant				Transition State			
O	-1.07347	-2.60653	0.67440	O	-1.01409	-1.84535	0.47538
O	0.62427	-0.42921	-0.81512	O	0.73698	-0.65939	-0.79297
C	1.69781	-1.37298	-1.07119	C	1.76268	-1.66895	-0.89415
H	2.64732	-0.90917	-0.81235	H	2.66727	-1.32965	-0.39283
H	1.52415	-2.27237	-0.48378	H	1.40399	-2.59962	-0.45606
H	1.63769	-1.57788	-2.13486	H	1.93838	-1.79066	-1.95870
C	0.41868	-0.04111	0.39206	C	0.23892	-0.42165	0.39646
C	-0.74898	0.83808	0.61993	C	-0.68610	0.74672	0.47002
H	-1.58741	0.19032	0.89641	H	-1.34106	0.75878	-0.39913
H	-0.54957	1.52704	1.43985	H	-1.27146	0.70432	1.38821
H	-1.49241	-2.16944	-0.08562	H	-1.67606	-1.69680	-0.24136
O	1.19666	-0.43321	1.30113	O	0.99384	-0.73260	1.41198
H	0.95839	-0.06944	2.27670	H	0.64387	-0.35164	2.27284
H	-1.35563	-2.10157	1.45689	H	-1.48458	-1.76916	1.34186
O	-2.05837	-1.27687	-1.64507	O	-2.61525	-1.32928	-1.63261
H	-1.20463	-0.89049	-1.87782	H	-3.30914	-1.96706	-1.83668
H	-2.27537	-1.86331	-2.37850	H	-3.07053	-0.48387	-1.54293
H	-0.99551	1.37119	-0.29559	H	-0.06768	1.64792	0.47475
O	-1.79726	-1.20146	3.01745	O	-2.09405	-1.42787	2.90101
H	-1.04633	-0.66809	3.31874	H	-1.41030	-0.86159	3.29831
H	-1.97660	-1.81151	3.74175	H	-2.14264	-2.20592	3.46792
O	0.60658	0.34303	3.55548	O	0.07178	0.23324	3.65075
H	1.24693	0.07103	4.22765	H	-0.05966	1.18933	3.61093
H	0.52225	1.30416	3.62804	H	0.64483	0.07462	4.41166

Step 2, Reactant				Transition State			
O	-0.71729	-1.25636	0.46785	O	-0.89202	-1.26096	0.66667
O	0.97284	-0.41546	-0.82243	O	0.56582	-0.41240	-0.78939
C	1.72138	-1.62605	-0.99811	C	1.35572	-1.57275	-1.08419
H	2.63219	-1.60440	-0.40014	H	2.35711	-1.47055	-0.66688

H	1.11937	-2.49694	-0.73558	H	0.88159	-2.47762	-0.69929
H	1.97631	-1.66310	-2.05470	H	1.41491	-1.62500	-2.16985
C	0.37163	-0.25166	0.40267	C	0.13002	-0.29659	0.54075
C	-0.21834	1.13427	0.49374	C	-0.39952	1.10846	0.73498
H	-0.89045	1.30217	-0.34779	H	-1.18486	1.30425	0.00398
H	-0.77446	1.23509	1.42756	H	-0.81534	1.20689	1.73972
H	-1.38518	-1.13878	-0.31477	H	-1.19291	-1.06745	-1.27806
O	1.23654	-0.57248	1.42387	O	1.19723	-0.58985	1.39388
H	0.92755	-0.17081	2.26245	H	0.99511	-0.23579	2.28252
H	-1.21207	-1.21945	1.41729	H	-1.32615	-1.15692	1.54256
O	-2.26971	-0.95894	-1.49138	O	-1.85938	-1.22405	-1.99760
H	-2.06336	-1.60301	-2.18083	H	-1.40470	-1.23600	-2.86075
H	-3.20057	-1.10097	-1.27689	H	-2.29488	-2.08560	-1.85496
H	0.59177	1.86302	0.46919	H	0.41000	1.82715	0.60610
O	-1.77738	-1.08537	2.68234	O	-1.88316	-0.81799	3.17348
H	-1.15512	-0.54497	3.21318	H	-1.09713	-0.37768	3.54510
H	-1.83771	-1.94052	3.12721	H	-1.98840	-1.62451	3.69045
O	0.21958	0.45266	3.78250	O	0.51958	0.44942	3.88670
H	0.09293	1.40920	3.80371	H	0.49742	1.41417	3.89377
H	0.66005	0.22732	4.61101	H	1.03445	0.19586	4.66225

Step 3, Reactant				Transition State			
O	-0.95367	0.72565	-1.15215	O	-1.43988	0.16994	0.47903
O	-0.53256	-0.53171	0.68635	O	0.56409	-0.57409	-0.75226
C	0.31625	-1.32319	1.55092	C	1.05455	-1.61609	0.10415
H	0.58649	-2.25501	1.05615	H	1.93860	-1.23952	0.61475
H	1.19620	-0.73080	1.79012	H	0.28746	-1.90618	0.82792
H	-0.26212	-1.51669	2.45101	H	1.32256	-2.47292	-0.51310
C	0.10717	0.12813	-0.54388	C	-0.29973	0.74142	0.17333
C	0.70674	-0.94506	-1.41325	H	-0.14823	-0.96312	-1.33798
H	1.52131	-1.45433	-0.89848	O	0.58520	1.00532	1.11761
H	-0.06401	-1.66599	-1.68794	H	0.58361	0.38709	1.89297
H	-1.39593	-1.08791	0.37665	H	-1.44657	-0.37923	1.33547
O	0.98203	1.04662	-0.04745	O	-1.37644	-1.59297	-2.17830
H	1.89389	0.67233	0.03424	H	-1.24262	-2.52075	-2.40731
H	-1.24385	1.49215	-0.59779	H	-2.16568	-1.58062	-1.62238
O	-2.51773	-1.78424	-0.02874	O	-1.59741	-1.22604	2.61882
H	-2.41427	-2.73702	0.09918	H	-0.70911	-1.17988	3.01806
H	-2.64198	-1.65689	-0.97963	H	-1.73985	-2.15537	2.40227
H	1.09736	-0.46726	-2.31216	O	0.99303	-0.57699	3.24866
O	-1.62304	2.78535	0.46216	H	1.28586	-0.09383	4.03128
H	-2.46498	2.67874	0.92048	H	1.70992	-1.18559	3.02937
H	-0.95652	2.75390	1.15945	C	-0.37111	1.75649	-0.91676
O	3.46566	0.08826	0.24543	H	-0.89765	2.62506	-0.51528
H	4.12849	0.77412	0.10109	H	0.63012	2.04647	-1.22637
H	3.67359	-0.59806	-0.39990	H	-0.93256	1.35514	-1.75902

4-Water Mechanism, Group tBu

Step 1, Reactant				Transition State			
O	-0.48134	-2.45261	1.12919	O	-1.05603	-1.44440	0.55662
O	0.25578	-0.45740	-0.93906	O	0.83149	-0.57432	-0.74101
C	1.29356	-1.30213	-1.49892	C	1.71767	-1.71246	-0.72304
H	2.16778	-0.69049	-1.71424	H	2.65283	-1.44492	-0.23444
H	1.53554	-2.08989	-0.78878	H	1.23750	-2.54396	-0.20937
H	0.86267	-1.70571	-2.40937	H	1.88832	-1.95462	-1.76781
C	0.44419	0.05870	0.21968	C	0.32547	-0.16865	0.39688
C	-0.63501	0.96168	0.75997	C	-0.39270	1.17167	0.30812
H	0.07477	-2.30152	1.91219	H	-1.64528	-1.50218	-0.23048
O	1.55121	-0.15693	0.78781	O	1.01516	-0.49688	1.45834
H	1.76780	0.28630	1.72321	H	0.60215	-0.25186	2.33053
H	-0.04319	-3.15310	0.61724	H	-1.59719	-1.39364	1.38087
O	0.96091	-1.91441	3.52809	O	-2.41565	-1.80405	-1.75873
H	1.38897	-1.04642	3.50097	H	-3.11742	-2.46533	-1.73907
H	0.23237	-1.80494	4.15003	H	-2.82348	-1.01685	-2.13846
O	0.62654	-4.51626	-0.47067	O	-2.28993	-1.39164	2.96582
H	0.68759	-4.24329	-1.39336	H	-1.52782	-1.04912	3.46657
H	0.06644	-5.30080	-0.48294	H	-2.43035	-2.28766	3.29251
O	2.27256	0.67634	2.98886	O	0.11071	-0.29415	3.93672
H	3.23686	0.75088	2.97208	H	0.07168	0.56025	4.38466
H	1.93966	1.53178	3.29327	H	0.67791	-0.85053	4.48539
C	-1.01114	0.55881	2.19361	C	-1.00594	1.56956	1.64978
H	-0.15926	0.58405	2.87365	H	-0.23750	1.76966	2.39982
H	-1.74795	1.27996	2.55342	H	-1.57022	2.49272	1.50364
H	-1.45648	-0.43620	2.21935	H	-1.69299	0.80992	2.02698
C	-1.87381	0.90646	-0.13358	C	-1.46488	1.16625	-0.78216
H	-1.65293	1.24435	-1.14711	H	-2.34619	0.60533	-0.46556
H	-2.28130	-0.10552	-0.17875	H	-1.77061	2.19813	-0.96715
H	-2.63091	1.56637	0.29374	H	-1.08998	0.74855	-1.71858
C	-0.03554	2.38247	0.75185	C	0.71247	2.18309	-0.05896
H	0.27659	2.67160	-0.25429	H	1.09053	2.00674	-1.06712
H	-0.80702	3.07622	1.09110	H	0.28450	3.18662	-0.01707
H	0.82051	2.45682	1.42606	H	1.54452	2.13438	0.64747

Step 2, Reactant				Transition State			
O	-0.73220	-1.17367	0.41669	O	-1.10565	-1.00164	0.68422
O	0.98383	-0.40213	-0.88310	O	0.45312	-0.38483	-0.78085
C	1.76164	-1.60491	-0.93713	C	1.25523	-1.56515	-0.92568
H	2.67345	-1.50044	-0.34965	H	2.25395	-1.40457	-0.52127
H	1.18251	-2.45866	-0.58354	H	0.78659	-2.42040	-0.43460
H	2.01401	-1.74359	-1.98611	H	1.31919	-1.74946	-1.99710
C	0.33429	-0.15110	0.29796	C	-0.02012	-0.11824	0.51423
C	-0.25711	1.27954	0.26636	C	-0.46647	1.36467	0.56440
H	-1.52587	-1.11859	-0.24000	H	-1.28524	-1.15052	-1.29003
O	1.17924	-0.40968	1.35570	O	1.00412	-0.41917	1.41399
H	0.82750	-0.08866	2.20971	H	0.77354	-0.16409	2.32629
H	-1.07549	-1.31849	1.42107	H	-1.33690	-1.08913	1.63606

O	-2.72504	-1.22815	-1.12776	O	-1.84419	-1.50915	-2.02760
H	-3.18411	-2.06652	-0.98768	H	-1.25957	-1.86681	-2.72278
H	-3.37426	-0.54027	-0.93096	H	-2.40044	-2.23238	-1.68079
O	-1.49895	-1.51464	2.73121	O	-1.64182	-1.28629	3.35066
H	-0.90206	-1.00981	3.32182	H	-0.86701	-0.87070	3.77004
H	-1.40268	-2.44350	2.97825	H	-1.58845	-2.21696	3.59652
O	0.39668	0.04472	3.98258	O	0.74926	-0.06353	4.18811
H	0.15583	0.90357	4.35054	H	0.76155	0.80231	4.61314
H	1.03637	-0.33500	4.59736	H	1.43150	-0.58029	4.63308
C	-1.37717	1.41821	1.30218	C	-1.22501	1.63519	1.86849
H	-1.68137	2.46604	1.34884	H	-2.15312	1.06151	1.91988
H	-2.25246	0.82343	1.02826	H	-0.62526	1.41031	2.75415
H	-1.05389	1.12279	2.30361	H	-1.48312	2.69607	1.91112
C	-0.81792	1.60253	-1.12376	C	-1.40029	1.66481	-0.61358
H	-1.54054	0.85710	-1.46144	H	-1.77610	2.68646	-0.51802
H	-1.32905	2.56685	-1.07408	H	-0.88216	1.58330	-1.57096
H	-0.02316	1.67496	-1.86721	H	-2.26047	0.99038	-0.62162
C	0.86985	2.26776	0.59005	C	0.76405	2.27269	0.49022
H	1.73051	2.11420	-0.06537	H	1.37003	2.05068	-0.39136
H	0.50140	3.28490	0.43907	H	0.43983	3.31441	0.42605
H	1.19907	2.17514	1.62746	H	1.39100	2.16755	1.37834

Step 3, Reactant				Transition State			
O	-1.10450	-0.06206	-1.28270	O	-1.66797	-0.15930	1.24455
O	-0.75292	0.27042	0.91230	O	0.23114	-0.51869	-0.25478
C	-0.05882	0.56141	2.14548	C	1.39962	-1.25985	0.11892
H	0.28884	-0.36073	2.60768	H	2.20943	-0.55013	0.27444
H	0.76909	1.23035	1.92128	H	1.22238	-1.83626	1.02971
H	-0.78009	1.06581	2.78514	H	1.64937	-1.93094	-0.70321
C	-0.04986	0.05756	-0.43334	C	-0.54358	0.49873	1.05675
C	0.79963	-1.23070	-0.43118	C	-0.68418	1.83044	0.34045
H	-1.63951	-0.33351	1.04614	H	-0.47314	-1.14553	-0.58588
O	0.61917	1.22232	-0.68439	O	0.38720	0.47437	1.98861
H	1.44864	1.34020	-0.16967	H	0.35372	-0.30666	2.59807
H	-1.57184	0.80873	-1.32447	H	-1.51972	-1.09449	1.60750
O	-2.80144	-1.00721	1.27599	O	-1.64553	-2.12978	-1.12896
H	-2.62397	-1.94252	1.44820	H	-1.36836	-3.05053	-1.21406
H	-3.34388	-0.98718	0.47492	H	-2.35286	-2.14110	-0.47124
O	-2.31559	2.34946	-1.31856	O	-1.22030	-2.58165	1.98651
H	-3.12570	2.36642	-0.79544	H	-0.47479	-2.48156	2.60759
H	-1.71643	2.95680	-0.86770	H	-0.85183	-3.00812	1.20198
O	2.77827	2.13466	0.69751	O	0.71056	-1.59053	3.67377
H	3.20813	2.78356	0.12779	H	0.52093	-1.44934	4.60953
H	3.48051	1.52265	0.94751	H	1.64356	-1.83400	3.62777
C	2.13590	-1.03985	0.29586	C	-1.36562	2.77691	1.34496
H	2.64009	-2.00798	0.33400	H	-2.35455	2.40935	1.62668
H	2.78813	-0.35418	-0.24962	H	-0.76161	2.89743	2.24668
H	2.02965	-0.68471	1.32135	H	-1.48312	3.75574	0.87532

C	1.10716	-1.57030	-1.89781	C	-1.56515	1.68285	-0.90127
H	1.82092	-2.39680	-1.92219	H	-1.69233	2.66760	-1.35614
H	0.20893	-1.87519	-2.43575	H	-1.10744	1.02295	-1.64037
H	1.55453	-0.71752	-2.41426	H	-2.55359	1.29655	-0.64651
C	0.01502	-2.38257	0.20306	C	0.69029	2.38411	-0.03734
H	-0.12452	-2.23681	1.27775	H	1.21071	1.71653	-0.72666
H	-0.96445	-2.50213	-0.26645	H	0.55342	3.34845	-0.53152
H	0.57482	-3.30938	0.06019	H	1.31533	2.54055	0.84351

(e) Reactant and transition state structures of the 2-water mechanism for 20 alkyl groups.

Group C2H5

Reactant				Transition State			
O	-2.11805	-0.28384	-1.77220	O	0.56295	0.33309	-1.22897
O	-1.00237	0.55824	0.81904	O	1.98095	-0.76501	0.06461
C	-2.00499	1.56364	1.13934	C	2.33362	-1.67727	1.10606
H	-1.50710	2.50445	1.36306	H	1.94950	-1.33638	2.06918
H	-2.67834	1.66004	0.28879	H	1.96016	-2.67851	0.88434
H	-2.51860	1.17106	2.01034	H	3.42126	-1.69637	1.13686
C	-0.24135	0.73212	-0.18379	C	0.65001	-0.79021	-0.38887
H	-2.58075	-0.66487	-1.00327	H	2.16451	1.10050	-0.40305
O	-0.31469	1.85284	-0.79838	O	0.51058	-1.97237	-1.12702
H	0.30304	1.91431	-1.54964	H	-0.42256	-2.12352	-1.32640
H	-2.56052	0.55640	-1.93556	H	0.97667	0.10508	-2.07468
O	-3.24465	-1.43922	0.53941	O	2.81463	1.84869	-0.32301
H	-3.83371	-0.81407	0.97820	H	3.27648	1.77764	0.53315
H	-2.45668	-1.45679	1.09605	H	2.34220	2.70125	-0.35409
C	0.72358	-0.34520	-0.50991	C	-0.36608	-0.64085	0.73258
C	1.33935	-0.24420	-1.89787	C	-1.80658	-0.53767	0.24213
H	0.19113	-1.28562	-0.35685	H	-0.08817	0.25428	1.29528
H	1.49016	-0.28420	0.27188	H	-0.25953	-1.49970	1.39770
H	1.99679	-1.09841	-2.05407	H	-1.94350	0.32035	-0.41708
H	1.94585	0.65838	-2.00713	H	-2.47636	-0.42159	1.09519
H	0.57003	-0.25668	-2.67164	H	-2.11974	-1.43862	-0.29273

Group C3H7

Reactant				Transition State			
O	-2.18420	-0.37620	-1.73501	O	0.69768	0.52753	-1.30563
O	-0.96231	0.50669	0.79009	O	1.90345	-0.76590	0.02182
C	-1.94052	1.51311	1.17565	C	2.08200	-1.74257	1.04909
H	-1.42409	2.44615	1.39014	H	1.68785	-1.38298	2.00132
H	-2.65431	1.63078	0.36178	H	1.60106	-2.68289	0.77401
H	-2.41395	1.10978	2.06418	H	3.15534	-1.89853	1.13726
C	-0.25173	0.69132	-0.24723	C	0.60088	-0.61024	-0.48695
H	-2.65302	-0.68992	-0.93954	H	2.28217	1.11731	-0.34475
O	-0.36534	1.81402	-0.85342	O	0.33816	-1.75115	-1.25505
H	0.21554	1.88711	-1.63270	H	-0.60789	-1.80255	-1.44340
H	-2.64386	0.43066	-1.99153	H	1.12963	0.26278	-2.13098
O	-3.40243	-1.34860	0.61075	O	2.95454	1.83383	-0.19331

H	-3.97171	-0.66772	0.98854	H	3.37748	1.70181	0.67588
H	-2.67095	-1.42254	1.23554	H	2.51023	2.70201	-0.20053
C	0.71012	-0.37231	-0.62121	C	-0.43593	-0.34672	0.59319
C	1.26451	-0.27722	-2.03955	C	-1.82414	0.00005	0.05799
C	2.17890	-1.46178	-2.33124	C	-2.80960	0.22053	1.20188
H	1.63239	-2.40332	-2.24045	H	-2.47514	1.03550	1.84914
H	2.58128	-1.39705	-3.34309	H	-3.80117	0.47560	0.82304
H	3.01727	-1.48573	-1.63105	H	-2.90245	-0.67945	1.81515
H	0.20255	-1.32333	-0.44377	H	-0.05824	0.47466	1.21028
H	1.51754	-0.30059	0.11909	H	-0.49822	-1.23652	1.22481
H	1.83132	0.65201	-2.15683	H	-1.76576	0.89907	-0.55942
H	0.43632	-0.25655	-2.75265	H	-2.19717	-0.80514	-0.58396

Group C4H9

Reactant				Transition State			
O	-2.18646	-0.35357	-1.74563	O	0.66411	0.53173	-1.28897
O	-0.97237	0.48999	0.79549	O	1.89256	-0.75245	0.02730
C	-1.95187	1.49307	1.18665	C	2.09090	-1.73426	1.04620
H	-1.43599	2.42377	1.41238	H	1.70095	-1.38583	2.00426
H	-2.66200	1.61862	0.37074	H	1.61874	-2.67826	0.76870
H	-2.42937	1.08135	2.06914	H	3.16671	-1.87832	1.12423
C	-0.25490	0.68675	-0.23494	C	0.58697	-0.61325	-0.47803
H	-2.66385	-0.67097	-0.95672	H	2.25108	1.13405	-0.33930
O	-0.36443	1.81662	-0.82841	O	0.34271	-1.75304	-1.25437
H	0.22317	1.89936	-1.60172	H	-0.59477	-1.79263	-1.48475
H	-2.62789	0.46755	-1.98863	H	1.09449	0.27856	-2.11883
O	-3.42962	-1.34462	0.57878	O	2.92211	1.85273	-0.19210
H	-4.00018	-0.66667	0.95987	H	3.34789	1.72408	0.67620
H	-2.70637	-1.43178	1.21141	H	2.47591	2.71993	-0.20024
C	0.70890	-0.37256	-0.61564	C	-0.45091	-0.37242	0.60660
C	1.26789	-0.26194	-2.03031	C	-1.85321	-0.08342	0.07595
C	2.18429	-1.44118	-2.34726	C	-2.84446	0.16506	1.21097
H	1.62001	-2.37178	-2.23261	H	-2.49005	1.00468	1.81792
H	2.99661	-1.46975	-1.61430	H	-2.86645	-0.71068	1.86782
H	0.20083	-1.32525	-0.44926	H	-0.09595	0.47012	1.20840
H	1.51289	-0.30729	0.12896	H	-0.47736	-1.25485	1.25055
H	1.84015	0.66673	-2.13754	H	-1.82977	0.78961	-0.58249
H	0.44386	-0.23210	-2.74997	H	-2.21563	-0.92800	-0.52247
C	2.75679	-1.34963	-3.75708	C	-4.24834	0.45860	0.69236
H	3.33785	-0.43206	-3.88198	H	-4.94835	0.63467	1.51196
H	3.41238	-2.19555	-3.97325	H	-4.24871	1.34588	0.05328
H	1.95630	-1.34432	-4.50158	H	-4.62723	-0.37928	0.10067

Group CH3

Reactant				Transition State			
O	-2.30300	-0.49698	-1.65550	O	0.77437	0.50784	-1.35487
O	-0.96353	0.52861	0.74752	O	1.97646	-0.77838	-0.01387
C	-1.92585	1.56275	1.09900	C	2.13870	-1.70245	1.06344

H	-1.39760	2.50182	1.24800	H	1.77032	-1.27635	1.99861
H	-2.65785	1.64028	0.29658	H	1.62175	-2.63919	0.84763
H	-2.37966	1.21369	2.02015	H	3.20725	-1.88988	1.14630
C	-0.29552	0.64131	-0.32637	C	0.66507	-0.59052	-0.48453
H	-2.73482	-0.77139	-0.82555	H	2.36144	1.11020	-0.38392
O	-0.42738	1.72356	-0.99955	O	0.32036	-1.75023	-1.18906
H	0.11306	1.72580	-1.80904	H	-0.63746	-1.76753	-1.31377
H	-2.77013	0.30157	-1.92434	H	1.21314	0.20196	-2.16257
O	-3.38546	-1.33761	0.80825	O	3.03143	1.82769	-0.23083
H	-3.93856	-0.64328	1.18543	H	3.45190	1.69690	0.63980
H	-2.60760	-1.36061	1.37862	H	2.58600	2.69533	-0.24031
C	0.65110	-0.42916	-0.68107	C	-0.33092	-0.23751	0.59644
H	0.79126	-0.45987	-1.76030	H	0.02139	0.63542	1.14765
H	0.28948	-1.37916	-0.29528	H	-0.46373	-1.07438	1.28111
H	1.60486	-0.18297	-0.20292	H	-1.28920	-0.00551	0.12989

Group cyclohexane

Reactant				Transition State			
O	-2.40974	-1.04974	-1.08694	O	0.70017	0.30462	-1.47902
O	-0.78450	0.87928	0.47403	O	1.88705	-0.64491	0.12808
C	-1.84972	1.84927	0.68385	C	2.07067	-1.45000	1.29345
H	-1.50882	2.82813	0.35440	H	1.54987	-1.02230	2.15289
H	-2.72530	1.52152	0.12549	H	1.72493	-2.46951	1.11540
H	-2.03026	1.83146	1.75332	H	3.14132	-1.46023	1.48857
C	-0.35694	0.65961	-0.70051	C	0.62488	-0.69329	-0.49319
H	-2.51787	-1.10164	-0.11967	H	2.19341	1.15317	-0.49487
O	-0.80593	1.40029	-1.64811	O	0.52972	-1.96088	-1.08036
H	-0.42933	1.15904	-2.51354	H	-0.37828	-2.11030	-1.37373
H	-2.99792	-0.33818	-1.36367	H	1.22292	-0.04811	-2.21396
O	-2.52307	-1.20593	1.73588	O	2.82129	1.91805	-0.40160
H	-3.04653	-0.47951	2.09493	H	3.24553	1.87183	0.47581
H	-1.60963	-0.96220	1.93120	H	2.32723	2.75690	-0.46449
C	0.69949	-0.35914	-0.90451	C	-0.52937	-0.37284	0.45639
C	2.05722	0.38140	-0.99993	C	-0.32726	0.98713	1.13660
C	0.71975	-1.42240	0.19491	C	-1.89209	-0.42109	-0.24651
H	0.49108	-0.81990	-1.87706	H	-0.52036	-1.15616	1.22367
C	3.17344	-0.63235	-1.25060	C	-1.45610	1.27109	2.12907
H	2.23324	0.90845	-0.05617	H	-0.31628	1.76978	0.36889
H	2.01944	1.12323	-1.80113	H	0.64053	1.01828	1.64504
C	1.84589	-2.42150	-0.07178	C	-3.02122	-0.13408	0.74647
H	0.88462	-0.93343	1.16083	H	-1.91110	0.32626	-1.04701
H	-0.24796	-1.92799	0.23696	H	-2.06436	-1.39973	-0.70541
C	3.19830	-1.71495	-0.17143	C	-2.82059	1.21210	1.44202
H	4.13024	-0.10639	-1.28875	H	-1.30403	2.24937	2.59217
H	3.01808	-1.09763	-2.23049	H	-1.42315	0.52548	2.93249
H	1.86281	-3.16879	0.72468	H	-3.98179	-0.15594	0.22566
H	1.64195	-2.95181	-1.00906	H	-3.04482	-0.93011	1.50000
H	3.98758	-2.43940	-0.38650	H	-3.61942	1.38473	2.16808

H	3.43551	-1.25435	0.79469	H	-2.88252	2.01419	0.69674

Group Et2CH

Reactant				Transition State			
O	-2.51022	-0.39518	-1.72778	O	0.55773	0.22216	-1.32196
O	-0.98728	0.55392	0.74201	O	1.96643	-0.52518	0.22191
C	-1.96093	1.59468	1.04142	C	2.71233	-1.66924	0.64510
H	-1.43735	2.54073	1.16050	H	2.14240	-2.28477	1.34061
H	-2.68332	1.63880	0.22837	H	3.02031	-2.27038	-0.21099
H	-2.42410	1.27784	1.96966	H	3.59331	-1.27410	1.14863
C	-0.30755	0.61919	-0.32851	C	0.64408	-0.69181	-0.24907
H	-2.82236	-0.71564	-0.86186	H	2.24294	1.02398	-0.90860
O	-0.46373	1.65582	-1.06646	O	0.51286	-2.00090	-0.70672
H	0.08039	1.62810	-1.87360	H	-0.42421	-2.22709	-0.76853
H	-2.87316	0.49345	-1.80971	H	0.87739	-0.23154	-2.11610
O	-3.22590	-1.43466	0.79788	O	2.91797	1.73528	-1.09181
H	-3.74013	-0.80157	1.31273	H	3.39454	1.94308	-0.26608
H	-2.35534	-1.43098	1.21493	H	2.46252	2.53989	-1.40243
C	0.68719	-0.45280	-0.59932	C	-0.39219	-0.28587	0.81053
C	1.99090	-0.08096	0.15360	C	-1.83553	-0.63257	0.40839
C	2.51450	1.32241	-0.13443	C	-2.33005	-0.12004	-0.94403
H	2.60530	1.49386	-1.21080	H	-2.16185	0.95525	-1.04115
H	1.86158	2.09531	0.27979	H	-1.83596	-0.61218	-1.78374
H	3.50120	1.45192	0.31267	H	-3.40294	-0.30404	-1.03437
C	0.14683	-1.82848	-0.18157	C	-0.04654	-0.90157	2.17446
H	-0.02063	-1.82915	0.89958	H	-0.05143	-1.99403	2.08684
H	-0.82140	-1.98585	-0.66192	H	0.96915	-0.60684	2.44696
H	0.88410	-0.43240	-1.67653	H	-0.30367	0.80453	0.89004
H	2.73524	-0.81849	-0.14891	C	-0.99362	-0.47522	3.29487
C	1.09780	-2.95759	-0.56572	H	-1.10382	0.61312	3.31832
H	2.02976	-2.91606	0.00024	H	-1.98724	-0.91264	3.18475
H	0.62999	-3.92285	-0.36433	H	-0.60016	-0.79320	4.26259
H	1.34134	-2.91623	-1.63068	H	-1.97290	-1.72071	0.46920
H	1.81279	-0.21345	1.22474	H	-2.48383	-0.21678	1.18192

Group EtMe2C

Reactant				Transition State			
O	2.01278	-0.71611	-1.76608	O	-1.05123	0.41144	1.32856
O	0.37730	0.73978	0.30726	O	-1.43824	-0.94544	-0.40231
C	1.50889	0.97502	1.19276	C	-1.49911	-2.32300	-0.78044
H	1.27344	0.58051	2.17888	H	-2.23184	-2.37233	-1.58443
H	2.38696	0.49170	0.76768	H	-0.53702	-2.68268	-1.14587
H	1.62045	2.05376	1.21370	H	-1.83056	-2.94263	0.05330
C	-0.00346	-0.44938	0.07287	C	-0.41503	-0.50846	0.46716
H	2.62498	-0.98179	-1.07096	H	-2.55262	0.60515	0.12127
O	0.58813	-1.39220	0.70763	O	0.02138	-1.60963	1.19853
H	0.25363	-2.27593	0.47089	H	0.86530	-1.40185	1.61884
H	2.06187	0.25722	-1.78741	H	-1.50667	-0.10615	2.00846

O	1.97448	2.10439	-1.85746	O	-3.23002	1.25172	-0.21347
H	1.09954	2.28827	-1.49371	H	-3.42652	1.04565	-1.14711
H	2.58617	2.46321	-1.20347	H	-2.83063	2.14227	-0.17479
C	-1.18779	-0.64171	-0.82633	C	0.69457	0.24941	-0.30229
C	-1.26279	-2.08288	-1.33404	C	1.32264	-0.63058	-1.40475
H	-2.11055	-2.15579	-2.01668	H	1.94606	0.04400	-2.00055
H	-0.35636	-2.35188	-1.88125	C	0.06135	1.46528	-0.99642
C	-2.43217	-0.27988	0.03863	H	0.84076	2.01401	-1.52991
H	-2.41553	0.79833	0.21660	H	-0.39984	2.14733	-0.27943
C	-2.55735	-1.02227	1.36520	C	2.18937	-1.81427	-0.97369
H	-2.55622	-2.10573	1.23040	H	3.01154	-1.49340	-0.32937
H	-1.74831	-0.76237	2.05393	H	1.62384	-2.58018	-0.44205
H	-3.49664	-0.74916	1.84902	H	2.63127	-2.28085	-1.85734
C	-1.10366	0.33215	-2.00810	H	-0.69374	1.15759	-1.72394
H	-0.23994	0.11249	-2.63749	H	0.52729	-0.97144	-2.07513
H	-2.00996	0.21277	-2.60459	C	1.76645	0.75085	0.67290
H	-1.04989	1.36732	-1.66829	H	1.34706	1.46877	1.38006
H	-1.42776	-2.81021	-0.53492	H	2.24734	-0.04959	1.24172
H	-3.29439	-0.49367	-0.59868	H	2.55401	1.25234	0.10437

Group H

Reactant				Transition State			
O	-2.16137	-0.58541	-1.63963	O	0.80509	0.60870	-1.23962
O	-0.92205	0.55304	0.72883	O	2.03728	-0.81312	-0.04271
C	-1.85899	1.56568	1.20675	C	2.11740	-1.78045	1.00571
H	-1.32477	2.50531	1.32739	H	1.48843	-1.47660	1.84691
H	-2.66594	1.65388	0.48118	H	1.80768	-2.76292	0.64600
H	-2.21373	1.18405	2.15745	H	3.15826	-1.81587	1.31880
C	-0.37441	0.71119	-0.39459	C	0.73650	-0.56126	-0.47589
H	-2.67623	-0.82496	-0.84633	H	2.48327	1.11156	-0.39659
O	-0.54140	1.79080	-1.04691	O	0.30763	-1.65330	-1.22788
H	-0.05185	1.78511	-1.88945	H	-0.65646	-1.63369	-1.28328
H	-2.70831	0.05366	-2.10928	H	1.14441	0.37546	-2.11728
O	-3.45495	-1.27237	0.75559	O	3.18011	1.80610	-0.26487
H	-3.98297	-0.52856	1.06915	H	3.61838	1.66749	0.59589
H	-2.72619	-1.33127	1.38520	H	2.75517	2.68427	-0.26689
H	0.29429	-0.07077	-0.73873	H	0.07019	-0.36447	0.36806

Group iBu2CH

Reactant				Transition State			
O	3.40675	-1.34743	-0.05905	O	0.91994	-0.66459	-1.49441
O	0.70075	-2.12532	-1.12992	O	1.08954	-2.01981	0.32595
C	1.21173	-2.75589	-2.33796	C	1.38932	-3.30136	-0.23594
H	0.64160	-2.38882	-3.18947	H	0.54091	-3.97723	-0.12534
H	2.27053	-2.52262	-2.43842	H	1.66747	-3.22246	-1.28986
H	1.05077	-3.81723	-2.18205	H	2.23736	-3.68247	0.33002
C	0.73420	-0.85935	-1.02138	C	0.20530	-1.20756	-0.39787
H	3.16007	-2.28956	-0.02154	H	2.51880	-0.79645	-0.31148

O	1.23157	-0.20935	-2.00794	O	-0.83527	-2.01437	-0.86083
H	1.22676	0.75600	-1.87867	H	-1.46246	-1.46808	-1.35252
H	3.58899	-1.17135	-0.98841	H	0.92819	-1.31095	-2.21486
O	2.64779	-4.04480	0.24846	O	3.36345	-0.34524	-0.05113
H	2.79228	-4.55717	-0.55566	H	3.50686	-0.48643	0.90439
H	1.68872	-4.02663	0.35161	H	3.26416	0.61268	-0.21248
C	0.20441	-0.25996	0.24061	C	-0.21457	-0.02403	0.49580
C	0.06588	1.27466	0.23962	C	-1.53324	0.65278	0.06719
H	-0.30002	1.62562	-0.73358	H	-2.33800	-0.08990	0.03298
C	-1.10781	-0.96520	0.66280	C	-0.25751	-0.33623	2.00787
H	-0.96131	-2.04877	0.64887	H	0.70216	-0.75305	2.32725
C	1.28267	2.10661	0.68599	C	-1.59648	1.51017	-1.21534
H	0.90015	3.12780	0.78410	H	-2.49181	2.12792	-1.08281
C	-2.35009	-0.60733	-0.16092	C	-1.38751	-1.21933	2.56525
H	-2.52373	0.47085	-0.07721	H	-2.33000	-0.93771	2.08336
H	0.96309	-0.56443	0.97361	H	0.59563	0.70322	0.37467
C	2.43042	2.14958	-0.32195	C	-0.41003	2.46417	-1.34824
H	2.10094	2.52261	-1.29867	H	0.51250	1.92473	-1.57686
H	3.21242	2.82747	0.02902	H	-0.58602	3.17954	-2.15593
H	2.89436	1.16570	-0.44789	H	-0.25221	3.02969	-0.42502
C	-2.20250	-0.95424	-1.64284	C	-1.15982	-2.71727	2.34927
H	-1.95974	-2.01394	-1.77386	H	-0.21197	-3.02451	2.80477
H	-3.13858	-0.75586	-2.17064	H	-1.96080	-3.29109	2.82424
H	-1.43058	-0.35712	-2.13917	H	-1.12972	-2.98828	1.29456
H	-1.27692	-0.67878	1.70399	H	-1.78862	1.31879	0.89776
H	-0.74003	1.49373	0.94422	H	-0.33952	0.64356	2.49032
C	1.79688	1.66927	2.05772	C	-1.82018	0.71820	-2.50650
H	0.97917	1.56622	2.77659	H	-2.03861	1.40105	-3.33215
H	2.32450	0.71258	1.99905	H	-0.94120	0.13617	-2.79276
H	2.50313	2.40552	2.44884	H	-2.67577	0.04097	-2.40923
C	-3.55888	-1.33092	0.43188	C	-1.52886	-0.94554	4.06484
H	-3.43289	-2.41511	0.34662	H	-0.59156	-1.17759	4.58250
H	-3.68740	-1.08718	1.48958	H	-1.76856	0.10331	4.25808
H	-4.47501	-1.05534	-0.09593	H	-2.31578	-1.56312	4.50565

Group iBut

Reactant				Transition State			
O	-2.26215	-0.25637	-0.71004	O	-0.18433	-1.64292	-0.04939
O	0.53805	-0.04003	0.20901	O	0.16704	0.47938	-0.56338
C	0.88150	1.11434	-0.60957	C	0.87001	1.71900	-0.47143
H	1.79629	0.89795	-1.15728	H	0.84997	2.10471	0.54976
H	0.05102	1.31902	-1.28341	H	1.90176	1.60217	-0.80780
H	1.02631	1.92086	0.10113	H	0.35150	2.41288	-1.13004
C	0.28075	-1.14930	-0.35301	C	0.79380	-0.63834	0.02393
H	-2.09839	0.44707	-0.05527	H	-1.59990	-0.31126	-0.08226
O	0.42898	-1.22117	-1.62521	O	1.88514	-0.94866	-0.79760
H	0.21476	-2.10326	-1.97988	H	2.53417	-1.46143	-0.30001
H	-2.03034	0.13997	-1.55716	H	-0.24378	-1.92959	-0.97296

O	-1.72985	1.68538	1.26398	O	-2.56540	-0.11911	0.04897
H	-0.98035	1.30573	1.73832	H	-2.68795	0.83924	0.18435
H	-1.37188	2.47788	0.84688	H	-2.88195	-0.59559	0.83940
C	-0.07077	-2.30864	0.49171	C	1.15640	-0.40549	1.48711
H	-0.93508	-2.79979	0.03814	H	0.34866	0.19073	1.92235
H	-0.33390	-1.93902	1.48349	H	2.06446	0.20578	1.51069
C	1.11675	-3.29879	0.57490	C	1.35818	-1.66089	2.34591
H	1.32894	-3.65249	-0.43929	H	0.40339	-2.19202	2.39818
C	2.36210	-2.62055	1.13865	C	2.41079	-2.61973	1.78874
H	3.17002	-3.34767	1.24359	H	3.35860	-2.09717	1.61071
H	2.72106	-1.81532	0.49075	H	2.60835	-3.41989	2.50599
H	2.15247	-2.19778	2.12601	H	2.08754	-3.09663	0.85902
C	0.69210	-4.48483	1.43425	C	1.74369	-1.22242	3.75847
H	-0.19609	-4.97261	1.02642	H	2.71328	-0.71435	3.74859
H	1.49774	-5.22040	1.48408	H	1.00496	-0.53405	4.17694
H	0.46727	-4.15538	2.45287	H	1.82165	-2.08584	4.42332

Group iPrEtCH

Reactant				Transition State			
O	-2.48064	-0.35211	-1.75476	O	0.62288	0.14697	-1.30827
O	-1.01328	0.53232	0.78173	O	2.00960	-0.52370	0.28994
C	-1.98480	1.57291	1.08916	C	2.80748	-1.61819	0.74853
H	-1.45647	2.51113	1.24412	H	2.24277	-2.28001	1.40459
H	-2.68965	1.64502	0.26290	H	3.20621	-2.18622	-0.09253
H	-2.46913	1.23562	1.99918	H	3.62814	-1.16959	1.30618
C	-0.30792	0.62154	-0.27031	C	0.72540	-0.77177	-0.24531
H	-2.79783	-0.71398	-0.90699	H	2.05624	1.21867	-0.60396
O	-0.44472	1.67915	-0.98378	O	0.71933	-2.08366	-0.72051
H	0.10804	1.66345	-1.78518	H	-0.14419	-2.27107	-1.10929
H	-2.84944	0.53696	-1.79624	H	1.13753	-0.20995	-2.04797
O	-3.27769	-1.44343	0.72185	O	2.52239	2.09772	-0.58382
H	-3.82031	-0.79523	1.18636	H	2.98572	2.18935	0.26975
H	-2.44043	-1.44383	1.20195	H	1.85947	2.80974	-0.66330
C	0.68098	-0.45060	-0.56084	C	-0.37630	-0.43833	0.77812
C	2.03454	-0.09346	0.13851	C	-1.83214	-0.77051	0.35289
C	2.51866	1.31024	-0.22249	C	-2.25371	-0.19527	-1.00114
H	2.48486	1.48340	-1.30212	H	-1.77279	-0.71842	-1.83231
H	1.91529	2.07977	0.26971	H	-3.33473	-0.30640	-1.12011
H	3.55038	1.44002	0.10950	H	-2.00784	0.86580	-1.08262
C	1.99327	-0.27725	1.65315	C	-2.22293	-2.25268	0.43284
H	1.26245	0.39223	2.11602	H	-1.81325	-2.84949	-0.38741
H	1.75199	-1.30263	1.93905	H	-1.91685	-2.71931	1.37065
H	2.97380	-0.03550	2.06982	H	-3.31044	-2.33640	0.36053
C	0.12789	-1.83162	-0.17746	C	-0.03508	-1.02405	2.15830
H	-0.13463	-1.84274	0.88312	H	0.05535	-2.11283	2.09205
H	-0.79584	-1.99593	-0.73668	H	0.94353	-0.64643	2.46164
H	0.85869	-0.41387	-1.64096	H	-0.32602	0.65461	0.86882
H	2.74192	-0.81226	-0.28263	C	-1.04803	-0.65567	3.24083

C	1.11957	-2.94899	-0.48350	H	-1.21866	0.42495	3.26105
H	1.99751	-2.90109	0.16401	H	-2.01270	-1.14486	3.09159
H	0.64542	-3.92000	-0.33043	H	-0.67521	-0.95401	4.22294
H	1.45813	-2.89798	-1.52187	H	-2.43959	-0.25507	1.10276

Group iPr

Reactant				Transition State			
O	-2.59132	-1.00934	-1.03497	O	-0.03810	-0.29241	-1.57166
O	-0.81558	0.83812	0.39601	O	-0.88930	0.91221	0.08537
C	-1.82328	1.84926	0.68024	C	-1.54917	1.96568	-0.63060
H	-1.45134	2.82058	0.36205	H	-1.03258	2.91316	-0.47845
H	-2.73757	1.58021	0.15326	H	-1.60841	1.73907	-1.69665
H	-1.95698	1.80967	1.75592	H	-2.55267	2.02376	-0.21334
C	-0.47264	0.62002	-0.80771	C	0.33265	0.47717	-0.45405
H	-2.68546	-1.04252	-0.06514	H	-1.77161	-0.68519	-0.66278
O	-0.95250	1.39125	-1.71073	O	1.10415	1.53660	-0.94076
H	-0.64589	1.16234	-2.60666	H	1.47262	2.03352	-0.19759
H	-3.18071	-0.30013	-1.31460	H	0.74295	-0.67126	-1.99564
O	-2.67461	-1.11703	1.77897	O	-2.62947	-1.18061	-0.62938
H	-3.17755	-0.36843	2.12131	H	-2.86326	-1.33355	0.30601
H	-1.75683	-0.90304	1.98647	H	-2.52666	-2.04286	-1.07508
C	0.53604	-0.44763	-1.05516	C	1.03730	-0.35457	0.62317
C	0.53305	-0.93907	-2.49813	H	0.31509	-1.13028	0.89769
C	1.90927	0.11823	-0.64532	C	1.36010	0.48211	1.86070
H	2.17385	0.96924	-1.27643	H	1.75238	-0.16868	2.64437
H	1.91588	0.42975	0.39936	H	2.13269	1.22788	1.64766
H	2.65519	-0.66466	-0.78494	H	0.47942	0.99311	2.25151
H	0.26548	-1.25628	-0.37234	C	2.30308	-1.01403	0.07900
H	-0.45835	-1.26942	-2.81189	H	2.77336	-1.60250	0.86893
H	1.21854	-1.78320	-2.57571	H	2.09979	-1.69072	-0.75407
H	0.89241	-0.16490	-3.18351	H	3.02160	-0.25940	-0.25113

Group Pr2CH

Reactant				Transition State			
O	-2.50977	-0.39013	-1.73801	O	0.53335	-0.02341	-1.49878
O	-0.98507	0.55501	0.74066	O	2.05275	-0.40734	0.07176
C	-1.95716	1.59659	1.04238	C	2.90116	-1.40693	0.64262
H	-1.43208	2.54175	1.16221	H	2.40112	-1.94679	1.44616
H	-2.68040	1.64301	0.23022	H	3.23843	-2.11062	-0.11913
H	-2.41977	1.27910	1.97068	H	3.75772	-0.86878	1.04582
C	-0.30535	0.62121	-0.32983	C	0.73320	-0.74739	-0.30360
H	-2.81719	-0.71845	-0.87336	H	2.15400	0.96926	-1.29940
O	-0.46337	1.65748	-1.06808	O	0.69778	-2.11910	-0.54597
H	0.08454	1.63200	-1.87279	H	-0.21831	-2.42564	-0.53587
H	-2.87007	0.50060	-1.80788	H	0.86665	-0.56652	-2.22865
O	-3.21505	-1.44234	0.78566	O	2.74829	1.69538	-1.63464
H	-3.72956	-0.80934	1.30039	H	3.28720	2.03502	-0.89596
H	-2.34362	-1.43592	1.20092	H	2.20384	2.42298	-1.98855

C	0.68825	-0.45187	-0.60292	C	-0.29752	-0.25757	0.72590
C	1.99361	-0.08303	0.14762	C	-1.71884	-0.77492	0.44909
C	2.51913	1.32688	-0.11461	C	-2.31035	-0.54369	-0.94313
H	2.55531	1.50595	-1.19510	H	-2.20328	0.51152	-1.21314
H	1.83268	2.06916	0.30671	H	-1.76036	-1.11458	-1.69616
C	0.14433	-1.82555	-0.18531	C	0.14200	-0.61552	2.15259
H	-0.01772	-1.83166	0.89792	H	0.22410	-1.70575	2.24560
H	-0.82793	-1.98187	-0.66144	H	1.13935	-0.20362	2.33183
H	0.88192	-0.43056	-1.68053	H	-0.29641	0.83467	0.62712
H	2.74497	-0.80958	-0.16938	C	-0.78954	-0.08925	3.24515
C	1.07759	-2.97111	-0.57124	H	-0.99912	0.97069	3.06104
H	2.02004	-2.88866	-0.02414	H	-1.74919	-0.61087	3.21017
H	1.31882	-2.89655	-1.63683	H	-1.76585	-1.84615	0.69328
H	1.82590	-0.23028	1.21976	H	-2.37929	-0.28631	1.17031
C	3.90406	1.52214	0.49338	C	-3.78267	-0.94416	-0.98108
H	4.62184	0.82359	0.05586	H	-4.36677	-0.35255	-0.27079
H	4.27121	2.53612	0.32332	H	-4.21069	-0.79627	-1.97503
H	3.88087	1.34820	1.57250	H	-3.90518	-1.99846	-0.71674
C	0.43764	-4.32446	-0.27682	C	-0.17585	-0.26213	4.63167
H	-0.48836	-4.44957	-0.84417	H	-0.85032	0.09257	5.41417
H	1.10842	-5.14518	-0.53911	H	0.04296	-1.31536	4.82953
H	0.19465	-4.41501	0.78547	H	0.76145	0.29450	4.71610

Group PrEtCH

Reactant				Transition State			
O	-2.66714	0.91702	1.16399	O	-0.16893	-1.39607	0.06077
O	-0.92314	-1.39276	-0.19312	O	0.33666	0.77510	0.11631
C	-1.67598	-2.25325	0.71180	C	1.17643	1.77576	-0.46340
H	-0.97998	-2.93267	1.19931	H	2.10907	1.88992	0.09100
H	-2.20085	-1.63336	1.43470	H	1.39537	1.54617	-1.50655
H	-2.36588	-2.78703	0.06698	H	0.60759	2.70282	-0.40705
C	-0.04374	-0.59999	0.26747	C	0.86894	-0.50648	0.40428
H	-2.95601	0.47309	0.34635	H	-1.46250	0.08180	0.01047
O	0.15371	-0.61191	1.53296	O	1.96993	-0.70217	-0.42650
H	0.85083	0.00623	1.81772	H	2.59411	-1.31099	-0.01393
H	-3.14044	0.46497	1.87024	H	-0.15955	-1.49281	-0.90320
O	-3.42736	-0.27831	-1.28319	O	-2.39336	0.43113	-0.02177
H	-2.55198	-0.45262	-1.65029	H	-2.41318	1.30030	0.42055
H	-3.79527	-1.15494	-1.11934	H	-2.99262	-0.17827	0.44759
C	0.66212	0.28511	-0.70289	C	1.13227	-0.65626	1.90842
C	-0.11570	1.62481	-0.81426	C	1.36538	-2.10946	2.35819
H	0.23795	2.08988	-1.73715	H	0.48142	-2.70913	2.13250
H	-1.17676	1.40343	-0.95625	H	1.44827	-2.07397	3.44810
C	2.14401	0.46303	-0.36499	C	2.24686	0.29248	2.39076
H	2.54412	1.18535	-1.08326	H	2.99050	0.44576	1.60101
H	2.27073	0.92173	0.62262	H	2.78374	-0.19495	3.21141
C	0.08492	2.58461	0.35485	C	2.60736	-2.80174	1.79419
H	-0.57080	3.44916	0.23472	H	2.82246	-3.71137	2.35803

H	-0.15326	2.12073	1.31543	H	2.46915	-3.10849	0.75313
H	1.11336	2.94776	0.39686	H	3.49385	-2.16214	1.85760
C	2.93780	-0.83905	-0.43887	C	1.73911	1.64577	2.89331
H	2.52618	-1.56435	0.27243	H	1.09430	2.11167	2.14334
H	2.81790	-1.27284	-1.43640	H	1.11357	1.47660	3.77618
H	0.56660	-0.22989	-1.66159	H	0.19102	-0.33753	2.37049
C	4.41629	-0.61450	-0.14132	C	2.88615	2.58811	3.24196
H	4.97935	-1.54800	-0.20051	H	3.49073	2.80524	2.35642
H	4.85201	0.08866	-0.85611	H	2.51913	3.53716	3.63909
H	4.55242	-0.20100	0.86151	H	3.54403	2.14095	3.99269

Group PrMeCH

Reactant				Transition State			
O	-2.75819	0.38971	0.95359	O	-0.22544	-1.50842	0.23364
O	-0.59080	-1.53880	0.41352	O	0.14635	0.57219	-0.38513
C	-0.91998	-2.44966	1.50041	C	0.86401	1.80374	-0.48255
H	-0.02537	-2.63386	2.09115	H	0.74557	2.39259	0.42833
H	-1.70914	-1.99862	2.10014	H	1.92150	1.62335	-0.68004
H	-1.26144	-3.35320	1.00661	H	0.42880	2.34439	-1.32132
C	-0.17771	-0.36921	0.67870	C	0.76675	-0.50825	0.26695
H	-3.03444	-0.40324	0.45826	H	-1.62317	-0.19521	0.03657
O	0.03998	-0.07608	1.90857	O	1.85565	-0.88369	-0.52522
H	0.35966	0.83771	2.01694	H	2.44542	-1.44944	-0.00933
H	-2.80003	0.12763	1.87988	H	-0.24976	-1.86155	-0.66799
O	-3.40690	-1.89104	-0.59205	O	-2.58951	0.00807	0.15607
H	-2.58239	-1.99570	-1.08288	H	-2.69841	0.96953	0.28340
H	-3.44909	-2.67095	-0.02584	H	-2.90411	-0.45004	0.95862
C	0.13293	0.55752	-0.44210	C	1.13255	-0.28348	1.74427
C	1.65912	0.49722	-0.65810	C	2.39128	0.56376	1.96350
H	1.94464	1.26197	-1.37912	H	3.17671	0.32550	1.24406
H	2.20083	0.68630	0.27007	H	2.78960	0.36258	2.95912
C	-0.66824	0.21835	-1.70063	C	-0.07239	0.25892	2.52137
H	-0.36518	-0.76841	-2.06625	H	-0.94072	-0.38407	2.34177
H	-1.72932	0.15836	-1.43987	H	-0.32821	1.25523	2.13963
C	-0.48590	1.25737	-2.80478	C	0.16619	0.34591	4.02778
H	-0.71329	2.25082	-2.40389	H	0.50641	-0.62867	4.39516
H	0.55665	1.27752	-3.13283	H	0.96825	1.05919	4.23701
H	-0.13326	1.55750	-0.08235	H	1.34828	-1.29466	2.11000
C	-1.38756	0.96144	-3.99909	C	-1.09551	0.76966	4.77377
H	-1.25256	1.70167	-4.79043	H	-1.90351	0.05041	4.61394
H	-1.16503	-0.02364	-4.41821	H	-0.91859	0.84337	5.84901
H	-2.44022	0.97017	-3.70420	H	-1.44322	1.74568	4.42344
H	1.94575	-0.48209	-1.04692	H	2.18014	1.63274	1.90340

Group sBut

Reactant				Transition State			
O	0.77284	-1.89683	-1.56173	O	-0.72145	-1.29909	0.29686
O	0.05326	0.10052	0.45976	O	0.30069	0.58002	-0.33124

C	0.01674	1.24473	-0.43933	C	1.28707	1.10987	-1.22151
H	0.63990	2.03758	-0.03165	H	2.27974	1.09840	-0.77160
H	0.36875	0.92263	-1.41838	H	1.30161	0.55465	-2.15991
H	-1.02727	1.53754	-0.46867	H	0.98709	2.13900	-1.41182
C	1.15944	-0.48140	0.68726	C	0.53651	-0.65975	0.30039
H	-0.16741	-1.63871	-1.57471	H	-1.64907	0.32073	-0.10088
O	2.21975	0.04413	0.19542	O	1.45115	-1.37389	-0.47138
H	3.02888	-0.45238	0.41916	H	1.77765	-2.12433	0.04260
H	1.21667	-1.24293	-2.11297	H	-0.84242	-1.70124	-0.57619
O	-1.94964	-1.20252	-1.39499	O	-2.51940	0.80227	-0.13057
H	-2.01958	-1.00344	-0.45340	H	-2.36293	1.75718	-0.00658
H	-2.09946	-0.35435	-1.82927	H	-3.08400	0.47748	0.59591
C	1.14707	-1.66451	1.59152	C	0.95424	-0.47329	1.76160
H	0.24028	-2.21669	1.32744	H	0.08466	-0.01260	2.24429
C	1.01019	-1.12841	3.03016	C	2.14939	0.46977	1.87897
H	1.90206	-0.56321	3.30956	H	2.43744	0.58160	2.92525
H	0.90041	-1.97080	3.71218	H	3.01085	0.07250	1.33432
C	2.38166	-2.55152	1.40252	C	1.23005	-1.82427	2.43821
H	3.26764	-2.02106	1.77076	H	2.21251	-2.19280	2.11815
H	2.52651	-2.74274	0.33598	H	0.48688	-2.55671	2.11192
C	2.24622	-3.87972	2.14024	C	1.20093	-1.73512	3.96235
H	1.34223	-4.40561	1.82322	H	1.96423	-1.05398	4.34393
H	3.10371	-4.51823	1.92248	H	0.22658	-1.37924	4.30756
H	2.20080	-3.73948	3.22141	H	1.37860	-2.71534	4.40927
H	0.13359	-0.48782	3.13002	H	1.91966	1.46378	1.49164

Group tBuCH2_2_CH

Reactant				Transition State			
O	-3.19832	-2.94150	0.62304	O	1.07426	0.01253	-1.21897
O	-1.68801	0.26862	-0.47586	O	1.95639	-0.46212	0.83784
C	-2.93752	0.20064	-1.22396	C	3.23664	-1.07748	0.63246
H	-3.51118	1.05214	-0.87424	H	3.21209	-2.12652	0.92489
H	-2.70643	0.28486	-2.28419	H	3.55619	-0.98743	-0.40902
H	-3.43603	-0.73947	-0.99673	H	3.92990	-0.53305	1.27139
C	-0.80678	-0.62896	-0.63903	C	0.93526	-0.80369	-0.06989
H	-3.20310	-2.05315	1.02302	H	2.36854	1.20375	-0.14693
O	-1.07787	-1.58523	-1.45354	O	1.12207	-2.13678	-0.42336
H	-0.34913	-2.22958	-1.52475	H	0.38231	-2.41560	-0.97805
H	-2.68321	-2.84642	-0.18521	H	1.71156	-0.40826	-1.81390
O	-3.32977	-0.45485	1.95704	O	2.89207	2.04624	-0.15029
H	-3.97573	0.12953	1.54269	H	3.12899	2.26335	0.77192
H	-2.49343	0.02073	1.88312	H	2.33139	2.76208	-0.50692
C	0.42816	-0.59189	0.17952	C	-0.42592	-0.49801	0.58001
C	0.94969	0.82863	0.42348	C	-0.69183	-1.42539	1.79519
H	0.11600	1.45314	0.76164	C	-1.62974	-2.65498	1.67910
C	0.05677	-1.32692	1.50979	C	-0.45679	1.00490	0.97168
H	0.03337	-0.57422	2.30405	H	-0.29919	1.08444	2.05244
C	1.66373	1.50075	-0.76409	H	0.38068	1.52753	0.50769

C	1.02118	-2.46420	1.88703	H	-1.16573	-0.69209	-0.20517
H	1.16842	-1.18206	-0.36476	H	-1.11753	-0.80586	2.59107
C	1.97358	2.94374	-0.35464	H	0.27438	-1.77642	2.17634
H	2.58627	2.96770	0.55150	C	-1.70234	1.83235	0.59869
H	2.52020	3.45896	-1.14939	C	-1.60963	-3.34036	3.05232
H	1.05172	3.49906	-0.15838	H	-0.60420	-3.69649	3.29632
C	0.58035	-2.99569	3.25429	H	-1.92580	-2.64880	3.83918
H	-0.44958	-3.36318	3.21462	H	-2.28674	-4.19932	3.06300
H	1.22544	-3.82090	3.56842	C	-3.06949	-2.23670	1.37101
H	0.63550	-2.21060	4.01383	H	-3.14900	-1.77098	0.38487
H	1.65355	0.76499	1.25898	H	-3.71867	-3.11774	1.37279
H	-0.95073	-1.75415	1.45192	H	-3.44772	-1.53500	2.11941
C	2.97974	0.77784	-1.07037	C	-1.20205	-3.68204	0.62808
H	3.62694	0.76126	-0.18827	H	-1.85405	-4.55834	0.69550
H	2.81595	-0.25362	-1.39506	H	-1.30862	-3.28606	-0.38671
H	3.51300	1.29450	-1.87360	H	-0.17229	-4.01374	0.77650
C	0.78666	1.51634	-2.02042	C	-2.97330	1.27007	1.23330
H	0.60104	0.50573	-2.40263	H	-3.81431	1.94835	1.05845
H	-0.17519	2.00194	-1.83102	H	-3.23197	0.30279	0.80349
H	1.29213	2.06682	-2.81875	H	-2.85469	1.14741	2.31472
C	0.92771	-3.59738	0.85977	C	-1.47266	3.25409	1.12367
H	-0.10372	-3.95335	0.77034	H	-2.31434	3.90183	0.86164
H	1.27036	-3.28538	-0.13201	H	-1.36918	3.25552	2.21306
H	1.55332	-4.43879	1.17055	H	-0.56366	3.68768	0.69466
C	2.46085	-1.95274	1.98244	C	-1.87072	1.89256	-0.92259
H	2.82464	-1.57227	1.02285	H	-0.98221	2.32259	-1.39557
H	2.54019	-1.14908	2.72075	H	-2.04005	0.90172	-1.35318
H	3.12624	-2.76438	2.29022	H	-2.72975	2.51833	-1.18296

Group tBuCH2Me2C

Reactant				Transition State			
O	2.40971	-1.16582	-1.62466	O	1.72732	0.40873	-0.88509
O	0.64009	1.01735	-0.29622	O	2.00517	-1.37795	0.51256
C	1.74861	1.55014	0.48264	C	3.11206	-2.10093	-0.04258
H	1.46656	1.55634	1.53412	H	3.77470	-2.31241	0.79482
H	2.62682	0.93038	0.30924	H	2.78008	-3.03525	-0.49376
H	1.89024	2.55695	0.10463	H	3.64736	-1.50082	-0.78319
C	0.23568	-0.16827	-0.08527	C	1.12152	-0.77439	-0.39723
H	2.44094	-0.26059	-1.98592	H	2.92489	0.31778	0.79225
O	0.81782	-0.83601	0.84072	O	0.92865	-1.65409	-1.46167
H	0.45559	-1.73662	0.93026	H	0.31198	-1.25252	-2.08747
H	2.91471	-1.12387	-0.80533	H	2.29861	0.17061	-1.62842
O	2.41401	1.42018	-2.72781	O	3.54299	0.86565	1.34199
H	1.52468	1.75073	-2.55182	H	3.59734	0.46027	2.22902
H	2.99006	1.98659	-2.20065	H	3.15840	1.75928	1.43117
C	-0.92370	-0.67258	-0.88641	C	-0.16565	-0.38304	0.36422
C	-1.01740	-2.20042	-0.80469	C	-0.75152	-1.51903	1.24828
H	-1.86267	-2.51873	-1.41636	H	-1.65689	-1.06680	1.67067

H	-0.11181	-2.65828	-1.21079	C	0.17493	0.75273	1.34863
C	-2.22107	0.05459	-0.40232	H	-0.72346	1.01313	1.91284
H	-3.02291	-0.47641	-0.92623	H	0.51721	1.64837	0.82775
C	-2.61797	0.18613	1.08564	C	-1.15803	-2.94264	0.78582
H	-1.18754	-2.58093	0.20296	H	0.93991	0.44433	2.06574
H	-2.18747	1.06792	-0.81473	H	-0.06815	-1.65516	2.09378
C	-1.72729	1.18509	1.83864	C	0.04506	-3.87962	0.62121
H	-0.73266	0.78751	2.05578	H	0.66425	-3.87893	1.52403
H	-1.61713	2.11897	1.27946	H	-0.30739	-4.90278	0.45593
H	-2.18279	1.42062	2.80469	H	0.66990	-3.59998	-0.22475
C	-2.62422	-1.14799	1.83681	C	-2.01905	-3.50683	1.92895
H	-3.08017	-1.00930	2.82151	H	-1.47173	-3.48738	2.87661
H	-3.20053	-1.90591	1.29837	H	-2.93615	-2.92356	2.05390
H	-1.61096	-1.52600	1.99585	H	-2.29916	-4.54322	1.72009
C	-4.04794	0.74624	1.07374	C	-2.00588	-2.96372	-0.48970
H	-4.73416	0.05236	0.57994	H	-1.42334	-2.69723	-1.37330
H	-4.39982	0.90719	2.09613	H	-2.40412	-3.97139	-0.64558
H	-4.08878	1.70266	0.54387	H	-2.85352	-2.27618	-0.41205
C	-0.70973	-0.27015	-2.35807	C	-1.19747	0.17308	-0.62863
H	0.17181	-0.76029	-2.77333	H	-1.51990	-0.54982	-1.37809
H	-1.58810	-0.59193	-2.92061	H	-2.08665	0.48357	-0.07479
H	-0.60910	0.81053	-2.46457	H	-0.79939	1.05097	-1.14291

Group tBuCH2MeCH

Reactant				Transition State			
O	1.39217	1.49287	-1.17400	O	1.49597	0.79699	-1.44739
O	2.16200	-0.47419	0.85231	O	2.55407	0.00470	0.30860
C	3.58416	-0.47484	0.54012	C	2.77863	-0.85665	1.42313
H	3.91811	-1.50263	0.41571	H	1.93866	-0.82766	2.12145
H	3.73877	0.10739	-0.36714	H	2.95970	-1.88092	1.09190
H	4.05424	-0.00670	1.39817	H	3.67010	-0.47550	1.91787
C	1.33953	-0.94854	0.00813	C	1.51832	-0.31743	-0.59359
H	1.86904	1.87918	-0.41652	H	1.92864	1.89723	0.12963
O	1.81893	-1.48273	-1.05443	O	1.94115	-1.45275	-1.29362
H	1.12512	-1.84005	-1.63835	H	1.19035	-1.82461	-1.77552
H	2.08494	1.19895	-1.77585	H	2.33840	0.80627	-1.92561
O	2.67320	2.57532	1.08917	O	1.66345	2.72153	0.61453
H	3.62881	2.49541	0.98576	H	1.81399	2.58892	1.56989
H	2.45932	1.97456	1.81302	H	0.70896	2.86680	0.46663
C	-0.10632	-0.95749	0.35946	C	0.13103	-0.45657	0.09020
C	-0.28527	-2.22416	1.24195	C	-0.14096	-1.91853	0.49269
H	0.46072	-2.16529	2.04084	H	0.77615	-2.34394	0.90350
C	-1.66481	-2.42667	1.90802	C	-1.27176	-2.19659	1.52059
H	-0.04758	-3.10692	0.63732	H	-0.36038	-2.49852	-0.41256
C	-2.18224	-1.11898	2.50962	C	-1.36716	-1.09393	2.57838
H	-2.42504	-0.38609	1.73477	H	-1.70975	-0.14842	2.14832
H	-3.09198	-1.30821	3.08632	H	-2.08000	-1.38496	3.35558
H	-1.44040	-0.67640	3.18177	H	-0.39763	-0.92160	3.05693

C	-2.70114	-3.00855	0.93870	C	-2.63745	-2.38631	0.84647
H	-2.98104	-2.31009	0.15010	H	-2.99848	-1.48219	0.35544
H	-2.32226	-3.92202	0.47065	H	-2.58819	-3.18260	0.09761
H	-3.61107	-3.26545	1.48915	H	-3.38252	-2.67461	1.59449
C	-1.45098	-3.44732	3.03407	C	-0.91993	-3.51735	2.21958
H	-0.76379	-3.05760	3.79025	H	0.01031	-3.42124	2.78750
H	-2.40168	-3.68085	3.52107	H	-1.71515	-3.81385	2.90969
H	-1.03296	-4.37869	2.63971	H	-0.78899	-4.32005	1.48686
C	-0.98429	-0.90072	-0.89019	H	0.21083	0.15713	0.99338
H	-1.02156	-1.86924	-1.39759	C	-0.99038	0.12148	-0.77346
H	-1.99962	-0.63182	-0.60546	H	-1.11726	-0.45842	-1.69290
H	-0.62099	-0.14339	-1.58661	H	-1.92812	0.09482	-0.22055
H	-0.25710	-0.06905	0.97681	H	-0.79782	1.15973	-1.04221

Group tBuCH2

Reactant				Transition State			
O	-2.24479	-0.61664	-1.74378	O	0.83217	0.50566	-1.16965
O	-0.99122	0.42355	0.72994	O	1.74080	-1.18971	0.06445
C	-1.98608	1.44644	1.01952	C	2.56782	-1.88900	-0.87464
H	-1.47934	2.39466	1.18551	H	2.12931	-2.85400	-1.12762
H	-2.67630	1.50562	0.17909	H	2.72514	-1.30039	-1.78215
H	-2.48235	1.09989	1.91957	H	3.52250	-2.03906	-0.37433
C	-0.26346	0.53695	-0.30530	C	0.53830	-0.67034	-0.42941
H	-2.68582	-0.89253	-0.91934	H	2.48344	0.65243	-0.07418
O	-0.39015	1.60688	-1.00198	O	-0.03656	-1.61901	-1.27563
H	0.18542	1.61414	-1.78730	H	-0.97080	-1.40376	-1.39109
H	-2.61286	0.25198	-1.93962	H	1.04902	0.25575	-2.07876
O	-3.39683	-1.46499	0.68702	O	3.17744	1.28267	0.25060
H	-3.96440	-0.77153	1.04393	H	3.39635	1.06397	1.17643
H	-2.64451	-1.49301	1.29053	H	2.80632	2.18526	0.22279
C	0.72137	-0.52816	-0.59511	C	-0.34448	-0.22872	0.73030
C	2.08297	-0.30917	0.13177	C	-0.63520	-1.21367	1.88185
C	2.95962	-1.50336	-0.25237	C	-1.81801	-0.62272	2.66095
H	3.10408	-1.54996	-1.33504	H	-2.71184	-0.56722	2.03295
H	3.93956	-1.40754	0.22195	H	-2.04811	-1.24391	3.53085
H	2.50716	-2.44200	0.07835	H	-1.58657	0.38657	3.01519
C	2.74472	0.98736	-0.33866	C	-1.02262	-2.60664	1.37735
H	2.86030	0.99625	-1.42637	H	-0.18289	-3.10255	0.88476
H	2.16591	1.86771	-0.04394	H	-1.33449	-3.22674	2.22299
H	3.73653	1.07621	0.11161	H	-1.85472	-2.55538	0.66874
C	1.88894	-0.28076	1.64868	C	0.55445	-1.33195	2.84299
H	1.32282	0.59780	1.96905	H	1.40966	-1.82024	2.37538
H	1.36496	-1.17609	1.99458	H	0.86979	-0.34397	3.19299
H	2.86563	-0.24464	2.13789	H	0.26274	-1.92139	3.71734
H	0.88333	-0.55046	-1.67536	H	-1.29081	0.07760	0.27063
H	0.28108	-1.47145	-0.26800	H	0.11072	0.67531	1.14744

Group tBuMeCH

Reactant				Transition State			
O	-2.50237	-0.38862	-1.73435	O	0.45377	0.41801	-0.99099
O	-0.98435	0.55073	0.76779	O	1.90205	-0.40687	0.47929
C	-1.95105	1.59907	1.06329	C	2.86588	-1.45001	0.63751
H	-1.42018	2.54068	1.18572	H	3.65338	-1.02491	1.25812
H	-2.66846	1.65010	0.24618	H	2.43788	-2.31769	1.13959
H	-2.42134	1.28543	1.98897	H	3.28299	-1.74755	-0.32503
C	-0.29547	0.61266	-0.29682	C	0.65619	-0.68178	-0.13262
H	-2.81164	-0.71068	-0.86773	H	2.00651	1.35284	-0.30976
O	-0.45083	1.64838	-1.03748	O	0.80263	-1.86019	-0.86467
H	0.08863	1.61682	-1.84721	H	-0.03417	-2.07400	-1.29561
H	-2.84219	0.51043	-1.79995	H	0.91635	0.23031	-1.82173
O	-3.27220	-1.40385	0.77894	O	2.65534	2.10952	-0.30712
H	-3.81319	-0.75281	1.24136	H	3.15026	2.08650	0.53304
H	-2.43331	-1.40194	1.25610	H	2.17692	2.95750	-0.36250
C	0.68555	-0.47294	-0.57722	C	-0.45563	-0.69763	0.93451
C	2.06485	-0.12341	0.10369	C	-1.90575	-1.05231	0.46034
C	3.12265	-1.04772	-0.50728	C	-2.87772	-0.46272	1.49614
H	3.19052	-0.90133	-1.58868	H	-2.79769	0.62766	1.52385
H	4.09622	-0.81439	-0.06868	H	-3.90567	-0.72115	1.22716
H	2.91148	-2.10009	-0.30952	H	-2.69124	-0.84598	2.50156
C	2.45769	1.32779	-0.19508	C	-2.28073	-0.43115	-0.89299
H	2.41711	1.53778	-1.26876	H	-1.71581	-0.84678	-1.73148
H	1.81369	2.04328	0.32521	H	-3.33926	-0.62860	-1.08468
H	3.48128	1.50048	0.14458	H	-2.13158	0.65040	-0.88957
C	2.01307	-0.33156	1.61860	C	-2.15698	-2.56807	0.39557
H	1.22917	0.26981	2.08647	H	-1.47542	-3.09261	-0.27957
H	1.84922	-1.37967	1.87683	H	-2.07046	-3.03190	1.38035
H	2.97026	-0.02642	2.04941	H	-3.17386	-2.74454	0.03449
C	0.10573	-1.82796	-0.16635	C	-0.01055	-1.58031	2.10644
H	-0.13659	-1.85282	0.89668	H	0.21925	-2.59479	1.77162
H	-0.80070	-2.04027	-0.73415	H	0.87641	-1.17083	2.59048
H	0.83005	-2.61436	-0.37482	H	-0.79585	-1.64968	2.85901
H	0.85398	-0.44873	-1.65870	H	-0.48959	0.34205	1.28063

Group tBu

Reactant				Transition State			
O	-1.25614	-1.51527	-0.66240	O	-0.35447	-1.35353	0.20203
O	0.51557	0.52946	0.58057	O	0.22219	0.71886	-0.23029
C	0.60611	1.36288	-0.60924	C	1.06916	1.86087	-0.36444
H	1.65461	1.53736	-0.84030	H	1.01733	2.48692	0.52782
H	0.09635	0.85463	-1.42580	H	2.09976	1.56263	-0.55737
H	0.10156	2.28387	-0.33743	H	0.69186	2.42091	-1.21891
C	1.01461	-0.63814	0.57274	C	0.72168	-0.45898	0.35985
H	-1.70071	-0.70982	-0.34007	H	-1.63419	0.05255	0.04272
O	1.66274	-0.99318	-0.47438	O	1.80702	-0.86474	-0.42097
H	2.01435	-1.89916	-0.41591	H	2.32904	-1.52377	0.05482
H	-0.91514	-1.28065	-1.53267	H	-0.37288	-1.61964	-0.72908

O	-2.46218	0.78624	0.44321	O	-2.59526	0.29200	0.13743
H	-1.83532	0.96813	1.15440	H	-2.67934	1.25375	0.27846
H	-2.36190	1.53113	-0.16140	H	-2.95097	-0.17210	0.91882
C	0.91589	-1.45586	1.82628	C	1.03577	-0.35856	1.87728
C	1.03358	-2.95132	1.52188	C	1.15123	-1.77469	2.46253
H	2.01858	-3.21596	1.12615	H	1.47356	-1.69850	3.50337
H	0.91035	-3.49406	2.46011	H	0.19668	-2.30053	2.43666
H	0.25957	-3.28020	0.82625	H	1.89308	-2.38065	1.93265
C	-0.40094	-1.14942	2.54572	C	-0.10845	0.38091	2.57734
H	-0.42329	-1.73184	3.46832	H	0.07838	0.38987	3.65391
H	-0.47798	-0.09240	2.80497	H	-0.18524	1.41644	2.23719
H	-1.25799	-1.43354	1.93225	H	-1.06737	-0.11549	2.40595
C	2.11272	-0.99754	2.69067	C	2.36104	0.37087	2.13899
H	2.09267	-1.57719	3.61544	H	2.54254	0.36728	3.21648
H	3.06088	-1.18261	2.18169	H	3.20340	-0.13406	1.66004
H	2.03452	0.06294	2.93608	H	2.34815	1.40978	1.81278