Intramolecular hydrogen migration in Alkylperoxy and Hydroperoxyalkylperoxy radicals: Accurate treatment of hindered rotors

Supporting Information

Contents

1 Geometries of ROO Radicals

This section contain the structure of ROO species in cartesian coordinates.

	Cartesian Coordinates (Å)		
H	-1.874325	0.579357	-0.000356
C	-1.096560	-0.183311	-0.000002
O	0.157655	0.543638	0.000001
O	1.186324	-0.278601	0.000001
H	-1.149233	-0.799619	0.897630
H	-1.148914	-0.800162	-0.897275

Table 1: CH_3OO

	Cartesian Coordinates (Å)		
C	1.746322	-0.182743	-0.000175
C	0.415263	0.538551	0.000172
O	-0.634572	-0.479904	0.000307
O	-1.835405	0.059406	-0.000269
H	0.265547	1.152499	0.890547
H	0.265151	1.152802	-0.889908
H	2.559611	0.546952	-0.001103
H	1.850552	-0.811086	0.886663
H	1.849441	-0.812035	-0.886486

Table 2: CH_3CH_2OO

Cartesian Coordinates (Å)			
C	1.081626	0.537047	-0.000203
C	-0.128117	-0.379440	0.000061
O	-1.322954	0.460610	0.000300
O	-2.425697	-0.259255	-0.000193
H	-0.176561	-1.010791	-0.890620
H	-0.176165	-1.010746	0.890802
C	2.392640	-0.255949	0.000045
H	1.034079	1.186909	-0.879241
H	1.034056	1.187399	0.878474
H	3.251966	0.417839	-0.000620
H	2.472673	-0.895093	0.884124
H	2.472278	-0.896311	-0.883191

Table 3: $CH_3CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	-1.573431	-0.831450	0.025099
C	-0.372728	0.022005	-0.341947
O	0.778893	-0.625722	0.322510
O	1.928954	-0.161144	-0.116687
H	-0.155334	-0.036036	-1.411278
C	-0.458262	1.470105	0.110097
H	-2.468815	-0.443071	-0.465786
H	-1.427702	-1.866010	-0.291458
H	-1.740967	-0.818514	1.104944
H	-1.270663	1.979248	-0.414785
H	-0.648954	1.528621	1.184958
H	0.476191	1.986728	-0.112677

Table 4: $(CH_3)_2CHOO$

Cartesian Coordinates (Å)			
C	-0.497722	-0.364651	0.000142
C	0.790283	0.437465	0.000167
O	1.903651	-0.508787	0.000439
O	3.067540	0.107356	-0.000551
H	0.897446	1.061171	-0.890610
H	0.897238	1.061415	0.890809
C	-1.738913	0.537500	0.000194
H	-0.511269	-1.017190	-0.879303
H	-0.511273	-1.017264	0.879530
C	-3.047765	-0.256814	-0.000333
H	-1.710841	1.194768	0.877093
H	-1.710503	1.195375	-0.876240
H	-3.914302	0.409125	-0.000275
H	-3.120489	-0.898173	-0.883673
H	-3.120839	-0.898772	0.882543

Table 5: $CH_3CH_2CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	-2.074674	-0.933822	0.041894
C	-0.917116	0.000685	-0.337118
C	0.389933	-0.569191	0.198569
O	1.490660	0.236498	-0.325817
O	2.653772	-0.156083	0.150405
H	0.447978	-0.524892	1.289623
H	0.562145	-1.596181	-0.132117
C	-1.155557	1.431977	0.160975
H	-0.835329	0.020888	-1.430610
H	-3.018828	-0.554315	-0.356166
H	-1.926600	-1.942795	-0.353076
H	-2.180771	-1.009306	1.129077
H	-2.069133	1.845923	-0.273654
H	-1.265124	1.451068	1.250616
H	-0.325311	2.088395	-0.106324

Table 6: $(CH_3)_2CHCH_2OO$

Cartesian Coordinates (Å)			
C	-1.469968	-1.263783	-0.081443
C	-0.261426	-0.491416	0.422332
C	0.972674	-0.593002	-0.468466
C	2.208492	0.106673	0.103271
H	-1.753907	-0.913951	-1.075364
H	-2.320082	-1.133737	0.591504
H	-1.234316	-2.329241	-0.137997
H	-0.018868	-0.773515	1.450619
O	-0.635786	0.933179	0.606884
H	1.180247	-1.657454	-0.621846
H	0.715083	-0.176011	-1.446245
H	2.021999	1.171830	0.254918
H	2.499772	-0.323966	1.066172
H	3.058499	0.008294	-0.576005
O	-0.970097	1.513935	-0.526874

Table 7: $CH_3CH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	1.524166	-0.000868	-0.945000
C	0.369140	0.000231	0.048702
C	0.316544	1.270166	0.891018
O	-0.833784	-0.001467	-0.851336
O	-1.972202	-0.000081	-0.196345
C	0.316946	-1.268116	0.893946
H	2.475883	-0.001319	-0.408566
H	1.486657	-0.887379	-1.581766
H	1.487857	0.885248	-1.582451
H	1.182247	1.312284	1.556580
H	0.326550	2.157332	0.253637
H	-0.590870	1.283354	1.495801
H	1.183314	-1.309887	1.558657
H	-0.589861	-1.279534	1.499675
H	0.325332	-2.156188	0.257885

Table 8: $(CH_3)_3COO$

Cartesian Coordinates (Å)			
C	-0.158613	0.464485	-0.000078
C	-1.389910	-0.422164	0.000187
O	-2.564240	0.447443	0.000678
O	-3.684272	-0.245139	-0.000649
H	-1.455288	-1.051674	-0.890529
H	-1.454666	-1.051858	0.890835
C	1.139091	-0.353541	0.000197
H	-0.189267	1.116009	-0.879730
H	-0.189302	1.116526	0.879192
C	2.399972	0.518642	-0.000309
H	1.156483	-1.011988	0.877774
H	1.156356	-1.012811	-0.876765
C	3.694783	-0.298216	0.000002
H	2.381662	1.176728	-0.876967
H	2.381776	1.177571	0.875718
H	4.574177	0.350976	-0.000506
H	3.757234	-0.941051	0.883468
H	3.756990	-0.942105	-0.882713

Table 9: $CH_3CH_2CH_2CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	2.651975	-0.952068	-0.000614
C	1.505479	0.009913	0.338666
C	0.171617	-0.546828	-0.196298
C	-1.044134	0.253357	0.236855
O	-2.227776	-0.473758	-0.220162
O	-3.337667	0.178390	0.056617
H	-1.120001	0.339406	1.324103
H	-1.093936	1.248108	-0.207860
H	0.043303	-1.575739	0.155771
H	0.203842	-0.588975	-1.291090
C	1.806268	1.421288	-0.187853
H	1.428778	0.065815	1.432962
H	3.599688	-0.594068	0.410696
H	2.467020	-1.951607	0.402697
H	2.774410	-1.046473	-1.084783
H	2.769002	1.778180	0.188013
H	1.855307	1.425734	-1.282158
H	1.048897	2.148594	0.115476

Table 10: $(CH_3)_2CHCH_2CH_2OO$

Cartesian Coordinates (Å)			
C	1.870580	1.123174	-0.000162
C	0.808803	0.007571	0.000003
C	-0.561242	0.691483	-0.000175
O	-1.607600	-0.328900	-0.000012
O	-2.810052	0.207587	0.000003
H	-0.715083	1.304153	0.891653
H	-0.715017	1.303801	-0.892258
C	0.964275	-0.859023	1.263623
C	0.964373	-0.859488	-1.263286
H	2.873873	0.688652	-0.000065
H	1.783517	1.759642	-0.885986
H	1.783477	1.759948	0.885439
H	1.948358	-1.335529	1.279818
H	0.870096	-0.253650	2.170501
H	0.206220	-1.643942	1.302083
H	1.948432	-1.336051	-1.279198
H	0.206280	-1.644382	-1.301543
H	0.870326	-0.254439	-2.170393

Table 11: $(CH_3)_3CCH_2OO$

Cartesian Coordinates (Å)			
C	-1.952588	-1.271371	-0.225801
C	-0.831648	-0.491198	0.442347
O	-1.240334	0.930343	0.573217
O	-1.416926	1.510633	-0.595606
C	0.514832	-0.582595	-0.267244
C	1.664615	0.111048	0.472278
H	-2.096577	-0.922386	-1.249641
H	-2.889407	-1.147180	0.321452
H	-1.704495	-2.335239	-0.248573
H	-0.734240	-0.773125	1.494355
H	0.747618	-1.645553	-0.400815
H	0.397671	-0.156358	-1.268795
H	1.408750	1.163295	0.628188
H	1.772775	-0.331054	1.470137
C	2.994785	0.011196	-0.278968
H	3.797251	0.511979	0.268669
H	3.292823	-1.031914	-0.425014
H	2.925934	0.477252	-1.266524

Table 12: $CH_3CH_2CH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	0.891035	1.716211	0.087442
C	0.331630	0.367876	0.515520
O	1.427091	-0.631219	0.474417
O	1.911750	-0.794825	-0.739741
C	-0.868535	-0.155076	-0.288576
C	-1.325430	-1.528064	0.225206
H	1.138786	1.708094	-0.975301
H	1.797333	1.941102	0.653772
H	0.167766	2.510640	0.277466
H	0.094609	0.370222	1.584100
C	-2.032134	0.846990	-0.268280
H	-0.520673	-0.267125	-1.321491
H	-0.513618	-2.256436	0.204186
H	-1.692057	-1.459077	1.255189
H	-2.141048	-1.913352	-0.392046
H	-2.888858	0.435714	-0.808089
H	-2.359492	1.053945	0.756615
H	-1.772866	1.797006	-0.739676

Table 13: $(CH_3)_2CHCH(CH_3)OO$

Cartesian Coordinates (Å)			
C	1.487991	-0.660820	0.955096
C	0.284812	-0.411709	0.050850
O	0.629452	0.739978	-0.852322
O	0.891729	1.850946	-0.201887
C	-0.960270	-0.027364	0.863265
C	-2.218054	0.289051	0.049025
H	1.687649	0.218084	1.569179
H	2.377449	-0.881951	0.360662
H	1.291145	-1.511447	1.612228
C	0.061446	-1.548665	-0.939307
H	-1.160882	-0.848687	1.559855
H	-0.689500	0.840077	1.470866
H	-2.026701	1.080210	-0.679209
H	-2.592736	-0.584778	-0.489425
H	-3.016686	0.632567	0.710972
H	0.983803	-1.769258	-1.480536
H	-0.249295	-2.450780	-0.406605
H	-0.709244	-1.294388	-1.667877

Table 14: $CH_3CH_2C(CH_3)_2OO$

Cartesian Coordinates (Å)			
C	1.487991	-0.660820	0.955096
C	0.284812	-0.411709	0.050850
O	0.629452	0.739978	-0.852322
O	0.891729	1.850946	-0.201887
C	-0.960270	-0.027364	0.863265
C	-2.218054	0.289051	0.049025
H	1.687649	0.218084	1.569179
H	2.377449	-0.881951	0.360662
H	1.291145	-1.511447	1.612228
C	0.061446	-1.548665	-0.939307
H	-1.160882	-0.848687	1.559855
H	-0.689500	0.840077	1.470866
H	-2.026701	1.080210	-0.679209
H	-2.592736	-0.584778	-0.489425
H	-3.016686	0.632567	0.710972
H	0.983803	-1.769258	-1.480536
H	-0.249295	-2.450780	-0.406605
H	-0.709244	-1.294388	-1.667877

Table 15: $CH_3CH_2CH_2CH_2CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	-3.258540	-0.954938	-0.012583
C	-2.114067	0.016654	-0.332054
C	-0.774094	-0.552052	0.172866
C	0.466137	0.244537	-0.254885
C	1.747309	-0.432338	0.195861
O	2.865838	0.405653	-0.231171
O	4.025053	-0.112985	0.117206
H	1.812263	-0.527367	1.282545
H	1.888968	-1.415358	-0.259682
H	0.441070	1.254564	0.163268
H	0.484037	0.349892	-1.345011
H	-0.675812	-1.581974	-0.191786
H	-0.807341	-0.618041	1.268583
C	-2.412620	1.410805	0.237409
H	-2.044643	0.105327	-1.424789
H	-4.211168	-0.584721	-0.401482
H	-3.079015	-1.941457	-0.449853
H	-3.370304	-1.084942	1.069351
H	-3.372414	1.783678	-0.130982
H	-2.467394	1.380417	1.331364
H	-1.650126	2.142626	-0.039488

Table 16: $(CH_3)_2CHCH_2CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	1.487991	-0.660820	0.955096
C	0.284812	-0.411709	0.050850
O	0.629452	0.739978	-0.852322
O	0.891729	1.850946	-0.201887
C	-0.960270	-0.027364	0.863265
C	-2.218054	0.289051	0.049025
H	1.687649	0.218084	1.569179
H	2.377449	-0.881951	0.360662
H	1.291145	-1.511447	1.612228
C	0.061446	-1.548665	-0.939307
H	-1.160882	-0.848687	1.559855
H	-0.689500	0.840077	1.470866
H	-2.026701	1.080210	-0.679209
H	-2.592736	-0.584778	-0.489425
H	-3.016686	0.632567	0.710972
H	0.983803	-1.769258	-1.480536
H	-0.249295	-2.450780	-0.406605
H	-0.709244	-1.294388	-1.667877

Table 17: $(CH_3)_2CH(CH_2)_4OO$

Cartesian Coordinates (Å)			
C	0.914506	1.499309	-0.681102
C	0.345980	0.388852	0.199503
C	0.161785	0.847768	1.641786
O	1.425135	-0.652874	0.335297
O	1.818042	-1.152174	-0.814484
C	-0.885547	-0.313530	-0.425481
C	-1.399745	-1.489015	0.419714
H	1.061950	1.145691	-1.702258
H	1.878154	1.828671	-0.285991
H	0.243056	2.359438	-0.696985
C	-2.028080	0.663751	-0.742063
H	-0.517594	-0.720438	-1.373312
H	-0.594205	-2.173345	0.691534
H	-1.883468	-1.146928	1.339241
H	-2.142699	-2.055780	-0.147515
H	1.080108	1.309740	2.010135
H	-0.639256	1.587079	1.704179
H	-0.085596	0.012216	2.297425
H	-2.860655	0.120487	-1.196556
H	-2.411918	1.146151	0.162284
H	-1.726689	1.444602	-1.442825

Table 18: $(CH_3)_2CHC(CH_3)_2OO$

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Cartesian Coordinates (Å)			
C	-1.138819	0.268100	0.094796
O	-0.077567	-0.560324	-0.084251
O	1.147239	0.226159	-0.070421
H	1.420049	0.109688	0.852081
H	-1.085451	1.252303	-0.355421
H	-2.059055	-0.297267	0.171932

Table 19: CH_2OOH

Cartesian Coordinates (Å)			
C	-0.454216	0.469400	0.026568
O	0.502294	-0.494605	-0.141499
O	1.819685	0.110971	-0.016165
H	1.971436	0.014320	0.936039
H	-0.214595	1.438003	-0.402896
C	-1.833956	-0.085420	0.059514
H	-2.541220	0.700899	0.332269
H	-2.147773	-0.494409	-0.913157
H	-1.914641	-0.893628	0.792566

Table 20: $CH_3CH(.)OOH$

Cartesian Coordinates (Å)			
C	-0.090707	-0.242592	-0.140785
O	-1.214038	0.526094	-0.017351
O	-2.387187	-0.337386	0.002447
H	-2.467964	-0.507127	0.953114
H	-0.187822	-1.106079	-0.794767
C	1.174864	0.537835	-0.022782
C	2.401708	-0.374739	0.100083
H	1.300178	1.201617	-0.894052
H	1.103662	1.199651	0.847743
H	3.318105	0.215944	0.168097
H	2.335139	-1.005511	0.989905
H	2.493311	-1.031180	-0.769899

Table 21: $CH_3CH_2CH(.)OOH$

Cartesian Coordinates (Å)			
C	2.075978	-0.967658	0.169760
C	0.994059	-0.006970	-0.344459
C	-0.360269	-0.542276	0.006492
O	-1.398939	0.211067	-0.444302
O	-2.631407	-0.203462	0.234543
H	-2.588119	0.347775	1.030776
H	-0.565888	-1.603017	0.126694
H	1.079285	0.036195	-1.443803
C	1.203710	1.423647	0.185142
H	3.069587	-0.614457	-0.116582
H	2.043512	-1.040743	1.260968
H	1.946156	-1.972842	-0.240541
H	2.173301	1.812662	-0.137667
H	0.426765	2.096207	-0.182477
H	1.177303	1.436922	1.279083

Table 22: $(CH_3)_2CHCH(.)OOH$

Cartesian Coordinates (Å)

Table 23: $(CH_3)_3CCH(.)OOH$

Cartesian Coordinates (Å)			
C	1.496004	-0.551355	-0.097891
C	0.630060	0.604443	0.247348
O	-0.656121	0.566944	-0.387107
O	-1.418981	-0.498193	0.240350
H	-1.353967	-1.191043	-0.431233
H	1.597211	-0.851098	-1.134679
H	2.060693	-1.084496	0.655516
H	1.040411	1.548595	-0.141035
H	0.500080	0.709508	1.328752

Table 24: $HOOCH_2CH_2(.)$

Cartesian Coordinates (Å)			
C	-0.423359	1.495642	-0.110293
C	-0.418010	0.075897	0.340185
O	0.622918	-0.684160	-0.320104
O	1.903039	-0.214624	0.171698
H	2.169003	0.381225	-0.542286
H	-0.536912	1.715971	-1.166491
H	-0.314910	2.318238	0.584263
C	-1.699058	-0.679235	-0.024161
H	-0.238828	0.014606	1.418066
H	-2.557098	-0.221164	0.471770
H	-1.865514	-0.650575	-1.103553
H	-1.620839	-1.721853	0.291095

Table 25: $HOOCH(CH_3)CH_2(.)$

Cartesian Coordinates (Å)			
C	0.285469	-0.432557	1.501349
C	0.400741	0.018945	0.082315
O	-0.704340	-0.539115	-0.705982
O	-1.965166	-0.019655	-0.212049
H	-2.253724	-0.750411	0.351548
H	0.371702	-1.488030	1.734561
H	0.043782	0.257026	2.300134
C	1.609982	-0.622577	-0.611998
C	0.410116	1.541597	-0.046978
H	2.534979	-0.263224	-0.156541
H	1.573762	-1.710074	-0.520436
H	1.613219	-0.362190	-1.672769
H	1.254989	1.965469	0.502512
H	0.493405	1.829900	-1.096856
H	-0.513909	1.959252	0.353966

Table 26: $HOOC(CH_3)_2CH_2(.)$

Cartesian Coordinates (Å)			
C	1.014202	0.268014	0.600229
C	-0.147297	0.984803	0.005690
O	-1.078053	0.116221	-0.670918
O	-1.779327	-0.646871	0.345618
H	-1.301170	-1.486967	0.311980
C	1.942195	-0.531827	-0.248573
H	1.232453	0.399758	1.653877
H	0.160579	1.649067	-0.815547
H	-0.687501	1.577241	0.748673
H	2.346233	-1.396219	0.287264
H	1.443388	-0.888002	-1.154448
H	2.810457	0.064379	-0.573482

Table 27: $CH_3CH(.)CH_2OOH$

Cartesian Coordinates (Å)			
C	-2.281617	-0.104235	0.044901
C	-1.017721	0.519939	-0.438810
C	0.210537	0.540634	0.408332
O	0.667197	-0.804760	0.727926
O	1.108766	-1.449750	-0.497655
H	0.328041	-1.975894	-0.718130
H	-0.998926	1.011017	-1.405884
H	-0.043767	0.878975	1.424842
C	1.342167	1.393710	-0.150297
H	-2.840217	-0.582298	-0.766300
H	-2.083111	-0.853483	0.816644
H	-2.960847	0.641848	0.487877
H	2.201840	1.367221	0.521678
H	1.653304	1.017083	-1.125804
H	1.015783	2.431323	-0.261843

Table 28: $CH_3CH(.)CH(CH_3)OOH$

Cartesian Coordinates (Å)			
C	-2.255343	0.134632	0.126871
C	-0.969543	-0.184035	0.811107
C	0.307506	-0.415689	0.056666
C	1.505349	-0.562405	0.995975
O	0.545748	0.677974	-0.885272
O	0.735005	1.915908	-0.153091
H	-0.151393	2.299112	-0.204785
H	-0.965959	-0.319418	1.887309
C	0.203348	-1.614169	-0.903873
H	-2.829670	0.886746	0.679643
H	-2.087077	0.506101	-0.887515
H	-2.911147	-0.746215	0.044821
H	2.417851	-0.725432	0.418939
H	1.628559	0.341722	1.592373
H	1.359191	-1.411604	1.669050
H	1.117114	-1.695852	-1.497168
H	0.070688	-2.534683	-0.331427
H	-0.642084	-1.501535	-1.584821

Table 29: $CH_3CH(.)C(CH_3)_2OOH$

Cartesian Coordinates (Å)			
C	1.198044	1.413508	-0.222245
C	0.825079	-0.006068	0.063612
C	-0.377067	-0.270213	0.911222
O	-1.582980	0.331771	0.412838
O	-1.969603	-0.393305	-0.784017
H	-1.604782	0.176603	-1.475519
C	1.804620	-1.097580	-0.214873
H	-0.294510	0.202788	1.902939
H	-0.543742	-1.342329	1.054542
H	1.652166	1.522860	-1.213382
H	0.329152	2.073671	-0.164869
H	1.941754	1.790213	0.500326
H	2.308787	-0.948822	-1.176437
H	2.603939	-1.141077	0.544586
H	1.323844	-2.079515	-0.229049

Table 30: $(CH_3)_2C(.)CH_2OOH$

Cartesian Coordinates (Å)			
C	1.906783	-0.360695	-0.994265
C	0.916817	0.226850	-0.042787
C	-0.506886	0.413774	-0.472360
C	-1.059266	1.826273	-0.256413
O	-1.420410	-0.418150	0.287945
O	-1.028060	-1.804768	0.087720
H	-1.780512	-2.121479	-0.430080
C	1.246761	0.246498	1.414636
H	-0.609800	0.143747	-1.531477
H	1.915726	-1.461376	-0.924099
H	1.676802	-0.111269	-2.034464
H	2.926193	-0.022362	-0.779789
H	-2.113106	1.871209	-0.541199
H	-0.970393	2.125374	0.789448
H	-0.499086	2.535582	-0.868854
H	2.248501	0.653651	1.592878
H	0.528810	0.826694	1.997884
H	1.239368	-0.772622	1.831566

Table 31: $(CH_3)_2C(.)CH(CH_3)OOH$

Cartesian Coordinates (Å)			
C	-1.952498	-0.628924	-0.962764
C	-0.987227	0.133372	-0.111622
C	-1.519341	1.264864	0.714128
C	0.391280	-0.407620	0.203669
O	1.337371	0.696491	0.335190
O	1.470897	1.372708	-0.940454
C	0.446420	-1.017842	1.618256
H	0.816404	2.079216	-0.847406
C	0.925710	-1.402894	-0.829358
H	-2.789398	0.006522	-1.267206
H	-1.490502	-1.030954	-1.867947
H	-2.392309	-1.487792	-0.427170
H	1.467305	-1.328218	1.853260
H	0.122567	-0.297177	2.370740
H	-0.205645	-1.893010	1.668594
H	-2.226928	0.915689	1.483992
H	-0.720886	1.804389	1.227415
H	-2.078869	1.977843	0.096041
H	1.939811	-1.695549	-0.550575
H	0.305726	-2.301304	-0.871822
H	0.960518	-0.948980	-1.819668

Table 32: $(CH_3)_2C(.)C(CH_3)_2OOH$

Cartesian Coordinates (Å)			
C	-2.494778	-0.280909	0.013665
C	-1.237685	0.519203	-0.020219
C	0.019695	-0.367449	0.024754
O	1.132101	0.520798	-0.038005
O	2.330315	-0.300715	-0.080817
H	2.731166	-0.064329	0.766821
H	-2.860575	-0.772875	-0.879494
H	-3.013851	-0.471444	0.944457
H	-1.196262	1.213513	0.824278
H	-1.183165	1.116510	-0.937269
H	0.044602	-1.053333	-0.828321
H	0.055360	-0.953771	0.950899

Table 33: $HOOCH_2CH_2CH_2(.)$

Cartesian Coordinates (Å)			
C	-2.050316	-0.898755	-0.263003
C	-0.822230	-0.044984	-0.303609
C	0.260521	-0.642630	0.627496
O	1.496244	0.069852	0.625586
O	2.011554	0.051859	-0.733703
H	2.807412	-0.492522	-0.609990
H	-2.069643	-1.876151	-0.740497
H	-2.906166	-0.620352	0.347998
C	-1.110459	1.420545	0.053587
H	-0.394580	-0.085487	-1.316496
H	0.441368	-1.699536	0.375763
H	-0.047663	-0.579954	1.680182
H	-1.808712	1.866500	-0.664911
H	-1.562190	1.498962	1.052929
H	-0.187315	2.009795	0.053130

Table 34: $HOOCH_2CH(CH_3)CH_2(.)$

Cartesian Coordinates (Å)			
C	-1.885261	-0.154293	1.185169
C	-0.913850	-0.005621	0.052239
C	0.510362	-0.092888	0.663484
O	1.456681	0.059441	-0.394476
O	2.775478	-0.132871	0.183983
H	3.131422	0.762908	0.105634
H	-2.191933	-1.136459	1.526239
H	-2.203102	0.707989	1.760149
C	-1.101859	1.364694	-0.631571
C	-1.106760	-1.146607	-0.968555
H	0.660103	-1.064178	1.145737
H	0.656346	0.699934	1.407753
H	-2.108481	1.445795	-1.049517
H	-0.967750	2.180586	0.085460
H	-0.379369	1.500229	-1.438361
H	-2.107592	-1.100333	-1.405434
H	-0.370435	-1.078191	-1.770730
H	-0.992277	-2.122550	-0.487586

Table 35: $HOOCH_2C(CH_3)_2CH_2(.)$

Cartesian Coordinates (Å)			
C	2.239396	-0.264014	0.097970
C	1.109070	0.533797	-0.450406
C	-0.143163	0.523909	0.440452
O	-0.592582	-0.816074	0.704626
O	-0.992519	-1.427577	-0.558098
H	-1.942761	-1.517947	-0.407985
H	3.262906	-0.029926	-0.165951
H	2.039521	-1.182849	0.633728
H	0.807307	0.150857	-1.438742
H	1.412994	1.574470	-0.613331
C	-1.269023	1.408764	-0.085603
H	0.134896	0.838058	1.453142
H	-2.137603	1.352531	0.575387
H	-0.945107	2.451521	-0.134688
H	-1.569030	1.097759	-1.088259

Table 36: $HOOCH(CH_3)CH_2CH_2(.)$

Cartesian Coordinates (Å)			
C	-2.130505	-0.709933	0.052479
C	-1.034051	-0.105643	0.856872
C	0.141756	0.463226	0.027420
C	1.263412	0.969728	0.937068
O	0.649394	-0.550572	-0.876262
O	1.117959	-1.694925	-0.106971
H	2.067075	-1.638337	-0.279000
H	-3.155281	-0.681021	0.400030
H	-1.892475	-1.327814	-0.803583
H	-0.607371	-0.861907	1.534210
H	-1.419446	0.692397	1.501393
C	-0.317912	1.551066	-0.946101
H	2.094807	1.350363	0.337681
H	0.904963	1.780114	1.576902
H	1.630847	0.167661	1.579223
H	0.519774	1.899437	-1.554158
H	-1.099080	1.172789	-1.606896
H	-0.718832	2.399630	-0.386366

Table 37: $HOOCH(CH_3)_2CH_2CH_2(.)$

Cartesian Coordinates (Å)			
C	-1.923021	0.429062	0.366253
C	-0.597001	0.785931	-0.223734
C	0.539544	-0.118559	0.285396
O	1.728355	0.335529	-0.354799
O	2.799798	-0.562038	0.047597
H	3.349310	0.046152	0.560564
C	-2.762602	-0.673818	-0.182703
H	-2.191708	0.859136	1.326006
H	-0.335325	1.822210	0.014105
H	-0.626327	0.698972	-1.315967
H	0.357306	-1.165598	0.021547
H	0.644303	-0.041848	1.374796
H	-3.811400	-0.566854	0.108224
H	-2.713186	-0.709389	-1.276886
H	-2.439717	-1.666394	0.173956

Table 38: $CH_3CH(.)(CH_2)_2OOH$

Cartesian Coordinates (Å)			
C	3.295272	-0.151709	-0.109829
C	1.930856	0.024314	0.462160
C	0.727429	-0.546484	-0.211936
C	-0.588387	0.102113	0.235425
O	-1.602319	-0.729619	-0.352463
O	-2.892342	-0.298709	0.158993
H	-3.120154	-1.063069	0.705487
H	1.837050	0.339580	1.497554
H	0.647764	-1.629161	-0.012047
H	0.818614	-0.454623	-1.301820
C	-0.736806	1.554123	-0.198776
H	-0.677814	0.024088	1.328007
H	4.027741	0.494402	0.380457
H	3.659094	-1.187660	-0.000638
H	3.313380	0.065613	-1.184320
H	-1.709806	1.942096	0.103915
H	0.044089	2.169414	0.255216
H	-0.652859	1.631808	-1.286320

Table 39: $CH_3CH(.)CH_2CH(CH_3)OOH$

Cartesian Coordinates (Å)			
C	3.161233	-0.236550	-0.003828
C	1.873906	0.511814	0.030666
C	0.636499	-0.396458	-0.047952
C	-0.662855	0.394539	0.029634
O	-1.721146	-0.554342	-0.061301
O	-2.965454	0.197780	-0.068452
H	4.081679	0.254808	-0.293436
H	3.226269	-1.243972	0.390461
H	-3.363888	-0.124960	0.751162
H	1.848584	1.247010	-0.783884
H	1.813338	1.111259	0.956956
H	0.660982	-1.124314	0.769709
H	0.651810	-0.964261	-0.982619
H	-0.741108	1.110014	-0.797266
H	-0.737571	0.946840	0.975820

Table 40: $HOOCH_2CH_2CH_2CH_2(.)$

Cartesian Coordinates (Å)			
C	1.805658	1.461823	0.207139
C	1.589739	0.082531	-0.327134
C	2.796152	-0.833500	0.000852
C	0.286268	-0.550491	0.199333
C	-0.959513	0.201601	-0.252381
O	-2.072776	-0.506177	0.287616
O	-3.273488	0.157240	-0.193204
H	-0.959201	1.235341	0.113453
H	2.394200	2.186460	-0.342817
H	1.545660	1.698646	1.233746
H	-3.628200	0.495184	0.640345
H	1.523736	0.140940	-1.422118
H	0.311954	-0.579933	1.294746
H	0.212521	-1.586254	-0.145754
H	-1.032871	0.219610	-1.346174
H	3.725459	-0.411496	-0.388918
H	2.907938	-0.953360	1.082324
H	2.659092	-1.825417	-0.440986

Table 41: $HOO(CH_2)_2CH(CH_3)CH_2(.)$

Cartesian Coordinates (Å)			
C	-3.826756	-0.206843	-0.107634
C	-2.495702	0.441730	0.059604
C	-1.240805	-0.364929	0.114313
C	0.037208	0.473832	-0.031088
C	1.297441	-0.377721	0.048518
O	2.399315	0.513710	-0.096046
O	3.605089	-0.298688	-0.099036
H	-2.453620	1.481198	0.370893
H	4.032259	0.027937	0.704392
H	-1.267861	-1.138779	-0.666435
H	-1.193373	-0.926019	1.066189
H	0.071784	1.234579	0.755702
H	0.026369	1.003621	-0.987993
H	1.323273	-1.123792	-0.754204
H	1.365300	-0.900519	1.011806
H	-4.605319	0.519017	-0.355119
H	-3.808728	-0.968454	-0.896802
H	-4.153639	-0.725379	0.809948

Table 42: $CH_3CH(.)(CH_2)_3OOH$

Cartesian Coordinates (Å)			
C	2.224858	-1.285853	-0.247883
C	1.622165	0.004609	0.209096
C	0.251099	0.010922	0.817213
C	-0.869455	-0.008562	-0.237960
O	-2.097428	-0.005196	0.482941
O	-3.169465	-0.095732	-0.497632
H	-3.596169	0.761372	-0.362841
C	2.231167	1.286756	-0.262815
H	0.112165	0.902164	1.439194
H	0.112892	-0.863038	1.462977
H	-0.809752	-0.909351	-0.858217
H	-0.815181	0.872942	-0.888953
H	3.318091	-1.265648	-0.172286
H	1.858928	-2.135392	0.335896
H	1.997046	-1.503780	-1.305580
H	3.324695	1.259217	-0.195158
H	1.997173	1.497983	-1.320615
H	1.876258	2.143723	0.317202

Table 43: $(CH_3)_2C(.)(CH_2)_2OOH$

Cartesian Coordinates (Å)			
C	-2.830460	-1.283214	-0.271794
C	-2.239026	0.001131	0.216188
C	-2.833949	1.289144	-0.257698
C	-0.866914	-0.000592	0.819832
C	0.277951	-0.000043	-0.226301
C	1.649789	-0.002359	0.435567
O	2.609395	-0.010940	-0.617490
O	3.923072	-0.089132	0.003756
H	4.291187	0.762139	-0.269268
H	-0.747009	-0.882767	1.461478
H	-0.746508	0.878827	1.465311
H	0.192724	0.880448	-0.870558
H	0.195395	-0.880406	-0.870358
H	1.785402	-0.892052	1.061484
H	1.791271	0.888650	1.061541
H	-2.550350	-1.502552	-1.316812
H	-2.500623	-2.136948	0.328090
H	-3.925527	-1.254711	-0.250463
H	-2.551254	1.522885	-1.298985
H	-3.928929	1.256050	-0.240631
H	-2.509861	2.136616	0.354269

Table 44: $(CH_3)_2C(.)(CH_2)_3OOH$

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	Cartesian Coordinates (Å)		
C	-0.009141	0.004200	0.013715
H	-0.004399	-0.105370	1.108562
C	1.423642	0.040372	-0.479213
H	2.012529	-0.881927	-0.280995
O	1.917075	0.990169	-1.033404
O	-0.770026	1.113327	-0.397436
O	-0.231995	2.280459	0.274165
H	0.486828	2.509329	-0.338392
H	-0.514359	-0.872552	-0.409647

Table 45: $HOOCH_2CHO$

	Cartesian Coordinates (Å)		
C	-0.035137	-0.006605	0.058167
H	-0.018148	-0.063488	1.157564
C	1.411288	0.033542	-0.412457
H	2.005384	-0.876961	-0.177058
O	1.908023	0.966974	-0.991499
O	-0.755774	1.138779	-0.355954
O	-0.184724	2.295841	0.303166
H	0.544157	2.492687	-0.308520
C	-0.773419	-1.213602	-0.520553
H	-1.791381	-1.242115	-0.131285
H	-0.817283	-1.145966	-1.609481
H	-0.267625	-2.141589	-0.244458

Table 46: $HOOCH(CH_3)CHO$

	Cartesian Coordinates (Å)		
C	-0.004985	0.009838	0.074200
H	0.020923	-0.004310	1.173030
C	1.428071	0.007031	-0.458885
O	1.883270	0.977376	-1.024028
O	-0.769180	1.091525	-0.402476
O	-0.235939	2.299700	0.195666
H	0.518108	2.455873	-0.398779
H	-0.533214	-0.888269	-0.265270
C	2.228712	-1.256337	-0.238454
H	2.092488	-1.642431	0.775737
H	1.879072	-2.031185	-0.929295
H	3.283380	-1.062158	-0.428225

Table 47: $HOOCH_2C(CH_3)O$

	Cartesian Coordinates (Å)		
C	-0.015840	-0.049023	-0.019676
H	0.018823	-0.036883	1.079595
C	1.434366	-0.033030	-0.528882
O	1.856394	0.901709	-1.175196
O	-0.738738	1.078244	-0.481078
O	-0.155177	2.268110	0.101700
H	0.578348	2.408022	-0.521395
C	2.308889	-1.218056	-0.177858
H	2.124392	-1.570285	0.840325
H	2.087764	-2.048347	-0.856380
H	3.355684	-0.941356	-0.297045
C	-0.802797	-1.265156	-0.511078
H	-0.371156	-2.192315	-0.130842
H	-1.832331	-1.191142	-0.158828
H	-0.812904	-1.299182	-1.602686

Table 48: $HOOCH(CH_3)C(CH_3)O$

Cartesian Coordinates (Å)			
C	0.005922	-0.005985	0.003796
H	0.018572	-0.025697	1.097763
C	1.440618	-0.005920	-0.576118
H	1.379592	0.218334	-1.643039
H	2.024123	0.775992	-0.082771
C	2.108536	-1.353063	-0.423919
O	1.836861	-2.302704	-1.122129
O	-0.735262	-1.165399	-0.327253
O	-0.786929	-1.272894	-1.773204
H	-0.037332	-1.880089	-1.917339
H	-0.513510	0.899846	-0.328100
H	2.865311	-1.457323	0.380187

Table 49: $HOOCH_2CH_2CHO$

Cartesian Coordinates (Å)			
C	-0.018942	0.007379	0.006367
C	0.004678	-0.057664	1.559331
H	1.049024	-0.107936	1.875449
H	-0.438467	0.856860	1.961470
C	-0.693733	-1.278778	2.112489
O	-0.228167	-2.393621	2.039447
O	0.286485	-1.252219	-0.584008
O	1.564023	-1.714183	-0.080266
H	1.251604	-2.287925	0.644617
H	0.736132	0.741568	-0.299627
H	-1.676372	-1.126563	2.602867
C	-1.377337	0.380385	-0.577816
H	-1.675406	1.375318	-0.239288
H	-1.322141	0.388112	-1.667578
H	-2.146242	-0.337570	-0.282495

Table 50: $HOOCH(CH_3)CH_2CHO$

Cartesian Coordinates (Å)			
C	-0.057427	0.011022	-0.009808
H	-0.114775	-0.030513	1.082514
C	1.409621	-0.024828	-0.495998
H	1.428051	0.239042	-1.555152
H	1.978821	0.726637	0.057601
C	2.031118	-1.408665	-0.362966
O	1.723941	-2.296451	-1.134511
O	-0.820060	-1.111655	-0.410843
O	-0.788867	-1.184961	-1.859229
H	-0.029072	-1.788788	-1.971378
H	-0.524125	0.941840	-0.351704
C	3.022267	-1.638582	0.752862
H	3.900547	-1.000852	0.607128
H	2.581224	-1.355370	1.714195
H	3.325619	-2.684036	0.775638

Table 51: $HOOCH_2CH_2C(CH_3)O$

Cartesian Coordinates (Å)			
C	-0.025588	-0.011501	-0.038102
C	-0.101218	-0.044225	1.512929
H	0.921341	-0.022210	1.895679
H	-0.612031	0.858878	1.856254
C	-0.753755	-1.300492	2.075151
O	-0.190444	-2.375965	2.000079
O	0.390820	-1.256250	-0.588999
O	1.650818	-1.643018	0.011685
H	1.310263	-2.200141	0.739226
H	0.703262	0.762950	-0.308034
C	-1.359062	0.274007	-0.721173
H	-1.741679	1.250835	-0.416304
H	-1.226330	0.277359	-1.804355
H	-2.100515	-0.489970	-0.475285
C	-2.102457	-1.167727	2.742680
H	-2.818390	-0.697274	2.061459
H	-2.465987	-2.146721	3.051329
H	-2.020227	-0.511379	3.615680

Table 52: $HOOCH(CH_3)CH_2C(CH_3)O$

Cartesian Coordinates (Å)			
C	0.028244	-0.102663	0.030746
H	0.048811	-0.294746	1.106081
C	1.453357	-0.023422	-0.556932
C	2.249833	-1.307801	-0.392250
O	1.836623	-2.385525	-0.031861
O	-0.799920	-1.077255	-0.592930
O	-0.906312	-2.237335	0.265737
H	-0.016852	-2.625293	0.157076
H	-0.463439	0.862936	-0.137299
H	3.323477	-1.202123	-0.661128
C	2.228937	1.104027	0.155056
H	3.245810	1.194511	-0.236307
H	1.727563	2.062186	-0.003507
H	2.293211	0.930131	1.232947
C	1.390503	0.253145	-2.077356
H	0.956331	1.241274	-2.253332
H	2.386086	0.240950	-2.530660
H	0.767209	-0.490613	-2.575990

Table 53: $HOOCH_2C(CH_3)_2CHO$

Cartesian Coordinates (Å)			
C	-1.180939	0.715070	0.388019
H	-1.344127	0.452692	1.439784
H	-1.643548	1.690774	0.195313
C	0.302426	0.735945	0.043531
H	0.772037	1.551903	0.600347
H	0.428051	0.978824	-1.014944
C	1.011436	-0.580843	0.356843
H	0.555833	-1.414487	-0.191208
H	0.903755	-0.850855	1.417408
C	2.487525	-0.574473	0.046804
O	3.094556	0.368198	-0.395548
O	-1.780187	-0.277985	-0.443363
O	-3.163076	-0.412057	-0.024647
H	-3.615766	-0.074962	-0.809994
H	3.010733	-1.533335	0.260583

Table 54: $HOO(CH_2)_3CHO$

Cartesian Coordinates (Å)			
C	-1.035913	0.332385	-0.523783
H	-1.472369	0.324152	-1.531163
C	0.481413	0.160349	-0.657106
H	0.873474	1.013159	-1.218633
H	0.680867	-0.723404	-1.267979
C	1.232615	0.025299	0.668418
H	0.832245	-0.801852	1.267497
H	1.118333	0.914281	1.302701
C	2.714653	-0.205247	0.504315
O	3.292333	-0.265679	-0.551732
O	-1.474148	-0.857307	0.155612
O	-2.926138	-0.873410	0.157476
H	-3.087888	-1.606477	-0.452038
H	3.272845	-0.321194	1.460392
C	-1.484206	1.593984	0.206386
H	-1.097072	1.620621	1.227314
H	-1.135459	2.484165	-0.324930
H	-2.572722	1.627096	0.256613

Table 55: $HOOCH(CH_3)(CH_2)_2CHO$

Cartesian Coordinates (Å)			
C	-1.711807	0.687157	0.406485
H	-1.801898	0.371873	1.452513
H	-2.320019	1.588240	0.259676
C	-0.259814	0.940917	0.024567
H	0.101174	1.800041	0.596284
H	-0.206438	1.233290	-1.027790
C	0.648995	-0.262178	0.273458
H	0.318133	-1.127815	-0.309683
H	0.584184	-0.583328	1.322560
C	2.116538	0.009139	-0.027492
O	2.519116	1.115310	-0.310264
O	-2.184942	-0.358511	-0.442543
O	-3.523480	-0.701336	0.000863
H	-4.041779	-0.392646	-0.755059
C	3.049912	-1.185841	0.043196
H	2.908129	-1.742843	0.973874
H	2.826772	-1.874246	-0.778707
H	4.083239	-0.851425	-0.039397

Table 56: $HOO(CH_3)_3C(CH_3)O$

Cartesian Coordinates (Å)			
C	-1.535841	0.562611	-0.233954
H	-2.110792	1.084514	-1.010235
C	-0.048841	0.655332	-0.594641
H	0.238880	1.710031	-0.594487
H	0.082380	0.305720	-1.621748
C	0.887089	-0.133957	0.322190
H	0.605626	-1.191965	0.348440
H	0.812875	0.209043	1.361784
C	2.352215	-0.024331	-0.078487
O	2.724491	0.719269	-0.958279
O	-1.843603	-0.839899	-0.327420
O	-3.280429	-1.003109	-0.192901
H	-3.507108	-1.259579	-1.097256
C	-1.909114	1.129244	1.131948
H	-1.380119	0.610609	1.934587
H	-1.663609	2.193991	1.180483
H	-2.979805	1.014334	1.302444
C	3.325049	-0.903758	0.686524
H	3.188728	-0.794692	1.766458
H	3.138625	-1.955513	0.445353
H	4.347318	-0.647418	0.411495

Table 57: $HOOCH(CH_3)(CH_2)_2C(CH_3)O$

Cartesian Coordinates (Å)			
C	-0.536856	0.503211	0.045554
H	-0.531454	1.150866	-0.837044
C	0.760129	-0.312103	0.103682
H	0.814301	-0.981432	-0.762293
H	0.749115	-0.953873	0.992823
C	2.014396	0.578592	0.130411
H	1.952391	1.259137	0.990695
H	2.097041	1.182171	-0.776491
C	3.280405	-0.231949	0.281691
O	4.206386	-0.214306	-0.487511
C	-1.772205	-0.387873	-0.000378
H	-1.767708	-1.030433	-0.890478
H	-1.833502	-1.025726	0.889016
H	-0.607578	1.157384	0.920495
O	-2.895910	0.485741	-0.038443
O	-4.083404	-0.351197	-0.001267
H	-4.471839	-0.134291	-0.859737
H	3.307432	-0.884982	1.185022

Table 58: $HOO(CH_2)_4CHO$

Cartesian Coordinates (Å)			
C	0.981808	-0.542918	-0.027241
H	1.015417	-1.135391	-0.948278
C	-0.312939	0.275771	0.026823
H	-0.344819	0.988689	-0.802304
H	-0.336979	0.879878	0.939257
C	-1.563464	-0.600132	-0.024196
H	-1.582264	-1.309319	0.813654
H	-1.562268	-1.226727	-0.926660
C	-2.870049	0.185358	-0.013885
O	-2.889427	1.394875	-0.043633
C	-4.148536	-0.632003	0.038788
H	-4.157172	-1.397643	-0.742600
H	-4.216842	-1.153634	0.999172
H	-5.009344	0.025518	-0.075093
C	2.220084	0.342712	0.032935
H	2.245326	1.048422	-0.807664
H	2.253078	0.913858	0.967542
H	1.019588	-1.251602	0.806784
O	3.344934	-0.530153	-0.031816
O	4.532793	0.292760	0.117351
H	4.928458	0.185355	-0.758374

Table 59: $HOO(CH_2)_4C(CH_3)O$

4 Transition States for intramolecular hydrogen migration in ROO radicals

	Cartesian Coordinates (Å)		
C	-0.123375	0.000003	0.068277
O	-0.064190	0.000006	1.446323
O	1.442028	-0.000011	1.347298
H	1.212525	0.000001	0.100337
H	-0.443944	-0.938010	-0.386075
H	-0.443962	0.938008	-0.386079

Table 60: (1,3p) hydogen migration in CH_3OO

	Cartesian Coordinates (Å)		
O	0.076230	0.023142	-0.017167
O	0.089178	0.039414	1.483028
C	1.477692	0.001881	1.456126
C	2.176459	1.201185	2.021902
H	1.346654	0.029477	0.131669
H	1.885222	-0.992639	1.658039
H	3.251976	1.151488	1.837606
H	1.774705	2.118034	1.586173
H	2.017041	1.247535	3.106107

Table 61: (1,3s) hydogen migration in CH_3CH_2OO

	Cartesian Coordinates (Å)		
C	0.011666	0.008164	0.021027
C	0.029080	-0.005196	1.524011
O	1.281370	-0.010273	2.123375
O	0.989957	1.341670	2.705944
H	-0.109822	1.203758	2.066967
H	-0.706716	-0.620287	2.052184
C	-1.392547	0.184985	-0.562710
H	0.686670	0.796473	-0.325104
H	0.448317	-0.940053	-0.323419
H	-1.364108	0.156055	-1.653753
H	-2.067994	-0.607401	-0.227587
H	-1.826444	1.143244	-0.264819

Table 62: (1,3s) hydogen migration in $CH_3CH_2CH_2OO$

	Cartesian Coordinates (Å)		
C	-0.010022	-0.006542	0.012334
C	0.004483	0.003483	1.520895
O	1.255474	0.001055	2.126042
O	0.977639	1.373683	2.665559
H	-0.124792	1.224839	2.038994
H	-0.733954	-0.605058	2.054496
C	-1.425272	0.236726	-0.524534
H	0.647501	0.806186	-0.316340
C	0.582631	-1.334243	-0.501730
H	-1.426971	0.235152	-1.617083
H	-2.114211	-0.546434	-0.191784
H	-1.821866	1.199015	-0.189894
H	0.637256	-1.324650	-1.593776
H	1.589942	-1.487902	-0.109768
H	-0.037893	-2.184528	-0.201786

Table 63: (1,3s) hydogen migration in $(CH_3)_2CHCH_2OO$

Cartesian Coordinates (Å)			
C	0.009292	0.012862	-0.013855
C	0.001468	-0.003728	1.504183
O	1.232871	-0.052517	2.145172
O	0.960317	1.299566	2.738674
H	-0.116611	1.205295	2.058757
H	-0.763177	-0.607658	2.004332
C	-1.434372	0.207146	-0.507054
C	0.917488	1.139176	-0.537131
C	0.551767	-1.357889	-0.486906
H	-1.469344	0.180583	-1.599286
H	-2.095454	-0.581142	-0.134069
H	-1.838210	1.170340	-0.182308
H	0.570911	-1.392492	-1.580198
H	1.567917	-1.520374	-0.120622
H	-0.076906	-2.180301	-0.133548
H	0.972604	1.102218	-1.628443
H	0.534383	2.121426	-0.248620
H	1.927059	1.041166	-0.135041

Table 64: (1,3s) hydogen migration in $(CH_3)_3CCH_2OO$

Cartesian Coordinates (Å)			
C	0.038746	0.006215	0.010524
C	-0.026995	0.020328	1.516696
O	1.231562	0.058735	2.133272
O	0.967552	1.471017	2.554141
H	-0.145444	1.269396	1.945035
C	-1.022853	-0.857224	2.231858
H	-0.946265	0.167365	-0.433124
H	0.726899	0.773990	-0.345224
H	0.412528	-0.967460	-0.330230
H	-2.031906	-0.718801	1.837326
H	-0.744524	-1.910130	2.098452
H	-1.018277	-0.641074	3.300910

Table 65: (1,3t) hydogen migration in $(CH_3)_2CHOO$

Cartesian Coordinates (Å)			
C	-0.028467	0.021161	-0.018797
C	-0.027818	-0.009306	1.505787
O	1.359082	0.080200	1.858323
O	1.961224	-0.847876	0.972293
H	1.194452	-0.635237	0.076350
H	-0.762374	-0.580665	-0.547734
H	0.192603	0.980402	-0.483310
H	-0.457900	-0.948093	1.870687
H	-0.521336	0.842021	1.982630

Table 66: (1,4p) hydogen migration in CH_3CH_2OO

Cartesian Coordinates (Å)			
C	0.014002	-0.018460	-0.024019
C	0.012852	-0.000205	1.505574
O	1.415264	-0.003505	1.841657
O	1.958332	-0.971237	0.957647
H	1.194043	-0.733067	0.068465
H	-0.755936	-0.592391	-0.533281
H	0.276886	0.920114	-0.511253
H	-0.442003	-0.927903	1.873641
C	-0.618716	1.217262	2.157207
H	-1.686306	1.256207	1.927478
H	-0.504344	1.169791	3.242811
H	-0.146824	2.133132	1.795206

Table 67: (1,4p) hydogen migration in $(CH_3)_2CHOO$

	Cartesian Coordinates (Å)		
C	0.007540	0.001984	-0.019337
C	-0.013550	-0.011242	1.517644
O	1.406752	0.005355	1.845994
O	1.980961	-0.913788	0.927053
H	1.204354	-0.675493	0.049102
H	-0.744117	-0.577020	-0.549901
H	0.255265	0.954495	-0.485512
C	-0.668011	-1.283690	2.058192
C	-0.591850	1.257890	2.133112
H	-1.653068	1.348253	1.888160
H	-0.493587	1.230550	3.221448
H	-0.066645	2.138102	1.758394
H	-1.726206	-1.325228	1.786128
H	-0.166759	-2.164229	1.653873
H	-0.587790	-1.309165	3.146899

Table 68: (1,4p) hydogen migration in $(CH_3)_3COO$

	Cartesian Coordinates (Å)		
C	0.009254	-0.009564	0.019672
C	0.030487	-0.028494	1.550115
O	1.417778	0.036379	1.884473
O	1.990971	-0.917406	1.001746
H	1.201790	-0.673388	0.098440
C	-1.065881	-0.753010	-0.715764
H	0.293018	0.952920	-0.410386
H	-0.414929	-0.960148	1.920533
H	-0.446353	0.832765	2.027623
H	-0.856969	-0.800621	-1.787385
H	-1.179863	-1.772447	-0.336156
H	-2.039233	-0.253631	-0.603497

Table 69: (1,4s) hydogen migration in $CH_3CH_2CH_2OO$

	Cartesian Coordinates (Å)		
C	2.229538	-0.082072	-0.152644
C	0.857215	-0.164051	0.447601
C	-0.341543	0.423371	-0.312252
O	-1.425780	-0.448363	0.047035
O	-0.851995	-1.742910	-0.066296
H	0.254787	-1.374316	0.296724
H	0.807079	0.003486	1.526448
H	-0.151082	0.331133	-1.390237
C	-0.738577	1.842969	0.054136
H	2.948262	-0.681668	0.411598
H	2.233337	-0.420954	-1.192542
H	2.604450	0.951716	-0.145521
H	-1.636168	2.140071	-0.493417
H	-0.941518	1.920303	1.124436
H	0.063257	2.539118	-0.204446

Table 70: (1,4s) hydogen migration in $CH_3CH_2CH(CH_3)OO$

	Cartesian Coordinates (Å)		
C	-2.289284	-0.096889	-0.025197
C	-0.915987	-0.300826	-0.595385
C	0.335032	0.384103	0.005975
O	1.374292	-0.576084	-0.327740
O	0.799474	-1.833236	0.006939
H	-0.332033	-1.489695	-0.300797
H	-0.878494	-0.315054	-1.687300
C	0.255765	0.564640	1.522377
C	0.716609	1.674823	-0.712400
H	-3.015632	-0.745113	-0.521914
H	-2.328708	-0.295142	1.047897
H	-2.631048	0.937269	-0.179019
H	1.661542	2.062038	-0.322428
H	0.830212	1.498001	-1.783422
H	-0.051533	2.437192	-0.559178
H	1.211504	0.944763	1.888907
H	-0.526318	1.275479	1.801136
H	0.057562	-0.390280	2.010299

Table 71: (1,4s) hydogen migration in $CH_3CH_2C(CH_3)_2OO$

Cartesian Coordinates (Å)			
C	0.046650	0.000593	0.006185
C	-0.014031	0.001176	1.510371
C	1.329080	0.036436	2.264973
O	1.068094	0.840957	3.413906
O	0.368634	1.947521	2.861403
H	-0.191035	1.250784	1.995753
C	-1.074175	-0.866068	2.145634
H	2.102009	0.497324	1.639335
H	1.669188	-0.936688	2.633879
H	-0.940952	0.170165	-0.431390
H	0.730449	0.765736	-0.370589
H	0.400110	-0.970527	-0.370626
H	-2.067002	-0.642799	1.746617
H	-0.871721	-1.928054	1.943912
H	-1.091380	-0.729193	3.228852

Table 72: (1,4t) hydogen migration in $(CH_3)_2CHCH_2OO$

Cartesian Coordinates (Å)			
C	0.070254	-0.068671	-0.024344
C	0.007668	-0.025983	1.480600
C	1.344100	0.011682	2.186023
C	-1.080836	0.838420	2.174215
O	-1.379157	0.068261	3.356106
O	-1.514791	-1.257810	2.856243
H	-0.641717	-1.091428	1.985475
C	-2.333889	1.113021	1.353132
H	-0.660628	1.776318	2.557401
H	0.783000	-0.827445	-0.358564
H	-0.897838	-0.284151	-0.479157
H	0.417250	0.894150	-0.427769
H	1.992185	-0.805614	1.859245
H	1.867053	0.953048	1.962288
H	1.216428	-0.050790	3.268305
H	-3.052379	1.658627	1.968064
H	-2.108849	1.719007	0.471571
H	-2.796908	0.178284	1.033974

Table 73: (1,4t) hydogen migration in $(CH_3)_2CHCH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-0.025500	-0.027278	0.023339
C	-0.018357	0.055655	1.528183
C	1.421764	-0.023104	2.091346
O	2.044253	-1.194861	1.583922
O	2.262087	-0.988368	0.203085
H	1.204192	-0.688375	-0.146233
H	-0.461650	0.997939	1.877246
H	-0.596574	-0.764407	1.959636
H	2.008837	0.857126	1.810002
H	1.421591	-0.141022	3.177133
H	-0.769072	-0.670740	-0.439512
H	0.161823	0.896623	-0.520891

Table 74: (1,5p) hydogen migration in $CH_3CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	-0.004434	0.002755	-0.028891
C	-0.006173	0.000315	1.477429
C	1.431465	-0.007683	2.069434
O	2.137193	-1.095693	1.466691
O	2.350233	-0.777916	0.108361
H	1.276953	-0.537244	-0.230814
H	-0.517723	0.888836	1.870838
H	-0.527331	-0.881067	1.860104
H	1.945700	0.921514	1.798715
C	1.469221	-0.240176	3.570274
H	-0.686219	-0.678708	-0.530930
H	0.096429	0.968614	-0.520497
H	2.499461	-0.238345	3.930254
H	0.918593	0.548667	4.088049
H	1.015579	-1.201986	3.821487

Table 75: (1,5p) hydogen migration in $CH_3CH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-0.031123	-0.049116	-0.031714
C	0.001628	0.022250	1.472098
C	1.451657	0.040014	2.062871
O	2.134399	-1.089901	1.473977
O	2.309803	-0.874113	0.090017
H	1.236222	-0.626754	-0.231795
H	-0.509547	0.924788	1.832617
H	-0.512442	-0.841740	1.898707
C	2.188492	1.348686	1.775678
C	1.436510	-0.285635	3.553945
H	-0.730515	-0.751216	-0.478169
H	0.060510	0.886483	-0.579446
H	2.451297	-0.273940	3.956570
H	0.839325	0.451659	4.095581
H	1.007963	-1.275349	3.724840
H	3.211739	1.285249	2.152286
H	2.236677	1.556131	0.707669
H	1.685114	2.180778	2.274911

Table 76: (1,5p) hydogen migration in $CH_3CH_2C(CH_3)_2OO$

Cartesian Coordinates (Å)			
C	0.033520	-0.014989	-0.012302
C	0.013720	0.003038	1.497727
C	1.463649	-0.027910	2.052094
O	2.163514	-1.126864	1.490212
O	2.375824	-0.835738	0.123123
H	1.303787	-0.582634	-0.211609
C	-0.737421	1.220958	2.069498
H	-0.469704	-0.912108	1.853418
H	1.991625	0.904992	1.823498
H	1.468821	-0.203874	3.130626
H	-0.662224	-0.682256	-0.515339
H	0.159212	0.948479	-0.506037
H	-1.775785	1.231325	1.731699
H	-0.738606	1.202174	3.163509
H	-0.269474	2.155470	1.746195

Table 77: (1,5p) hydogen migration in $(CH_3)_2CHCH_2OO$

Cartesian Coordinates (Å)			
C	0.038700	0.001012	-0.001073
C	-0.004810	-0.007434	1.514639
C	1.464350	0.001593	2.044914
O	2.186290	-1.089355	1.496707
O	2.382465	-0.816535	0.122348
H	1.303692	-0.568311	-0.203014
C	-0.703350	1.261729	2.050885
C	-0.716182	-1.272726	2.024511
H	1.965709	0.940950	1.788255
H	1.488961	-0.151543	3.127109
H	-0.661103	-0.648009	-0.523235
H	0.184150	0.969739	-0.477746
H	-1.742765	1.299442	1.715927
H	-0.701885	1.271273	3.145576
H	-0.202947	2.169041	1.701488
H	-1.744593	-1.312991	1.655113
H	-0.194558	-2.171461	1.689694
H	-0.751101	-1.289169	3.117873

Table 78: (1,5p) hydogen migration in $(CH_3)_3CCH_2OO$

Cartesian Coordinates (Å)			
C	0.029814	-0.017704	0.007465
C	0.030203	-0.016575	1.522114
C	1.463970	0.007308	2.093640
O	2.197378	-1.071807	1.527684
O	2.397805	-0.765946	0.161528
H	1.294454	-0.528066	-0.175019
H	-0.511616	0.854100	1.916316
H	-0.470721	-0.914180	1.896457
H	1.970400	0.952179	1.870040
H	1.470180	-0.171067	3.171278
C	-0.970489	-0.888133	-0.709494
H	0.176904	0.968606	-0.437774
H	-0.803864	-0.889142	-1.789129
H	-0.924406	-1.921607	-0.354265
H	-1.996420	-0.531393	-0.537343

Table 79: (1,5s) hydogen migration in $CH_3CH_2CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	-0.060485	-0.011916	-0.011983
C	-0.000998	-0.011387	1.494511
C	1.357374	0.016959	2.162188
C	1.400399	0.966824	3.386095
H	0.727299	0.595636	4.167611
O	0.914363	2.243240	2.956251
O	-0.467327	2.113750	2.694933
H	-0.462980	1.195544	1.961133
H	1.644184	-0.987243	2.502964
H	2.118752	0.353825	1.451203
C	2.799587	1.193982	3.933340
H	-0.722058	-0.674149	1.977556
H	-1.086942	0.078643	-0.375014
H	0.525524	0.810621	-0.432004
H	0.350122	-0.945843	-0.422691
H	2.768950	1.872272	4.787792
H	3.237002	0.246537	4.257111
H	3.445733	1.630292	3.167645

Table 80: (1,5s) hydogen migration in $CH_3CH_2CH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	0.040417	0.046398	0.035005
C	-0.028192	-0.005755	1.546114
C	1.311541	-0.004902	2.272192
C	1.317869	0.959321	3.477643
O	0.909686	2.248395	3.036289
O	-0.460868	2.155959	2.703585
H	-0.440371	1.214581	1.962444
H	1.558220	-1.013201	2.632847
H	2.107241	0.305472	1.589929
H	0.649767	0.617309	4.274878
H	2.325931	1.094564	3.875984
C	-1.078204	-0.937522	2.116868
H	-0.950195	0.181221	-0.406977
H	0.683683	0.860111	-0.309309
H	0.452779	-0.891387	-0.366252
H	-2.065937	-0.733900	1.695063
H	-0.831289	-1.983518	1.885323
H	-1.152552	-0.848792	3.203512

Table 81: (1,5t) hydogen migration in $(CH_3)_2CHCH_2CH_2OO$

Cartesian Coordinates (Å)			
C	-0.080117	0.045099	-0.077852
C	0.026814	-0.037439	1.458366
C	1.446977	-0.022708	2.027297
O	2.215704	-1.180355	1.675270
O	2.697311	-1.027257	0.355522
H	1.780573	-1.224989	-0.296466
H	-0.507508	0.814328	1.894822
H	-0.480507	-0.941613	1.813679
H	1.999719	0.870638	1.717668
H	1.413551	-0.057998	3.119963
H	-1.139482	0.164377	-0.348861
H	0.424105	0.951411	-0.432024
C	0.480252	-1.156333	-0.797929
H	0.624281	-1.060102	-1.872585
H	0.096858	-2.129269	-0.490285

Table 82: (1,6p) hydrogen migration in $CH_3CH_2CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	0.004105	0.024896	0.002380
C	0.013129	0.029439	1.516556
C	1.420210	0.007039	2.144529
C	2.275457	1.253357	1.905464
O	2.640795	1.438695	0.532648
O	1.543899	1.993032	-0.161833
H	0.806547	1.095388	-0.274255
H	1.320104	-0.115617	3.229305
H	1.971923	-0.867107	1.780467
H	1.776675	2.161716	2.260295
H	3.236575	1.152720	2.417887
H	-0.548374	-0.845180	1.878469
H	-0.535441	0.908365	1.877366
C	-1.311984	0.268126	-0.688826
H	0.611059	-0.769667	-0.439958
H	-1.195881	0.325274	-1.773545
H	-2.018531	-0.547711	-0.476688
H	-1.779162	1.195396	-0.343934

Table 83: (1,6s) hydrogen migration in $CH_3CH_2CH_2CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	0.030663	0.006385	-0.028102
C	0.034099	0.003881	1.497805
C	1.418949	0.035298	2.174895
C	2.257274	1.288217	1.915296
O	2.632811	1.443614	0.539811
O	1.547704	1.998240	-0.169674
H	0.788408	1.089438	-0.271732
H	1.272552	-0.038551	3.259028
H	2.003807	-0.843512	1.885716
H	1.740210	2.198144	2.237294
H	3.213198	1.217294	2.442325
H	-0.503243	-0.892437	1.844610
H	-0.551568	0.861153	1.849175
C	-1.315601	0.323286	-0.642489
C	0.796699	-1.112998	-0.701761
H	-1.246394	0.437113	-1.727368
H	-2.028936	-0.490433	-0.443166
H	-1.743171	1.239717	-0.226775
H	0.756971	-1.017040	-1.789301
H	1.847443	-1.125411	-0.404932
H	0.363874	-2.089360	-0.437447

Table 84: (1,6t) hydrogen migration in $(CH_3)_2CHCH_2CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	1.513996	-1.245823	-0.128821
H	0.196419	-1.443021	0.308792
O	-0.930443	-1.472179	0.490882
O	-1.427728	-0.681314	-0.567203
C	-1.636331	0.654963	-0.100126
C	-0.399928	1.327866	0.497842
C	0.887897	1.252477	-0.354071
C	1.898520	0.188237	0.119956
H	2.073438	-2.000208	0.422839
H	1.335077	-1.516779	-1.169944
H	2.104170	0.340918	1.185585
H	2.855379	0.372395	-0.394993
H	0.635646	1.075059	-1.405434
H	1.391981	2.222681	-0.319608
H	-0.212906	0.902643	1.487554
H	-0.675004	2.374820	0.666093
H	-1.967701	1.171749	-1.006425
H	-2.456053	0.661365	0.627425

Table 85: (1,7p) hydrogen migration in $CH_3(CH_2)_4OO$

Cartesian Coordinates (Å)			
C	1.516011	-0.104473	-0.349548
H	0.577956	-0.977970	0.136041
O	-0.334297	-1.663095	0.383898
O	-1.279184	-1.254107	-0.579860
C	-2.154244	-0.281610	-0.000644
C	-1.453564	0.945465	0.584451
C	-0.412960	1.630122	-0.331086
C	1.053179	1.289719	0.002115
C	2.846747	-0.555349	0.197647
H	1.356262	-0.360514	-1.400956
H	1.231246	1.478932	1.068315
H	1.701937	2.000708	-0.535341
H	-0.616021	1.387666	-1.380228
H	-0.525839	2.714548	-0.241812
H	-0.983072	0.662878	1.529957
H	-2.247660	1.655105	0.841131
H	-2.793600	-0.006285	-0.845503
H	-2.773164	-0.761758	0.766121
H	3.045299	-1.602915	-0.040615
H	3.666811	0.038961	-0.231079
H	2.896681	-0.434982	1.284058

Table 86: (1,7s) hydogen migration in $CH_3CH_2(CH_2)_4OO$

Cartesian Coordinates (Å)			
C	0.010220	-0.053650	-0.033393
C	0.045973	-0.038889	1.489323
C	1.424378	0.020117	2.180523
C	2.145474	1.381428	2.052209
C	3.259905	1.449045	1.007849
O	2.902244	0.943038	-0.282667
O	1.764460	1.626706	-0.753645
H	0.879127	0.906860	-0.425816
C	-1.308903	0.391920	-0.631716
C	0.615336	-1.279503	-0.686837
H	-0.554661	0.802741	1.853200
H	-0.472769	-0.947574	1.836003
H	2.068799	-0.785032	1.813436
H	1.258521	-0.189988	3.241344
H	1.414983	2.165928	1.837452
H	2.607319	1.650322	3.008556
H	4.103858	0.810550	1.287738
H	3.618145	2.479817	0.905177
H	-1.247529	0.472324	-1.720093
H	-2.101440	-0.335536	-0.401473
H	-1.628370	1.358541	-0.232865
H	0.603216	-1.192220	-1.775716
H	1.650592	-1.436013	-0.378167
H	0.041996	-2.178148	-0.415544

Table 87: (1,7t) hydogen migration in $(CH_3)_2CH(CH_2)_4OO$

5 Transition States for intramolecular hydrogen migration in OOQOOH radicals

Cartesian Coordinates (Å)			
O	0.002282	-0.000520	-0.001538
O	-0.000010	0.000137	1.421933
C	1.382700	0.000029	1.751538
H	1.462370	-0.210953	2.820450
H	1.859087	0.956678	1.508424
C	1.950276	-1.088849	0.835951
H	1.020323	-0.734783	-0.066567
H	1.778164	-2.129653	1.114127
O	3.247916	-0.830067	0.489503
O	3.828059	-2.049388	-0.039637
H	4.529181	-1.663543	-0.584039

Table 88: Transition state for reaction $HOOCH_2CH_2OO \rightarrow HOOCH_2CHO + OH$

Cartesian Coordinates (Å)			
O	0.005755	-0.075383	-0.045729
O	0.024960	-0.043978	1.380375
C	1.418771	0.040543	1.709101
H	1.476089	-0.220917	2.770570
C	1.988370	-1.073727	0.809135
H	1.063014	-0.751727	-0.108314
H	1.771736	-2.098393	1.113821
O	3.300352	-0.882295	0.471190
O	3.851384	-2.152763	0.038594
H	4.484729	-1.833017	-0.619948
C	2.015773	1.416978	1.449804
H	1.504968	2.151835	2.074727
H	3.080826	1.429646	1.692205
H	1.885746	1.697261	0.404342

Table 89: Transition state for reaction $HOOCH_2CH(CH_3)OO \rightarrow HOOCH(CH_3)CHO + OH$

Cartesian Coordinates (Å)			
O	0.005173	0.001305	-0.003680
O	0.000498	0.000574	1.420714
C	1.382550	-0.000373	1.750084
H	1.462373	-0.217777	2.818472
H	1.856351	0.957154	1.509329
C	1.960586	-1.094774	0.833064
H	1.042502	-0.731820	-0.063878
O	3.239534	-0.715934	0.476467
O	3.877396	-1.763203	-0.304731
H	4.279880	-1.212290	-0.990746
C	1.741630	-2.531961	1.225180
H	2.385800	-2.797359	2.072447
H	0.698767	-2.657001	1.519661
H	1.964931	-3.207760	0.400828

Table 90: Transition state for reaction $HOOCH(CH_3)CH_2OO \rightarrow HOOCH_2C(CH_3)O + OH$

Cartesian Coordinates (Å)			
O	0.043372	0.092917	0.075674
O	0.084259	-0.148426	1.478363
C	1.472597	-0.054119	1.798441
C	2.122791	-0.914657	0.682911
H	1.155126	-0.487611	-0.122446
O	3.355549	-0.357809	0.399974
O	4.078997	-1.173692	-0.562377
H	4.361981	-0.474666	-1.168580
C	2.044444	-2.415346	0.778399
H	2.729008	-2.793934	1.546445
H	1.023642	-2.697283	1.039477
H	2.310517	-2.878997	-0.170555
H	1.817144	0.975818	1.645702
C	1.679775	-0.497689	3.234270
H	1.152341	0.178508	3.910272
H	1.303755	-1.509353	3.395148
H	2.743374	-0.469880	3.481954

Table 91: Transition state for reaction $HOOCH(CH_3)CH(CH_3)OO \rightarrow HOOCH(CH_3)C(CH_3)O + OH$

Cartesian Coordinates (Å)			
C	-0.138296	0.090990	-0.210858
H	0.013519	0.411288	0.825037
H	0.773670	0.262280	-0.786810
C	-0.572906	-1.386563	-0.289767
H	-0.574103	-1.698015	-1.337440
H	0.151187	-2.009966	0.247671
C	-1.969863	-1.570419	0.262393
H	-2.429103	-0.303190	0.143793
H	-2.079433	-1.769779	1.330898
O	-1.133592	0.903592	-0.817688
O	-2.260374	0.881897	0.041381
O	-2.674195	-2.468867	-0.521000
O	-3.951771	-2.725166	0.110743
H	-4.546857	-2.303517	-0.526623

Table 92: Transition state for reaction $HOOCH_2CH_2CH_2OO \rightarrow HOOCH_2CH_2CHO + OH$

Cartesian Coordinates (Å)			
C	-0.002468	0.017974	-0.021131
H	0.009995	-0.019399	1.074130
C	1.446924	0.000619	-0.564611
H	1.411385	0.147355	-1.647934
H	2.005758	0.836772	-0.128551
C	2.138384	-1.314911	-0.284213
H	1.059388	-2.101605	-0.073456
H	2.702760	-1.414022	0.645870
O	-0.663890	-1.160041	-0.492137
O	-0.099210	-2.267243	0.184197
O	2.869682	-1.710537	-1.392467
O	3.617042	-2.902183	-1.047452
H	3.152626	-3.559375	-1.586501
C	-0.810912	1.205892	-0.515381
H	-1.819342	1.176699	-0.099554
H	-0.335693	2.141323	-0.210644
H	-0.884226	1.193120	-1.605540

Table 93: Transition state for reaction $HOOCH_2CH_2CH(CH_3)OO \rightarrow HOOCH(CH_3)CH_2CHO + OH$

Cartesian Coordinates (Å)			
C	0.499029	0.748152	-0.044905
C	0.525393	2.030905	-0.901606
C	-0.712303	-0.108600	-0.411915
C	0.505541	1.100177	1.454186
C	1.756604	-0.103758	-0.377162
O	1.731963	-1.329017	0.338925
O	0.708621	-2.127509	-0.233752
O	-1.816995	0.185061	0.367311
O	-2.965580	-0.494785	-0.195669
H	-0.365940	2.632844	-0.710812
H	0.556959	1.799422	-1.969897
H	1.403314	2.637061	-0.658577
H	-0.210955	-1.346414	-0.216626
H	-0.963295	-0.151427	-1.475338
H	-0.376641	1.680835	1.727454
H	1.392155	1.696272	1.687960
H	0.531135	0.199355	2.068836
H	2.661880	0.410787	-0.044252
H	1.822168	-0.309001	-1.451847
H	-3.160434	-1.120990	0.516989

Table 94: Transition state for reaction $HOOCH_2C(CH_3)_2CH_2OO \rightarrow HOOCH_2CH_2C(CH_3)O + OH$

Cartesian Coordinates (Å)			
C	0.000115	0.000559	-0.000638
H	0.000667	0.001295	1.094138
H	1.028762	0.000747	-0.367735
C	-0.788459	-1.198437	-0.569012
H	-0.625917	-1.244115	-1.648152
H	-0.407320	-2.126726	-0.126752
C	-2.280235	-1.050360	-0.312399
H	-2.321323	0.274113	-0.103942
O	-0.575642	1.210066	-0.474527
O	-1.829511	1.346598	0.169355
O	-2.936588	-1.347889	-1.509520
O	-4.357047	-1.081628	-1.372916
H	-4.423239	-0.262055	-1.885011
C	-2.861927	-1.676298	0.934282
H	-3.909288	-1.403498	1.055945
H	-2.792964	-2.769368	0.873769
H	-2.308110	-1.339386	1.812715

Table 95: Transition state for reaction $HOOCH(CH_3)CH_2CH_2OO \rightarrow HOOCH(CH_3)CH_2C(CH_3)O + OH$

Cartesian Coordinates (Å)			
C	-0.000149	0.000077	-0.000006
H	0.000286	0.000013	1.095859
C	1.456237	-0.001069	-0.528457
H	1.427477	0.130097	-1.613342
H	1.994768	0.850747	-0.096440
C	2.179190	-1.301552	-0.218391
H	1.115358	-2.078909	0.024875
O	-0.633283	-1.206276	-0.436685
O	-0.049129	-2.278027	0.277047
O	2.787101	-1.729013	-1.402832
O	3.356882	-3.051204	-1.215304
H	2.695894	-3.585914	-1.679682
C	3.035357	-1.373655	1.025196
H	3.408107	-2.384582	1.184361
H	3.894621	-0.698377	0.930226
H	2.451064	-1.073968	1.897531
C	-0.828636	1.153441	-0.541167
H	-1.839903	1.118671	-0.132566
H	-0.374568	2.108297	-0.265811
H	-0.892075	1.101294	-1.630729

Table 96: Transition state for reaction $HOOCH(CH_3)CH_2CH(CH_3)OO \rightarrow HOOCH_2C(CH_3)_2CHO + OH$

Cartesian Coordinates (Å)			
O	-0.002066	-0.006204	0.002546
H	-0.010310	0.063479	0.968544
O	1.424478	-0.008738	-0.247113
C	1.792240	-1.268879	-0.690766
H	1.081955	-1.678853	-1.412740
H	1.743184	-2.118871	0.357647
C	3.262705	-1.262746	-1.064257
H	3.454806	-2.130489	-1.699872
H	3.464586	-0.369369	-1.666186
C	4.187562	-1.279826	0.171410
H	3.792947	-0.580765	0.911824
H	5.181210	-0.915006	-0.104763
C	4.351707	-2.673236	0.800834
H	5.111310	-3.256829	0.271920
H	4.636539	-2.595702	1.855456
O	3.186500	-3.496701	0.672166
O	2.084392	-2.832148	1.251860

Table 97: Transition state for reaction $HOO(CH_2)_4OO \rightarrow HOO(CH_2)_3CHO + OH$

Cartesian Coordinates (Å)			
O	-3.363425	0.343027	-0.106232
H	-3.278111	0.898146	-0.895331
O	-2.243307	-0.555314	-0.295755
C	-1.273435	-0.256073	0.647821
H	-1.698916	-0.074524	1.637729
H	-0.689435	0.911199	0.303171
C	-0.133165	-1.249035	0.535186
H	0.448055	-1.200415	1.458741
H	-0.555141	-2.258923	0.475311
C	0.764552	-0.987162	-0.694139
H	0.123369	-0.748778	-1.545168
H	1.303399	-1.901850	-0.957136
C	1.802716	0.139941	-0.492963
H	2.021644	0.607560	-1.459479
O	1.312767	1.166352	0.394828
O	0.107263	1.695926	-0.108130
C	3.096906	-0.329861	0.160636
H	3.625894	-1.014225	-0.506627
H	3.746680	0.522379	0.368470
H	2.900725	-0.847360	1.103391

Table 98: Transition state for reaction $HOO(CH_2)_3CH(CH_3)OO \rightarrow HOOCH(CH_3)(CH_2)_2CHO + OH$

Cartesian Coordinates (Å)			
O	-0.002021	0.001236	-0.003242
H	-0.003600	0.004102	0.965209
O	1.427713	0.001882	-0.255389
C	1.840548	-1.267762	-0.672965
H	1.620772	-2.091063	0.360346
C	3.363288	-1.223862	-0.739282
H	3.704028	-2.075551	-1.333268
H	3.653264	-0.316750	-1.283222
C	4.026392	-1.231460	0.652618
H	3.479928	-0.543973	1.301310
H	5.047829	-0.846294	0.579186
C	4.091180	-2.625091	1.298730
H	4.945851	-3.195158	0.922204
H	4.169655	-2.548369	2.388437
O	2.982992	-3.464270	0.950775
O	1.782390	-2.815149	1.307471
C	1.091762	-1.844306	-1.850599
H	0.016414	-1.802257	-1.683444
H	1.325274	-1.276080	-2.760523
H	1.386203	-2.884075	-2.003930

Table 99: Transition state for reaction $HOOCH(CH_3)(CH_2)_3OO \rightarrow HOO(CH_3)_3C(CH_3)O + OH$

	Cartesian Coordinates (Å)		
O	-3.004257	0.544250	-0.771859
H	-2.664591	1.143422	-1.452719
O	-1.967597	-0.472565	-0.787898
C	-1.141006	-0.330923	0.331602
H	-0.534118	0.857052	0.203272
C	0.018276	-1.300882	0.137941
H	0.518128	-1.428741	1.100790
H	-0.397810	-2.277889	-0.136500
C	1.016075	-0.839433	-0.944493
H	0.447826	-0.452357	-1.792240
H	1.581019	-1.699427	-1.315746
C	2.027263	0.224746	-0.463995
H	2.338448	0.839678	-1.316098
O	1.448990	1.101218	0.526299
O	0.288527	1.708012	0.005966
C	-1.846285	-0.316909	1.666582
H	-2.655676	0.411817	1.668702
H	-2.269152	-1.307326	1.880366
H	-1.138418	-0.062137	2.457388
C	3.252444	-0.361622	0.227147
H	2.965660	-1.026573	1.045901
H	3.848796	-0.931394	-0.489167
H	3.873974	0.436687	0.637284

Table 100: Transition state for reaction $HOOCH(CH_3)(CH_2)_2CH(CH_3)OO \rightarrow HOOCH(CH_3)(CH_2)_2C(CH_3)O + OH$

	Cartesian Coordinates (Å)		
C	0.001227	-0.000979	-0.000954
H	0.006305	0.002914	1.093004
H	1.333376	-0.003518	-0.222256
C	-0.617640	1.199952	-0.675794
H	-0.652302	1.020916	-1.755861
H	-1.661003	1.276145	-0.341775
C	1.480913	2.683431	-1.078877
H	1.549589	2.000764	-1.929990
H	1.581743	3.693226	-1.490769
C	2.696890	2.467919	-0.175827
H	3.615203	2.482532	-0.773899
H	2.763685	3.248248	0.589034
O	2.658350	1.269416	0.604066
O	2.512993	0.161794	-0.258431
O	-0.545998	-1.164286	-0.518421
O	-0.192953	-2.269846	0.345717
H	0.500059	-2.696233	-0.180125
C	0.102208	2.533406	-0.396254
H	-0.557761	3.329314	-0.751564
H	0.198623	2.679151	0.685152

Table 101: Transition state for reaction $HOO(CH_2)_5OO \rightarrow HOO(CH_2)_4CHO + OH$

6 Geometries of OOQOOH molecules

In this section we give the B3LYP/6-31G(d) optimized geometries of the low energy conformers for which hindered rotor scans were performed to calculate the configuration integral of $\mathcal{A}_i$ regions. Also the B3LYP/CBSB7 optimized geometry of the lowest energy conformer is given.

6.1 Reactants for 1,4-hydrogen shift in OOQOOH

For all OOQOOH molecules undergoin 1,4-hydrogen shift we have chosen four low energy conformers to calculate the hindered rotor contribution to the partition function. For each of these conformers the B3LYP/6-31G(d) optimized geometry is given below. In addition to the B3LYP/6-31G(d) energy of the four conformers B3LYP/CBSB7 optimized geometry of the lowest energy conformer is also given. Thus for each of the four reactants we give five geometries each.

	Cartesian Coordinates (Å)		
O	-0.004436	0.001206	-0.010397
H	-0.024263	0.035241	0.961815
O	1.430882	-0.004290	-0.213356
C	1.842889	-1.341323	-0.413613
H	2.925850	-1.257071	-0.539033
H	1.404170	-1.759606	-1.329057
C	1.501308	-2.271046	0.745919
H	1.973822	-3.245312	0.610980
H	0.424613	-2.384865	0.863797
O	2.033567	-1.772034	2.001759
O	1.296902	-0.790260	2.489830

Table 102: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOOCH_2CH_2OO$

	Cartesian Coordinates (Å)		
O	-0.002688	0.010650	-0.008119
H	-0.033431	0.013961	0.964822
O	1.435671	0.005061	-0.192464
C	1.845329	-1.328272	-0.413788
H	2.928224	-1.244253	-0.546372
H	1.397896	-1.727715	-1.333051
C	1.519513	-2.286751	0.734943
H	0.439005	-2.363027	0.858642
O	2.032842	-1.735035	1.993741
O	1.260577	-0.782064	2.479062
C	2.167337	-3.649476	0.570026
H	1.903334	-4.303886	1.401906
H	1.823258	-4.115555	-0.356040
H	3.255578	-3.561847	0.528917

Table 103: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOOCH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
O	-0.011671	0.014217	0.044917
H	0.009406	0.034097	1.017873
O	1.417174	-0.016433	-0.211004
C	1.817287	-1.365669	-0.435171
H	2.904893	-1.260223	-0.511363
C	1.489509	-2.266173	0.759379
H	1.963041	-3.242349	0.647925
H	0.413678	-2.379672	0.890669
O	2.037696	-1.741362	1.998106
O	1.305214	-0.760583	2.492406
C	1.240129	-1.939331	-1.727181
H	1.524433	-1.302643	-2.566123
H	1.616475	-2.948789	-1.914441
H	0.150896	-1.971727	-1.673909

Table 104: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOOCH(CH_3)CH_2OO$

Cartesian Coordinates (Å)			
O	-0.014299	-0.073884	-0.062053
H	-0.056665	-0.043610	0.909950
O	1.423329	-0.029047	-0.231468
C	1.918478	-1.351481	-0.427382
H	1.459201	-1.776251	-1.330891
C	1.529840	-2.284783	0.735727
H	0.442907	-2.312730	0.807551
O	2.001407	-1.722890	2.007765
O	1.216694	-0.763874	2.461145
C	3.417579	-1.160394	-0.626143
H	3.891379	-2.094875	-0.931633
H	3.585591	-0.419449	-1.408935
H	3.886736	-0.806874	0.293347
C	2.112359	-3.684157	0.648130
H	1.706043	-4.315376	1.439862
H	1.857191	-4.134310	-0.314260
H	3.199338	-3.668562	0.744947

Table 105: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOOCH(CH_3)CH(CH_3)OO$

Cartesian Coordinates (Å)			
O	-0.030800	0.159193	-0.145328
H	-0.180911	0.326287	0.802331
O	1.419499	-0.027573	-0.118964
C	1.681829	-1.191989	-0.881087
H	2.773901	-1.214097	-0.958214
H	1.252427	-1.097080	-1.887775
C	1.183960	-2.474274	-0.236447
H	1.348140	-3.331938	-0.895294
H	0.129082	-2.398823	0.034740
O	1.862465	-2.743054	1.024955
O	3.138832	-3.031307	0.825271

Table 106: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH_2OO$

Cartesian Coordinates (Å)			
O	0.367091	0.581012	-0.044783
H	-0.061081	0.031521	0.644676
O	1.685663	-0.021544	-0.087727
C	1.629385	-1.158085	-0.930776
H	2.671824	-1.319302	-1.235523
H	1.028714	-0.944806	-1.822329
C	1.157860	-2.435109	-0.236831
H	1.557433	-2.500583	0.778707
H	1.448296	-3.316208	-0.816913
O	-0.295123	-2.573903	-0.149582
O	-0.829223	-1.792593	0.772246

Table 107: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH_2OO$

Cartesian Coordinates (Å)			
O	0.108819	0.204078	0.015643
H	0.144093	-0.154016	0.928124
O	1.512193	0.057907	-0.327872
C	1.660986	-1.160683	-1.028284
H	2.737443	-1.211705	-1.227293
H	1.118590	-1.142825	-1.985056
C	1.194470	-2.383573	-0.241003
H	1.480544	-3.306841	-0.752587
H	0.116919	-2.363335	-0.070748
O	1.847221	-2.462897	1.054576
O	1.317914	-1.609453	1.920180

Table 108: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH_2OO$

Cartesian Coordinates (Å)			
O	-0.079794	-0.110977	0.059359
H	-0.093227	-0.133341	1.032989
O	1.360344	-0.000736	-0.154030
C	1.736405	-1.119265	-0.938755
H	1.427542	-2.054450	-0.452156
H	2.830296	-1.069591	-0.970107
C	1.188278	-1.076161	-2.355864
H	0.118325	-0.859550	-2.365425
H	1.393946	-2.013850	-2.880829
O	1.784154	0.004555	-3.131131
O	3.070778	-0.220330	-3.342692

Table 109: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH_2OO$

Cartesian Coordinates (Å)			
O	0.011162	-0.026065	0.043407
H	0.034662	-0.080232	1.015577
O	1.449650	-0.017452	-0.221643
C	1.675241	-0.986587	-1.229640
H	2.726239	-0.840091	-1.499418
H	1.045189	-0.779692	-2.104693
C	1.456492	-2.422353	-0.766163
H	0.482791	-2.504963	-0.276611
O	2.379258	-2.737916	0.341590
O	3.645435	-2.650129	-0.029736
C	1.611991	-3.447907	-1.879919
H	1.460899	-4.459365	-1.491426
H	0.872134	-3.267342	-2.666685
H	2.613222	-3.388846	-2.316423

Table 110: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
O	-0.010824	0.007822	0.009738
H	-0.006741	0.014014	0.989687
O	1.413929	-0.001177	-0.260614
C	1.876133	-1.338857	-0.205510
H	2.789781	-1.328865	-0.813894
H	1.148832	-2.014463	-0.670937
C	2.259387	-1.828693	1.196391
H	2.698245	-1.003542	1.765402
O	1.079615	-2.269298	1.970023
O	0.352023	-1.270243	2.431994
C	3.168021	-3.049879	1.161629
H	4.128604	-2.786073	0.708262
H	3.353987	-3.420910	2.173320
H	2.719110	-3.858156	0.574184

Table 111: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
O	0.000977	0.010909	0.002560
H	-0.008861	-0.017017	0.983285
O	1.440234	0.009619	-0.196022
C	1.843374	-1.325779	-0.417796
H	2.928679	-1.247404	-0.554171
H	1.393494	-1.727223	-1.337400
C	1.514653	-2.283673	0.733639
H	0.431745	-2.363338	0.851698
O	2.022575	-1.732002	1.993611
O	1.250505	-0.766056	2.467810
C	2.167501	-3.647531	0.572483
H	1.900324	-4.305584	1.403956
H	1.828937	-4.114759	-0.357987
H	3.258305	-3.558373	0.536560

Table 112: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
O	-0.012099	0.010074	-0.034478
H	-0.017676	0.042457	0.938884
O	1.430830	0.007538	-0.260838
C	1.720080	-1.169878	-0.994273
H	1.338239	-2.053325	-0.465875
H	2.814555	-1.205269	-1.022485
C	1.179908	-1.144493	-2.420733
H	0.146618	-0.788581	-2.419892
O	1.863917	-0.090671	-3.195480
O	3.164786	-0.308854	-3.281939
C	1.313288	-2.479849	-3.139616
H	0.723854	-3.246596	-2.626087
H	0.948823	-2.396820	-4.167730
H	2.359825	-2.797474	-3.167056

Table 113: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
O	-0.016421	-0.028036	-0.044953
H	-0.015711	-0.056801	0.928635
O	1.424406	0.024821	-0.278040
C	1.734731	-0.994374	-1.229052
H	1.071170	-0.878441	-2.099102
C	1.478227	-2.394573	-0.668595
H	1.658965	-3.165038	-1.421730
H	0.457037	-2.459755	-0.286693
O	2.321770	-2.688288	0.478231
O	3.467311	-3.246752	0.113403
C	3.180710	-0.724497	-1.634089
H	3.848803	-0.800989	-0.772478
H	3.503674	-1.453812	-2.382954
H	3.264140	0.280107	-2.057689

Table 114: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH_2OO$

Cartesian Coordinates (Å)			
O	-0.006120	-0.033675	0.006617
H	-0.018636	-0.010038	0.985858
O	1.421903	-0.011681	-0.242101
C	1.921614	-1.347518	-0.206131
H	1.182226	-2.013748	-0.665899
C	2.226914	-1.817266	1.222835
H	2.701218	-1.018877	1.799906
H	2.861176	-2.708279	1.212086
O	1.058471	-2.271534	1.974265
O	0.333277	-1.276323	2.452358
C	3.211420	-1.316644	-1.029383
H	3.644210	-2.318709	-1.112202
H	2.992156	-0.943177	-2.032663
H	3.953457	-0.652732	-0.572272

Table 115: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH_2OO$

Cartesian Coordinates (Å)			
O	-0.021308	-0.057058	-0.042809
H	-0.022630	-0.015526	0.937285
O	1.413597	-0.031261	-0.258617
C	1.876654	-1.368466	-0.406960
H	1.400273	-1.830038	-1.285869
C	1.497233	-2.244977	0.794270
H	1.969899	-3.228374	0.722159
H	0.415035	-2.350722	0.881470
O	1.990608	-1.695769	2.046083
O	1.240416	-0.686799	2.468391
C	3.382481	-1.238177	-0.620363
H	3.821036	-2.218223	-0.835604
H	3.581993	-0.575079	-1.466627
H	3.864681	-0.823227	0.269271

Table 116: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH_2OO$

Cartesian Coordinates (Å)			
O	0.029274	0.136348	-0.075197
H	-0.033180	0.069216	0.894054
O	1.473307	-0.016648	-0.236516
C	1.706780	-1.209919	-0.988677
H	2.801043	-1.209875	-1.065543
C	1.141620	-1.096840	-2.402245
H	0.090742	-0.801196	-2.387017
H	1.270064	-2.031744	-2.954572
O	1.803755	-0.045184	-3.160562
O	3.058373	-0.372868	-3.425123
C	1.223915	-2.469009	-0.270472
H	1.634466	-2.495905	0.744040
H	0.132130	-2.493131	-0.205284
H	1.559475	-3.368263	-0.797677

Table 117: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH_2OO$

Cartesian Coordinates (Å)			
O	0.018156	-0.049614	0.003140
H	0.024063	-0.182900	0.968077
O	1.457504	-0.010135	-0.237606
C	1.751499	-0.975825	-1.250114
H	1.080659	-0.799259	-2.103748
C	1.469420	-2.407466	-0.759627
H	0.455687	-2.412822	-0.350130
O	2.266722	-2.704874	0.442189
O	3.508569	-3.070106	0.164482
C	3.192295	-0.672368	-1.652393
H	3.872320	-0.804831	-0.807728
H	3.513337	-1.335642	-2.460358
H	3.259272	0.361679	-2.002278
C	1.625540	-3.490480	-1.815671
H	1.341190	-4.463392	-1.403455
H	0.968638	-3.274031	-2.664889
H	2.655292	-3.556544	-2.171586

Table 118: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH(CH_3)OO$

Cartesian Coordinates (Å)			
O	-0.051704	-0.164158	-0.024330
H	-0.108754	-0.065674	0.947132
O	1.380975	-0.047076	-0.213186
C	1.964706	-1.352917	-0.232324
H	1.259508	-2.041878	-0.712455
C	2.283977	-1.855228	1.189070
H	2.746747	-1.046673	1.762222
O	1.035213	-2.188616	1.910408
O	0.486278	-1.150090	2.510397
C	3.228305	-1.196937	-1.082473
H	3.700949	-2.163333	-1.277474
H	2.954577	-0.743516	-2.038491
H	3.957037	-0.542629	-0.590942
C	3.098864	-3.141514	1.246628
H	2.650691	-3.924165	0.624715
H	4.120077	-2.964231	0.899458
H	3.147302	-3.507056	2.276454

Table 119: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH(CH_3)OO$

Cartesian Coordinates (Å)			
O	-0.013502	-0.072646	-0.050669
H	-0.034821	-0.072188	0.930331
O	1.425505	-0.022935	-0.233526
C	1.915119	-1.346526	-0.429609
H	1.455790	-1.774010	-1.334307
C	1.523305	-2.281282	0.733803
H	0.434180	-2.316284	0.799401
O	1.987078	-1.720883	2.008775
O	1.204163	-0.747251	2.449104
C	3.417890	-1.163190	-0.628499
H	3.887780	-2.102972	-0.933120
H	3.592025	-0.422676	-1.414111
H	3.891465	-0.810568	0.292223
C	2.114531	-3.680341	0.649795
H	1.708942	-4.315534	1.442425
H	1.863848	-4.133558	-0.315244
H	3.203810	-3.659704	0.748888

Table 120: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH(CH_3)OO$

Cartesian Coordinates (Å)			
O	0.036181	0.146991	-0.131838
H	-0.026946	0.127309	0.839431
O	1.479743	-0.022175	-0.284382
C	1.708634	-1.255316	-0.974915
H	2.803765	-1.268096	-1.036063
C	1.166184	-1.177549	-2.408635
H	0.129231	-0.832719	-2.386207
O	1.836983	-0.067818	-3.114582
O	3.136221	-0.277394	-3.238976
C	1.208884	-2.460737	-0.179837
H	1.575369	-2.388875	0.849548
H	0.115651	-2.499335	-0.157720
H	1.582222	-3.396701	-0.605307
C	1.309401	-2.450484	-3.232722
H	0.681607	-3.247671	-2.824266
H	0.992279	-2.261694	-4.262883
H	2.349753	-2.788424	-3.248551

Table 121: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH(CH_3)OO$

6.2 Reactants for 1,5-hydrogen shift in OOQOOH

For all OOQOOH molecules undergoin 1,5-hydrogen shift we have chosen six low energy conformers to calculate the hindered rotor contribution to the partition function. For each of these conformers the B3LYP/6-31G(d) optimized geometry is given below. In addition to the B3LYP/6-31G(d) energy of the six conformers B3LYP/CBSB7 optimized geometry of the lowest energy conformer is also given. Thus for each of the five reactants we give five geometries each.

	Cartesian Coordinates (Å)		
C	0.004474	0.004355	-0.000871
C	0.006421	-0.004674	1.531667
C	1.419424	0.013181	-0.591735
O	1.644545	-1.109683	-1.510470
O	1.586045	-2.277963	-0.909801
O	0.847213	-1.011169	2.076399
O	0.280392	-2.297728	1.721466
H	-1.013837	-0.117358	1.912805
H	0.432307	0.918885	1.937954
H	2.181767	-0.073001	0.184049
H	1.620840	0.877474	-1.223498
H	0.807005	-2.508771	0.928194
H	-0.514925	-0.888633	-0.353396
H	-0.569145	0.864842	-0.355336

Table 122: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOOCH_2CH_2CH_2OO$

	Cartesian Coordinates (Å)		
C	0.001893	-0.018836	-0.009309
C	0.006345	0.003543	1.522505
C	1.417721	0.019764	-0.605051
O	1.619297	-1.127050	-1.527057
O	1.555031	-2.291877	-0.923727
O	0.851751	-0.990609	2.085289
O	0.296588	-2.286325	1.745517
H	-1.012755	-0.105751	1.907964
H	0.429796	0.935771	1.911694
H	2.158754	-0.134505	0.181936
H	0.814296	-2.497239	0.946113
H	-0.495732	-0.932821	-0.337192
H	-0.595004	0.819137	-0.381346
C	1.736665	1.245475	-1.439229
H	2.750522	1.195676	-1.840369
H	1.034050	1.342959	-2.270438
H	1.657004	2.139690	-0.816340

Table 123: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOOCH_2CH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	0.000033	0.000112	-0.000022
C	0.000012	-0.000164	1.542660
C	1.481284	0.000159	-0.446412
C	-0.714607	1.253851	-0.532225
C	-0.754466	-1.266193	-0.425102
O	-1.002395	-1.269226	-1.871722
O	-2.077423	-1.960071	-2.193715
O	1.711091	0.055496	-1.847666
O	1.706861	-1.300336	-2.364785
H	0.557502	0.859507	1.923675
H	0.463411	-0.904917	1.948087
H	-1.018444	0.064042	1.934308
H	2.017428	-0.860405	-0.033134
H	1.955637	0.913904	-0.072140
H	-0.254099	2.155785	-0.119720
H	-1.770976	1.255302	-0.248331
H	-0.652094	1.309325	-1.619390
H	-1.739276	-1.319019	0.040346
H	-0.189918	-2.175081	-0.203039
H	0.814431	-1.347713	-2.743589

Table 124: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOOCH_2C(CH_3)_2CH_2OO$

Cartesian Coordinates (Å)			
C	0.040773	0.008792	-0.020869
C	0.013205	0.042832	1.518107
C	1.460837	-0.035070	-0.596694
O	1.644487	-1.160469	-1.521905
O	1.553159	-2.327752	-0.922959
O	0.828244	-0.994124	2.071078
O	0.246907	-2.271137	1.710603
H	-1.019491	-0.117285	1.847799
H	2.210732	-0.163149	0.184947
H	1.708765	0.824066	-1.218589
H	0.776893	-2.493748	0.922672
H	-0.490163	-0.886339	-0.349271
H	-0.512849	0.865919	-0.412580
C	0.555731	1.331498	2.127167
H	-0.049228	2.181961	1.803791
H	0.521770	1.274077	3.216153
H	1.592547	1.512280	1.831178

Table 125: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOOCH(CH_3)CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	0.023695	0.000198	-0.011378
C	0.013293	0.036714	1.527984
C	1.435914	0.003840	-0.615911
O	1.604019	-1.153621	-1.533302
O	1.530360	-2.314509	-0.924298
O	0.843819	-0.991267	2.075807
O	0.274295	-2.275067	1.722111
H	-1.014741	-0.134556	1.867047
H	2.180380	-0.163571	0.164867
H	0.790915	-2.485573	0.921785
H	-0.488125	-0.910257	-0.326792
H	-0.561250	0.840587	-0.396533
C	0.546465	1.329555	2.136508
H	-0.059614	2.177248	1.807791
H	0.505529	1.274139	3.225406
H	1.585014	1.512787	1.848526
C	1.779286	1.211608	-1.467348
H	2.786152	1.127794	-1.880636
H	1.069729	1.318257	-2.291653
H	1.730878	2.115290	-0.855815

Table 126: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOOCH(CH_3)CH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-0.059313	-0.046822	0.078709
C	-0.385882	0.133042	1.565353
C	1.430129	-0.085318	-0.234304
O	1.935518	-1.414081	0.127563
O	3.204247	-1.559793	-0.208317
O	0.348362	-0.724866	2.426521
O	-0.053145	-2.089750	2.123418
H	-1.463934	0.014485	1.735558
H	-0.086498	1.130998	1.911460
H	2.010024	0.644635	0.338578
H	1.635236	0.041808	-1.300377
H	0.729984	-2.376077	1.613245
H	-0.523415	-0.964107	-0.299820
H	-0.507596	0.785261	-0.479185

Table 127: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	-0.076251	0.250088	0.133064
C	0.040826	0.001656	1.642749
C	1.268147	0.088381	-0.590786
O	1.187036	-0.869962	-1.698336
O	0.949456	-2.100471	-1.282265
O	0.718457	-1.207496	1.951825
O	-0.100479	-2.301336	1.457506
H	-0.952697	0.013254	2.108398
H	0.663905	0.764381	2.127449
H	2.046450	-0.284411	0.079924
H	1.606415	0.998596	-1.090448
H	0.329645	-2.453734	0.587546
H	-0.786048	-0.469671	-0.284858
H	-0.495074	1.247849	-0.039421

Table 128: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	0.075966	-0.080825	-0.032135
C	0.019282	0.105258	1.483626
C	1.492310	-0.049583	-0.587770
O	2.284194	-1.175236	-0.089870
O	1.857250	-2.320752	-0.598034
O	0.599654	1.332285	1.919358
O	-0.244730	2.407790	1.409767
H	0.631196	-0.647293	1.994982
H	-1.013432	0.027681	1.848255
H	2.045524	0.827024	-0.242461
H	1.506076	-0.103316	-1.679310
H	-0.574090	2.766471	2.253490
H	-0.388443	-1.037006	-0.300046
H	-0.503671	0.714198	-0.513936

Table 129: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	0.019696	-0.050145	0.037336
C	-0.069556	0.081523	1.559333
C	1.438352	-0.038655	-0.517529
O	2.227393	-1.189750	-0.070903
O	1.651505	-2.334438	-0.400255
O	0.672095	-0.901980	2.270371
O	0.058820	-2.187879	2.000721
H	-1.120385	0.061420	1.876423
H	0.380945	1.021303	1.904371
H	2.029035	0.811291	-0.163233
H	1.441329	-0.059461	-1.611755
H	0.710956	-2.567672	1.373727
H	-0.474097	-0.971491	-0.283378
H	-0.527806	0.783615	-0.421876

Table 130: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	-0.017105	-0.045828	-0.017552
C	0.000682	-0.020315	1.514759
C	1.361786	0.009971	-0.673159
O	1.913035	-1.362913	-0.554430
O	3.193446	-1.413165	-0.873969
O	0.907851	-0.939817	2.104472
O	0.445970	-2.278002	1.772109
H	-1.012159	-0.179402	1.907788
H	0.368176	0.946592	1.882707
H	2.055019	0.644485	-0.111995
H	1.076192	-2.490246	1.055559
H	-0.534874	-0.944544	-0.372225
H	-0.605981	0.811536	-0.367351
C	1.337187	0.395269	-2.144958
H	2.334927	0.284516	-2.577752
H	0.635856	-0.234946	-2.702793
H	1.025344	1.439761	-2.251887

Table 131: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-0.005684	-0.025292	-0.011633
C	0.002138	0.008745	1.521813
C	1.413199	0.006498	-0.606158
O	1.604372	-1.129644	-1.539641
O	1.545702	-2.302359	-0.938424
O	0.858114	-0.972824	2.090346
O	0.316237	-2.275370	1.742514
H	-1.017960	-0.103471	1.910467
H	0.420169	0.950039	1.902095
H	2.153419	-0.159535	0.181954
H	0.842718	-2.467934	0.935553
H	-0.504861	-0.943446	-0.333186
H	-0.602931	0.812883	-0.390487
C	1.741029	1.241489	-1.428405
H	2.757711	1.192763	-1.829711
H	1.039094	1.353241	-2.261676
H	1.663758	2.131220	-0.794457

Table 132: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-0.009734	0.006485	-0.011245
C	0.011863	-0.001760	1.516425
C	1.381721	-0.010333	-0.637998
O	2.084908	-1.261558	-0.264879
O	1.455678	-2.336654	-0.709797
O	0.709595	1.109529	2.075443
O	-0.062556	2.305061	1.753337
H	0.578157	-0.859543	1.897525
H	-1.008142	-0.044533	1.920772
H	2.018774	0.740302	-0.161505
H	-0.333090	2.568163	2.651431
H	-0.570227	-0.864779	-0.369502
H	-0.536352	0.903196	-0.354542
C	1.388718	0.139174	-2.152085
H	0.947326	1.101034	-2.433216
H	2.411368	0.102148	-2.540194
H	0.808401	-0.663269	-2.616820

Table 133: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-0.002066	-0.008205	0.000308
C	0.024807	0.007144	1.530846
C	1.371951	-0.020040	-0.667856
O	2.101381	-1.269192	-0.341828
O	1.420796	-2.350041	-0.684435
O	0.743194	-1.071744	2.116269
O	0.023950	-2.291802	1.807226
H	-1.000820	0.029507	1.921943
H	0.560133	0.887815	1.909324
H	2.035471	0.726443	-0.217463
H	0.595306	-2.658917	1.098566
H	-0.569968	-0.875037	-0.350058
H	-0.538510	0.885896	-0.342982
C	1.326455	0.133798	-2.182979
H	0.881487	1.098211	-2.449155
H	2.333943	0.089034	-2.607677
H	0.723541	-0.664816	-2.625158

Table 134: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2CH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-0.056996	-0.041961	-0.044125
C	-0.047032	-0.059450	1.509097
C	1.374237	-0.057706	-0.596213
O	1.966779	-1.389322	-0.439935
O	3.057800	-1.524770	-1.173088
O	0.970138	-0.831395	2.128516
O	0.665815	-2.241712	1.939893
H	-1.033037	-0.354395	1.891907
H	0.180972	0.946770	1.885272
H	2.029535	0.642858	-0.068897
H	1.395270	0.158431	-1.667643
H	1.318421	-2.450235	1.242789
C	-0.691082	1.297253	-0.481319
H	-0.828173	1.332143	-1.567805
H	-1.677454	1.420445	-0.019128
H	-0.075319	2.155822	-0.186346
C	-0.887128	-1.201811	-0.631369
H	-1.932308	-1.108733	-0.314754
H	-0.866632	-1.179698	-1.727694
H	-0.526034	-2.174570	-0.295411

Table 135: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2C(CH_3)_2CH_2OO$

Cartesian Coordinates (Å)			
C	-0.091181	-0.062690	-0.066035
C	-0.057057	-0.106109	1.491270
C	1.360218	-0.088115	-0.626982
O	1.721526	-1.308238	-1.351354
O	2.031734	-2.328954	-0.572675
O	0.956471	-0.895749	2.086554
O	0.632420	-2.297246	1.880997
H	-1.041424	-0.400584	1.878246
H	0.180752	0.893386	1.879750
H	2.104767	0.040713	0.161721
H	1.498386	0.668372	-1.403743
H	1.253614	-2.491069	1.144815
C	-0.726818	1.289888	-0.457909
H	-1.702008	1.413980	0.027701
H	-0.096747	2.136464	-0.157822
H	-0.884011	1.349101	-1.540867
C	-0.956922	-1.198809	-0.647316
H	-0.971286	-1.165569	-1.742308
H	-0.609076	-2.183484	-0.333357
H	-1.987456	-1.082846	-0.293120

Table 136: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2C(CH_3)_2CH_2OO$

Cartesian Coordinates (Å)			
C	-0.069993	0.002167	-0.056180
C	-0.043719	0.058777	1.487204
C	1.373258	-0.034988	-0.590099
O	2.114810	-1.191583	-0.099964
O	2.052274	-2.214356	-0.940401
O	0.731240	1.120093	2.041520
O	-0.085174	2.330520	2.034517
H	0.453863	-0.837652	1.877165
H	-1.062070	0.100355	1.892467
H	1.939120	0.823559	-0.218705
H	1.403171	-0.076035	-1.681312
H	-0.099139	2.513080	2.991368
C	-0.744044	1.248174	-0.663991
H	-0.804601	1.155462	-1.755129
H	-1.763362	1.357773	-0.278438
H	-0.200216	2.165142	-0.421707
C	-0.848791	-1.261429	-0.466636
H	-0.877700	-1.363481	-1.556710
H	-0.397568	-2.172343	-0.061300
H	-1.883415	-1.203260	-0.107483

Table 137: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2C(CH_3)_2CH_2OO$

Cartesian Coordinates (Å)			
C	-0.104368	-0.058164	-0.021138
C	-0.154943	-0.020829	1.530647
C	1.352455	-0.175587	-0.503296
O	1.906828	-1.515527	-0.295479
O	1.895150	-2.238315	-1.406556
O	0.811887	-0.807218	2.211664
O	0.460436	-2.211337	2.063478
H	-1.163253	-0.268473	1.887167
H	0.096191	0.988633	1.882826
H	2.016871	0.485898	0.060786
H	1.439137	0.018634	-1.574339
H	1.134281	-2.472587	1.405457
C	-0.637091	1.297869	-0.534988
H	-0.723865	1.297240	-1.627227
H	-1.633214	1.496757	-0.122943
H	0.015694	2.130242	-0.243908
C	-0.974476	-1.190979	-0.599090
H	-2.025235	-1.019087	-0.338460
H	-0.898905	-1.226727	-1.691819
H	-0.691307	-2.165957	-0.199821

Table 138: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH_2C(CH_3)_2CH_2OO$

Cartesian Coordinates (Å)			
C	-0.006078	-0.028352	-0.011693
C	-0.038626	-0.016945	1.525748
C	1.390893	-0.010071	-0.616892
O	1.947571	-1.364752	-0.539087
O	3.120416	-1.444097	-1.140934
O	0.866456	-0.968387	2.096983
O	0.438993	-2.303485	1.701260
H	0.408769	0.923146	1.880548
H	2.081438	0.649903	-0.083382
H	1.380088	0.255039	-1.677306
H	1.105955	-2.481149	1.009285
H	-0.549521	-0.900383	-0.393580
H	-0.542481	0.856946	-0.375646
C	-1.450782	-0.158862	2.088270
H	-1.425929	-0.106350	3.180677
H	-2.101074	0.640967	1.715642
H	-1.880473	-1.121858	1.798792

Table 139: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	-0.012436	-0.036861	-0.011769
C	-0.042672	-0.014494	1.527238
C	1.417131	-0.010483	-0.570710
O	1.654448	-1.091823	-1.532590
O	1.640179	-2.282423	-0.961026
O	0.833556	-1.006331	2.076605
O	0.356137	-2.319632	1.671605
H	0.435899	0.906942	1.889725
H	2.161518	-0.133460	0.219892
H	1.637279	0.882778	-1.159373
H	0.920660	-2.468498	0.881511
H	-0.508396	-0.950031	-0.355217
H	-0.594152	0.806177	-0.399667
C	-1.457008	-0.113957	2.092266
H	-1.427660	-0.070061	3.184996
H	-2.079544	0.710723	1.726752
H	-1.918878	-1.059884	1.796879

Table 140: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	0.042028	-0.053329	0.021170
C	0.023535	-0.046999	1.557320
C	1.421261	0.048677	-0.615687
O	2.184900	-1.197139	-0.514244
O	1.634829	-2.158284	-1.237844
O	0.684198	1.115967	2.082230
O	-0.064320	2.288684	1.645900
H	-1.025852	-0.022814	1.885228
H	2.052259	0.781581	-0.107269
H	1.351359	0.286203	-1.680342
H	-0.407960	2.591431	2.505646
H	-0.455646	-0.954562	-0.355118
H	-0.542219	0.806001	-0.325548
C	0.738878	-1.219812	2.226436
H	0.313208	-2.164260	1.872920
H	1.806116	-1.222698	1.990037
H	0.620647	-1.165893	3.312944

Table 141: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	-0.011553	-0.032835	-0.012965
C	-0.042836	-0.014124	1.522126
C	1.383353	-0.004833	-0.624919
O	2.168463	-1.200665	-0.312784
O	1.563910	-2.302506	-0.727661
O	0.711904	-1.092737	2.092749
O	0.082498	-2.345907	1.718503
H	0.531512	0.849919	1.887004
H	2.005415	0.802865	-0.228083
H	1.339175	0.066459	-1.716173
H	0.710381	-2.660061	1.033174
H	-0.542294	-0.915602	-0.381452
H	-0.552180	0.844913	-0.390085
C	-1.463511	0.042261	2.081074
H	-1.433198	0.056104	3.174555
H	-1.981499	0.943884	1.734895
H	-2.035496	-0.833738	1.763146

Table 142: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH_2CH_2OO$

Cartesian Coordinates (Å)			
C	-0.027217	-0.067872	-0.031942
C	-0.038617	-0.024001	1.504980
C	1.359764	-0.002574	-0.670266
O	1.921214	-1.371888	-0.562208
O	3.206096	-1.407775	-0.866138
O	0.890149	-0.945065	2.087969
O	0.481805	-2.296787	1.732245
H	0.393722	0.932354	1.834000
H	2.042899	0.630132	-0.095171
H	1.123596	-2.469933	1.015676
H	-0.535031	-0.973613	-0.385149
H	-0.614814	0.780991	-0.402676
C	1.349711	0.397877	-2.138570
H	2.352901	0.297705	-2.561234
H	0.658424	-0.230477	-2.710871
H	1.032772	1.441535	-2.238126
C	-1.441129	-0.180144	2.088844
H	-1.402526	-0.104815	3.179622
H	-2.110963	0.599919	1.708847
H	-1.856348	-1.156795	1.825037

Table 143: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-0.018369	-0.067764	-0.030609
C	-0.037800	-0.007128	1.506954
C	1.407758	-0.011924	-0.605276
O	1.622660	-1.128202	-1.556415
O	1.605375	-2.309527	-0.969100
O	0.846712	-0.982669	2.074324
O	0.377052	-2.307215	1.698221
H	0.439437	0.924631	1.844680
H	2.138112	-0.183198	0.190636
H	0.926528	-2.462151	0.898479
H	-0.494908	-1.001489	-0.343368
H	-0.625132	0.750953	-0.434837
C	1.732100	1.242154	-1.399888
H	2.756107	1.215383	-1.784211
H	1.042974	1.359102	-2.243066
H	1.630775	2.119068	-0.751644
C	-1.447043	-0.100272	2.085845
H	-1.408689	-0.035388	3.177290
H	-2.075831	0.714894	1.709819
H	-1.908059	-1.053330	1.812819

Table 144: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-0.028876	0.001594	-0.016652
C	-0.037781	-0.013442	1.516593
C	1.372648	-0.009543	-0.619728
O	2.062337	-1.273784	-0.262847
O	1.434913	-2.335091	-0.741692
O	0.705516	1.093247	2.058291
O	0.045181	2.331021	1.650032
H	0.571228	-0.853566	1.874969
H	2.006150	0.725994	-0.116570
H	-0.266137	2.644008	2.517779
H	-0.577858	-0.868439	-0.393883
H	-0.551324	0.899254	-0.364696
C	1.405735	0.170785	-2.130238
H	0.978974	1.142972	-2.398159
H	2.434424	0.131190	-2.501970
H	0.825486	-0.615758	-2.621595
C	-1.442148	-0.107071	2.107947
H	-1.396033	-0.101278	3.202300
H	-2.062152	0.731941	1.776975
H	-1.928340	-1.036194	1.791963

Table 145: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-0.024921	-0.051482	-0.018605
C	-0.033486	-0.019195	1.516987
C	1.361476	-0.023230	-0.660892
O	2.126698	-1.247466	-0.326875
O	1.493508	-2.348660	-0.695962
O	0.713117	-1.100702	2.093133
O	0.059090	-2.349281	1.748736
H	0.556644	0.841160	1.864997
H	1.992744	0.743206	-0.197863
H	0.665559	-2.676940	1.050029
H	-0.560814	-0.938065	-0.371610
H	-0.577319	0.822218	-0.386690
C	1.338243	0.134746	-2.176471
H	0.869818	1.086611	-2.447452
H	2.354216	0.121580	-2.582847
H	0.767622	-0.679685	-2.632333
C	-1.445509	0.064010	2.094898
H	-1.399228	0.088041	3.187715
H	-1.955181	0.969831	1.747129
H	-2.034675	-0.806609	1.794026

Table 146: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)CH_2CH(CH_3)OO$

6.3 Reactants for 1,6-hydrogen shift in OOQOOH

For all OOQOOH molecules undergoin 1,6-hydrogen shift we have chosen six low energy conformers to calculate the hindered rotor contribution to the partition function. For each of these conformers the B3LYP/6-31G(d) optimized geometry is given below. In addition to the B3LYP/6-31G(d) energy of the six conformers B3LYP/CBSB7 optimized geometry of the lowest energy conformer is also given. Thus for each of the four reactants we give five geometries each.

	Cartesian Coordinates (Å)		
C	-1.771947	0.724408	-0.041542
H	-2.049141	1.496769	0.685010
H	-2.621194	0.556575	-0.711584
C	-0.535191	1.139486	-0.838833
H	-0.826370	1.977870	-1.481417
H	-0.256279	0.326413	-1.514556
C	0.671641	1.578290	0.004914
H	1.413293	2.062072	-0.638805
H	0.355915	2.335900	0.733204
C	1.378853	0.480845	0.796588
H	0.697461	-0.114937	1.400494
H	2.178092	0.896460	1.412776
O	-1.587587	-0.433422	0.772305
O	-1.493143	-1.578228	-0.112592
H	-0.525969	-1.698927	-0.154497
O	2.093819	-0.432182	-0.100970
O	1.383668	-1.478214	-0.465916

Table 147: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOO(CH_2)_4OO$

	Cartesian Coordinates (Å)		
C	-1.888501	-1.045846	-0.042010
H	-1.844440	-1.953301	-0.655241
H	-2.875922	-0.991313	0.427475
C	-0.789826	-1.049083	1.021629
H	-1.031417	-1.843527	1.736578
H	-0.834791	-0.114001	1.586459
C	0.632389	-1.294447	0.493819
H	1.302002	-1.512876	1.332844
H	0.635256	-2.187050	-0.143706
C	1.263422	-0.162206	-0.320887
H	0.582802	0.201798	-1.088673
O	-1.775762	0.000339	-1.005695
O	-2.113513	1.244437	-0.342107
H	-1.224656	1.596843	-0.146392
O	1.504630	0.987976	0.585553
O	0.548667	1.889728	0.575007
C	2.628126	-0.510142	-0.891438
H	2.529986	-1.334242	-1.601875
H	3.057639	0.345674	-1.415011
H	3.317706	-0.817486	-0.101202

Table 148: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOO(CH_2)_3CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-1.593744	0.119979	0.347064
H	-2.142364	0.702471	1.095510
C	-0.489912	-0.663119	1.077617
H	-0.973267	-1.256665	1.861483
H	0.147525	0.055126	1.600073
C	0.374146	-1.607369	0.225870
H	0.977395	-2.237402	0.887580
H	-0.259129	-2.294025	-0.346310
C	1.317335	-0.940863	-0.773016
H	0.826171	-0.186025	-1.383669
H	1.814182	-1.683291	-1.400009
O	-1.066326	1.051226	-0.613260
O	-0.420597	2.127192	0.109727
H	0.515326	1.858964	0.045095
O	2.437041	-0.293806	-0.079707
O	2.224330	0.973217	0.203586
C	-2.576833	-0.737179	-0.443934
H	-3.031267	-1.487701	0.207769
H	-3.367698	-0.109971	-0.857776
H	-2.088410	-1.252797	-1.274110

Table 149: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOOCH(CH_3)(CH_2)_3OO$

Cartesian Coordinates (Å)			
C	-1.876075	-0.176844	0.257410
H	-2.678771	0.349442	0.785706
C	-0.720358	-0.390922	1.249825
H	-1.127863	-0.929454	2.112664
H	-0.411862	0.586709	1.629635
C	0.503588	-1.165938	0.734960
H	1.142227	-1.432334	1.584403
H	0.189255	-2.113731	0.285794
C	1.381860	-0.448877	-0.293888
H	0.782530	0.004911	-1.081415
O	-1.498664	0.640675	-0.863269
O	-1.324427	1.999194	-0.392823
H	-0.353746	2.042056	-0.300126
O	2.076843	0.672143	0.386415
O	1.472505	1.832862	0.267738
C	-2.435273	-1.452303	-0.365477
H	-2.740615	-2.151955	0.416826
H	-3.304819	-1.215784	-0.980445
H	-1.699236	-1.948349	-1.002581
C	2.493929	-1.319160	-0.855395
H	3.131636	-0.745405	-1.530091
H	3.113620	-1.729294	-0.053961
H	2.061553	-2.151538	-1.415499

Table 150: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOOCH(CH_3)(CH_2)_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-1.784907	0.705169	-0.051204
H	-2.077286	1.482111	0.668327
H	-2.628888	0.523669	-0.728098
C	-0.546659	1.132733	-0.842871
H	-0.842165	1.971797	-1.486843
H	-0.254920	0.320795	-1.518287
C	0.651704	1.581414	0.010035
H	1.392973	2.079141	-0.627655
H	0.322166	2.332184	0.742860
C	1.366894	0.486050	0.801105
H	0.686013	-0.123003	1.395534
H	2.155301	0.909240	1.430621
O	-1.592053	-0.442321	0.774522
O	-1.468934	-1.589942	-0.108070
H	-0.491764	-1.687415	-0.134333
O	2.105488	-0.409521	-0.093741
O	1.407546	-1.463305	-0.478276

Table 151: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOO(CH_2)_4OO$

Cartesian Coordinates (Å)			
C	-1.834487	0.649869	-0.052243
H	-2.131880	1.350726	0.739600
H	-2.678542	0.531374	-0.743429
C	-0.598643	1.144220	-0.803556
H	-0.892190	2.029152	-1.383280
H	-0.312117	0.383280	-1.537167
C	0.617926	1.518816	0.061095
H	1.423346	1.867985	-0.595137
H	0.366737	2.356291	0.727157
C	1.173558	0.403827	0.944898
H	0.470383	0.086356	1.715108
H	2.133726	0.678423	1.389402
O	-1.639838	-0.569683	0.665777
O	-1.435751	-1.625241	-0.314294
H	-0.468687	-1.747988	-0.234273
O	1.398137	-0.826713	0.180172
O	2.419839	-0.707862	-0.654046

Table 152: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOO(CH_2)_4OO$

Cartesian Coordinates (Å)			
C	-1.871832	-0.819495	0.085768
H	-2.232751	-1.523924	-0.675135
H	-2.591903	-0.800750	0.913934
C	-0.476653	-1.196950	0.588284
H	-0.526473	-2.178451	1.076443
H	-0.201302	-0.474630	1.363345
C	0.575082	-1.190736	-0.538781
H	0.671812	-2.182948	-0.997488
H	0.257773	-0.504175	-1.329462
C	1.957080	-0.751209	-0.078599
H	2.677137	-0.714979	-0.901689
H	2.357083	-1.359802	0.737757
O	-1.898837	0.425079	-0.608657
O	-1.569056	1.466214	0.353996
H	-0.669701	1.708223	0.053930
O	1.917358	0.593239	0.515663
O	1.445068	1.488191	-0.333710

Table 153: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOO(CH_2)_4OO$

Cartesian Coordinates (Å)			
C	1.809748	0.677046	-0.022526
H	2.694931	1.089349	-0.522024
H	1.875404	0.929889	1.044821
C	0.536315	1.258794	-0.674520
H	0.236405	0.594856	-1.494026
H	0.810482	2.211087	-1.146723
C	-0.659326	1.560135	0.247870
H	-0.318123	2.155249	1.107195
H	-1.375118	2.190369	-0.294806
C	-1.422032	0.369851	0.821750
H	-2.249208	0.705441	1.453964
H	-0.782691	-0.324454	1.366373
O	2.003203	-0.720407	-0.197332
O	1.114628	-1.432578	0.704536
H	0.365753	-1.634179	0.101968
O	-2.101531	-0.377683	-0.242212
O	-1.372059	-1.358404	-0.746516

Table 154: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOO(CH_2)_4OO$

Cartesian Coordinates (Å)			
C	-1.901066	-1.033616	-0.033606
H	-1.865352	-1.951542	-0.636309
H	-2.889402	-0.966350	0.437757
C	-0.800245	-1.037193	1.030283
H	-1.045302	-1.828717	1.751087
H	-0.837866	-0.096149	1.590197
C	0.620530	-1.293917	0.499722
H	1.292029	-1.518480	1.338873
H	0.614578	-2.189055	-0.138487
C	1.258086	-0.165776	-0.319818
H	0.575547	0.201986	-1.086788
O	-1.778477	-0.002179	-1.011190
O	-2.095271	1.253683	-0.352723
H	-1.190280	1.589900	-0.169201
O	1.519631	0.981039	0.581664
O	0.566420	1.893849	0.580509
C	2.618264	-0.530903	-0.898093
H	2.506348	-1.357652	-1.607233
H	3.057710	0.319687	-1.427396
H	3.310153	-0.846336	-0.109517

Table 155: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOO(CH_2)_3CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-2.007822	-0.886480	-0.017046
H	-2.039631	-1.761848	-0.679852
H	-2.976340	-0.802779	0.492186
C	-0.878757	-1.002605	1.007506
H	-1.144883	-1.810810	1.701506
H	-0.855170	-0.085924	1.605929
C	0.522772	-1.298807	0.444602
H	1.225156	-1.397282	1.280811
H	0.517746	-2.265150	-0.078628
C	1.090399	-0.269531	-0.537369
H	0.462313	-0.194490	-1.426831
O	-1.865871	0.197199	-0.936638
O	-2.011033	1.432218	-0.182108
H	-1.073469	1.704045	-0.116541
O	0.935896	1.100536	0.017857
O	1.628610	1.278248	1.131771
C	2.548231	-0.501694	-0.903308
H	2.658761	-1.485594	-1.371621
H	2.898359	0.256269	-1.610929
H	3.177412	-0.467338	-0.009412

Table 156: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOO(CH_2)_3CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	1.912249	-1.193747	-0.061590
H	2.157081	-1.886782	0.754010
H	2.515336	-1.460138	-0.939221
C	0.419631	-1.224973	-0.400023
H	0.160276	-2.227793	-0.761168
H	0.261354	-0.538406	-1.237948
C	-0.457308	-0.811833	0.798529
H	-0.742284	-1.684506	1.400041
H	0.121142	-0.151983	1.451732
C	-1.735657	-0.063949	0.420922
H	-2.234975	0.302421	1.324481
O	2.343641	0.060819	0.459408
O	2.195689	1.045781	-0.602255
H	1.426984	1.552418	-0.269767
O	-1.381746	1.156586	-0.349346
O	-0.575633	1.955926	0.323317
C	-2.711783	-0.812139	-0.473242
H	-3.077521	-1.701851	0.049952
H	-3.571806	-0.183776	-0.724552
H	-2.233990	-1.132662	-1.404128

Table 157: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOO(CH_2)_3CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	1.982800	0.931958	0.109435
H	2.880170	1.435685	-0.270355
H	1.779711	1.319097	1.117559
C	0.805092	1.190777	-0.855758
H	0.798360	0.394499	-1.609231
H	1.024584	2.117157	-1.402434
C	-0.594470	1.373372	-0.239620
H	-0.539215	2.114912	0.569955
H	-1.261481	1.801056	-0.999862
C	-1.285106	0.137205	0.340992
H	-0.646220	-0.369116	1.064752
O	2.422873	-0.417427	0.193196
O	1.491137	-1.166033	1.018878
H	0.923972	-1.575269	0.328519
O	-1.523124	-0.830325	-0.757467
O	-0.564418	-1.726780	-0.904952
C	-2.665186	0.428150	0.913828
H	-3.134339	-0.487810	1.284942
H	-2.575866	1.131629	1.748163
H	-3.320199	0.873918	0.157497

Table 158: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOO(CH_2)_3CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	1.509440	-0.483054	0.265172
H	1.685806	-1.188278	1.091146
C	0.422573	-1.053733	-0.658958
H	0.870221	-1.871083	-1.238495
H	0.136650	-0.286813	-1.387941
C	-0.819090	-1.613327	0.057316
H	-1.416224	-2.203553	-0.649195
H	-0.503312	-2.309758	0.847451
C	-1.745940	-0.595640	0.720967
H	-1.216205	0.111227	1.359636
H	-2.541029	-1.098055	1.279957
O	1.059390	0.672904	0.996116
O	0.872801	1.768998	0.057928
H	-0.100321	1.726917	-0.069978
O	-2.486717	0.172009	-0.284440
O	-1.890631	1.298482	-0.631752
C	2.827913	-0.212319	-0.456883
H	3.553590	0.218054	0.239887
H	3.241845	-1.142620	-0.862197
H	2.680851	0.493247	-1.278773

Table 159: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)(CH_2)_3OO$

Cartesian Coordinates (Å)			
C	-1.540142	0.436783	0.274366
H	-1.696534	1.047671	1.176016
C	-0.447783	1.071764	-0.595995
H	-0.876716	1.949563	-1.095165
H	-0.189838	0.365859	-1.392938
C	0.828123	1.527348	0.135758
H	1.510749	1.977766	-0.594027
H	0.584678	2.312195	0.865763
C	1.593266	0.445885	0.893794
H	1.015010	0.013779	1.710649
H	2.558936	0.809874	1.254287
O	-1.113969	-0.804256	0.872239
O	-0.884362	-1.778182	-0.186477
H	0.093305	-1.774132	-0.209921
O	1.871152	-0.713608	0.040360
O	2.778496	-0.439148	-0.884349
C	-2.868080	0.268828	-0.461352
H	-3.601049	-0.211579	0.193844
H	-3.262841	1.242594	-0.772492
H	-2.738544	-0.355682	-1.349635

Table 160: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)(CH_2)_3OO$

Cartesian Coordinates (Å)			
C	-1.693635	-0.069807	0.397043
H	-2.205612	0.299245	1.296195
C	-0.404910	-0.789307	0.826824
H	-0.667638	-1.648877	1.456585
H	0.152754	-0.094743	1.462492
C	0.475029	-1.224214	-0.361550
H	0.225953	-2.238098	-0.698070
H	0.301152	-0.555600	-1.210351
C	1.964617	-1.193191	-0.052466
H	2.573994	-1.470076	-0.918202
H	2.242279	-1.808805	0.808214
O	-1.410537	1.053132	-0.450115
O	-0.655491	2.023169	0.327452
H	0.229351	1.931678	-0.079846
O	2.398739	0.149186	0.362833
O	2.133684	1.055592	-0.560931
C	-2.655004	-0.928415	-0.422446
H	-2.975845	-1.794597	0.166261
H	-3.540373	-0.348695	-0.699399
H	-2.183751	-1.290454	-1.342220

Table 161: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)(CH_2)_3OO$

Cartesian Coordinates (Å)			
C	-1.548365	-0.173493	0.204556
H	-1.478646	-0.328208	1.290570
C	-0.480567	-1.022302	-0.535101
H	-0.092129	-0.427787	-1.370232
H	-0.982841	-1.884250	-0.992036
C	0.674694	-1.587427	0.311391
H	0.268474	-2.074357	1.209707
H	1.183363	-2.375642	-0.257908
C	1.734312	-0.600875	0.793857
H	2.491032	-1.106112	1.400841
H	1.313988	0.247734	1.333441
O	-1.426031	1.231179	-0.049572
O	-0.296769	1.752991	0.696769
H	0.412174	1.721823	0.017772
O	2.515311	-0.080375	-0.334303
O	2.000356	1.010665	-0.875582
C	-2.964452	-0.503388	-0.268929
H	-3.200930	-1.549650	-0.049705
H	-3.695117	0.135544	0.234157
H	-3.056040	-0.349854	-1.349750

Table 162: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)(CH_2)_3OO$

Cartesian Coordinates (Å)			
C	1.690054	-0.694308	0.234545
H	1.636293	-1.561818	0.909455
C	0.662553	-0.872442	-0.893714
H	1.050115	-1.636041	-1.580267
H	0.605542	0.054878	-1.475067
C	-0.738713	-1.318982	-0.441129
H	-1.311913	-1.664811	-1.311447
H	-0.643499	-2.186362	0.227597
C	-1.595078	-0.281868	0.294432
H	-1.028473	0.218110	1.080959
O	1.336417	0.367082	1.140857
O	1.465142	1.635681	0.440625
H	0.528391	1.795417	0.190367
O	-1.986420	0.774261	-0.668753
O	-1.182563	1.820697	-0.674812
C	3.121601	-0.541403	-0.275632
H	3.803603	-0.392893	0.567119
H	3.432724	-1.438459	-0.822921
H	3.204732	0.322138	-0.940594
C	-2.910763	-0.844351	0.814843
H	-2.709348	-1.614450	1.566610
H	-3.514053	-0.058804	1.279322
H	-3.492642	-1.298551	0.005458

Table 163: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)(CH_2)_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-1.748237	-0.609773	-0.250495
H	-1.725463	-1.414157	-1.000808
C	-0.703675	-0.892752	0.837549
H	-1.088722	-1.700880	1.472348
H	-0.628352	-0.011464	1.483602
C	0.694547	-1.312696	0.349038
H	1.317902	-1.539725	1.222142
H	0.620006	-2.241365	-0.233760
C	1.448859	-0.306533	-0.524612
H	0.895903	-0.096703	-1.441986
O	-1.398182	0.521944	-1.072130
O	-1.414661	1.721746	-0.246644
H	-0.453959	1.847971	-0.112470
O	1.430023	1.035032	0.114747
O	2.057290	1.052550	1.280291
C	-3.164907	-0.472924	0.304355
H	-3.863942	-0.243592	-0.505633
H	-3.482266	-1.404341	0.786690
H	-3.212928	0.334972	1.039788
C	2.887968	-0.700190	-0.820412
H	2.907301	-1.659501	-1.348526
H	3.374942	0.048975	-1.452464
H	3.456483	-0.801146	0.108438

Table 164: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)(CH_2)_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-2.004129	-0.277869	0.340703
H	-2.677437	0.083368	1.130034
C	-0.644934	-0.617350	0.973924
H	-0.785710	-1.418179	1.711235
H	-0.321575	0.266368	1.532332
C	0.432761	-1.003483	-0.057484
H	0.421800	-2.081785	-0.256944
H	0.227097	-0.501803	-1.008665
C	1.849539	-0.626902	0.366313
H	2.086739	-1.019619	1.361306
O	-1.879924	0.754560	-0.647961
O	-1.446042	1.969072	0.023165
H	-0.512642	2.013583	-0.267837
O	1.927028	0.836860	0.627945
O	1.534454	1.552752	-0.409509
C	-2.664610	-1.437050	-0.402905
H	-2.849138	-2.266724	0.288088
H	-3.620857	-1.119571	-0.828890
H	-2.032033	-1.800879	-1.219235
C	2.929514	-0.999222	-0.639565
H	3.916519	-0.679854	-0.290931
H	2.948035	-2.084961	-0.781268
H	2.726228	-0.524638	-1.604269

Table 165: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)(CH_2)_2CH(CH_3)OO$

Cartesian Coordinates (Å)			
C	-1.779510	-0.377438	0.236276
H	-1.523583	-0.723501	1.247647
C	-0.713717	-0.853632	-0.786470
H	-0.546336	-0.044356	-1.506715
H	-1.141053	-1.682478	-1.364498
C	0.624687	-1.361082	-0.218892
H	0.426739	-2.075806	0.592689
H	1.152851	-1.925045	-0.999101
C	1.598611	-0.318215	0.335771
H	1.110408	0.339142	1.056106
O	-1.921002	1.047276	0.280679
O	-0.794073	1.616197	0.995657
H	-0.189500	1.839199	0.254013
O	2.049885	0.546602	-0.781840
O	1.310423	1.625755	-0.963932
C	-3.181449	-0.867664	-0.131515
H	-3.213520	-1.962274	-0.119549
H	-3.918893	-0.485643	0.579898
H	-3.458799	-0.526315	-1.135171
C	2.876950	-0.922709	0.899582
H	3.561539	-0.139806	1.239112
H	2.635058	-1.562651	1.754455
H	3.389804	-1.532673	0.148092

Table 166: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)(CH_2)_2CH(CH_3)OO$

6.4 Reactants for 1,7-hydrogen shift in OOQOOH

For all OOQOOH molecules undergoin 1,7-hydrogen shift we have chosen six low energy conformers to calculate the hindered rotor contribution to the partition function. For each of these conformers the B3LYP/6-31G(d) optimized geometry is given below. In addition to the B3LYP/6-31G(d) energy of the six conformers B3LYP/CBSB7 optimized geometry of the lowest energy conformer is also given. Thus for each of the two reactants we give five geometries each.

	Cartesian Coordinates (Å)		
C	1.423842	0.862828	0.528821
H	0.921251	0.246011	1.272616
H	1.881396	1.729701	1.008669
C	0.515208	1.237987	-0.635520
H	1.020371	1.985526	-1.254612
H	0.363747	0.349186	-1.248729
C	-0.851791	1.785281	-0.181464
H	-1.395090	2.109556	-1.076238
H	-0.698806	2.690626	0.418316
C	-1.738437	0.814496	0.619300
H	-2.628165	1.359871	0.955422
H	-1.233966	0.481920	1.530037
C	-2.241637	-0.417928	-0.134278
H	-2.784686	-0.129542	-1.041246
H	-2.922371	-0.994868	0.503100
O	-1.234592	-1.283475	-0.646445
O	-0.539396	-1.862522	0.499089
H	0.383784	-1.763613	0.199841
O	2.576173	0.085704	0.058794
O	2.253993	-1.159751	-0.217479

Table 167: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOO(CH_2)_5OO$

	Cartesian Coordinates (Å)		
C	1.841354	0.850431	0.417287
H	1.444219	0.252666	1.236779
H	2.378156	1.715232	0.811071
C	0.776130	1.229232	-0.604423
H	1.195679	1.963536	-1.298895
H	0.522912	0.337989	-1.179496
C	-0.498446	1.802089	0.044308
H	-1.144200	2.174997	-0.756543
H	-0.234806	2.683932	0.640887
C	-1.292000	0.836635	0.944759
H	-2.102064	1.400439	1.421734
H	-0.665817	0.473389	1.763070
C	-1.941028	-0.388592	0.279120
H	-2.461837	-0.953764	1.062849
O	-1.002596	-1.276945	-0.340913
O	-0.147966	-1.825916	0.705514
H	0.721072	-1.744287	0.270105
O	2.899954	0.048045	-0.205758
O	2.519236	-1.193040	-0.420748
C	-2.929150	-0.059917	-0.836684
H	-3.383693	-0.976299	-1.216332
H	-3.720735	0.589369	-0.454882
H	-2.439062	0.446375	-1.671307

Table 168: B3LYP/CBSB7 optimized geometry of lowest energy conformer of $HOOCH(CH_3)(CH_2)_4OO$

Cartesian Coordinates (Å)			
C	1.407850	0.858981	0.534309
H	0.907995	0.222326	1.265768
H	1.848921	1.727006	1.033051
C	0.503584	1.241178	-0.633539
H	1.012066	1.996296	-1.245243
H	0.358164	0.354730	-1.255710
C	-0.868986	1.780918	-0.183798
H	-1.411887	2.100783	-1.083583
H	-0.724042	2.690151	0.416733
C	-1.753140	0.804631	0.615127
H	-2.653715	1.344272	0.939732
H	-1.251736	0.484431	1.534826
C	-2.236704	-0.439102	-0.136012
H	-2.783075	-0.158928	-1.046562
H	-2.914677	-1.021568	0.503409
O	-1.220050	-1.293943	-0.646420
O	-0.514978	-1.854246	0.505748
H	0.409637	-1.733092	0.197182
O	2.575405	0.107848	0.061204
O	2.270464	-1.145414	-0.225048

Table 169: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOO(CH_2)_5OO$

Cartesian Coordinates (Å)			
C	-1.411112	0.859421	0.533311
H	-1.855031	1.727953	1.028629
H	-0.911223	0.226379	1.267936
C	-0.505457	1.240127	-0.633979
H	-0.358329	0.352589	-1.254192
H	-1.013763	1.993519	-1.247945
C	0.866086	1.781832	-0.183536
H	0.719786	2.690894	0.416920
H	1.409049	2.102339	-1.083062
C	1.750981	0.806576	0.615847
H	1.248834	0.484570	1.534508
H	2.650089	1.347604	0.942177
C	2.237695	-0.435786	-0.135594
H	2.916577	-1.016949	0.504040
H	2.783967	-0.154085	-1.045736
O	1.223112	-1.292568	-0.646678
O	0.519265	-1.855151	0.505110
H	-0.405713	-1.733638	0.197709
O	-2.576206	0.104430	0.060568
O	-2.267846	-1.148485	-0.223660

Table 170: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOO(CH_2)_5OO$

Cartesian Coordinates (Å)			
C	1.993101	0.220759	0.685255
H	1.295114	-0.171659	1.427884
H	2.965547	0.405473	1.151333
C	1.481846	1.461227	-0.046117
H	1.513868	2.293060	0.672092
H	2.201244	1.707356	-0.837079
C	0.069423	1.318467	-0.634452
H	0.021260	0.404229	-1.236375
H	-0.107703	2.149044	-1.329439
C	-1.044049	1.285467	0.426987
H	-1.315030	2.305105	0.731864
H	-0.699969	0.776827	1.334273
C	-2.305303	0.560041	-0.044932
H	-2.742242	1.042866	-0.928960
H	-3.062038	0.541319	0.750903
O	-2.054984	-0.763538	-0.507628
O	-1.548483	-1.529933	0.623643
H	-0.618826	-1.652145	0.338041
O	2.268624	-0.864480	-0.258626
O	1.257176	-1.701703	-0.406762

Table 171: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOO(CH_2)_5OO$

Cartesian Coordinates (Å)			
C	1.991475	0.221333	0.685818
H	1.292640	-0.172021	1.427146
H	2.963158	0.406287	1.153388
C	1.480485	1.461989	-0.045469
H	1.511931	2.293673	0.672930
H	2.200334	1.708376	-0.835940
C	0.068436	1.319046	-0.634662
H	0.020798	0.404839	-1.236685
H	-0.108414	2.149653	-1.329671
C	-1.045623	1.285758	0.426209
H	-1.318195	2.305381	0.729705
H	-0.701314	0.778757	1.334322
C	-2.305694	0.558133	-0.045532
H	-2.743045	1.039688	-0.930047
H	-3.062638	0.539006	0.750104
O	-2.053442	-0.765424	-0.507136
O	-1.545569	-1.530075	0.624688
H	-0.616312	-1.652762	0.337962
O	2.268838	-0.862974	-0.258576
O	1.258495	-1.701331	-0.407902

Table 172: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOO(CH_2)_5OO$

	Cartesian Coordinates (Å)		
C	-1.869733	0.629373	-0.615862
H	-1.216150	0.077218	-1.293217
H	-2.424991	1.391107	-1.170938
C	-1.127508	1.197059	0.589387
H	-1.803285	1.860776	1.142433
H	-0.863493	0.368671	1.251197
C	0.148536	1.968614	0.201723
H	0.556091	2.418937	1.116986
H	-0.121741	2.812408	-0.449253
C	1.259737	1.158483	-0.493795
H	2.044921	1.863345	-0.797982
H	0.895085	0.701955	-1.420816
C	1.941197	0.068542	0.348841
H	2.268846	0.506015	1.303752
O	1.045345	-0.944843	0.827882
O	0.499201	-1.653176	-0.332571
H	-0.444959	-1.682319	-0.064659
O	-2.913765	-0.308101	-0.188537
O	-2.406872	-1.467975	0.190236
C	3.144673	-0.553784	-0.360959
H	3.903082	0.207261	-0.576978
H	3.594304	-1.325279	0.271328
H	2.839606	-1.017052	-1.303952

Table 173: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)(CH_2)_4OO$

	Cartesian Coordinates (Å)		
C	-1.834366	0.844123	0.420638
H	-2.364241	1.710321	0.827721
H	-1.437093	0.234861	1.233987
C	-0.771972	1.229507	-0.604339
H	-0.517891	0.339084	-1.184759
H	-1.197628	1.966300	-1.296516
C	0.504918	1.803358	0.041317
H	0.243531	2.689509	0.637176
H	1.150510	2.173139	-0.764836
C	1.300542	0.838491	0.942538
H	0.676186	0.485227	1.769722
H	2.118789	1.403688	1.409671
C	1.939434	-0.395333	0.279370
H	2.462968	-0.958291	1.066115
O	0.998386	-1.281497	-0.337706
O	0.135379	-1.813610	0.714819
H	-0.734498	-1.715357	0.269671
O	-2.901119	0.056802	-0.206056
O	-2.526576	-1.190956	-0.426559
C	2.928959	-0.072536	-0.840392
H	3.728081	0.572082	-0.459253
H	3.377689	-0.992971	-1.224774
H	2.439955	0.440828	-1.674697

Table 174: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)(CH_2)_4OO$

	Cartesian Coordinates (Å)		
C	-2.292633	-0.439415	0.592426
H	-1.745009	0.159879	1.322742
H	-3.252169	-0.754158	1.013410
C	-1.501479	-1.631328	0.056067
H	-1.463961	-2.381038	0.859249
H	-2.082101	-2.080855	-0.759276
C	-0.080023	-1.292463	-0.422185
H	-0.125474	-0.439592	-1.108796
H	0.298338	-2.137143	-1.010052
C	0.890780	-0.970657	0.729544
H	1.316991	-1.895850	1.139898
H	0.353973	-0.491721	1.555202
C	2.040439	-0.027289	0.342655
H	2.606825	0.222242	1.251512
O	1.559330	1.191897	-0.235993
O	0.734439	1.867765	0.756643
H	-0.137472	1.808366	0.312266
O	-2.677208	0.459376	-0.498497
O	-1.839935	1.466819	-0.670756
C	2.993926	-0.589582	-0.710402
H	3.778370	0.137927	-0.939031
H	3.465924	-1.504580	-0.336583
H	2.466693	-0.825933	-1.640334

Table 175: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)(CH_2)_4OO$

	Cartesian Coordinates (Å)		
C	-2.293028	-0.439106	0.592357
H	-1.745473	0.159616	1.323218
H	-3.252788	-0.753786	1.012872
C	-1.502122	-1.631096	0.055781
H	-1.464981	-2.380957	0.858837
H	-2.082747	-2.080300	-0.759744
C	-0.080457	-1.292674	-0.422120
H	-0.125499	-0.440147	-1.109166
H	0.297983	-2.137708	-1.009438
C	0.889914	-0.970420	0.729816
H	1.315569	-1.895531	1.140962
H	0.352869	-0.490783	1.554902
C	2.040080	-0.027751	0.342770
H	2.606570	0.221771	1.251564
O	1.559822	1.191639	-0.236269
O	0.735435	1.868544	0.755987
H	-0.136688	1.808515	0.312115
O	-2.677115	0.460367	-0.498101
O	-1.838455	1.466595	-0.670865
C	2.993576	-0.590804	-0.709945
H	3.779096	0.135880	-0.937681
H	3.464178	-1.506554	-0.336096
H	2.466623	-0.826065	-1.640316

Table 176: B3LYP/6-31G(d) optimized geometry of low energy conformer of $HOOCH(CH_3)(CH_2)_4OO$