Supporting Information for:

IMPROVEMENT OF THE MODELLING OF THE LOW-TEMPERATURE OXIDATON OF N-BUTANE - STUDY OF THE PRIMARY REACTIONS

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Optimized geometries (Cartesian coordinates) at the B3LYP/6-311G(d,p) level of theory.

Content

1) Species of Table 1 and 2

1-propyl radical

C	-1.30123	-0.286193	0.020152
H	-2.26778	0.188613	-0.097757
H	-1.28225	-1.35711	0.18863
C	-0.057894	0.524517	0.146217
H	0.021679	0.929209	1.17087
H	-0.125382	1.41015	-0.498395
C	1.22409	-0.256275	-0.172081
H	2.11178	0.368443	-0.042631
H	1.21418	-0.621585	-1.20252
H	1.32665	-1.12319	0.487553

2-propyl radical

C	-0.010383	-0.197518	1.29797
C	-0.010383	0.535062	0
H	-0.223134	0.463766	2.14173
H	-0.752102	-1.0062	1.30443
H	0.962717	-0.676058	1.50346
C	-0.010383	-0.197518	-1.29797
H	0.211936	1.59682	0
H	-0.223134	0.463766	-2.14173
H	0.962717	-0.676058	-1.50346
H	-0.752102	-1.0062	-1.30443

1-butyl radical

C	-1.99842	0.130304	-0.01222
H	-2.86743	-0.446258	-0.304842
H	-2.16374	1.12827	0.378158
C	-0.644866	-0.488785	0.03593
H	-0.54877	-1.23958	-0.759713
H	-0.524646	-1.05793	0.976138
C	0.509102	0.521427	-0.065348
H	0.403543	1.26232	0.73605
H	0.416522	1.07407	-1.0067
C	1.8907	-0.131817	0.017914
H	2.0369	-0.853758	-0.791685
H	2.68832	0.612401	-0.054365
H	2.01986	-0.666501	0.964264

2-butyl radical

C	-0.570938	-0.505259	0.092413
C	0.581185	0.442779	0.051401
H	-0.436795	-1.27873	-0.677416
H	-0.567278	-1.06058	1.04836
C	1.98527	-0.042637	-0.068456
H	0.407202	1.47632	0.336947
H	2.68057	0.769494	-0.295279
H	2.34076	-0.517476	0.862161
H	2.08408	-0.803326	-0.852905
C	-1.93705	0.168678	-0.082527
H	-2.75015	-0.560437	-0.031569
H	-2.10849	0.913972	0.700235
H	-2.00069	0.679398	-1.04752

1-propylperoxy radical

C	-4.80E-05	2.00E-06	-0.000281

C	-0.000156	-0.00022	1.53053
H	1.01931	-0.000875	1.92826
H	-0.509246	0.884694	1.91921
H	-0.51338	-0.881084	1.92245
H	-1.02277	0.044449	-0.385548
H	0.518697	0.886904	-0.381096
C	0.674683	-1.21824	-0.611947
O	-0.025569	-2.45428	-0.258596
H	0.701424	-1.17028	-1.70187
H	1.68129	-1.37891	-0.219436
O	-1.18977	-2.5404	-0.871063

2-propylperoxy radical

O	-0.001032	-0.003536	4.90E-05
O	-0.00015	0.001065	1.31585
C	1.37065	0.000561	1.87134
H	1.89027	-0.80646	1.34898
C	2.02778	1.33906	1.57906
H	1.4938	2.14959	2.08202
H	3.06223	1.33321	1.93218
H	2.029	1.52798	0.504841
C	1.20025	-0.315889	3.34636
H	0.688018	-1.27006	3.48386
H	2.1789	-0.376283	3.82802
H	0.620211	0.465	3.84447

1-butylperoxy radical

C	-0.011917	0.015319	0.002751
H	0.072767	-0.07014	1.08738
H	0.981314	0.098691	-0.444098
C	-0.828702	-1.11686	-0.599497
H	-1.83252	-1.07514	-0.164398
H	-0.381167	-2.06105	-0.266065
O	-0.615927	1.32033	-0.273114
O	-1.72847	1.49154	0.412903
C	-0.908031	-1.08467	-2.12997
H	0.105062	-1.14318	-2.54599
H	-1.31522	-0.11956	-2.447
C	-1.76376	-2.21757	-2.70212
H	-2.79113	-2.16249	-2.32979
H	-1.80343	-2.17124	-3.79335
H	-1.36297	-3.19784	-2.42544

2-butylperoxy radical

O	-0.114559	0.128016	0.024403
O	-0.064538	0.153123	1.33922
C	1.31792	0.025112	1.84761
H	1.75786	-0.798033	1.27794
C	2.05942	1.32406	1.57791
H	1.60837	2.15063	2.13314
H	3.10471	1.22984	1.88299
H	2.02923	1.55603	0.512347
C	1.18005	-0.335591	3.32129
H	2.18259	-0.31251	3.76143
H	0.605787	0.454991	3.81682
C	0.528152	-1.69932	3.56671
H	0.44549	-1.90388	4.63674
H	-0.474985	-1.73667	3.13749
H	1.11666	-2.5048	3.11738

1-hydroperoxy-2-propyl radical

H	0.003182	-0.054565	-0.006882
O	-0.003429	0.025594	0.956595
O	1.42966	0.012702	1.22668
C	1.78214	1.33028	1.7077
C	3.20096	1.26425	2.14172
H	1.11561	1.57291	2.54506
H	1.62955	2.06349	0.907776
C	3.60529	0.49151	3.34746
H	3.96737	1.61673	1.46018
H	3.7653	-0.570645	3.10689
H	4.54045	0.865215	3.77463
H	2.83042	0.519995	4.11997

1-hydroperoxy-3-propyl radical

H	-0.005512	-0.049826	-0.031408
O	-0.021871	-0.043466	0.935227
O	1.40794	0.005047	1.20817
C	1.76206	-1.22302	1.83892
H	2.85384	-1.16005	1.88904
H	1.48226	-2.06321	1.19213
C	1.15933	-1.38353	3.23692
H	1.45076	-2.36631	3.62731
H	0.06484	-1.42185	3.11752
C	1.5486	-0.300466	4.18072
H	1.56377	-0.472628	5.24937

H	1.65686	0.714271	3.81967

2-hydroperoxy-1-propyl radical

H	-0.015472	0.007542	0.01203
O	0.000903	0.009673	0.978191
O	1.44156	-0.004339	1.20893
C	1.74726	-1.21158	1.94395
H	1.01217	-1.26802	2.7628
C	3.10725	-0.987213	2.49711
H	3.3362	-0.04636	2.97988
H	3.87382	-1.74717	2.42354
C	1.62596	-2.45371	1.06569
H	2.33703	-2.40434	0.236838
H	1.83032	-3.35597	1.64859
H	0.614818	-2.53089	0.663493

1-hydroperoxy-2-butyl radical

H	0.041435	-0.034163	-0.038886
O	0.023915	-0.041318	0.927758
O	1.45356	-0.009187	1.21249
C	1.73785	1.27678	1.81118
C	3.15817	1.24505	2.24438
H	1.05848	1.41036	2.66223
H	1.54885	2.06877	1.07779
C	3.60436	0.40521	3.39223
H	3.90954	1.67675	1.59025
H	3.67319	-0.645195	3.06419
H	2.82677	0.405048	4.16701
C	4.95073	0.834398	3.98883
H	5.24658	0.174034	4.80778
H	5.74196	0.803059	3.2339
H	4.90198	1.85478	4.37868

1-hydroperoxy-3-butyl radical

H	-0.019542	-0.001948	0.028619
O	0.006084	0.017728	0.994861
O	1.44689	-0.006049	1.20615
C	1.76623	-1.24927	1.82776
H	2.86113	-1.2377	1.83272
H	1.42229	-2.07541	1.19398
C	1.21647	-1.37988	3.24798
H	1.47625	-2.37895	3.62582
H	0.116	-1.36738	3.18174

C	1.70615	-0.324376	4.18147
H	1.91154	0.65571	3.7648
C	1.56881	-0.472692	5.65763
H	1.88148	-1.46785	5.99755
H	2.15973	0.27124	6.19793
H	0.52328	-0.351193	5.98933

1-hydroperoxy-4-butyl radical

H	0.036716	0.020616	-0.056082
O	-0.011567	0.036757	0.90935
O	1.40796	-0.015338	1.23048
C	1.74901	1.22413	1.85143
H	1.505	2.05126	1.17406
H	2.83948	1.15237	1.93611
C	1.10222	1.42352	3.21728
H	0.017011	1.45701	3.08981
H	1.40846	2.40682	3.5954
C	1.47361	0.334531	4.23401
H	2.57476	0.31061	4.33487
H	1.20666	-0.646145	3.82563
C	0.84673	0.52563	5.57093
H	0.741402	-0.303759	6.25943
H	0.603297	1.51736	5.93539

2-hydroperoxy-1-butyl radical

C	-0.007536	0.044783	-0.06192
H	-0.080637	0.113573	1.03426
C	1.42182	-0.042256	-0.467617
H	2.12603	0.702474	-0.115198
H	1.77264	-0.806	-1.15032
O	-0.580423	1.33458	-0.411333
O	-0.616683	1.44984	-1.86092
H	0.164161	1.99824	-2.01681
C	-0.866612	-1.11898	-0.559863
H	-0.831301	-1.12358	-1.65281
H	-0.393967	-2.04808	-0.221468
C	-2.3168	-1.05503	-0.078741
H	-2.89641	-1.89181	-0.476592
H	-2.37652	-1.09778	1.01356
H	-2.79036	-0.12696	-0.403129

2-hydroperoxy-3-butyl radical

H	-0.05462	-0.13997	0.114237

O	0.0195	-0.074005	1.07547
O	1.47217	0.022734	1.21589
C	1.77867	1.33044	1.77656
C	3.19435	1.22292	2.22706
H	1.11604	1.45424	2.64417
C	3.59105	0.326048	3.34611
H	3.96489	1.66782	1.60525
H	3.77142	-0.700011	2.99172
H	4.51305	0.664185	3.8281
H	2.80441	0.257076	4.1039
C	1.52949	2.43945	0.762151
H	0.487666	2.42693	0.437629
H	1.73679	3.41752	1.20463
H	2.17454	2.30816	-0.111257

2-hydroperoxy-4-butyl radical

H	-0.047149	0.104983	0.095828
O	0.016655	0.112624	1.05995
O	1.46121	-0.013864	1.22035
C	1.7438	-1.2895	1.81992
H	2.83607	-1.2318	1.89223
C	1.15142	-1.39205	3.2344
H	1.40015	-2.37726	3.64587
H	0.05456	-1.37892	3.12868
C	1.60252	-0.310224	4.15147
H	1.62011	-0.46308	5.22309
H	1.76106	0.689272	3.76792
C	1.34547	-2.44744	0.910077
H	1.77828	-2.31588	-0.084844
H	1.70754	-3.39535	1.31637
H	0.259495	-2.50995	0.815935

1-hydroperoxy-2-propylperoxy radical

O	-2.02499	-0.305757	0.706566
H	-1.82638	0.645583	0.759943
O	-1.46828	-0.584081	-0.603173
C	-0.170635	-1.11308	-0.426181
H	0.170883	-1.29981	-1.4488
H	-0.206833	-2.06312	0.122451
C	0.797924	-0.175259	0.299146
H	0.447035	0.005085	1.31549
O	0.801765	1.13332	-0.365014
O	-0.248544	1.86437	-0.045288

C	2.23234	-0.670662	0.275227
H	2.29679	-1.64873	0.757514
H	2.59495	-0.767117	-0.750926
H	2.88619	0.019315	0.810451

1-hydroperoxy-3-propylperoxy radical

C	0.004474	0.004355	-0.000871
C	0.006421	-0.004674	1.53167
C	1.41942	0.013181	-0.591735
O	1.64454	-1.10968	-1.51047
O	1.58604	-2.27796	-0.909801
O	0.847213	-1.01117	2.0764
O	0.280392	-2.29773	1.72147
H	-1.01384	-0.117358	1.91281
H	0.432307	0.918885	1.93795
H	2.18177	-0.073001	0.184049
H	1.62084	0.877474	-1.2235
H	0.807005	-2.50877	0.928194
H	-0.514925	-0.888633	-0.353396
H	-0.569145	0.864842	-0.355336

2-hydroperoxy-1-propylperoxy radical

O	0.42166	1.67059	-0.504114
H	-0.548076	1.68914	-0.585745
O	0.529494	0.931787	0.740987
C	0.772374	-0.440928	0.443864
H	0.731424	-0.890336	1.4419
C	-0.339684	-1.04547	-0.418051
H	-0.233164	-2.12909	-0.481287
H	-0.354407	-0.60719	-1.41566
O	-1.65098	-0.848324	0.175417
O	-2.1123	0.371853	-0.027201
C	2.14181	-0.666873	-0.192712
H	2.33632	-1.73215	-0.345042
H	2.20127	-0.154688	-1.15415
H	2.91663	-0.263278	0.46066

1-hydroperoxy-2-butylperoxy radical

O	-2.31775	-0.204566	0.95648
H	-2.06364	0.735104	0.948195
O	-1.99924	-0.542431	-0.417514
C	-0.715688	-1.13261	-0.438209
H	-0.558865	-1.36587	-1.49561

H	-0.704796	-2.06279	0.144012
C	0.401341	-0.224599	0.083533
H	0.238533	-0.004633	1.1398
O	0.34067	1.06644	-0.612204
O	-0.596784	1.85967	-0.131153
C	1.79413	-0.786945	-0.166597
H	1.80564	-1.82063	0.194941
H	1.96017	-0.83327	-1.24823
C	2.90809	0.018928	0.507131
H	3.88647	-0.414556	0.288375
H	2.91103	1.05241	0.154873
H	2.78301	0.032689	1.59363

1-hydroperoxy-3-butylperoxy radical

C	0.000696	-0.000213	0.000371
C	0.00012	-0.000133	1.53238
C	1.4189	0.00025	-0.59061
O	1.5859	-1.13929	-1.52846
O	1.48033	-2.31005	-0.942671
O	0.808989	-1.03069	2.08338
O	0.211856	-2.30157	1.72163
H	-1.02362	-0.080145	1.91271
H	0.453587	0.911312	1.93667
H	2.152	-0.189402	0.196063
H	0.72455	-2.51684	0.920175
H	-0.525827	-0.892379	-0.342204
H	-0.566962	0.862302	-0.36124
C	1.78045	1.22646	-1.40665
H	2.79314	1.14872	-1.80634
H	1.08346	1.3585	-2.23782
H	1.72879	2.11412	-0.771469

1-hydroperoxy-4-butylperoxy radical

C	-1.77218	0.724078	-0.042023
H	-2.04999	1.49628	0.684394
H	-2.62105	0.555689	-0.712363
C	-0.535241	1.13947	-0.838773
H	-0.826344	1.9778	-1.48141
H	-0.255985	0.326512	-1.51447
C	0.671243	1.57849	0.005371
H	1.41288	2.06263	-0.638062
H	0.355142	2.33587	0.733724
C	1.37849	0.481044	0.796793

H	0.697171	-0.115367	1.40009
H	2.17765	0.896304	1.41326
O	-1.58774	-0.433664	0.772164
O	-1.49263	-1.57844	-0.11245
H	-0.525361	-1.6988	-0.154127
O	2.09377	-0.431544	-0.101514
O	1.38435	-1.47827	-0.465605

2-hydroperoxy-1-butylperoxy radical

O	0.127679	1.69581	0.575188
H	1.10078	1.67335	0.552855
O	-0.143025	0.947479	-0.6397
C	-0.398228	-0.413548	-0.297923
H	-0.480592	-0.873842	-1.28957
C	0.7804	-1.0446	0.44773
H	0.648606	-2.12364	0.534537
H	0.916391	-0.598701	1.43265
O	2.02657	-0.895197	-0.284997
O	2.54591	0.310691	-0.148918
C	-1.70389	-0.594159	0.484392
H	-1.81886	-1.65487	0.736209
H	-1.61248	-0.048429	1.42757
C	-2.92735	-0.100922	-0.291232
H	-3.83314	-0.195564	0.312224
H	-2.80842	0.948087	-0.567243
H	-3.07492	-0.677324	-1.20962

2-hydroperoxy-3-butylperoxy radical

O	2.06987	-0.081092	0.897085
H	1.97706	-0.962184	0.494056
O	1.43181	0.711821	-0.133091
C	0.078427	0.967565	0.236194
H	0.064434	1.52463	1.18331
C	-0.700634	-0.337674	0.489015
H	-0.203411	-0.887205	1.28785
O	-0.628368	-1.20061	-0.696579
O	0.515502	-1.85314	-0.779689
C	-0.458932	1.82824	-0.901582
H	-1.4512	2.21438	-0.662373
H	0.209506	2.67586	-1.05827
H	-0.513911	1.2533	-1.82733
C	-2.17689	-0.147374	0.788141
H	-2.63568	-1.09967	1.05838

H	-2.30085	0.542461	1.6265
H	-2.70832	0.258068	-0.074535

2-hydroperoxy-4-butylperoxy radical

C	6.50E-05	0.000207	-7.50E-05
C	0.000223	-3.00E-05	1.53957
C	1.40985	-0.000299	-0.602341
O	1.60009	-1.10177	-1.55458
O	1.54549	-2.28292	-0.978781
O	0.84737	-1.03042	2.0551
O	0.288106	-2.31181	1.67582
H	-1.02256	-0.190087	1.88397
H	2.17667	-0.128688	0.162641
H	1.62773	0.876957	-1.21001
H	0.80829	-2.50432	0.873467
H	-0.51791	-0.898611	-0.339033
H	-0.578626	0.853676	-0.362459
C	0.525383	1.28679	2.16751
H	-0.103942	2.13042	1.87411
H	0.512365	1.20467	3.25537
H	1.55246	1.49722	1.85747

2) Species of Tables 3 and 4

2a) Alkylperoxy radicals

$CH_3CH_2OO.$

C	0.001455	0.001572	-0.001286
H	0.002078	0.00462	1.08971
H	1.03745	-0.001377	-0.349976
H	-0.481087	0.914084	-0.358113
C	-0.718674	-1.22906	-0.517114
H	-0.800012	-1.24319	-1.60526
H	-0.26158	-2.1561	-0.166805
O	-2.11246	-1.24746	-0.073414
O	-2.20391	-1.49485	1.21781

$CH_3CH_2CH_2OO.$

C	-4.80E-05	2.00E-06	-0.000281
C	-0.000156	-0.00022	1.53053
H	1.01931	-0.000875	1.92826
H	-0.509246	0.884694	1.91921
H	-0.51338	-0.881084	1.92245
H	-1.02277	0.044449	-0.385548
H	0.518697	0.886904	-0.381096
C	0.674683	-1.21824	-0.611947
O	-0.025569	-2.45428	-0.258596
H	0.701424	-1.17028	-1.70187
H	1.68129	-1.37891	-0.219436
O	-1.18977	-2.5404	-0.871063

$CH_3CH_2CH_2CH_2OO.$

C	-0.011917	0.015319	0.002751
H	0.072767	-0.07014	1.08738
H	0.981314	0.098691	-0.444098
C	-0.828702	-1.11686	-0.599497
H	-1.83252	-1.07514	-0.164398
H	-0.381167	-2.06105	-0.266065
O	-0.615927	1.32033	-0.273114
O	-1.72847	1.49154	0.412903
C	-0.908031	-1.08467	-2.12997
H	0.105062	-1.14318	-2.54599
H	-1.31522	-0.11956	-2.447
C	-1.76376	-2.21757	-2.70212
H	-2.79113	-2.16249	-2.32979
H	-1.80343	-2.17124	-3.79335
H	-1.36297	-3.19784	-2.42544

$CH_3CH_2CH_2CH_2CH_2OO.$

C	-0.010179	0.010869	0.012751
H	0.055101	-0.068511	1.09922
H	0.990952	0.088555	-0.417081
C	-0.820116	-1.12226	-0.597032
H	-1.8308	-1.07426	-0.179128
H	-0.381132	-2.06538	-0.249738
O	-0.604771	1.31634	-0.280949
O	-1.72974	1.49429	0.382716
C	-0.872501	-1.09803	-2.12846
H	0.147549	-1.16421	-2.5288
H	-1.2704	-0.132673	-2.45978
C	-1.72306	-2.22803	-2.71879

H	-2.74017	-2.1598	-2.31504
H	-1.32636	-3.19403	-2.38302
C	-1.77844	-2.20278	-4.24864
H	-0.779315	-2.30643	-4.68325
H	-2.39553	-3.01671	-4.63825
H	-2.20107	-1.26141	-4.61275

$(CH_3)_2CHCH_2OO.$

C	-0.004086	-0.000852	0.003048
H	-0.01491	0.007618	1.0961
H	1.02497	-0.007512	-0.361101
C	-0.818501	-1.1586	-0.570148
H	-0.83781	-1.01116	-1.65569
O	-0.573842	1.29481	-0.356341
O	-0.371969	1.57436	-1.62939
C	-0.10594	-2.48406	-0.27057
H	-0.03431	-2.66106	0.807831
H	-0.656959	-3.32157	-0.705366
H	0.906749	-2.50071	-0.683183
C	-2.2588	-1.15279	-0.044323
H	-2.28126	-1.31761	1.03841
H	-2.75383	-0.20176	-0.251034
H	-2.84453	-1.94702	-0.514207

$(CH_3)_2CHCH_2CH_2OO.$

C	-0.017505	0.019906	0.017847
H	-1.30E-05	-0.054733	1.10649
H	1.00183	0.101833	-0.36177
C	-0.805598	-1.11928	-0.610998
H	-1.82371	-1.06665	-0.213109
H	-0.374658	-2.06128	-0.247914
O	-0.6033	1.32167	-0.308224
O	-1.75529	1.50173	0.306852
C	-0.847858	-1.12814	-2.15109
H	-1.19172	-0.139546	-2.47758
C	-1.86608	-2.16608	-2.64204
H	-2.86444	-1.96321	-2.24457
H	-1.93346	-2.16533	-3.73345
H	-1.5796	-3.17595	-2.328
C	0.531633	-1.38426	-2.77411
H	1.26441	-0.623937	-2.4913
H	0.923719	-2.36022	-2.46681
H	0.469587	-1.38166	-3.86568

$(CH_3)_2CH_2CH_2CH_2CH_2OO.$

C	-0.004022	0.024553	-0.007905
H	0.136861	-0.09803	1.06729
H	0.962982	0.154841	-0.498844
C	-0.816708	-1.11026	-0.612007
H	-1.80185	-1.10607	-0.133806
H	-0.329096	-2.04699	-0.322358
O	-0.657821	1.32032	-0.20266
O	-1.74081	1.43029	0.540823
C	-0.960179	-1.01744	-2.13587
H	0.032165	-1.09596	-2.60107
H	-1.3396	-0.022005	-2.3892
C	-1.89178	-2.07137	-2.76286
H	-2.86823	-1.98427	-2.2672
C	-2.09757	-1.78071	-4.25586
H	-1.15088	-1.85567	-4.80214
H	-2.79629	-2.49221	-4.70497
H	-2.49505	-0.774257	-4.41482
C	-1.3843	-3.50579	-2.55659
H	-0.394009	-3.63722	-3.00733
H	-1.30839	-3.77027	-1.49892
H	-2.05858	-4.22811	-3.02523

2b) Hydroperoxyalkylperoxy radicals

$HOOCH_2CH_2CH(CH_3)OO.$

C	0.000696	-0.000213	0.000371
C	0.00012	-0.000133	1.53238
C	1.4189	0.00025	-0.59061
O	1.5859	-1.13929	-1.52846
O	1.48033	-2.31005	-0.942671
O	0.808989	-1.03069	2.08338
O	0.211856	-2.30157	1.72163
H	-1.02362	-0.080145	1.91271
H	0.453587	0.911312	1.93667
H	2.152	-0.189402	0.196063
H	0.72455	-2.51684	0.920175
H	-0.525827	-0.892379	-0.342204
H	-0.566962	0.862302	-0.36124
C	1.78045	1.22646	-1.40665
H	2.79314	1.14872	-1.80634
H	1.08346	1.3585	-2.23782

H	1.72879	2.11412	-0.771469

$HOOCH(CH_3)CH_2CH_2OO.$

C	6.50E-05	0.000207	-7.50E-05
C	0.000223	-3.00E-05	1.53957
C	1.40985	-0.000299	-0.602341
O	1.60009	-1.10177	-1.55458
O	1.54549	-2.28292	-0.978781
O	0.84737	-1.03042	2.0551
O	0.288106	-2.31181	1.67582
H	-1.02256	-0.190087	1.88397
H	2.17667	-0.128688	0.162641
H	1.62773	0.876957	-1.21001
H	0.80829	-2.50432	0.873467
H	-0.51791	-0.898611	-0.339033
H	-0.578626	0.853676	-0.362459
C	0.525383	1.28679	2.16751
H	-0.103942	2.13042	1.87411
H	0.512365	1.20467	3.25537
H	1.55246	1.49722	1.85747

2c) Transition states of the isomerizations of the alkylperoxy radicals

$CH_3CH_2OO. \rightarrow CH_2(.)CH_2OOH$

C	0	0	0
H	0	0	1.0952
H	1.0264	0	-0.377064
C	-0.878846	-1.12611	-0.533711
H	-0.795624	-1.34194	-1.59734
H	-1.04088	-1.99759	0.094657
H	-1.92516	-0.21637	-0.420579
O	-0.613871	1.19375	-0.503834
O	-1.98806	0.966617	-0.240437

$CH_3CH_2CH_2OO. \rightarrow CH_3CH(.)CH_2OOH$

C	0	0	0
H	0	0	1.09971
H	1.04501	0	-0.323109
C	-0.741996	1.18624	-0.538898
C	-0.129434	2.58337	-0.412436
H	-0.615418	1.36625	-1.88832
H	-0.475616	3.16133	0.449683
H	0.965437	2.51427	-0.405864

O	-0.585211	3.27471	-1.57641
O	-0.358147	2.32353	-2.60654
H	-0.463226	-0.938076	-0.315838
H	-1.82414	1.16819	-0.395581

$(CH_3)_2CHCH_2OO. \rightarrow (CH_3)_2C(.)CH_2OOH$

C	0	0	0
H	0	0	1.09995
H	1.04322	0	-0.326634
C	-0.749392	1.19084	-0.535353
C	-0.071274	2.56703	-0.390555
H	-0.535294	1.34997	-1.86136
H	-0.434132	3.16653	0.450695
H	1.01667	2.44776	-0.330992
O	-0.435016	3.26723	-1.57904
O	-0.195551	2.29904	-2.59096
H	-0.464674	-0.93748	-0.317355
C	-2.24511	1.19724	-0.331483
H	-2.48538	1.26243	0.739782
H	-2.70257	2.05493	-0.829006
H	-2.70558	0.282115	-0.712756

$CH_3CH_2CH_2OO. \rightarrow CH_2(.)CH_2CH_2OOH$

C	0	0	0
H	0	0	1.40635
H	1.04702	0	-0.291378
C	-0.780556	1.27134	-0.214088
C	-1.65824	1.61023	1.01588
H	-0.104354	2.1109	-0.390041
H	-2.08406	2.6131	0.940136
H	-2.45647	0.873318	1.15173
O	-0.831152	1.63664	2.17052
O	-0.433835	0.305836	2.43063
H	-1.44501	1.18878	-1.08471
H	-0.517505	-0.935383	-0.205105

$CH_3CH_2CH_2CH_2OO. \rightarrow CH_3CH(.)CH_2CH_2OOH$

C	-0.000439	-0.000726	0.000236
C	0.00015	0.000263	1.50936
H	1.01521	-0.000999	-0.402564
H	-0.521085	-0.874513	-0.401971
H	-0.508568	0.89153	-0.391287
H	0.594031	-1.18947	1.86328

H	0.650518	0.746758	1.96493
C	-1.31742	-0.218069	2.22601
C	-1.61288	-1.72294	2.43185
H	-1.29969	0.259056	3.2084
H	-2.46493	-1.87553	3.09794
H	-1.79192	-2.23153	1.479
O	-0.506176	-2.32211	3.09109
O	0.571184	-2.32488	2.17668
H	-2.15044	0.217472	1.65701

$(CH_3)_2CHCH_2CH_2OO. \rightarrow (CH_3)_2C(.)CH_2CH_2OOH$

C	0	0	0
C	0	0	1.51547
H	1.01739	0	-0.399851
H	-0.520353	-0.870687	-0.406536
H	-0.504464	0.897819	-0.384894
H	0.58486	-1.18145	1.82361
C	-1.34632	-0.285442	2.17081
C	-1.61277	-1.79942	2.3106
H	-1.37709	0.154853	3.17086
H	-2.48341	-1.99563	2.9404
H	-1.74772	-2.27939	1.33583
O	-0.514382	-2.39849	2.98692
O	0.59065	-2.34524	2.1072
H	-2.1641	0.158959	1.58668
C	0.833108	1.08474	2.16346
H	1.83255	1.13814	1.72402
H	0.361751	2.06919	2.02519
H	0.93899	0.920956	3.2388

$CH_3CH_2CH_2CH_2OO. \rightarrow CH_2(.)CH_2CH_2CH_2OOH$

C	-0.000229	9.20E-05	-0.00033
H	0.000739	6.10E-05	1.09342
H	1.03546	0.00041	-0.356518
C	-0.780188	-1.20723	-0.524105
H	-1.79972	-1.16234	-0.12444
H	-0.315483	-2.10431	-0.098888
O	-0.599682	1.25791	-0.337227
O	-0.276524	1.57572	-1.67575
C	-0.833351	-1.35654	-2.05815
H	-1.29749	-2.3242	-2.29934
H	0.185922	-1.40511	-2.45796
C	-1.59537	-0.257045	-2.75562

H	-1.48507	-0.194254	-3.83672
H	-2.61077	-0.07237	-2.40484
H	-0.952839	0.892123	-2.29161

$CH_3CH_2CH_2CH_2CH_2OO. \rightarrow CH_3CH(.)CH_2CH_2CH_2OOH$

C	0	0	0
H	0	0	1.09382
H	1.03594	0	-0.355794
C	-0.778965	-1.20819	-0.524396
H	-1.80055	-1.15966	-0.130532
H	-0.319172	-2.10453	-0.092017
O	-0.600126	1.2559	-0.33914
O	-0.283428	1.56727	-1.67914
C	-0.821998	-1.36381	-2.05727
H	-1.27962	-2.3348	-2.29998
H	0.201231	-1.40799	-2.45035
C	-1.5837	-0.270231	-2.77613
H	-2.58834	-0.098815	-2.38042
H	-0.964993	0.849345	-2.29691
C	-1.48366	-0.22049	-4.27836
H	-1.93883	-1.11509	-4.72817
H	-1.99944	0.649881	-4.69042
H	-0.440991	-0.190071	-4.60865

$(CH_3)_2CHCH_2CH_2CH_2OO. \rightarrow (CH_3)_2C(.)CH_2CH_2CH_2OOH$

C	0	0	0
H	0	0	1.09386
H	1.03546	0	-0.356118
C	-0.782187	-1.20483	-0.525954
H	-1.79054	-1.17989	-0.100768
H	-0.302563	-2.10476	-0.123191
O	-0.597316	1.25766	-0.34439
O	-0.246484	1.58165	-1.67105
C	-0.850552	-1.34019	-2.06058
H	-1.34452	-2.2934	-2.30491
H	0.169048	-1.41968	-2.45502
C	-1.57249	-0.220207	-2.80392
H	-0.921313	0.852323	-2.32307
C	-1.30992	-0.197822	-4.29434
H	-1.75807	-1.07954	-4.77651
H	-1.74402	0.687261	-4.76643
H	-0.239261	-0.215327	-4.51516
C	-3.01032	0.032885	-2.40153

H	-3.43536	0.86622	-2.96585
H	-3.62831	-0.854944	-2.60243
H	-3.10283	0.26662	-1.33894

2d) Transition states of the isomerizations of the hydroperoxyalkylperoxy radicals

$HOOCH_2CH_2CH(CH_3)OO. \rightarrow HOOCH(.)CH_2CH(CH_3)OOH$

C	0	0	0
H	0	0	1.09597
C	1.45591	0	-0.526055
H	1.43005	0.109102	-1.61409
H	1.98895	0.863936	-0.112435
C	2.17558	-1.28786	-0.193115
H	1.11349	-2.09333	0.032062
H	2.73081	-1.34153	0.746165
O	-0.626874	-1.20921	-0.438052
O	-0.043814	-2.27866	0.282022
O	2.92973	-1.70259	-1.27885
O	3.70149	-2.86311	-0.884919
H	3.25975	-3.5494	-1.40649
C	-0.830912	1.15024	-0.543632
H	-1.84334	1.11029	-0.138546
H	-0.382263	2.10687	-0.265587
H	-0.890588	1.09882	-1.63349

$HOOCH(CH_3)CH_2CH_2OO. \rightarrow HOOC(.)(CH_3)CH_2CH_2OOH$

C	0	0	0
H	0	0	1.09478
H	1.02883	0	-0.366578
C	-0.788793	-1.19828	-0.569577
H	-0.625726	-1.2433	-1.64867
H	-0.40827	-2.12703	-0.12775
C	-2.28064	-1.04974	-0.313617
H	-2.32127	0.274604	-0.104291
O	-0.575007	1.21007	-0.473366
O	-1.82914	1.3467	0.169975
O	-2.93651	-1.34619	-1.51127
O	-4.35693	-1.07942	-1.3752
H	-4.42251	-0.259478	-1.88678
C	-2.86322	-1.67628	0.932349
H	-3.91053	-1.40311	1.05367
H	-2.79469	-2.76933	0.871136
H	-2.30971	-1.34019	1.81129

2e) Hydroperoxyalkyl radicals

$CH_2(.)CH_2OOH$

C	-0.003609	-0.007514	0.008879
H	-0.011775	-0.007976	1.10678
H	1.04932	-0.013195	-0.317029
C	-0.753779	-1.15376	-0.551967
H	-1.0594	-1.13301	-1.58973
H	-0.950372	-2.03502	0.042612
O	-0.6165	1.18651	-0.493704
O	0.265219	2.2887	-0.141523
H	-0.313332	2.78546	0.452694

$CH_3CH(.)CH_2OOH$

H	0.003182	-0.054565	-0.006882
O	-0.003429	0.025594	0.956595
O	1.42966	0.012702	1.22668
C	1.78214	1.33028	1.7077
C	3.20096	1.26425	2.14172
H	1.11561	1.57291	2.54506
H	1.62955	2.06349	0.907776
C	3.60529	0.49151	3.34746
H	3.96737	1.61673	1.46018
H	3.7653	-0.570645	3.10689
H	4.54045	0.865215	3.77463
H	2.83042	0.519995	4.11997

$(CH_3)_2C(.)CH_2OOH$

C	-0.228821	0.201412	0.341862
H	-0.703518	0.782482	1.13994
H	0.853444	0.166914	0.517536
C	-0.815774	-1.16129	0.221543
O	-0.477606	0.871491	-0.917482
O	0.017458	2.23892	-0.785084
C	-0.025147	-2.25057	-0.427373
H	-0.297694	-3.23555	-0.032978
H	-0.208745	-2.28789	-1.51328
H	1.05052	-2.10964	-0.291355
C	-2.28922	-1.33843	0.393932
H	-2.53294	-2.33591	0.77586
H	-2.71113	-0.593116	1.07305
H	-2.81976	-1.23093	-0.565334

H	0.769319	2.20812	-1.39209

$CH_2(.)CH_2CH_2OOH$

H	-0.005512	-0.049826	-0.031408
O	-0.021871	-0.043466	0.935227
O	1.40794	0.005047	1.20817
C	1.76206	-1.22302	1.83892
H	2.85384	-1.16005	1.88904
H	1.48226	-2.06321	1.19213
C	1.15933	-1.38353	3.23692
H	1.45076	-2.36631	3.62731
H	0.06484	-1.42185	3.11752
C	1.5486	-0.300466	4.18072
H	1.56377	-0.472628	5.24937
H	1.65686	0.714271	3.81967

$CH_3CH(.)CH_2CH_2OOH$

H	-0.019542	-0.001948	0.028619
O	0.006084	0.017728	0.994861
O	1.44689	-0.006049	1.20615
C	1.76623	-1.24927	1.82776
H	2.86113	-1.2377	1.83272
H	1.42229	-2.07541	1.19398
C	1.21647	-1.37988	3.24798
H	1.47625	-2.37895	3.62582
H	0.116	-1.36738	3.18174
C	1.70615	-0.324376	4.18147
H	1.91154	0.65571	3.7648
C	1.56881	-0.472692	5.65763
H	1.88148	-1.46785	5.99755
H	2.15973	0.27124	6.19793
H	0.52328	-0.351193	5.98933

$(CH_3)_2C(.)CH_2CH_2OOH$

H	-0.002507	0.017019	-0.020998
O	-0.016181	0.031324	0.945522
O	1.41572	-0.001614	1.214
C	1.7573	1.22922	1.84484
H	1.47293	2.06731	1.19543
H	2.84986	1.17733	1.89383
C	1.14746	1.39886	3.25011
H	0.059471	1.41491	3.13514
H	1.45054	2.39517	3.60103

C	1.5587	0.351883	4.23972
C	0.807899	-0.938559	4.31015
H	1.19364	-1.67165	3.58321
H	0.889991	-1.39855	5.30165
H	-0.251782	-0.803845	4.07641
C	2.91661	0.428143	4.86381
H	3.68674	-0.079004	4.25644
H	3.24919	1.463	4.99556
H	2.93463	-0.0616	5.84366

$CH_2(.)CH_2CH_2CH_2OOH$

H	0.036716	0.020616	-0.056082
O	-0.011567	0.036757	0.90935
O	1.40796	-0.015338	1.23048
C	1.74901	1.22413	1.85143
H	1.505	2.05126	1.17406
H	2.83948	1.15237	1.93611
C	1.10222	1.42352	3.21728
H	0.017011	1.45701	3.08981
H	1.40846	2.40682	3.5954
C	1.47361	0.334531	4.23401
H	2.57476	0.31061	4.33487
H	1.20666	-0.646145	3.82563
C	0.84673	0.52563	5.57093
H	0.741402	-0.303759	6.25943
H	0.603297	1.51736	5.93539

$CH_3CH(.)CH_2CH_2CH_2OOH$

H	-0.043978	-0.037337	0.079314
O	0.017994	-0.04584	1.04407
O	1.46462	0.016384	1.20112
C	1.77342	1.27086	1.80927
H	1.38477	2.08417	1.18463
H	2.86851	1.28996	1.76476
C	1.27773	1.3949	3.2451
H	0.186092	1.33421	3.24494
H	1.53994	2.39705	3.60641
C	1.85754	0.33119	4.1866
H	1.63615	-0.664737	3.78312
H	2.96192	0.405567	4.16734
C	1.36302	0.434182	5.59056
C	1.56625	-0.672785	6.56755
H	1.05114	1.40696	5.96014

H	2.61654	-0.746889	6.89832
H	0.959794	-0.540571	7.46721
H	1.31713	-1.6466	6.12864

$(CH_3)_2C(.)CH_2CH_2CH_2OOH$

H	0.037156	0.01167	-0.056303
O	-0.008051	0.039825	0.908995
O	1.41244	-0.00946	1.22656
C	1.75763	1.23915	1.82638
H	1.51233	2.05514	1.13549
H	2.8483	1.16749	1.90872
C	1.11586	1.46149	3.19155
H	0.029869	1.47345	3.0663
H	1.4084	2.45716	3.54493
C	1.51709	0.388729	4.23488
H	2.6086	0.417461	4.35448
H	1.2695	-0.59171	3.81501
C	0.856651	0.560256	5.56953
C	-0.541813	0.067064	5.76769
H	-0.750363	-0.815756	5.15642
H	-0.733747	-0.188816	6.81603
H	-1.2961	0.826152	5.49555
C	1.40964	1.54999	6.54581
H	2.49864	1.63089	6.47002
H	1.00459	2.56558	6.38945
H	1.15996	1.28025	7.57811

2f) Ketohydroperoxydes

$(O)CHCH_2CH(CH_3)OOH$

C	-0.004949	0.005678	-0.002709
O	0.00067	0.005655	1.20384
H	0.952827	0.008105	-0.568907
C	-1.24021	0.016261	-0.866079
H	-1.18843	-0.835154	-1.55786
H	-1.18738	0.911055	-1.49818
C	-2.56411	0.014904	-0.102073
H	-2.54515	0.80523	0.656286
C	-2.89939	-1.32082	0.547885
H	-2.94453	-2.11376	-0.203158
H	-2.13187	-1.5669	1.28251
H	-3.86552	-1.26736	1.05299
O	-3.65781	0.266458	-0.999496

O	-3.50726	1.61084	-1.531
H	-4.22134	2.06335	-1.06134

(O)C(CH_3)CH_2CH_2OOH

H	-0.031853	0.041053	-0.007785
O	-0.016733	0.023145	0.969522
O	1.40819	-0.027212	1.21792
C	1.9843	1.23448	0.904846
H	1.2233	2.01031	1.01902
H	2.76109	1.39886	1.65911
C	2.64144	1.27459	-0.480776
H	3.36685	0.452907	-0.551653
H	3.23046	2.1945	-0.580755
C	1.73277	1.14002	-1.6928
O	0.608672	0.680984	-1.63293
C	2.31044	1.59734	-3.01445
H	3.32798	1.22085	-3.15146
H	1.67191	1.26754	-3.8325
H	2.37004	2.69115	-3.02293

2g) Transition states for the formation of cyclic ethers

CH_2(.)CH_2OOH → oxirane + OH

C	0	0	0
H	0	0	1.09312
H	1.0182	0	-0.398832
C	-0.948712	-0.934579	-0.632297
H	-0.836001	-1.20835	-1.67184
H	-1.85158	-1.2217	-0.112179
O	-0.826725	0.981605	-0.556658
O	-0.316463	2.53072	0.093583
H	-1.22015	2.87584	0.129775

CH_3CH(.)CH_2OOH → 2-methyl-oxirane + OH

C	0	0	0
H	0	0	1.09542
H	1.02142	0	-0.392536
C	-0.928556	-0.955767	-0.634382
H	-0.738691	-1.22386	-1.66704
O	-0.815357	0.986688	-0.562135
O	-0.081913	2.54209	-0.19115
H	-0.277695	2.8995	-1.06875
C	-2.16358	-1.44619	0.024414

H	-3.0444	-1.30393	-0.609322
H	-2.08586	-2.52689	0.214871
H	-2.33456	-0.945377	0.978527

$(CH_3)_2C(.)CH_2OOH \rightarrow$ 2,2-dimethyl-oxirane + OH

C	0	0	0
H	0	0	1.09559
H	1.02515	0	-0.387138
C	-0.917203	-0.974216	-0.633179
O	-0.807323	0.993422	-0.557948
O	-0.134751	2.53802	-0.05083
H	-1.00649	2.9537	0.00274
C	-2.12608	-1.4504	0.09636
H	-3.02907	-1.35611	-0.515787
H	-2.02244	-2.51831	0.339922
H	-2.27693	-0.905045	1.02834
C	-0.672659	-1.43403	-2.02915
H	-0.372346	-2.49268	-2.0299
H	-1.57819	-1.36442	-2.6404
H	0.1182	-0.857591	-2.5094

$CH_2(.)CH_2CH_2OOH \rightarrow$ oxetane + OH

C	0	0	0
H	0	0	1.09164
H	1.03331	0	-0.361967
C	-0.870689	-1.07146	-0.665253
H	-1.60597	-1.47892	0.030591
H	-0.292807	-1.89956	-1.08656
O	-0.694787	1.16016	-0.502356
O	0.166311	2.40022	0.261575
C	-1.53033	-0.206511	-1.70654
H	-1.02982	-0.024881	-2.6492
H	-2.59235	-0.004245	-1.67395
H	-0.588558	3.00274	0.299978

$CH_3CH(.)CH_2CH_2OOH \rightarrow$ 2-methyl-oxetane + OH

C	0	0	0
H	0	0	1.09185
H	1.03499	0	-0.359106
C	-0.861173	-1.08203	-0.657198
H	-1.61233	-1.46937	0.035263
H	-0.27969	-1.92587	-1.0437
O	-0.694108	1.15762	-0.499854

O	0.110118	2.38664	0.342648
C	-1.51027	-0.252884	-1.73613
H	-0.928969	-0.067111	-2.63332
H	-0.61339	3.02108	0.254994
C	-2.97773	-0.033652	-1.81156
H	-3.21579	0.87368	-2.37297
H	-3.47636	-0.871196	-2.32539
H	-3.41758	0.046717	-0.814393

$(CH_3)_2C(.)CH_2CH_2OOH \rightarrow$ 2,2-dimethyl-oxetane + OH

C	0	0	0
H	0	0	1.0922
H	1.03684	0	-0.353439
C	-0.857528	-1.09521	-0.643823
H	-1.56009	-1.52602	0.073106
H	-0.26379	-1.90974	-1.07319
O	-0.688832	1.15872	-0.498136
O	0.162288	2.38157	0.299175
C	-1.58709	-0.281962	-1.69266
H	-0.55987	3.02093	0.24432
C	-3.05698	-0.061808	-1.57198
H	-3.36999	0.83364	-2.11645
H	-3.61602	-0.911111	-1.99834
H	-3.36064	0.041554	-0.528526
C	-0.948514	-0.095886	-3.02913
H	-1.22828	-0.916672	-3.70931
H	-1.2745	0.837151	-3.49661
H	0.14088	-0.082644	-2.95982

$CH_2(.)CH_2CH_2CH_2OOH \rightarrow$ oxolane + OH

C	0	0	0
H	0	0	1.09252
H	1.03997	0	-0.351789
C	-0.765343	-1.1991	-0.551038
H	-1.72892	-1.28208	-0.038287
H	-0.208196	-2.12303	-0.36309
O	-0.659595	1.18121	-0.455254
O	0.094047	2.33867	0.47607
C	-1.0021	-0.96904	-2.05472
H	-1.65138	-1.76099	-2.45379
H	-0.051906	-1.02807	-2.59371
C	-1.61549	0.377652	-2.22468
H	-1.22865	1.08152	-2.94878

H	-2.623	0.550103	-1.86663
H	-0.54309	3.03555	0.269033

$CH_3CH(.)CH_2CH_2CH_2OOH \rightarrow$ 2-methyl-oxolane + OH

C	-0.02336	0.001958	-0.07439
H	-0.060389	0.126887	1.01077
H	1.02878	-0.063759	-0.381773
C	-0.796739	-1.24016	-0.512178
H	-1.77564	-1.24995	-0.021872
H	-0.262819	-2.14388	-0.199212
O	-0.633161	1.13288	-0.691697
O	0.152368	2.37931	0.08019
C	-0.987981	-1.18876	-2.03617
H	-1.61434	-2.03259	-2.36186
H	-0.019993	-1.29746	-2.53768
C	-1.60939	0.119705	-2.39414
H	-0.562076	3.01646	-0.052462
H	-2.60729	0.305234	-2.0086
C	-1.15383	0.942777	-3.54614
H	-1.56641	0.567316	-4.49614
H	-1.47794	1.98138	-3.44449
H	-0.064386	0.931208	-3.63648

$(CH_3)_2C(.)CH_2CH_2CH_2OOH \rightarrow$2,2-dimethyl-oxolane + OH

C	0	0	0
H	0	0	1.09318
H	1.04225	0	-0.347483
C	-0.761184	-1.20853	-0.537891
H	-1.7218	-1.28855	-0.020964
H	-0.20242	-2.12755	-0.330372
O	-0.665374	1.17094	-0.460268
O	-0.019735	2.316	0.559902
C	-0.991537	-1.0218	-2.04789
H	-1.64061	-1.82531	-2.42634
H	-0.035271	-1.10822	-2.57371
C	-1.60081	0.325638	-2.3077
H	-0.316595	3.07294	0.03745
C	-3.04179	0.544962	-1.97408
H	-3.22521	1.58528	-1.69119
H	-3.67915	0.330696	-2.84751
H	-3.38171	-0.092013	-1.15554
C	-0.986762	1.228	-3.32745
H	-1.30746	0.948297	-4.34442

H	-1.29117	2.26687	-3.17274
H	0.104095	1.18121	-3.30339

2h) Cyclic ethers

oxirane

C	0.038239	-0.032368	0.029152
H	0.010291	-0.005069	1.11599
H	1.03166	-0.00354	-0.412443
C	-1.0646	-0.658713	-0.708791
H	-0.878442	-1.08797	-1.6905
H	-1.89993	-1.08981	-0.161985
O	-0.948611	0.763241	-0.629444

2-methyl-oxirane

C	0.054714	-0.058636	0.04266
H	0.001874	-0.016209	1.12862
H	1.05749	-0.022432	-0.377114
C	-1.0302	-0.709196	-0.702548
H	-0.784336	-1.1224	-1.68061
O	-0.92936	0.720071	-0.648443
C	-2.22108	-1.3255	-0.017735
H	-3.12292	-1.1929	-0.622122
H	-2.06969	-2.39876	0.133488
H	-2.39109	-0.85606	0.953709

2,2-dimethyl-oxirane

C	0.058111	-0.063947	0.039661
H	0.01912	-0.026919	1.12643
H	1.05649	-0.013486	-0.390025
C	-1.02348	-0.725841	-0.705653
O	-0.940884	0.711135	-0.636943
C	-2.19508	-1.32133	0.043221
H	-3.11326	-1.21385	-0.542244
H	-2.03821	-2.38767	0.232558
H	-2.33976	-0.814074	0.998559
C	-0.746341	-1.30334	-2.07589
H	-0.504178	-2.36855	-2.01091
H	-1.62618	-1.19548	-2.71745
H	0.087028	-0.783709	-2.55166

oxetane

C	-0.029868	-0.008185	-0.027945

H	-0.246562	0.186872	1.02744
H	1.05495	-0.050743	-0.169915
C	-0.835512	-1.15157	-0.677013
H	-1.54046	-1.65727	-0.017161
H	-0.242389	-1.89396	-1.21093
O	-0.644682	0.977664	-0.891893
C	-1.4388	-0.035915	-1.554
H	-1.20992	-0.095456	-2.62309
H	-2.51145	0.142133	-1.42568

2-methyl-oxetane

C	-0.087325	0.013158	-0.043105
H	-0.2796	0.193589	1.01853
H	0.994714	0.004095	-0.215672
C	-0.857786	-1.14894	-0.695687
H	-1.6119	-1.60884	-0.054718
H	-0.25446	-1.92773	-1.16244
O	-0.754583	0.985468	-0.881643
C	-1.42027	-0.062973	-1.64112
H	-0.998787	-0.115865	-2.65328
C	-2.91871	0.138139	-1.70861
H	-3.15216	1.07647	-2.21898
H	-3.39219	-0.679697	-2.26161
H	-3.34785	0.178887	-0.703984

2,2-dimethyl-oxetane

C	-0.123879	0.016615	0.016483
H	-0.408025	0.160167	1.0639
H	0.967938	0.036976	-0.062176
C	-0.823122	-1.14341	-0.711797
H	-1.54046	-1.70712	-0.113964
H	-0.163077	-1.83774	-1.23325
O	-0.741984	0.998867	-0.845514
C	-1.4467	-0.038005	-1.60666
C	-2.9519	0.144069	-1.47686
H	-3.25581	1.09136	-1.93085
H	-3.48903	-0.66732	-1.97833
H	-3.24835	0.160385	-0.425646
C	-0.985048	-0.03057	-3.05691
H	-1.44543	-0.84977	-3.61841
H	-1.26158	0.913552	-3.53433
H	0.100755	-0.135473	-3.11518

oxolane

C	-0.075493	0.003247	-0.054155
H	-0.216074	0.18641	1.01426
H	1.00272	0.01276	-0.266056
C	-0.715508	-1.301	-0.535887
H	-1.64175	-1.49777	0.012659
H	-0.058674	-2.16515	-0.417725
O	-0.717553	1.05577	-0.784227
C	-1.0252	-0.9649	-2.00174
H	-1.80928	-1.5894	-2.43438
H	-0.124856	-1.07781	-2.61325
C	-1.42891	0.511167	-1.90534
H	-1.17072	1.08455	-2.80022
H	-2.50758	0.616377	-1.73048

2-methyl-oxolane

C	-0.284329	-0.061832	0.150399
H	-0.81108	-0.279227	1.08719
H	0.695978	0.356136	0.40029
C	-0.185786	-1.30968	-0.741566
H	-0.177568	-2.23756	-0.166197
H	0.726385	-1.28061	-1.34481
O	-1.04105	0.910784	-0.583716
C	-1.41882	-1.16036	-1.64159
H	-2.3195	-1.50962	-1.12508
H	-1.3352	-1.70179	-2.58636
C	-1.48711	0.358188	-1.83445
H	-0.775896	0.654081	-2.62192
C	-2.8581	0.925684	-2.1591
H	-2.81943	2.01662	-2.19454
H	-3.20801	0.562743	-3.13009
H	-3.58109	0.634235	-1.39258

2,2-dimethyl-oxolane

H	-0.043978	-0.037337	0.079314
O	0.017994	-0.04584	1.04407
O	1.46462	0.016384	1.20112
C	1.77342	1.27086	1.80927
H	1.38477	2.08417	1.18463
H	2.86851	1.28996	1.76476
C	1.27773	1.3949	3.2451
H	0.186092	1.33421	3.24494
H	1.53994	2.39705	3.60641

C	1.85754	0.33119	4.1866
H	1.63615	-0.664737	3.78312
H	2.96192	0.405567	4.16734
C	1.36302	0.434182	5.59056
C	1.56625	-0.672785	6.56755
H	1.05114	1.40696	5.96014
H	2.61654	-0.746889	6.89832
H	0.959794	-0.540571	7.46721
H	1.31713	-1.6466	6.12864

3) Species involved in the isomerization of one hydroperoxyalkyl radical into another hydroperoxyalkyl radical

1-hydroperoxy-4-butyl radical

H	0.036716	0.020616	-0.056082
O	-0.011567	0.036757	0.90935
O	1.40796	-0.015338	1.23048
C	1.74901	1.22413	1.85143
H	1.505	2.05126	1.17406
H	2.83948	1.15237	1.93611
C	1.10222	1.42352	3.21728
H	0.017011	1.45701	3.08981
H	1.40846	2.40682	3.5954
C	1.47361	0.334531	4.23401
H	2.57476	0.31061	4.33487
H	1.20666	-0.646145	3.82563
C	0.84673	0.52563	5.57093

H	0.741402	-0.303759	6.25943
H	0.603297	1.51736	5.93539

$CH_2(.)CH_2CH_2CH_2OOH \rightarrow$ butanal + OH

H	0	0	0
O	0	0	0.967287
O	1.49696	0	1.18858
C	1.82042	1.17127	1.83486
H	1.64073	2.06465	1.22925
H	3.13829	0.997281	2.06289
C	1.48243	1.24221	3.31995
H	0.471592	0.87901	3.51945
H	1.53048	2.28914	3.63917
C	2.58811	0.418056	4.019
H	2.35461	-0.646041	3.93475
H	2.67119	0.652406	5.08486
C	3.86179	0.724413	3.24558
H	4.34342	1.67824	3.45967
H	4.56572	-0.080546	3.05128

butanal

C	-0.022214	-0.103647	0.030971
O	-0.159881	-0.214375	1.22286
C	1.29912	0.095541	-0.672504
H	1.39536	-0.714071	-1.41114
H	1.20863	1.01095	-1.27563
C	2.51402	0.154613	0.251647
H	2.5563	-0.765611	0.841662
H	2.37071	0.962724	0.97501
C	3.82794	0.354295	-0.507483
H	4.6766	0.39547	0.179859
H	4.01139	-0.464087	-1.21081
H	3.82073	1.28688	-1.08048
H	-0.906259	-0.144899	-0.645264

4) Species involved in the beta-scission reactions

1-hydroperoxy-3-butyl radical

H	-0.019542	-0.001948	0.028619
O	0.006084	0.017728	0.994861
O	1.44689	-0.006049	1.20615
C	1.76623	-1.24927	1.82776
H	2.86113	-1.2377	1.83272
H	1.42229	-2.07541	1.19398
C	1.21647	-1.37988	3.24798
H	1.47625	-2.37895	3.62582
H	0.116	-1.36738	3.18174
C	1.70615	-0.324376	4.18147
H	1.91154	0.65571	3.7648
C	1.56881	-0.472692	5.65763
H	1.88148	-1.46785	5.99755
H	2.15973	0.27124	6.19793

H	0.52328	-0.351193	5.98933

2-hydroperoxy-4-butyl radical

H	-0.047149	0.104983	0.095828
O	0.016655	0.112624	1.05995
O	1.46121	-0.013864	1.22035
C	1.7438	-1.2895	1.81992
H	2.83607	-1.2318	1.89223
C	1.15142	-1.39205	3.2344
H	1.40015	-2.37726	3.64587
H	0.05456	-1.37892	3.12868
C	1.60252	-0.310224	4.15147
H	1.62011	-0.46308	5.22309
H	1.76106	0.689272	3.76792
C	1.34547	-2.44744	0.910077
H	1.77828	-2.31588	-0.084844
H	1.70754	-3.39535	1.31637
H	0.259495	-2.50995	0.815935

$CH_3CH(.)CH_2CH_2OOH \rightarrow$ propene + HCHO + OH

C	-0.066542	0.032619	-0.042921
C	0.086499	-0.046584	1.30871
C	2.27467	-0.120267	1.90324
O	2.3596	-0.081244	3.26101
O	1.84405	1.23239	3.68966
H	2.28055	1.28462	4.55117
C	-0.060157	1.31201	-0.822654
H	-0.128369	-0.887734	-0.619871
H	-0.069229	-0.989344	1.82051
H	-0.00348	0.840722	1.9255
H	2.69901	0.732649	1.37786
H	2.52711	-1.11958	1.56759
H	-0.956038	1.40304	-1.44872
H	-0.02145	2.18217	-0.162252
H	0.798185	1.36884	-1.50522

$CH_2(.)CH_2CH(OOH)CH_3 \rightarrow$ ethene + CH_3CHO + OH

C	2.40538	-0.226698	0.145957
C	1.49053	0.535537	-0.517277
C	-0.462907	0.518402	0.56997
O	-0.812104	-0.782157	0.748609
O	-0.913708	-1.43786	-0.595218
H	-1.62703	-2.05748	-0.389929

H	3.05057	0.194371	0.909269
H	2.45887	-1.29825	-0.00553
H	0.975336	0.12922	-1.37928
H	1.54519	1.61832	-0.463957
C	-1.37781	1.40508	-0.22304
H	-0.076745	0.876009	1.51967
H	-2.35989	1.4904	0.263126
H	-0.955502	2.40865	-0.30854
H	-1.53548	1.00496	-1.22561