The Cartesian coordinates of all thelocated reactants and transition states

1. 9c, 12c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-7.823496	1.215727	0.547621
2	8	0	-6.795833	1.036411	-1.488322
3	6	0	-1.642325	1.922856	-0.372665
4	6	0	-0.377177	2.220664	0.453039
5	6	0	-2.927550	1.879552	0.474473
6	6	0	0.907637	2.269320	-0.393552
7	6	0	-4.187399	1.574992	-0.355848
8	6	0	2.176659	2.552555	0.445432
9	6	0	-5.456386	1.537222	0.506381
10	6	0	2.784554	-2.884201	-0.443916
11	6	0	1.577222	-3.537108	0.252625
12	6	0	3.420305	2.679601	-0.400037
13	6	0	3.780456	-2.231497	0.545010
14	6	0	0.586698	-4.193471	-0.727754
15	6	0	4.545115	1.943536	-0.340017
16	6	0	4.856315	0.795331	0.600582
17	6	0	4.993891	-1.661378	-0.147969
18	6	0	-6.707503	1.240495	-0.273852
19	6	0	5.443708	-0.393316	-0.133292
20	6	0	-0.619194	-4.840819	-0.025928
21	1	0	-1.751892	2.686129	-1.158471
22	1	0	-1.518216	0.960364	-0.892443
23	1	0	-0.502784	3.181507	0.976683
24	1	0	-0.267115	1.454255	1.236409
25	1	0	-2.814988	1.119153	1.263356
26	1	0	-3.052747	2.844213	0.991100
27	1	0	0.804879	3.044714	-1.168228
28	1	0	1.036980	1.315701	-0.925695
29	1	0	-4.069157	0.613097	-0.872095
30	1	0	-4.304965	2.329989	-1.144469
31	1	0	2.291085	1.766627	1.202352
32	1	0	2.022472	3.492596	1.000453
33	1	0	-5.607440	2.493577	1.027094
34	1	0	-5.370883	0.780850	1.299551
35	1	0	2.433938	-2.120875	-1.153816
36	1	0	3.314091	-3.642591	-1.041057
37	1	0	1.934979	-4.295730	0.966848
38	1	0	1.045776	-2.778515	0.848892

39	1	0	3.376852	3.471187	-1.151043
40	1	0	3.258324	-1.462080	1.127116
41	1	0	4.103641	-2.998915	1.267499
42	1	0	1.117211	-4.953296	-1.321151
43	1	0	0.232010	-3.436565	-1.443323
44	1	0	5.346140	2.182541	-1.041685
45	1	0	3.970300	0.505304	1.171658
46	1	0	5.597459	1.142857	1.342196
47	1	0	5.556204	-2.386348	-0.740312
48	1	0	6.339026	-0.166139	-0.714976
49	1	0	-0.295209	-5.622170	0.673993
50	1	0	-1.302983	-5.301583	-0.749024
51	1	0	-1.188577	-4.096651	0.546157
52	1	0	-8.634607	1.021625	0.029220

2. 9c,12t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	5.639770	1.542971	-3.682633
2	8	0	6.083342	2.745627	-1.787148
3	6	0	2.478242	-1.911974	-0.833615
4	6	0	1.090318	-2.377003	-0.354765
5	6	0	2.530455	-0.412259	-1.180238
6	6	0	1.038448	-3.876991	-0.013200
7	6	0	3.919850	0.047953	-1.656582
8	6	0	-0.346508	-4.356396	0.489655
9	6	0	3.948785	1.562404	-1.987181
10	6	0	-3.948556	1.672491	1.467176
11	6	0	-4.241622	3.175075	1.298953
12	6	0	-0.718657	-3.781537	1.836004
13	6	0	-3.678457	0.964979	0.128553
14	6	0	-4.525349	3.897070	2.629653
15	6	0	-1.835844	-3.115884	2.181670
16	6	0	-3.020087	-2.764897	1.303687
17	6	0	-3.381003	-0.516466	0.199010
18	6	0	5.306045	2.029892	-2.427427
19	6	0	-3.320402	-1.278697	1.302477
20	6	0	-4.816628	5.396949	2.452849
21	1	0	3.222624	-2.129158	-0.051724
22	1	0	2.776310	-2.499029	-1.716376
23	1	0	0.791527	-1.791730	0.526485

24	1	0	0.344933	-2.159470	-1.135917
25	1	0	1.787420	-0.194199	-1.963020
26	1	0	2.233221	0.173873	-0.297209
27	1	0	1.796314	-4.102932	0.753203
28	1	0	1.313193	-4.461998	-0.903327
29	1	0	4.215736	-0.519662	-2.547871
30	1	0	4.663886	-0.165484	-0.876196
31	1	0	-0.320428	-5.455095	0.568212
32	1	0	-1.106484	-4.120278	-0.265578
33	1	0	3.669567	2.147465	-1.106094
34	1	0	3.227996	1.769876	-2.787597
35	1	0	-4.801201	1.192519	1.970451
36	1	0	-3.080963	1.545768	2.131779
37	1	0	-3.387297	3.659794	0.800603
38	1	0	-5.104863	3.304907	0.627248
39	1	0	0.030654	-3.943294	2.614554
40	1	0	-4.544287	1.117220	-0.537309
41	1	0	-2.836308	1.466471	-0.377292
42	1	0	-3.663782	3.767323	3.301817
43	1	0	-5.379844	3.413802	3.126963
44	1	0	-1.924348	-2.777010	3.215607
45	1	0	-3.904282	-3.305498	1.684305
46	1	0	-2.867943	-3.110560	0.275300
47	1	0	-3.199860	-0.991484	-0.768558
48	1	0	-3.490483	-0.833505	2.283228
49	1	0	-3.965063	5.912256	1.989756
50	1	0	-5.017635	5.881739	3.415826
51	1	0	-5.691715	5.554892	1.809011
52	1	0	6.537592	1.841955	-3.944944

3. 9t, 12c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-7.140337	5.534593	-0.500779
2	8	0	-5.860819	6.141080	1.296071
3	6	0	-1.561424	2.988563	0.892510
4	6	0	-0.613446	1.903734	0.347786
5	6	0	-2.849637	3.149486	0.064061
6	6	0	0.679681	1.766379	1.173772
7	6	0	-3.791957	4.231506	0.621286
8	6	0	1.689282	0.726953	0.621809
9	6	0	-5.064945	4.384564	-0.222282

10	6	0	0.806298	-6.854084	-0.689209
11	6	0	0.047611	-7.187263	0.607784
12	6	0	1.204098	-0.702120	0.673930
13	6	0	1.286693	-5.382490	-0.774970
14	6	0	-0.426555	-8.651260	0.678096
15	6	0	1.752732	-1.669309	1.426816
16	6	0	1.270446	-3.104087	1.495632
17	6	0	2.369921	-5.050011	0.223096
18	6	0	-6.011323	5.431894	0.296690
19	6	0	2.368170	-4.098677	1.174684
20	6	0	-1.196124	-8.974774	1.970221
21	1	0	-1.827570	2.747670	1.933253
22	1	0	-1.029643	3.952168	0.925054
23	1	0	-1.146282	0.941905	0.325324
24	1	0	-0.351876	2.140708	-0.695924
25	1	0	-2.582305	3.395100	-0.975837
26	1	0	-3.379776	2.184708	0.027274
27	1	0	0.425631	1.500454	2.210296
28	1	0	1.178954	2.746359	1.213115
29	1	0	-3.266743	5.194823	0.666008
30	1	0	-4.067487	3.987886	1.655903
31	1	0	2.626234	0.808456	1.189764
32	1	0	1.929252	0.996921	-0.419400
33	1	0	-5.616896	3.435363	-0.278071
34	1	0	-4.819449	4.643175	-1.262159
35	1	0	0.156906	-7.062774	-1.552325
36	1	0	1.675536	-7.523316	-0.785497
37	1	0	0.690540	-6.970864	1.473322
38	1	0	-0.825277	-6.520845	0.696586
39	1	0	0.343791	-0.948510	0.048235
40	1	0	1.679198	-5.208488	-1.789411
41	1	0	0.422709	-4.716400	-0.659555
42	1	0	0.445475	-9.317347	0.594046
43	1	0	-1.064577	-8.868074	-0.192190
44	1	0	2.621245	-1.431304	2.046070
45	1	0	0.408606	-3.234746	0.832333
46	1	0	0.909660	-3.306784	2.519198
47	1	0	3.261467	-5.676282	0.142038
48	1	0	3.256598	-4.007783	1.802504
49	1	0	-0.570967	-8.799823	2.855455
50	1	0	-1.521278	-10.022074	1.991322
51	1	0	-2.090003	-8.344349	2.064013
52	1	0	-7.752062	6.220003	-0.153909

4. 9t,12t

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	6.790272	3.219704	0.045934
2	8	0	7.322354	1.088960	0.686106
3	6	0	2.822216	-1.652704	-0.228825
4	6	0	1.377497	-1.940997	-0.679042
5	6	0	3.237320	-0.182652	-0.421355
6	6	0	0.961402	-3.410222	-0.476576
7	6	0	4.686994	0.098252	0.014053
8	6	0	-0.446853	-3.756323	-1.025119
9	6	0	5.076423	1.569936	-0.179030
10	6	0	-4.236997	1.412666	0.176035
11	6	0	-4.399880	2.942339	0.099170
12	6	0	-1.579855	-3.049382	-0.320355
13	6	0	-4.007524	0.909929	1.611325
14	6	0	-4.618040	3.464740	-1.333283
15	6	0	-2.570082	-3.669051	0.342354
16	6	0	-3.724878	-3.002241	1.068059
17	6	0	-3.834660	-0.582769	1.782580
18	6	0	6.489280	1.879634	0.233114
19	6	0	-3.880314	-1.520805	0.822575
20	6	0	-4.778177	4.992978	-1.401210
21	1	0	2.933852	-1.925147	0.831998
22	1	0	3.513542	-2.301444	-0.788781
23	1	0	0.692889	-1.280557	-0.127387
24	1	0	1.272320	-1.679958	-1.744429
25	1	0	3.112925	0.092235	-1.480738
26	1	0	2.551009	0.463836	0.148017
27	1	0	0.999831	-3.658214	0.594246
28	1	0	1.696468	-4.058652	-0.977028
29	1	0	5.376613	-0.538927	-0.555324
30	1	0	4.818876	-0.178317	1.068529
31	1	0	-0.599502	-4.842335	-0.956589
32	1	0	-0.466834	-3.504841	-2.098521
33	1	0	4.409932	2.231858	0.392037
34	1	0	4.961692	1.872831	-1.229644
35	1	0	-3.392554	1.107128	-0.459673
36	1	0	-5.133578	0.932409	-0.243286
37	1	0	-5.249210	3.250615	0.729014
38	1	0	-3.507343	3.425937	0.526759
39	1	0	-1.574950	-1.960211	-0.361643

40	1	0	-3.120250	1.414293	2.029308
41	1	0	-4.848275	1.239687	2.244555
42	1	0	-5.509981	2.982972	-1.761389
43	1	0	-3.769428	3.156685	-1.962565
44	1	0	-2.572751	-4.760861	0.383831
45	1	0	-3.625357	-3.187165	2.149585
46	1	0	-4.653603	-3.517276	0.768375
47	1	0	-3.656916	-0.905147	2.811696
48	1	0	-4.051591	-1.232388	-0.214709
49	1	0	-5.639667	5.326017	-0.807840
50	1	0	-4.930421	5.333762	-2.432457
51	1	0	-3.887310	5.500589	-1.008811
52	1	0	7.714219	3.411134	0.317952

5. Tsa1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-8.417561	2.903665	0.349724
2	8	0	-7.273107	3.642767	-1.488021
3	6	0	-2.147263	2.923702	-0.144341
4	6	0	-0.920858	2.523638	0.696457
5	6	0	-3.487087	2.657139	0.566624
6	6	0	0.420777	2.807415	-0.003246
7	6	0	-4.709640	3.054158	-0.280222
8	6	0	1.646823	2.397849	0.845560
9	6	0	-6.033118	2.787731	0.449738
10	6	0	3.410814	-3.717076	-1.228327
11	6	0	2.455387	-4.713603	-0.547668
12	6	0	2.960401	2.772370	0.201644
13	6	0	3.801182	-2.531243	-0.325063
14	6	0	2.071342	-5.902681	-1.448444
15	6	0	4.022580	1.983151	-0.042283
16	6	0	4.165522	0.509833	0.266917
17	6	0	4.790142	-1.579178	-0.985762
18	6	0	-7.249951	3.162771	-0.350744
19	6	0	5.067957	-0.216556	-0.710934
20	6	0	1.108339	-6.889570	-0.767185
21	1	0	-2.079462	3.992456	-0.399648
22	1	0	-2.127995	2.376428	-1.099375
23	1	0	-0.947939	3.062188	1.656868

24	1	0	-0.983812	1.451633	0.941951
25	1	0	-3.552347	1.588832	0.826963
26	1	0	-3.505817	3.208873	1.519665
27	1	0	0.487993	3.880545	-0.239545
28	1	0	0.455932	2.276594	-0.966026
29	1	0	-4.699781	2.502735	-1.229715
30	1	0	-4.648427	4.117692	-0.546405
31	1	0	1.600990	1.320732	1.052663
32	1	0	1.571689	2.899018	1.825440
33	1	0	-6.076270	3.338898	1.399912
34	1	0	-6.126781	1.726477	0.720959
35	1	0	2.941434	-3.333297	-2.147196
36	1	0	4.322605	-4.246550	-1.545099
37	1	0	2.922393	-5.093959	0.374437
38	1	0	1.540232	-4.186282	-0.235636
39	1	0	3.036391	3.821245	-0.092330
40	1	0	2.898921	-1.994653	-0.004100
41	1	0	4.272394	-2.912596	0.595478
42	1	0	2.985291	-6.433552	-1.754242
43	1	0	1.612143	-5.521251	-2.372819
44	1	0	4.900848	2.417146	-0.517548
45	1	0	3.182580	0.043541	0.444220
46	1	0	4.715486	0.399690	1.224079
47	1	0	5.524462	-2.090153	-1.618063
48	1	0	4.452739	-0.695962	-1.857203
49	1	0	1.553716	-7.310975	0.143392
50	1	0	0.854953	-7.723650	-1.432351
51	1	0	0.171983	-6.393028	-0.481254
52	1	0	-9.205564	3.152287	-0.180925

6. Tsa2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	8.768065	-0.624602	-1.990616
2	8	0	9.257819	-1.244407	0.156958
3	6	0	3.480407	-1.820885	-1.247473
4	6	0	2.038215	-1.388051	-0.923798
5	6	0	4.544290	-0.879988	-0.651667
6	6	0	0.973894	-2.317307	-1.534492
7	6	0	5.984203	-1.316855	-0.975343
8	6	0	-0.482216	-1.900741	-1.203602
9	6	0	7.034810	-0.357095	-0.360268

10	6	0	-5.909265	1.670059	0.573670
11	6	0	-7.408366	1.956524	0.777910
12	6	0	-0.832882	-2.070920	0.255748
13	6	0	-5.508968	0.266825	1.053571
14	6	0	-7.829021	3.357434	0.294876
15	6	0	-1.282213	-1.136215	1.115849
16	6	0	-1.552056	0.325153	0.828975
17	6	0	-4.033526	-0.094079	0.940611
18	6	0	8.444792	-0.783805	-0.651207
19	6	0	-2.993410	0.846770	0.783702
20	6	0	-9.325391	3.645162	0.503724
21	1	0	3.646321	-2.841679	-0.869478
22	1	0	3.610784	-1.869957	-2.339793
23	1	0	1.905049	-1.347967	0.166864
24	1	0	1.875598	-0.363416	-1.293809
25	1	0	4.379879	0.140179	-1.031772
26	1	0	4.413427	-0.830175	0.440194
27	1	0	1.142237	-3.347041	-1.182630
28	1	0	1.094904	-2.338540	-2.627477
29	1	0	6.127039	-1.355566	-2.062606
30	1	0	6.154343	-2.332513	-0.591095
31	1	0	-1.161343	-2.526838	-1.803915
32	1	0	-0.645454	-0.866531	-1.532349
33	1	0	6.921347	-0.317057	0.726958
34	1	0	6.881307	0.650951	-0.764834
35	1	0	-5.302774	2.418262	1.097661
36	1	0	-5.658246	1.779478	-0.492361
37	1	0	-8.007137	1.198557	0.247641
38	1	0	-7.658403	1.854546	1.846091
39	1	0	-0.691805	-3.085760	0.636099
40	1	0	-5.761216	0.159872	2.121520
41	1	0	-6.106455	-0.496887	0.532461
42	1	0	-7.580716	3.460220	-0.772115
43	1	0	-7.231498	4.114549	0.823862
44	1	0	-1.487179	-1.456816	2.139004
45	1	0	-1.049421	0.654567	-0.088088
46	1	0	-1.090859	0.939223	1.620251
47	1	0	-3.828902	-1.150673	1.179110
48	1	0	-3.695247	0.314076	-0.245815
49	1	0	-9.946450	2.922774	-0.042133
50	1	0	-9.592419	4.649001	0.151880
51	1	0	-9.594899	3.579990	1.566074
52	1	0	9.685940	-0.926453	-2.165663

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7. Tsa3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	5.647440	1.319540	-3.735339
2	8	0	6.016767	2.666482	-1.922661
3	6	0	2.505800	-2.016825	-0.744696
4	6	0	1.114297	-2.491476	-0.285215
5	6	0	2.527744	-0.541630	-1.186447
6	6	0	1.096201	-3.968066	0.150478
7	6	0	3.917921	-0.075588	-1.654778
8	6	0	-0.294984	-4.470298	0.611764
9	6	0	3.918116	1.414511	-2.081843
10	6	0	-3.980095	1.854406	1.454044
11	6	0	-4.358985	3.345687	1.386552
12	6	0	-0.733671	-3.794474	1.906894
13	6	0	-3.448996	1.312255	0.116404
14	6	0	-4.903718	3.899007	2.716846
15	6	0	-1.726821	-2.810715	2.150785
16	6	0	-2.702982	-2.467518	1.035406
17	6	0	-3.050583	-0.147065	0.097635
18	6	0	5.273115	1.885888	-2.525632
19	6	0	-3.108084	-1.010280	1.124237
20	6	0	-5.277749	5.389196	2.644314
21	1	0	3.226834	-2.160585	0.074836
22	1	0	2.851076	-2.650239	-1.576619
23	1	0	0.770206	-1.855845	0.543511
24	1	0	0.393769	-2.348374	-1.105341
25	1	0	1.802407	-0.395721	-2.001804
26	1	0	2.189861	0.091575	-0.352166
27	1	0	1.822197	-4.118425	0.964555
28	1	0	1.434226	-4.596890	-0.685838
29	1	0	4.252597	-0.690792	-2.499558
30	1	0	4.645215	-0.218408	-0.843162
31	1	0	-0.236249	-5.554022	0.785130
32	1	0	-1.028273	-4.314198	-0.187752
33	1	0	3.606567	2.048377	-1.246613
34	1	0	3.209989	1.552362	-2.908254
35	1	0	-4.860951	1.271451	1.761543
36	1	0	-3.220858	1.708469	2.236257
37	1	0	-3.477071	3.933154	1.085825
38	1	0	-5.113307	3.495519	0.597840
39	1	0	-0.017902	-3.948581	2.722893

40	1	0	-4.209467	1.479081	-0.664879
41	1	0	-2.580345	1.916635	-0.194967
42	1	0	-4.151520	3.747432	3.505465
43	1	0	-5.786080	3.313555	3.016176
44	1	0	-1.767033	-4.136224	2.575581
45	1	0	-3.604471	-3.085627	1.196234
46	1	0	-2.350304	-2.688780	0.013328
47	1	0	-2.680345	-0.507684	-0.865517
48	1	0	-3.447246	-0.691323	2.107355
49	1	0	-4.406096	6.002219	2.380352
50	1	0	-5.663271	5.752043	3.604842
51	1	0	-6.050939	5.565231	1.884988
52	1	0	6.542379	1.624361	-4.000753

8. Tsa4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	5.908477	3.552258	0.465262
2	8	0	6.603451	1.477649	1.126663
3	6	0	2.630720	-1.730361	-0.438841
4	6	0	1.189133	-2.160480	-0.769293
5	6	0	2.806703	-0.202742	-0.361425
6	6	0	1.042041	-3.677189	-0.987881
7	6	0	4.208657	0.220085	0.113394
8	6	0	-0.427000	-4.128203	-1.160350
9	6	0	4.396072	1.742938	0.085114
10	6	0	-3.884443	1.536200	0.113534
11	6	0	-3.996516	3.064424	-0.041989
12	6	0	-1.247095	-3.917821	0.113285
13	6	0	-3.199449	1.119464	1.426012
14	6	0	-4.801641	3.496051	-1.282194
15	6	0	-2.586690	-3.644877	0.128122
16	6	0	-3.307500	-2.826485	1.166407
17	6	0	-3.079991	-0.367535	1.675271
18	6	0	5.718976	2.190627	0.643050
19	6	0	-3.444710	-1.357551	0.844983
20	6	0	-4.908413	5.023130	-1.431826
21	1	0	2.932463	-2.178469	0.520560
22	1	0	3.316048	-2.137115	-1.198803
23	1	0	0.523901	-1.834177	0.045256
24	1	0	0.840371	-1.630799	-1.669180

25	1	0	2.603275	0.240316	-1.349001
26	1	0	2.048015	0.207658	0.323184
27	1	0	1.483903	-4.165249	-0.105519
28	1	0	1.624907	-3.961118	-1.877120
29	1	0	5.003471	-0.259915	-0.472919
30	1	0	4.332635	-0.138692	1.143812
31	1	0	-0.480853	-5.185889	-1.452690
32	1	0	-0.874759	-3.488374	-1.935244
33	1	0	3.635114	2.295662	0.654303
34	1	0	4.291010	2.083603	-0.954818
35	1	0	-3.323889	1.126324	-0.739688
36	1	0	-4.890589	1.093589	0.067597
37	1	0	-4.466366	3.489406	0.859021
38	1	0	-2.986613	3.500577	-0.098169
39	1	0	-0.623109	-3.499330	0.916131
40	1	0	-2.199082	1.571719	1.531406
41	1	0	-3.802094	1.564610	2.235362
42	1	0	-5.810941	3.061288	-1.226144
43	1	0	-4.332681	3.071089	-2.182406
44	1	0	-2.315004	-5.147061	-0.167578
45	1	0	-2.798149	-3.000785	2.130982
46	1	0	-4.267797	-3.375526	1.268609
47	1	0	-2.708529	-0.637181	2.667301
48	1	0	-3.809196	-1.132359	-0.156197
49	1	0	-5.403712	5.471001	-0.560447
50	1	0	-5.485487	5.298397	-2.322886
51	1	0	-3.914627	5.480901	-1.521792
52	1	0	6.788723	3.828862	0.801369

9. Tsb1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-6.183797	7.619546	0.312568
2	8	0	-6.983685	5.500770	-0.011561
3	6	0	-2.634819	2.431575	0.455881
4	6	0	-1.165776	2.039564	0.700012
5	6	0	-2.887389	3.947370	0.556630
6	6	0	-0.927482	0.520902	0.596400
7	6	0	-4.360786	4.327487	0.325667
8	6	0	0.520210	0.076812	0.932549
9	6	0	-4.593401	5.840965	0.428244

10	6	0	3.073060	-5.186982	-0.909393
11	6	0	3.814786	-4.412306	0.194645
12	6	0	1.547888	0.653449	-0.034962
13	6	0	2.058265	-4.325853	-1.701997
14	6	0	4.827240	-5.273833	0.972976
15	6	0	1.946684	0.182749	-1.313825
16	6	0	1.441497	-1.176993	-1.760820
17	6	0	2.714380	-3.259532	-2.548286
18	6	0	-6.026552	6.246176	0.217937
19	6	0	2.457708	-1.938926	-2.580973
20	6	0	5.557763	-4.493658	2.079245
21	1	0	-2.944231	2.078404	-0.539887
22	1	0	-3.275515	1.908411	1.182583
23	1	0	-0.528187	2.566966	-0.024355
24	1	0	-0.859424	2.387036	1.699543
25	1	0	-2.568462	4.302146	1.549468
26	1	0	-2.253551	4.469697	-0.176899
27	1	0	-1.184470	0.179506	-0.416661
28	1	0	-1.612715	0.002696	1.283397
29	1	0	-4.997185	3.810876	1.056261
30	1	0	-4.685576	3.975441	-0.662458
31	1	0	0.562782	-1.019204	0.926047
32	1	0	0.766218	0.399896	1.953327
33	1	0	-3.981735	6.384574	-0.305740
34	1	0	-4.280963	6.221807	1.411171
35	1	0	2.540894	-6.038283	-0.459463
36	1	0	3.806870	-5.614771	-1.610375
37	1	0	4.335643	-3.551976	-0.250283
38	1	0	3.077102	-3.997094	0.900550
39	1	0	1.862494	1.673214	0.205008
40	1	0	1.479788	-4.993944	-2.360274
41	1	0	1.334727	-3.886376	-1.003155
42	1	0	5.564662	-5.687578	0.268635
43	1	0	4.306171	-6.136536	1.415287
44	1	0	2.734865	0.180488	-0.176496
45	1	0	0.591105	-0.909446	-2.419570
46	1	0	1.010588	-1.813254	-0.971598
47	1	0	3.492871	-3.634024	-3.216868
48	1	0	3.033657	-1.309758	-3.258040
49	1	0	6.111807	-3.643509	1.660489
50	1	0	6.273963	-5.130380	2.612687
51	1	0	4.847463	-4.097726	2.817027
52	1	0	-7.121950	7.874721	0.174507

10. Tsb2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-7.350681	4.852401	-0.215722
2	8	0	-5.986494	5.597580	1.462864
3	6	0	-1.478435	2.822948	0.748778
4	6	0	-0.470827	1.841731	0.120642
5	6	0	-2.827015	2.874755	0.007403
6	6	0	0.868863	1.796949	0.880534
7	6	0	-3.820801	3.866589	0.638412
8	6	0	1.963448	0.916742	0.226111
9	6	0	-5.161680	3.901498	-0.107235
10	6	0	1.060830	-6.972856	-0.189589
11	6	0	-0.117411	-6.903907	0.798393
12	6	0	1.587844	-0.555213	0.224284
13	6	0	1.762394	-5.610917	-0.429039
14	6	0	-0.792906	-8.267848	1.035316
15	6	0	1.993023	-1.454414	1.232684
16	6	0	1.371402	-2.840103	1.160685
17	6	0	2.512990	-5.107199	0.781398
18	6	0	-6.154589	4.864347	0.483912
19	6	0	2.353076	-3.951084	1.451348
20	6	0	-1.980787	-8.192942	2.009843
21	1	0	-1.652988	2.541485	1.798599
22	1	0	-1.037263	3.831418	0.768948
23	1	0	-0.920602	0.838242	0.089984
24	1	0	-0.285991	2.132002	-0.925881
25	1	0	-2.651661	3.149440	-1.044766
26	1	0	-3.271744	1.867223	-0.005928
27	1	0	0.703166	1.441832	1.907377
28	1	0	1.264812	2.819838	0.960890
29	1	0	-3.384247	4.874025	0.649895
30	1	0	-3.995500	3.599832	1.689186
31	1	0	2.894183	1.034428	0.793860
32	1	0	2.139358	1.265473	-0.801741
33	1	0	-5.629970	2.907115	-0.122925
34	1	0	-5.018782	4.176138	-1.162170
35	1	0	0.700937	-7.358349	-1.155171
36	1	0	1.802496	-7.699006	0.177994
37	1	0	0.233707	-6.500072	1.759090
38	1	0	-0.866196	-6.190836	0.417516
39	1	0	0.814192	-0.839596	-0.512061

40	1	0	2.476677	-5.737035	-1.258384
41	1	0	1.017245	-4.880416	-0.768458
42	1	0	-0.045658	-8.977221	1.422104
43	1	0	-1.134545	-8.675883	0.071784
44	1	0	2.732945	-1.165078	0.137552
45	1	0	0.801012	-3.028941	0.233965
46	1	0	0.623242	-2.816501	1.975733
47	1	0	3.286009	-5.789108	1.143076
48	1	0	3.001841	-3.749890	2.302886
49	1	0	-1.662069	-7.819610	2.991738
50	1	0	-2.439352	-9.178093	2.158968
51	1	0	-2.757748	-7.515443	1.632117
52	1	0	-7.991773	5.484140	0.177039

11. Tsb3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-6.838714	6.223570	-1.426406
2	8	0	-5.684631	6.916893	0.423068
3	6	0	-1.639235	3.432259	0.749511
4	6	0	-0.723164	2.248577	0.385627
5	6	0	-2.818767	3.614218	-0.223351
6	6	0	0.463256	2.083071	1.353905
7	6	0	-3.725465	4.803316	0.142277
8	6	0	1.452261	0.952905	0.968027
9	6	0	-4.892024	4.967875	-0.841031
10	6	0	0.173277	-6.903013	0.027113
11	6	0	0.501073	-8.179109	0.826879
12	6	0	0.871494	-0.438579	1.050452
13	6	0	0.088814	-5.622382	0.885881
14	6	0	0.575214	-9.442399	-0.051644
15	6	0	1.306720	-1.400868	1.879911
16	6	0	0.726875	-2.792301	1.968275
17	6	0	1.438541	-5.132473	1.400034
18	6	0	-5.798037	6.123608	-0.516164
19	6	0	1.776958	-3.884929	1.983433
20	6	0	0.890506	-10.716681	0.749798
21	1	0	-2.028447	3.289807	1.769442
22	1	0	-1.043442	4.357926	0.773094
23	1	0	-1.321544	1.325865	0.366793
24	1	0	-0.336838	2.390753	-0.636465

25	1	0	-2.427398	3.751893	-1.243744
26	1	0	-3.416935	2.689483	-0.244204
27	1	0	0.085285	1.895877	2.369673
28	1	0	1.020283	3.031402	1.394777
29	1	0	-3.134563	5.728574	0.164628
30	1	0	-4.120775	4.671180	1.158177
31	1	0	2.332993	1.012313	1.621791
32	1	0	1.809650	1.144297	-0.057147
33	1	0	-5.510096	4.059375	-0.875072
34	1	0	-4.524326	5.111602	-1.867159
35	1	0	-0.787205	-7.047625	-0.488106
36	1	0	0.927102	-6.761109	-0.762885
37	1	0	1.457293	-8.059121	1.358119
38	1	0	-0.266285	-8.322493	1.603965
39	1	0	0.040106	-0.660237	0.377382
40	1	0	-0.402364	-4.825549	0.312456
41	1	0	-0.559466	-5.808325	1.757255
42	1	0	1.341714	-9.297522	-0.827776
43	1	0	-0.380520	-9.569241	-0.582102
44	1	0	2.152172	-1.210210	2.541690
45	1	0	-0.082031	-2.908450	1.224726
46	1	0	0.240254	-2.915160	2.957194
47	1	0	2.184694	-5.923305	1.520029
48	1	0	2.191767	-4.335158	0.734191
49	1	0	1.855862	-10.629951	1.265065
50	1	0	0.937339	-11.597014	0.097706
51	1	0	0.122030	-10.904076	1.510899
52	1	0	-7.423286	6.981257	-1.206149

12. Tsb4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	6.419862	3.529594	-0.473665
2	8	0	6.912984	1.672993	0.768485
3	6	0	2.747443	-1.563823	-0.113637
4	6	0	1.402273	-2.063269	-0.673084
5	6	0	3.124052	-0.150430	-0.595783
6	6	0	1.038748	-3.480154	-0.189849
7	6	0	4.470873	0.338792	-0.033682
8	6	0	-0.276159	-4.043915	-0.787701
9	6	0	4.829162	1.747472	-0.526624

10	6	0	-4.171686	1.375004	0.129774
11	6	0	-4.171545	2.911132	0.236951
12	6	0	-1.518113	-3.291494	-0.375416
13	6	0	-4.439872	0.690658	1.478567
14	6	0	-3.913113	3.611768	-1.110301
15	6	0	-2.515761	-3.824477	0.347919
16	6	0	-3.789519	-3.124879	0.788141
17	6	0	-4.412766	-0.832915	1.475178
18	6	0	6.140127	2.258578	0.004127
19	6	0	-3.799724	-1.634394	0.492374
20	6	0	-3.908836	5.146047	-1.003232
21	1	0	2.708336	-1.572814	0.986640
22	1	0	3.544103	-2.268037	-0.399880
23	1	0	0.609268	-1.358118	-0.385690
24	1	0	1.441981	-2.056241	-1.774078
25	1	0	3.160620	-0.141663	-1.696559
26	1	0	2.328004	0.554079	-0.307657
27	1	0	0.961629	-3.483720	0.907458
28	1	0	1.860002	-4.165097	-0.450571
29	1	0	5.268584	-0.360202	-0.318025
30	1	0	4.439783	0.333594	1.063932
31	1	0	-0.374356	-5.098689	-0.494085
32	1	0	-0.186934	-4.031280	-1.886351
33	1	0	4.051263	2.472158	-0.246581
34	1	0	4.878790	1.779570	-1.624374
35	1	0	-3.214560	1.020892	-0.271403
36	1	0	-4.933747	1.060077	-0.599389
37	1	0	-5.136754	3.254861	0.642147
38	1	0	-3.403307	3.227727	0.960374
39	1	0	-1.607009	-2.255285	-0.696476
40	1	0	-3.675289	1.002992	2.208289
41	1	0	-5.400878	1.032214	1.891941
42	1	0	-4.680276	3.296344	-1.833297
43	1	0	-2.949528	3.268560	-1.515216
44	1	0	-2.442763	-4.866562	0.667843
45	1	0	-3.965211	-3.349227	1.861759
46	1	0	-4.630256	-3.590792	0.245155
47	1	0	-4.733847	-1.275638	2.438269
48	1	0	-5.088049	-1.157136	0.431209
49	1	0	-4.872323	5.518519	-0.631352
50	1	0	-3.722895	5.614138	-1.977418
51	1	0	-3.129087	5.491186	-0.311728
52	1	0	7.277419	3.853842	-0.121828

Supplemental files

Fig. S1 C18:2 isomerization schemes of the reactant C18:2-9c,12c,transition states(ts), intermediates(im), and the products(C18:2-9c,12t, C18:2-9t,12c, C18:2-9t,12t).

Fig. S2 Energy (E) curves of the IRC isomerization reaction schemes.

Fig. S3 C18:2-9c12t degradation scheme of reactant (C18:2-9c12t and O_2), transition states, and the product (aldehydes and olefinic alcohol).

Fig. S4 Energy (E) curves of the Hydroperoxide degradation reaction scheme.

Fig. S1

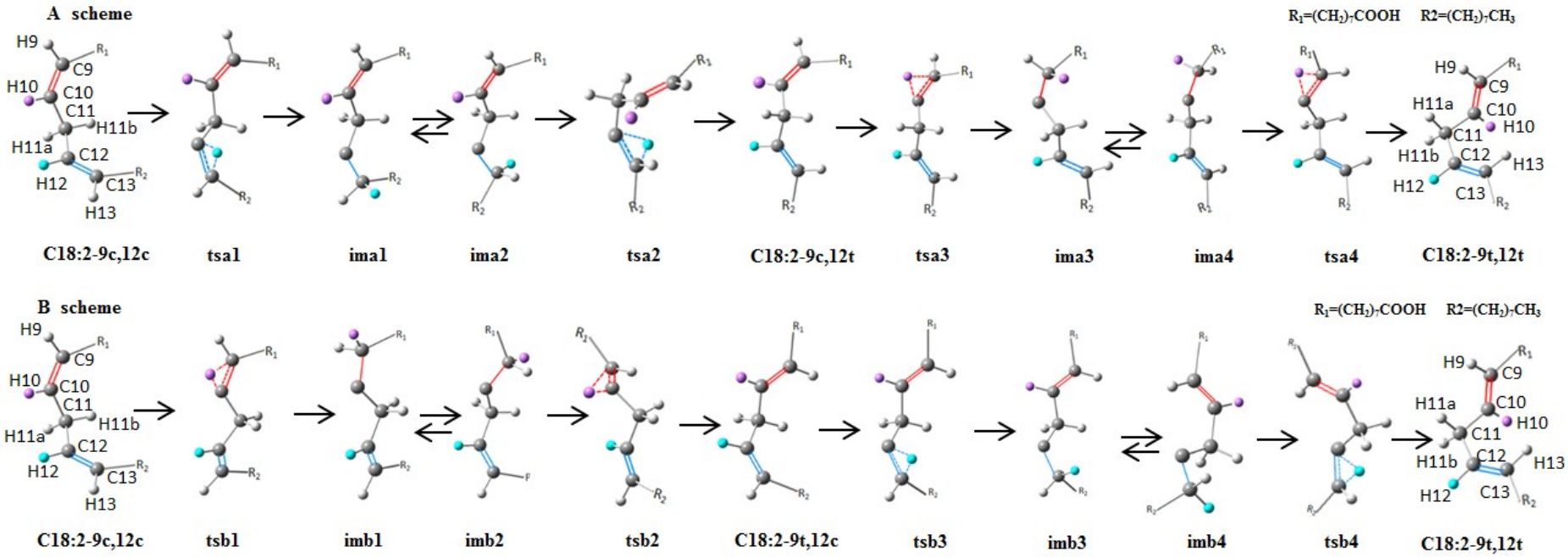
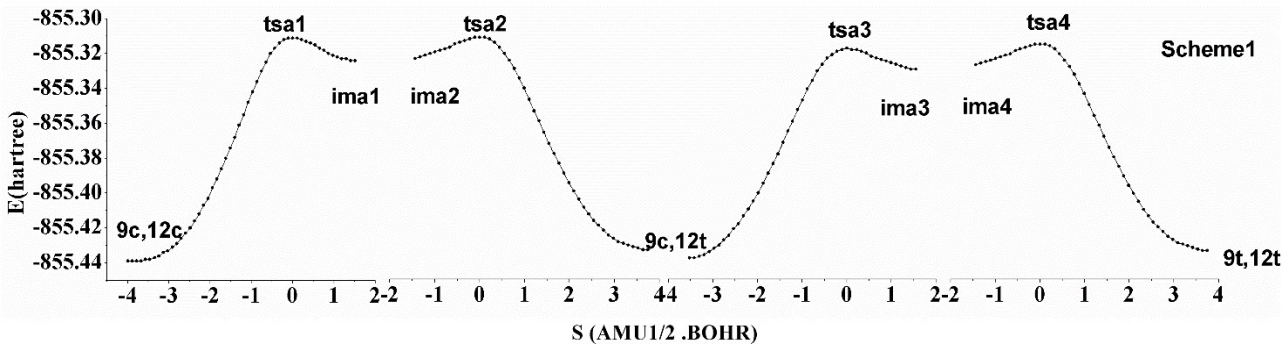

A scheme
R1=(CH2)7COOH R2=(CH2)7CH3
C18:2-9c,12c
tsa1
ima1
ima2
tsa2
C18:2-9c,12t
tsa3
ima3
ima4
tsa4
C18:2-9t,12t
B scheme
R1=(CH2)7COOH R2=(CH2)7CH3
C18:2-9c,12c
tsb1
imb1
imb2
tsb2
C18:2-9t,12c
tsb3
imb3
imb4
tsb4
C18:2-9t,12t

Fig. S2


-855.30
-855.32
-855.34
-855.36
-855.38
-855.40
-855.42
-855.44
E(hartree)
tsa1
tsa2
tsa3
tsa4
Scheme1
ima1
ima2
ima3
ima4
9c,12c
9c,12t
9t,12t
-4 -3 -2 -1 0 1 2-2 -1 0 1 2 3 44 -3 -2 -1 0 1 2-2 -1 0 1 2 3 4
S (AMU1/2 .BOHR)

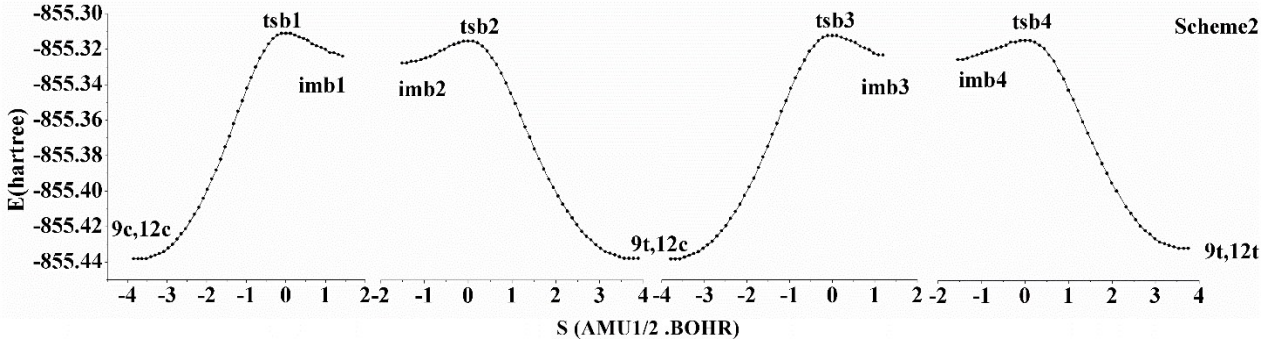
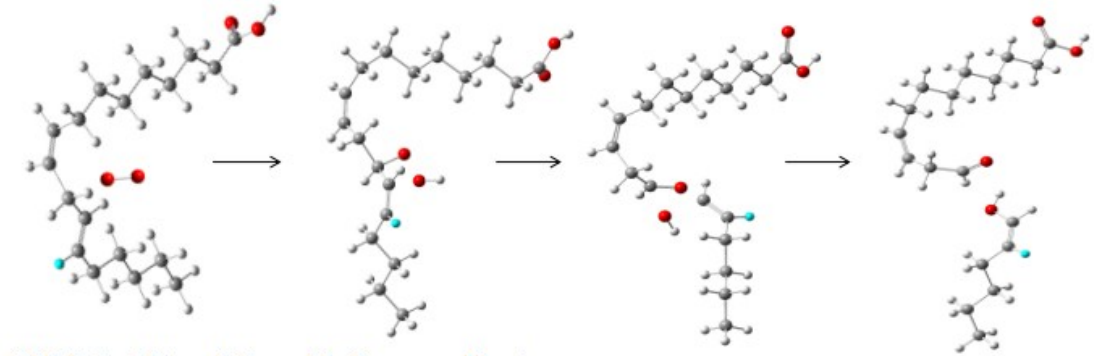
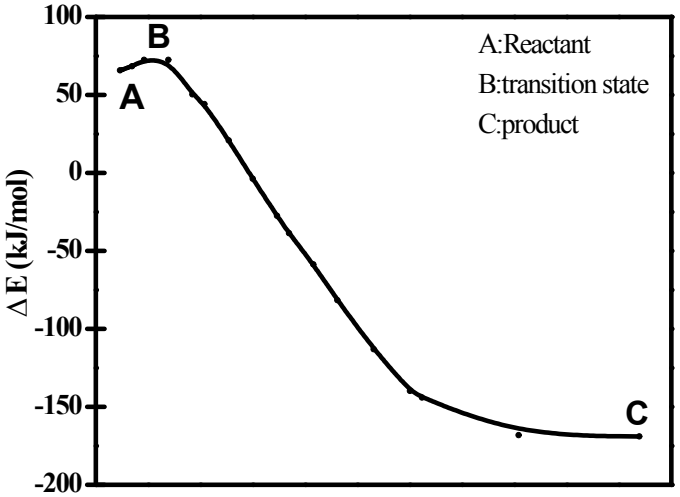

-855.30
-855.32
-855.34
-855.36
-855.38
-855.40
-855.42
-855.44
E(hartree)
tsb1
tsb2
tsb3
tsb4
Scheme2
imb1
imb2
imb3
imb4
9c,12c
9t,12c
9t,12t
-4 -3 -2 -1 0 1 2-2 -1 0 1 2 3 4-4 -3 -2 -1 0 1 2-2 -1 0 1 2 3 4
S (AMU1/2 .BOHR)

Fig. S3



C18:2-9c,12t and O_2 | **Hydroperoxide (peroxy group present at C11 position)** | **Transition state** | **product**

Fig.S4


100
50
0
-50
-100
-150
-200
ΔE (kJ/mol)
A
B
C
A:Reactant
B:transition state
C:product