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Supporting Information

Mechanisms of Air Oxidation of Ethoxylated Surfactants – Computational Estimations of Energies and Reaction Behaviors

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1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.984828	-0.357006	-0.000296
2	6	0	-1.755342	0.535587	0.000274
3	8	0	-0.594313	-0.286257	-0.000475
4	6	0	0.616440	0.450534	0.000525
5	6	0	1.765767	-0.545516	0.000639
6	8	0	2.975180	0.215141	-0.001125
7	1	0	-2.996658	-0.998120	0.886525
8	1	0	-2.996407	-0.997162	-0.887817
9	1	0	-3.894904	0.252406	-0.000111
10	1	0	-1.748580	1.188804	-0.887919
11	1	0	-1.748380	1.187455	0.889457
12	1	0	0.683511	1.094987	0.891279
13	1	0	0.684701	1.095671	-0.889654
14	1	0	1.694004	-1.185188	-0.889737
15	1	0	1.695605	-1.183527	0.892326
16	1	0	3.727941	-0.387996	0.001595

-308.9009562 -308.75968 -308.751605 -308.750661 -308.792136

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.942832	-0.377297	-0.062456
2	6	0	1.721327	0.519358	0.048709
3	8	0	0.554796	-0.288555	-0.042592
4	6	0	-0.648672	0.453952	0.064655
5	6	0	-1.791682	-0.499256	0.015740
6	8	0	-3.015779	0.119179	-0.099478
7	1	0	2.944848	-0.909318	-1.018665
8	1	0	2.951809	-1.117751	0.743295
9	1	0	3.858377	0.220150	0.004704
10	1	0	1.724512	1.063747	1.007933
11	1	0	1.717146	1.271755	-0.757374
12	1	0	-0.741294	1.185764	-0.756580
13	1	0	-0.646163	1.035870	1.010446
14	1	0	-1.743847	-1.436285	0.567962
15	1	0	-3.720369	-0.539470	-0.065048

-308.2393717 -308.112059 -308.10397 -308.103025 -308.145339

2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.968786	-0.333724	-0.072585
2	6	0	1.741601	0.556175	-0.000139
3	8	0	0.573893	-0.276075	-0.013539
4	6	0	-0.616378	0.376783	0.100508
5	6	0	-1.809414	-0.510128	0.147058
6	8	0	-2.949581	0.261870	-0.247726
7	1	0	2.960376	-0.930988	-0.989253
8	1	0	3.007220	-1.014301	0.783384
9	1	0	3.875552	0.280193	-0.068177
10	1	0	1.741808	1.156498	0.921248
11	1	0	1.696131	1.243135	-0.855839
12	1	0	-0.619185	1.343486	0.603839
13	1	0	-1.970998	-0.919745	1.163106
14	1	0	-1.644747	-1.363563	-0.527279
15	1	0	-3.748219	-0.215714	0.010043

-308.2399451 -308.112635 -308.104391 -308.103447 -308.146315

2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.037996	-0.280890	0.017738
2	6	0	1.772898	0.499045	-0.046991
3	8	0	0.632809	-0.258835	-0.032846
4	6	0	-0.593036	0.469939	-0.059044
5	6	0	-1.726832	-0.538859	0.034299
6	8	0	-2.941544	0.210436	0.010383
7	1	0	3.069176	-1.044243	-0.768611
8	1	0	3.162784	-0.803762	0.981750
9	1	0	3.897120	0.383868	-0.114084
10	1	0	1.692050	1.490110	0.402169
11	1	0	-0.671660	1.045580	-0.990112
12	1	0	-0.639112	1.167748	0.788695
13	1	0	-1.629390	-1.115665	0.964388
14	1	0	-1.667356	-1.235038	-0.813472
15	1	0	-3.689882	-0.396814	0.052966

-308.2413552 -308.114033 -308.105735 -308.104791 -308.147463

3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.462205	0.645836	-0.253355
2	6	0	2.439548	-0.313536	0.329174
3	8	0	1.162803	-0.008918	-0.228955
4	6	0	0.130444	-0.843026	0.247652
5	6	0	-1.179947	-0.349981	-0.331691
6	8	0	-2.166584	-1.289538	-0.106484
7	8	0	-1.509518	0.914043	0.383166
8	8	0	-2.689696	1.356863	-0.013653
9	1	0	3.198461	1.680541	-0.015238
10	1	0	3.512394	0.543558	-1.341584
11	1	0	4.453792	0.435536	0.160912
12	1	0	2.704611	-1.357643	0.095816
13	1	0	2.393330	-0.217780	1.425610
14	1	0	0.066451	-0.824816	1.346635
15	1	0	0.271652	-1.886543	-0.072166
16	1	0	-1.086671	-0.057535	-1.383887
17	1	0	-3.003559	-0.930676	-0.439376

-458.6248188 -458.487458 -458.477822 -458.476878 -458.52389

3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.926105	-0.705531	-0.330838
2	6	0	-2.065920	0.461013	0.136952
3	8	0	-0.814251	0.015206	0.707433
4	6	0	0.211705	-0.210093	-0.175204
5	6	0	1.308923	-1.003697	0.523222
6	8	0	2.404130	-1.272452	-0.335486
7	8	0	0.768099	1.084480	-0.695423
8	8	0	1.319253	1.813345	0.263582
9	1	0	-3.126743	-1.392865	0.496423
10	1	0	-2.446796	-1.267910	-1.139102
11	1	0	-3.883887	-0.331666	-0.709432
12	1	0	-1.864832	1.169314	-0.674790
13	1	0	-2.557237	1.008409	0.944901
14	1	0	-0.098533	-0.673904	-1.119973
15	1	0	0.889277	-1.969720	0.814246
16	1	0	1.607148	-0.464446	1.429439
17	1	0	2.892141	-0.452000	-0.487355

-458.6211596 -458.483584 -458.47391 -458.472966 -458.519942

3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.285098	-1.305487	-0.202679
2	6	0	1.225223	-0.458130	0.461868
3	8	0	0.038414	-0.555370	-0.232509
4	6	0	-1.103260	0.035194	0.403305
5	6	0	-2.306665	-0.266326	-0.475416
6	8	0	-3.441162	0.284149	0.191706
7	8	0	1.678104	0.966908	0.550830
8	8	0	1.934674	1.486448	-0.638608
9	1	0	2.410781	-0.988636	-1.240151
10	1	0	1.974364	-2.353220	-0.181824
11	1	0	3.236647	-1.203962	0.325200
12	1	0	1.097195	-0.678468	1.531327
13	1	0	-0.971294	1.117666	0.505098
14	1	0	-1.246533	-0.399492	1.402445
15	1	0	-2.404691	-1.353262	-0.603856
16	1	0	-2.159001	0.188726	-1.463869
17	1	0	-4.220087	0.182069	-0.368196

-458.6219399	-458.4847	-458.47484	-458.473896	-458.521339

4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.496166	0.692039	-0.254926
2	6	0	2.493278	-0.310886	0.288701
3	8	0	1.200464	0.026340	-0.204275
4	6	0	0.188931	-0.853743	0.241210
5	6	0	-1.152181	-0.359702	-0.283209
6	8	0	-2.070170	-1.414453	-0.176721
7	8	0	-1.515636	0.743915	0.538491
8	8	0	-2.711707	1.327361	-0.060445
9	1	0	3.239663	1.705990	0.066649
10	1	0	3.510272	0.669876	-1.348916
11	1	0	4.501469	0.456017	0.109724
12	1	0	2.755757	-1.334273	-0.026511
13	1	0	2.484282	-0.295175	1.390573
14	1	0	0.151154	-0.902308	1.340112
15	1	0	0.343962	-1.871571	-0.145717
16	1	0	-1.064736	-0.005567	-1.318981
17	1	0	-2.937096	-1.085506	-0.453404
18	1	0	-2.365498	2.190960	-0.340589

-459.2661662 -459.116966 -459.106885 -459.10594 -459.152821

4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.947109	-0.719885	-0.247283
2	6	0	-2.080168	0.494397	0.063025
3	8	0	-0.828673	0.122647	0.675734
4	6	0	0.202976	-0.207393	-0.209595
5	6	0	1.221620	-1.065311	0.539572
6	8	0	2.338509	-1.375021	-0.275067
7	8	0	0.789562	0.960726	-0.793928
8	8	0	1.455076	1.731096	0.248009
9	1	0	-3.144089	-1.294135	0.662935
10	1	0	-2.469981	-1.383041	-0.976554
11	1	0	-3.906041	-0.397227	-0.668189
12	1	0	-1.884046	1.089730	-0.837452
13	1	0	-2.574593	1.141989	0.792831
14	1	0	-0.157737	-0.723893	-1.110384
15	1	0	0.747904	-2.013768	0.804213
16	1	0	1.513517	-0.553639	1.463844
17	1	0	2.756477	-0.542965	-0.538463
18	1	0	0.698889	2.150521	0.694913

-459.2659524 -459.116234 -459.106296 -459.105352 -459.151604

4c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.219263	1.357570	-0.249420
2	6	0	-1.196344	0.488273	0.455952
3	8	0	0.003090	0.521549	-0.276253
4	6	0	1.152536	0.042189	0.425474
5	6	0	2.344836	0.195880	-0.505704
6	8	0	3.481898	-0.301394	0.198855
7	8	0	-1.641247	-0.850024	0.690239
8	8	0	-2.097229	-1.434360	-0.561657
9	1	0	-2.358245	1.021711	-1.278233
10	1	0	-1.872510	2.394271	-0.257100
11	1	0	-3.176265	1.301946	0.275398
12	1	0	-1.024401	0.818172	1.493115
13	1	0	1.031130	-1.009858	0.710990
14	1	0	1.313073	0.630085	1.340557
15	1	0	2.467977	1.254423	-0.772483
16	1	0	2.164486	-0.373382	-1.428376
17	1	0	4.267236	-0.198831	-0.351986
18	1	0	-1.275169	-1.828172	-0.899166

-459.2640291 -459.115076 -459.104714 -459.10377 -459.15145

H2O2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.718562	-0.118803	-0.053567
2	8	0	0.718562	0.118803	-0.053567
3	1	0	-1.025032	0.666260	0.428532
4	1	0	1.025032	-0.666259	0.428532

-151.5584105 -151.53197 -151.528735 -151.527791 -151.554288

4d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.846860	-0.416186	0.000039
2	6	0	-1.653777	0.523104	-0.000181
3	8	0	-0.460026	-0.256835	0.000106
4	6	0	0.720300	0.514588	0.000157
5	6	0	1.909232	-0.427152	-0.000092
6	8	0	3.058218	-0.041276	-0.000051
7	1	0	-2.834510	-1.055917	0.887595
8	1	0	-2.834570	-1.056312	-0.887233
9	1	0	-3.778647	0.158973	-0.000056
10	1	0	-1.667878	1.173926	-0.889379
11	1	0	-1.667992	1.174470	0.888611
12	1	0	0.786947	1.164896	0.888943
13	1	0	0.786698	1.165341	-0.888295
14	1	0	1.651041	-1.506605	-0.000161

-307.6858655 -307.568922 -307.561427 -307.560483 -307.600966

4e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.938079	-0.255558	-0.019125
2	6	0	1.637606	0.475022	0.262482
3	8	0	0.557431	-0.307909	-0.259761
4	6	0	-0.669883	0.302588	-0.189693
5	6	0	-1.766771	-0.401316	0.101245
6	8	0	-3.019191	0.167704	-0.023224
7	1	0	3.078298	-0.393774	-1.095480
8	1	0	2.939501	-1.240266	0.457978
9	1	0	3.784247	0.319695	0.371229
10	1	0	1.491039	0.622965	1.342350

11	1	0	1.632523	1.465730	-0.217367
12	1	0	-0.713695	1.359817	-0.451795
13	1	0	-1.716635	-1.456216	0.359759
14	1	0	-3.635382	-0.280731	0.567745

-307.6687741	-307.551548	-307.543896	-307.542951	-307.583275

4f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.056374	-0.217380	-0.001033
2	6	0	-1.860079	0.375819	0.000867
3	8	0	-0.693050	-0.330325	0.000770
4	6	0	0.505053	0.446299	-0.000527
5	6	0	1.672311	-0.527508	0.000909
6	8	0	2.859658	0.263946	-0.001252
7	1	0	-3.954306	0.388271	0.000012
8	1	0	-3.155500	-1.297472	-0.003312
9	1	0	-1.748092	1.459891	0.003156
10	1	0	0.550644	1.086033	0.890858
11	1	0	0.550578	1.083185	-0.893948
12	1	0	1.614171	-1.168993	-0.888936
13	1	0	1.615003	-1.165456	0.893341
14	1	0	3.629171	-0.317806	0.001385

-307.6666765	-307.549242	-307.541422	-307.540478	-307.584318

5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.088814	-0.527769	0.097325
2	6	0	1.084072	0.609807	0.014067
3	8	0	-0.173316	0.131747	-0.514798
4	6	0	-1.241720	0.087549	0.303988
5	8	0	-2.318119	-0.320279	-0.046830
6	1	0	2.226306	-0.992409	-0.883127
7	1	0	1.755727	-1.297715	0.800250
8	1	0	3.056961	-0.144648	0.437898
9	1	0	0.916315	1.068513	0.996869
10	1	0	1.420100	1.390740	-0.673497
11	1	0	-1.030925	0.466246	1.322355

-268.3958231	-268.305957	-268.300028	-268.299084	-268.335752

6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.531797	0.000007	-0.000053
2	8	0	0.677998	-0.000016	0.000013
3	1	0	-1.116487	0.941370	0.000108
4	1	0	-1.116713	-0.941279	0.000108

-	-	-	-	-
114.5115241	114.484851	114.481983	114.481039	114.50652

7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.170181	-0.149280	-0.000093
2	6	0	-0.231149	0.399919	-0.000188
3	8	0	-1.238275	-0.277324	0.000015
4	1	0	1.710571	0.223370	-0.879533
5	1	0	1.161183	-1.240981	-0.000326
6	1	0	1.708636	0.222443	0.881123
7	1	0	-0.308380	1.509919	0.000303

-	-	-	-	-
153.8451887	153.789774	153.785863	153.784918	153.814762

8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.727627	-0.353157	-0.114851
2	6	0	-0.516214	0.523249	-0.068732
3	8	0	-1.717718	-0.230296	-0.010835
4	8	0	1.843942	0.057418	0.118743
5	1	0	0.541227	-1.412974	-0.396875
6	1	0	-0.552749	1.095743	-1.003985
7	1	0	-0.419805	1.244838	0.753359
8	1	0	-1.846943	-0.565139	0.885733

-	-	-	-	-
229.0564999	228.995957	228.991087	228.990143	229.023338

Intermediate 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.492299	-0.547101	0.874706

2	6	0	1.958728	-0.508400	-0.521291
3	8	0	0.624873	-0.751974	-0.787251
4	6	0	-0.373627	-0.162327	0.018949
5	6	0	-1.669474	-0.944025	-0.201943
6	8	0	-2.709035	-0.480665	0.639933
7	8	0	-0.668628	1.158311	-0.405948
8	8	0	0.309440	2.070901	0.159555
9	1	0	2.279373	-1.507651	1.374264
10	1	0	2.093281	0.250254	1.511615
11	1	0	3.579112	-0.428212	0.839435
12	1	0	0.959311	2.119273	-0.564668
13	1	0	2.562925	-0.873759	-1.345983
14	1	0	-0.088486	-0.138047	1.074297
15	1	0	-1.490460	-1.990277	0.055035
16	1	0	-1.938555	-0.889299	-1.265774
17	1	0	-2.857253	0.456250	0.448937

-	-	-	-	-
458.6022851	458.46652	458.456487	458.455542	458.502428

Intermediate 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.914176	-0.181130	0.744387
2	6	0	2.097859	0.309685	-0.444339
3	8	0	0.924799	-0.506157	-0.667082
4	6	0	-0.200108	-0.140516	0.051201
5	6	0	-1.193036	-1.319857	-0.038789
6	8	0	-2.474595	-0.988965	0.297582
7	8	0	-0.766246	1.020255	-0.573286
8	8	0	-1.572549	1.701595	0.422993
9	1	0	3.220056	-1.222040	0.601482
10	1	0	2.351626	-0.110546	1.681350
11	1	0	3.815912	0.431874	0.852827
12	1	0	1.791099	1.354326	-0.326696
13	1	0	2.672096	0.228688	-1.370748
14	1	0	0.012937	0.123627	1.096559
15	1	0	-0.832927	-2.215355	0.495053
16	1	0	-1.238117	-1.594316	-1.115521
17	1	0	-2.397298	1.180824	0.369278

-	-	-	-	-
458.5907477	458.45521	458.445806	458.444861	458.490672

TS formation of 2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.878453	-3.058890	0.958151
2	6	0	2.418552	-3.459638	1.074642
3	8	0	1.600083	-2.304062	0.869162
4	6	0	0.204606	-2.572609	0.961631
5	6	0	-0.550843	-1.271607	0.736241
6	8	0	-1.912870	-1.590313	0.629022
7	8	0	-0.283300	-0.448690	1.869360
8	8	0	-0.482183	0.910596	1.516146
9	1	0	4.142254	-2.316376	1.717722
10	1	0	4.090562	-2.637703	-0.029236
11	1	0	4.517106	-3.936298	1.102535
12	1	0	2.160531	-4.220690	0.322793
13	1	0	2.204812	-3.880610	2.068542
14	1	0	-0.050092	-2.973863	1.952406
15	1	0	-0.101246	-3.296933	0.195229
16	1	0	-0.189445	-0.743045	-0.153321
17	1	0	-2.405985	-0.762141	0.542043
18	6	0	1.746527	5.959269	2.224961
19	6	0	2.202018	5.014103	1.126482
20	8	0	1.952865	3.677095	1.545863
21	6	0	2.336743	2.707814	0.591985
22	6	0	1.994663	1.344239	1.143982
23	8	0	2.345263	0.354891	0.254094
24	1	0	2.294803	5.766237	3.152069
25	1	0	0.678315	5.831217	2.423900
26	1	0	1.923294	6.998160	1.926672
27	1	0	1.658082	5.215534	0.189045
28	1	0	3.277396	5.144624	0.920234
29	1	0	3.422901	2.760357	0.392670
30	1	0	1.818299	2.862663	-0.368345
31	1	0	0.698520	1.281022	1.325084
32	1	0	2.330013	1.176529	2.177018
33	1	0	2.181227	-0.537777	0.624772

-767.5097727 -767.234622 -767.216495 -767.215551 -767.283912

TS formation of 2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.192645	2.158833	0.875706
2	6	0	2.638953	2.695182	-0.432609
3	8	0	1.397834	2.041730	-0.722180
4	6	0	0.761002	2.547175	-1.887260
5	6	0	-0.494908	1.728511	-2.134447

6	8	0	-1.268660	2.399804	-3.091132
7	8	0	-0.056608	0.455955	-2.601696
8	1	0	3.359834	1.079626	0.820371
9	1	0	2.500689	2.356855	1.699880
10	1	0	4.146284	2.648271	1.099887
11	1	0	2.464152	3.780055	-0.366870
12	1	0	3.341586	2.517103	-1.260940
13	1	0	1.420326	2.472816	-2.763851
14	1	0	0.473395	3.598211	-1.749270
15	1	0	-1.058412	1.571665	-1.204833
16	1	0	-2.022080	1.831890	-3.308431
17	8	0	-1.157573	-0.437818	-2.549834
18	6	0	-3.941559	-3.749268	-0.302256
19	6	0	-2.617251	-3.345989	-0.923103
20	8	0	-2.002307	-2.355798	-0.080233
21	6	0	-0.767036	-1.909386	-0.487147
22	6	0	-0.087668	-1.088981	0.599803
23	8	0	1.231415	-0.730932	0.241216
24	1	0	-4.608702	-2.886304	-0.218989
25	1	0	-3.791712	-4.169948	0.696566
26	1	0	-4.429672	-4.504615	-0.926773
27	1	0	-1.937990	-4.205623	-1.010643
28	1	0	-2.760293	-2.918669	-1.923967
29	1	0	-0.123813	-2.693706	-0.914146
30	1	0	-0.024555	-1.710962	1.503485
31	1	0	-0.704071	-0.214716	0.852517
32	1	0	1.228525	0.115097	-0.241074
33	1	0	-0.943282	-1.134979	-1.536498

-767.5099908 -767.234989 -767.216731 -767.215787 -767.284292

TS formation of 2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.639619	-2.757572	1.673910
2	6	0	-1.338167	-1.646540	0.908777
3	8	0	-0.397601	-1.034256	0.033314
4	6	0	-0.953245	0.021298	-0.727295
5	6	0	0.148191	0.650444	-1.564758
6	8	0	-0.457740	1.405035	-2.580170
7	8	0	0.916170	1.478492	-0.689794
8	8	0	2.037073	1.950420	-1.419357
9	1	0	0.195043	-2.356906	2.257139
10	1	0	-0.249287	-3.514689	0.986765
11	1	0	-1.341734	-3.242452	2.360464
12	1	0	-2.183232	-2.047406	0.324871
13	1	0	-1.743363	-0.891916	1.602330
14	1	0	-1.397244	0.792080	-0.079226

15	1	0	-1.731408	-0.347804	-1.411375
16	1	0	0.817425	-0.114822	-1.979579
17	1	0	0.245468	1.899516	-3.026450
18	6	0	3.667795	-0.900146	-0.738086
19	6	0	3.995905	0.557238	-0.542710
20	8	0	4.112585	0.880862	0.790676
21	6	0	4.569752	2.209108	1.066863
22	6	0	4.575885	2.380538	2.577612
23	8	0	5.117034	3.675532	2.833833
24	1	0	2.743250	-1.161700	-0.214603
25	1	0	4.475811	-1.533598	-0.349029
26	1	0	3.543213	-1.117820	-1.802962
27	1	0	4.826855	0.946857	-1.151696
28	1	0	2.981330	1.256939	-1.023311
29	1	0	3.898590	2.938894	0.599830
30	1	0	5.583352	2.348704	0.666284
31	1	0	5.190553	1.591933	3.033806
32	1	0	3.550655	2.288063	2.959536
33	1	0	5.049527	3.867598	3.776765

-767.5036345 -767.229513 -767.210716 -767.209772 -767.281487

TS1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.444980	-0.198937	-1.619785
2	6	0	-0.943118	-0.376568	-1.755167
3	8	0	-0.368867	-0.393486	-0.449563
4	6	0	1.029796	-0.555464	-0.451126
5	6	0	1.518913	-0.551928	0.975359
6	8	0	2.770472	-0.622558	1.218953
7	8	0	1.303864	1.339148	1.459445
8	8	0	2.515524	1.591994	1.847758
9	1	0	-2.677371	0.741039	-1.110529
10	1	0	-2.880845	-1.021030	-1.044136
11	1	0	-2.912555	-0.182583	-2.609828
12	1	0	-0.705214	-1.319111	-2.274694
13	1	0	-0.503115	0.446923	-2.339817
14	1	0	1.542584	0.235529	-1.020102
15	1	0	1.322500	-1.525119	-0.893462
16	1	0	0.789831	-0.884411	1.726959
17	1	0	2.978579	0.520428	1.652023

-458.6050472 -458.473271 -458.46405 -458.463106 -458.509306

TS1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.333905	1.179699	-0.716230
2	6	0	1.498367	0.603712	0.412608
3	8	0	0.366300	-0.059619	-0.163674
4	6	0	-0.453716	-0.704653	0.770766
5	6	0	-1.779512	-0.877242	0.377581
6	8	0	-2.498525	-1.871579	0.925820
7	8	0	-2.573090	0.863295	1.763629
8	8	0	-1.464734	1.025074	2.405635
9	1	0	1.752140	1.901266	-1.297803
10	1	0	2.674425	0.387203	-1.389528
11	1	0	3.212308	1.691417	-0.309266
12	1	0	2.083663	-0.120321	1.000588
13	1	0	1.157161	1.395799	1.093865
14	1	0	-0.755009	0.172861	1.744909
15	1	0	0.012255	-1.533033	1.317837
16	1	0	-2.207379	-0.305732	-0.439100
17	1	0	-3.445153	-1.693231	0.834458

-458.573114 -458.442327 -458.432676 -458.431732 -458.478282

TS2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.178484	-1.890474	0.110786
2	6	0	-1.546159	-0.688255	0.794211
3	8	0	-0.109875	-0.853945	0.937163
4	6	0	0.642567	-0.504025	-0.096955
5	6	0	2.025451	-0.383805	0.051390
6	8	0	2.755210	-0.497537	-1.153417
7	8	0	0.397014	1.950920	0.067144
8	8	0	1.618421	2.126983	0.463986
9	1	0	-1.968685	-2.809124	0.666409
10	1	0	-1.811355	-2.012404	-0.913390
11	1	0	-3.264441	-1.755160	0.064452
12	1	0	-1.733017	0.246334	0.256651
13	1	0	-1.907038	-0.576741	1.818564
14	1	0	0.173393	-0.363305	-1.067180
15	1	0	2.473527	-0.881259	0.916921
16	1	0	2.009349	0.911978	0.392380
17	1	0	3.390691	0.228015	-1.209657

-458.5747605 -458.444147 -458.434284 -458.43334 -458.480446

TS2b

Center	Atomic	Atomic	Coordinates (Angstroms)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.177472	-0.446641	0.176293
2	6	0	1.201337	0.445088	-0.577441
3	8	0	-0.133077	-0.122340	-0.615873
4	6	0	-0.930476	0.160398	0.456436
5	6	0	-2.083510	-0.955246	0.536296
6	8	0	-3.030689	-0.560569	1.427512
7	8	0	-1.594755	1.396051	0.222941
8	8	0	-2.324730	1.699486	1.388398
9	1	0	2.214101	-1.443937	-0.271925
10	1	0	1.905285	-0.550163	1.231935
11	1	0	3.182280	-0.012080	0.134087
12	1	0	1.149729	1.452144	-0.148557
13	1	0	1.486281	0.538762	-1.627820
14	1	0	-0.413995	0.213522	1.423490
15	1	0	-1.551230	-1.861090	0.868647
16	1	0	-2.453103	-1.067544	-0.493402
17	1	0	-2.892583	0.785925	1.520825

-	-	-	-	-
458.5864287	458.454702	458.446013	458.445069	458.489569

TS2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.574742	-0.006779	-1.912094
2	6	0	-1.701903	-0.509437	-0.492950
3	8	0	-0.601122	-1.186193	0.038397
4	6	0	0.436519	-0.335485	0.521273
5	6	0	1.525752	-1.201724	1.139548
6	8	0	2.642600	-0.426172	1.537711
7	8	0	-0.112463	0.456985	1.556307
8	8	0	-1.022837	1.374087	0.959134
9	1	0	-1.448267	-0.851718	-2.602387
10	1	0	-0.722716	0.667479	-2.038670
11	1	0	-2.482403	0.534232	-2.196822
12	1	0	-1.673447	0.608992	0.307052
13	1	0	-2.607503	-1.075878	-0.266111
14	1	0	0.818927	0.318462	-0.271281
15	1	0	1.880037	-1.906433	0.383859
16	1	0	1.094376	-1.771475	1.973090
17	1	0	2.361293	0.187887	2.230032

-	-	-	-	-
458.5878226	458.455755	458.447071	458.446127	458.48974

TS2d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.750462	0.321509	-0.100650
2	6	0	1.662666	-0.564979	-0.687793
3	8	0	0.797102	-1.111911	0.351622
4	6	0	-0.244155	-0.422141	0.849874
5	6	0	-1.951204	-0.926378	-0.342737
6	8	0	-2.642084	0.122716	-0.353278
7	8	0	-0.268643	0.933118	0.911452
8	8	0	-0.393075	1.536537	-0.428778
9	1	0	3.329807	-0.220557	0.652909
10	1	0	2.328948	1.221890	0.351306
11	1	0	3.431459	0.626259	-0.903138
12	1	0	1.052560	-0.023725	-1.412277
13	1	0	2.087179	-1.455728	-1.155673
14	1	0	-0.576487	-0.832440	1.802115
15	1	0	-2.258978	-1.785620	0.276428
16	1	0	-1.289533	-1.174747	-1.189685
17	1	0	-1.357969	1.352917	-0.582297
	-	-	-	-	-
458.578097	458.444192	458.434874	458.43393	458.479419	

TS2e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.020746	-0.237668	-0.392245
2	6	0	-1.913469	-0.731208	0.495106
3	8	0	-0.839137	-1.221434	0.016071
4	6	0	0.645244	-0.020837	-0.300606
5	6	0	1.767649	-0.921188	0.112065
6	8	0	3.047645	-0.424503	-0.291196
7	8	0	0.503788	1.039843	0.542094
8	8	0	-0.114881	2.150699	-0.176669
9	1	0	-3.214091	-0.953076	-1.200038
10	1	0	-2.748430	0.715737	-0.872861
11	1	0	-3.943675	-0.078160	0.174411
12	1	0	-0.807803	2.392036	0.461653
13	1	0	-2.001915	-0.595757	1.582940
14	1	0	0.479945	0.204931	-1.347767
15	1	0	1.633626	-1.880657	-0.389994
16	1	0	1.724487	-1.092279	1.195146
17	1	0	3.226469	0.395794	0.188199
	-	-	-	-	-
458.5718119	458.440748	458.429764	458.428819	458.479274	

TS3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.890130	-0.417366	0.644653
2	6	0	1.297964	0.301370	-0.549703
3	8	0	0.138271	-0.250404	-1.078575
4	6	0	-1.078674	0.138980	-0.413213
5	6	0	-2.245734	-0.450428	-1.169421
6	1	0	-3.182700	-0.169994	-0.682391
7	8	0	-1.163196	1.544923	-0.479808
8	8	0	-0.146972	2.076454	0.364002
9	1	0	2.171286	-1.439076	0.337871
10	1	0	1.150915	-0.497536	1.454419
11	8	0	3.029381	0.332776	1.049186
12	1	0	0.796442	1.489202	-0.055242
13	1	0	2.012797	0.528691	-1.343173
14	1	0	-1.039611	-0.164680	0.640293
15	1	0	-2.160729	-1.539808	-1.181087
16	1	0	-2.247582	-0.083092	-2.198518
17	1	0	3.441331	-0.093663	1.810548

-	-	-	-	-
458.5856509	458.454071	458.445165	458.444221	458.488534

TS3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.001002	0.221246	0.054582
2	6	0	1.723154	-0.028165	0.549911
3	8	0	0.665920	-0.002449	-0.258970
4	6	0	-0.631852	0.001774	0.368729
5	6	0	-1.664478	-0.094416	-0.742539
6	8	0	-2.932365	-0.164245	-0.096175
7	8	0	1.570992	2.195167	1.452219
8	8	0	2.681934	2.611815	0.935963
9	1	0	3.116934	0.218737	-1.028257
10	1	0	3.065055	1.518843	0.395754
11	1	0	3.824262	-0.212712	0.619279
12	1	0	1.544444	-0.337476	1.577131
13	1	0	-0.752089	0.927568	0.938307
14	1	0	-0.719532	-0.857748	1.044119
15	1	0	-1.470513	-0.990691	-1.348133
16	1	0	-1.588073	0.787906	-1.391808
17	1	0	-3.632105	-0.130955	-0.759547

-458.5791274	-458.44815	-458.438334	-458.43739	-458.485035