peroxy

sbphE501

[UB3LYP 6-311++G(d,p);Freq]
HF = -1236.5616337
S2 = 0.760047
[Thermochemistry]
Zero-point Correction = 0.178011
Enthalpy Correction = 0.194033
Free Energy Correction = 0.132038

Geometry:

C	-1.763179	0.096111	0.016930
C	-2.534518	-1.038895	-0.306334
C	-3.921724	-1.015231	-0.291064
C	-4.561930	0.172147	0.054196
C	-3.840198	1.320431	0.379961
C	-2.454604	1.274067	0.360804
H	-1.892988	2.156561	0.641369
H	-4.371877	2.223622	0.655337
H	-4.510226	-1.883948	-0.550771
H	-2.030500	-1.951269	-0.601285
O	-5.942482	0.314416	0.101673
O	-6.654107	-0.769025	-0.196453
C	-0.287379	0.052708	-0.004962
C	0.464767	1.176092	-0.392211
C	0.409986	-1.113068	0.357501
C	1.853595	1.135841	-0.414938
H	-0.044903	2.077820	-0.715407
C	1.799415	-1.151055	0.343295
H	-0.140804	-1.989429	0.682854
C	2.528932	-0.026293	-0.041303
H	2.431535	1.991431	-0.743400
H	2.336835	-2.049617	0.622009
S	4.358259	-0.054190	0.001243
O	4.702263	-1.477545	-0.236890
O	4.679173	0.430636	1.367728
O	4.756629	0.875860	-1.083787

Frequencies:

10.1385	34.6733	57.5697
67.4893	95.0041	122.7581
160.4090	181.9597	204.3525
251.7424	293.0093	341.8394
358.8485	391.9557	411.0496
423.5003	429.6971	486.1583
512.4400	518.1651	531.0668
566.6229	604.8130	635.9643
648.6050	656.7036	724.7935
744.2226	749.7468	825.4891
827.4324	836.3415	843.9685
868.2430	965.2003	970.8097
972.8552	985.2950	988.4503
1018.5820	1027.6299	1037.2351
1088.6187	1109.3891	1122.6314
1124.7994	1143.6375	1164.0243
1178.2891	1197.1769	1211.9987
1293.4373	1302.9741	1321.4512
1331.5443	1342.1333	1419.0696
1450.3977	1501.9627	1529.2765
1586.1499	1606.6042	1616.5797
1630.4580	3157.5824	3158.2736
3180.6310	3185.5458	3191.5461
3192.5512	3195.8164	3220.6147

phenyl

sbphE701

[UB3LYP 6-311++G(d,p);Freq]
HF = -1086.1130946
S2 = 0.75761
[Thermochemistry]
Zero-point Correction = 0.169606
Enthalpy Correction = 0.183566
Free Energy Correction = 0.126630

Geometry:

C	2.613405	0.000965	-0.003049
C	3.326624	-1.135458	0.414831
C	4.727568	-1.154394	0.428187
C	5.369945	-0.009496	0.020231
C	4.743287	1.140159	-0.398574
C	3.342172	1.131926	-0.408668
H	2.809576	2.009659	-0.758524
H	5.292579	2.017857	-0.722278
H	5.264622	-2.036139	0.761262
H	2.781387	-2.008880	0.755886
C	1.128727	0.006045	-0.014799
C	0.405388	-1.120785	-0.436405
C	0.406357	1.138843	0.390199
C	-0.986094	-1.116006	-0.450019
H	0.938942	-1.997851	-0.789060
C	-0.985708	1.143710	0.380426
H	0.939846	2.017167	0.739810
C	-1.688515	0.015081	-0.036875
H	-1.542675	-1.976440	-0.802290
H	-1.543737	2.019920	0.688738
S	-3.518836	-0.003627	0.011849
O	-3.899631	1.422272	-0.149663
O	-3.831559	-0.568585	1.349657
O	-3.901072	-0.882540	-1.122000

Frequencies:

10.0003	46.3133	64.6975
85.3129	134.3808	175.7575
202.3366	250.5361	321.9658
362.3076	393.3529	405.8949
415.1882	416.3706	485.1773
506.3853	523.4025	563.9053
603.9013	611.9001	647.5160
667.4773	693.0931	738.1516
767.2032	799.2093	801.0216
845.5414	851.3455	942.8521
958.9847	967.7054	971.8396
984.5238	991.2651	1021.0439
1038.7027	1050.5848	1104.4400
1109.1924	1120.3960	1164.2366
1174.9970	1179.2978	1198.1240
1284.1895	1293.1388	1310.5037
1314.4676	1324.4649	1376.9907
1425.9450	1473.8695	1519.2874
1583.1146	1588.4139	1608.5813
1628.5421	3151.9218	3152.6422
3157.1515	3157.6510	3174.1925
3176.1319	3189.2124	3190.2755

Ipso TS

sbphE401

[UB3LYP 6-311++G(d,p);Freq]
HF = -1236.5233281
S2 = 0.777871
[Thermochemistry]
Zero-point Correction = 0.176018
Enthalpy Correction = 0.191793
Free Energy Correction = 0.130475

Geometry:

C	3.916646	1.229070	-0.140049
C	4.633659	0.041964	0.182854
C	3.902540	-1.142081	0.484605
C	2.544880	1.212723	-0.187313
C	1.798695	0.033377	0.085132
C	2.531301	-1.137606	0.423470
H	4.487227	2.123111	-0.357792
H	4.460828	-2.025386	0.768219
H	1.990908	-2.039321	0.682710
H	2.018426	2.117609	-0.463200
O	5.949656	-0.274941	-0.986551
O	5.975458	0.101920	0.439385
C	0.336826	0.026180	0.034334
C	-0.380706	-1.161531	-0.229153
C	-0.411069	1.205669	0.246281
C	-1.766029	-1.169328	-0.277285
H	0.157291	-2.078719	-0.439543
C	-1.796442	1.194519	0.211481
H	0.100212	2.133457	0.475582
C	-2.485077	0.006896	-0.049810
H	-2.312542	-2.074767	-0.512134
H	-2.366702	2.100539	0.377627
S	-4.311894	-0.019022	-0.029505
O	-4.625558	-0.293124	1.395885
O	-4.666480	-1.120211	-0.956076
O	-4.695161	1.337448	-0.488478

Frequencies:

-368.6248	9.9037	34.8403
62.8402	68.7484	102.2408
154.7194	171.4553	186.9854
197.3136	255.9063	325.1498
349.5196	373.8000	382.0215
406.7935	422.0366	448.1393
477.7244	499.4954	520.0633
557.7182	570.0727	626.3856
628.0339	646.8764	704.0295
737.8447	745.0261	800.6099
805.3056	825.5432	837.9457
856.7585	863.7743	971.7687
972.7709	975.3817	980.1814
992.3816	1004.7064	1015.9151
1030.8871	1105.6002	1126.8011
1130.5174	1160.1913	1174.5367
1181.2728	1204.8088	1272.9203
1281.7135	1311.2508	1313.1851
1327.0617	1334.1192	1430.7761
1467.0363	1485.5334	1523.8418
1525.5831	1575.4716	1595.7805
1622.7892	3168.7338	3169.1322
3186.8016	3188.0504	3194.6572
3195.8616	3203.7216	3205.4868

phenoxyl

sbphE801

[UB3LYP 6-311++G(d,p);Freq]
HF = -1161.4182714
S2 = 0.776723
[Thermochemistry]
Zero-point Correction = 0.174253
Enthalpy Correction = 0.189192
Free Energy Correction = 0.129807

Geometry:

C	2.169962	0.002440	-0.008198
C	2.920157	1.191321	-0.251104
C	4.288122	1.199482	-0.249071
C	5.057704	-0.004312	0.014526
C	4.278470	-1.204419	0.266426
C	2.910727	-1.189755	0.247358
H	2.370478	-2.102792	0.467012
H	4.829921	-2.112880	0.482229
H	4.847107	2.105436	-0.455859
H	2.388013	2.107152	-0.478692
O	6.308573	-0.007275	0.023926
C	0.710960	0.004971	-0.020098
C	-0.025033	-1.174549	-0.279871
C	-0.025492	1.187590	0.223857
C	-1.410309	-1.170543	-0.297175
H	0.498414	-2.094613	-0.511800
C	-1.410820	1.187643	0.219667
H	0.496828	2.109052	0.452544
C	-2.115322	0.008905	-0.041060
H	-1.968973	-2.069105	-0.529882
H	-1.969894	2.096109	0.408909
S	-3.941122	-0.002915	0.013804
O	-4.322002	1.366566	-0.406940
O	-4.230541	-0.307610	1.438092
O	-4.322118	-1.079726	-0.930936

Frequencies:

8.8706	38.0651	65.9236
75.1814	108.6004	161.5279
193.5312	198.6232	264.4615
332.5536	365.2470	377.6629
391.7856	405.0935	408.8313
464.4670	486.5490	517.3302
525.0376	561.6828	579.1240
621.6002	632.7236	645.0968
726.2136	753.3875	755.0109
788.3637	815.7733	837.0122
842.5389	868.4884	972.6744
975.4452	979.0268	983.7189
986.3799	992.2080	1011.7722
1029.2215	1104.5821	1117.6177
1130.7810	1160.3303	1180.0241
1181.2885	1207.1921	1270.1529
1283.9333	1313.0816	1324.6971
1332.8957	1427.4709	1437.5624
1469.1654	1500.3872	1509.9659
1545.1757	1571.1166	1597.1065
1621.4822	3166.8732	3167.1982
3175.1164	3175.7063	3188.3276
3190.4476	3195.0666	3196.7329

Peroxyl->Phenoxyl vdW Complex

sbphE201

[UB3LYP 6-311++G(d,p);Freq]
HF = -1236.5156827
S2 = 1.309223
[Thermochemistry]
Zero-point Correction = 0.175151
Enthalpy Correction = 0.191446
Free Energy Correction = 0.128285

Geometry:

C	1.750233	0.049032	0.129464
C	2.490431	1.223825	-0.169766
C	3.862938	1.246145	-0.107349
C	4.595701	0.088712	0.293167
C	3.856869	-1.100320	0.571548
C	2.485036	-1.110152	0.496495
H	1.946856	-2.013738	0.754403
H	4.412884	-1.982912	0.865900
H	4.425337	2.138314	-0.357434
H	1.960199	2.112381	-0.489200
O	5.878441	0.127520	0.434074
O	6.742614	-0.366991	-1.130887
C	0.288514	0.033037	0.061829
C	-0.419794	-1.161003	-0.195886
C	-0.464949	1.212156	0.250746
C	-1.804048	-1.174079	-0.263651
H	0.124438	-2.078708	-0.387113
C	-1.849948	1.195403	0.198509
H	0.041035	2.143684	0.476776
C	-2.529977	0.002385	-0.059069
H	-2.344053	-2.084088	-0.495795
H	-2.426358	2.100481	0.347519
S	-4.357175	-0.031339	-0.064395
O	-4.739459	1.328013	-0.514746
O	-4.687872	-0.322130	1.353569
O	-4.692669	-1.124517	-1.007130

Frequencies:

-347.0159	9.8842	32.3948
46.6922	65.3848	77.6690
100.6676	136.4013	170.3664
191.5977	224.8028	290.3432
337.4160	374.1774	385.7114
401.7957	408.9290	415.3633
461.5480	487.5341	518.8229
537.6660	566.2648	583.9585
631.0731	634.8431	647.7557
729.2605	751.8270	762.0572
812.7788	836.7184	842.8533
851.2171	878.8234	972.9772
976.3610	980.5659	989.9409
993.0026	1002.0525	1018.0879
1031.6186	1105.7729	1126.2402
1130.8175	1161.2284	1174.7256
1182.1444	1205.2163	1288.4450
1301.9547	1313.8679	1326.0646
1332.8328	1338.0338	1429.8319
1470.9182	1488.2324	1521.6044
1525.6116	1577.0760	1603.6021
1626.1778	3168.7069	3168.8829
3180.3365	3181.2734	3193.9875
3195.1644	3196.2262	3198.3904