peroxy

sphE501

[UB3LYP 6-311++G(d,p);Freq]
HF = -1005.4513091
S2 = 0.759532
[Thermochemistry]
Zero-point Correction = 0.097507
Enthalpy Correction = 0.108840
Free Energy Correction = 0.058511

Geometry:

S	-2.307021	-0.073042	0.006076
C	-0.482289	0.053132	-0.037959
C	0.295728	-1.109923	-0.032134
C	1.682953	-1.037281	-0.014827
C	2.275938	0.223900	-0.000918
C	1.522015	1.397929	-0.009191
C	0.135165	1.304597	-0.025981
H	-0.486952	2.190880	-0.046860
H	2.028972	2.356129	-0.005226
H	2.304871	-1.921550	-0.015192
H	-0.204370	-2.070521	-0.058764
O	-2.605954	-1.226682	-0.877072
O	-2.600978	-0.314349	1.441298
O	-2.771584	1.240963	-0.501611
O	3.654878	0.422909	0.014439
O	4.410232	-0.670388	0.017307

Frequencies:

12.4671	66.5594	114.1287
140.8911	214.9970	237.4367
268.6999	358.8005	362.4787
413.7777	479.5561	487.5253
519.2632	540.4495	603.5982
636.4017	668.4223	707.0712
814.2672	825.2426	842.1116
953.6944	974.1600	982.5644
1026.5126	1086.0650	1103.7690
1107.7381	1145.3578	1163.7209
1177.4937	1188.8326	1308.6002
1346.7316	1429.5895	1492.5700
1596.6303	1617.7648	3177.5592
3191.2283	3198.8062	3217.2696

phenyl

sphE601

[UB3LYP 6-311++G(d,p);Freq] HF = -855.0007072 S2 = 0.757322 [Thermochemistry] Zero-point Correction = 0.089122 Enthalpy Correction = 0.098405 Free Energy Correction = 0.052785	Geometry: S -0.030402 -1.500881 0.000000 C 0.041129 0.332538 0.000000 C 0.040749 1.024998 1.210075 C 0.040749 2.429068 1.222022 C 0.036181 3.061006 0.000000 C 0.040749 2.429068 -1.222022 C 0.040749 1.024998 -1.210075 H 0.059905 0.462454 -2.136830 H 0.047401 2.974694 -2.160236 H 0.047401 2.974694 2.160236 H 0.059905 0.462454 2.136830 O 0.669284 -1.890340 1.250662 O -1.484820 -1.803102 0.000000 O 0.669284 -1.890340 -1.250662	Frequencies: 7.4720 121.4238 174.2738 284.4160 299.2445 347.2604 399.6616 455.5578 518.9745 525.7099 597.3087 608.6792 671.6658 701.3894 785.0037 788.2823 929.9713 958.6267 965.8168 996.8974 1045.3000 1086.4649 1090.3143 1161.5788 1168.3655 1171.1588 1289.1357 1309.4474 1373.1840 1460.2420 1552.3147 1609.2848 3150.5571 3150.9514 3181.6044 3182.3065

Ipso TS

sphE201

[UB3LYP 6-311++G(d,p);Freq]
HF = -1005.4110599
S2 = 0.777839
[Thermochemistry]
Zero-point Correction = 0.095294
Enthalpy Correction = 0.106400
Free Energy Correction = 0.055713

Geometry:

C	-1.651116	-1.233690	0.195897
C	-2.371217	-0.000001	0.209390
C	-1.651127	1.233693	0.195897
C	-0.278169	-1.222317	0.128175
C	0.423023	0.000013	0.093946
C	-0.278177	1.222334	0.128172
H	-2.222224	-2.152874	0.239930
H	-2.222244	2.152872	0.239930
H	0.293871	2.142049	0.130960
H	0.293877	-2.142032	0.130967
O	-3.689273	0.000000	-0.958009
O	-3.709436	-0.000006	0.515925
S	2.237313	0.000004	-0.049335
O	2.655129	1.250928	0.626658
O	2.655149	-1.250527	0.627378
O	2.450982	-0.000430	-1.519615

Frequencies:

-388.7180	4.0668	70.5085
149.9269	170.0272	191.0752
248.7930	311.4410	326.1915
393.5230	434.0215	455.0888
510.9626	515.7511	550.2545
622.0109	637.5604	690.5474
790.5273	799.3172	820.8595
865.7848	968.6607	973.2008
984.4180	1009.6725	1082.3784
1109.2341	1152.2095	1167.0943
1178.3817	1251.2108	1291.2653
1315.3210	1438.1485	1466.0471
1518.2948	1585.6708	3187.5548
3188.4422	3201.0598	3202.8002

phenoxyl

sph301

[UB3LYP 6-311++G(d,p);Freq]
HF = -930.3048808
S2 = 0.777296
[Thermochemistry]
Zero-point Correction = 0.093519
Enthalpy Correction = 0.103789
Free Energy Correction = 0.056182

Geometry:

S	-0.035585	-1.902222	0.000000
C	0.046494	-0.086814	0.000000
C	0.044378	0.617392	1.224694
C	0.044378	1.988954	1.235575
C	0.041581	2.754073	0.000000
C	0.044378	1.988954	-1.235575
C	0.044378	0.617392	-1.224694
H	0.060492	0.041899	-2.142757
H	0.049520	2.552774	-2.162265
H	0.049520	2.552774	2.162265
H	0.060492	0.041899	2.142757
O	0.651372	-2.302284	1.250664
O	-1.500215	-2.159132	0.000000
O	0.651372	-2.302284	-1.250664
O	0.041947	4.009512	0.000000

Frequencies:

12.7556	80.4638	162.8513
183.6661	265.7743	323.1172
331.4810	377.2784	453.4151
475.8190	516.6727	538.2660
562.8029	614.3143	652.3275
723.9092	786.6472	808.2812
853.1172	968.5462	970.4715
987.0641	994.4996	1073.6910
1103.3854	1148.1058	1170.8088
1178.3481	1272.0795	1293.6512
1412.2574	1440.6515	1489.3686
1512.1365	1585.8576	3170.8183
3171.0846	3191.1634	3193.0830

Peroxyl->Phenoxyl vdW Complex

sphE301

[UB3LYP 6-311++G(d,p);Freq]
HF = -1005.4042623
S2 = 1.353081
[Thermochemistry]
Zero-point Correction = 0.094427
Enthalpy Correction = 0.106071
Free Energy Correction = 0.054570

Geometry:

C	0.492585	0.000038	0.021701
C	-0.202753	-1.222432	0.097053
C	-1.569876	-1.229186	0.250882
C	-2.296053	0.000195	0.361408
C	-1.569769	1.229480	0.250574
C	-0.202626	1.222575	0.096816
H	0.365131	2.141301	0.012387
H	-2.135086	2.153044	0.304325
H	-2.135267	-2.152689	0.304891
H	0.364859	-2.141266	0.012816
O	-3.562073	0.000311	0.595207
O	-4.581764	-0.000485	-1.005720
S	2.310613	-0.000044	-0.092016
O	2.711584	-0.000678	1.339041
O	2.632328	-1.250566	-0.816784
O	2.632612	1.250954	-0.815840

Frequencies:

-240.5953	13.9090	59.6822
59.7182	127.4155	162.6071
227.9977	265.6264	328.9618
365.6115	391.9805	441.4443
483.5534	516.6440	546.9484
569.7956	625.3632	651.8514
729.9689	811.8093	836.4302
865.1345	972.0917	973.5999
992.4028	1007.5496	1082.9336
1109.2083	1152.6382	1167.5472
1183.9547	1291.6464	1315.0784
1335.0744	1447.0479	1474.2952
1515.0647	1594.6431	3178.4179
3179.0781	3196.0220	3197.7608