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Supporting Information

Table 1. Cartesian Coordinates (BLYP/6-31G*) of mono-substituted benzenes, para-substituted phenols, and para-substituted phenoxy radicals in CHEM3D format.

Benzene, BLYP/6-31G*, E = -232.13239

12												
C	1	0.00000	1.21831	0.70326	2	3	6	7	0	0	0	
C	2	0.00000	-1.21831	-0.70326	2	4	5	8	0	0	0	
C	3	0.00000	1.21831	-0.70326	2	1	5	9	0	0	0	
C	4	0.00000	-1.21831	0.70326	2	2	6	10	0	0	0	
C	5	0.00000	0.00000	-1.40652	2	2	3	11	0	0	0	
C	6	0.00000	0.00000	1.40652	2	1	4	12	0	0	0	
H	7	0.00000	2.16594	1.25074	5	1	0	0	0	0	0	
H	8	0.00000	-2.16594	-1.25074	5	2	0	0	0	0	0	
H	9	0.00000	2.16594	-1.25074	5	3	0	0	0	0	0	
H	10	0.00000	-2.16594	1.25074	5	4	0	0	0	0	0	
H	11	0.00000	0.00000	-2.50093	5	5	0	0	0	0	0	
H	12	0.00000	0.00000	2.50093	5	6	0	0	0	0	0	

Phenol, BLYP/6-31G*, E = -307.34235

13												
H	1	-0.86657	2.66976	0.00000	5	2	0	0	0	0	0	
O	2	0.05343	2.32961	0.00000	6	1	3	0	0	0	0	
C	3	0.00000	0.94700	0.00000	2	2	4	10	0	0	0	
C	4	1.22781	0.25407	0.00000	2	3	5	6	0	0	0	
H	5	2.15846	0.82677	0.00000	5	4	0	0	0	0	0	
C	6	1.22949	-1.14876	0.00000	2	4	7	8	0	0	0	
H	7	2.18510	-1.68201	0.00000	5	6	0	0	0	0	0	
C	8	0.02074	-1.87087	0.00000	2	6	9	12	0	0	0	
H	9	0.03000	-2.96418	0.00000	5	8	0	0	0	0	0	
C	10	-1.21577	0.23321	0.00000	2	3	11	12	0	0	0	
H	11	-2.16826	0.77646	0.00000	5	10	0	0	0	0	0	
C	12	-1.19885	-1.17209	0.00000	2	8	10	13	0	0	0	
H	13	-2.14662	-1.71905	0.00000	5	12	0	0	0	0	0	

Phenoxy Radical, BLYP/6-31G*, E = -306.71479

12												
O	1	0.00000	0.00000	2.32726	6	2	0	0	0	0	0	
C	2	0.00000	0.00000	1.05753	2	1	3	4	0	0	0	
C	3	0.00000	1.24876	0.29080	2	2	5	9	0	0	0	
C	4	0.00000	-1.24876	0.29080	2	2	6	10	0	0	0	
C	5	0.00000	1.23412	-1.09710	2	3	7	11	0	0	0	
C	6	0.00000	-1.23412	-1.09710	2	4	7	12	0	0	0	
C	7	0.00000	0.00000	-1.79953	2	5	6	8	0	0	0	
H	8	0.00000	0.00000	-2.89336	5	7	0	0	0	0	0	
H	9	0.00000	2.18092	0.86174	5	3	0	0	0	0	0	
H	10	0.00000	-2.18092	0.86174	5	4	0	0	0	0	0	
H	11	0.00000	2.17255	-1.66027	5	5	0	0	0	0	0	
H	12	0.00000	-2.17255	-1.66027	5	6	0	0	0	0	0	

Toluene, BLYP/6-31G*, E = -271.42271

15												
H	1	0.00986	-3.01303	0.00000	5	2	0	0	0	0	0	
C	2	0.00469	-1.91888	0.00000	2	1	3	7	0	0	0	
C	3	-1.21149	-1.21121	0.00000	2	2	4	5	0	0	0	
H	4	-2.16197	-1.75401	0.00000	5	3	0	0	0	0	0	

C	5	-1.21129	0.19311	0.00000	2	3	6	11	0	0	0
H	6	-2.16368	0.73458	0.00000	5	5	0	0	0	0	0
C	7	1.21670	-1.20857	0.00000	2	2	8	9	0	0	0
H	8	2.16940	-1.74738	0.00000	5	7	0	0	0	0	0
C	9	1.21085	0.19780	0.00000	2	7	10	11	0	0	0
H	10	2.16015	0.74403	0.00000	5	9	0	0	0	0	0
C	11	0.00000	0.92082	0.00000	2	5	9	12	0	0	0
C	12	-0.00613	2.44284	0.00000	1	11	13	14	15	0	0
H	13	-0.52626	2.84670	0.88714	5	12	0	0	0	0	0
H	14	-0.52626	2.84670	-0.88714	5	12	0	0	0	0	0
H	15	1.01879	2.84701	0.00000	5	12	0	0	0	0	0

p-Me-Phenol, BLYP/6-31G*, E = -346.63194

16											
H	1	-3.19456	-0.79059	0.00000	5	2	0	0	0	0	0
O	2	-2.44999	-1.42915	0.00000	6	1	3	0	0	0	0
C	3	-1.26800	-0.70733	0.00000	2	2	4	8	0	0	0
C	4	-1.23393	0.70178	0.00000	2	3	5	6	0	0	0
H	5	-2.16949	1.27369	0.00000	5	4	0	0	0	0	0
C	6	0.00000	1.37113	0.00000	2	4	7	12	0	0	0
H	7	0.00793	2.46661	0.00000	5	6	0	0	0	0	0
C	8	-0.06181	-1.43287	0.00000	2	3	9	10	0	0	0
H	9	-0.09904	-2.52512	0.00000	5	8	0	0	0	0	0
C	10	1.16146	-0.74515	0.00000	2	8	11	12	0	0	0
H	11	2.09314	-1.32069	0.00000	5	10	0	0	0	0	0
C	12	1.22232	0.66514	0.00000	2	6	10	13	0	0	0
C	13	2.55285	1.40178	0.00000	1	12	14	15	16	0	0
H	14	2.66160	2.05210	0.88709	5	13	0	0	0	0	0
H	15	2.66160	2.05210	-0.88709	5	13	0	0	0	0	0
H	16	3.40135	0.69822	0.00000	5	13	0	0	0	0	0

p-Me-Phenoxy Radical, BLYP/6-31G*, E = -346.00740

15											
O	1	0.01062	-2.83014	0.00000	6	2	0	0	0	0	0
C	2	0.00546	-1.56130	0.00000	2	1	3	7	0	0	0
C	3	-1.24124	-0.79116	0.00000	2	2	4	5	0	0	0
H	4	-2.17577	-1.35850	0.00000	5	3	0	0	0	0	0
C	5	-1.22785	0.59303	0.00000	2	3	6	11	0	0	0
H	6	-2.17140	1.15012	0.00000	5	5	0	0	0	0	0
C	7	1.24723	-0.78582	0.00000	2	2	8	9	0	0	0
H	8	2.18451	-1.34849	0.00000	5	7	0	0	0	0	0
C	9	1.22758	0.60091	0.00000	2	7	10	11	0	0	0
H	10	2.16787	1.16274	0.00000	5	9	0	0	0	0	0
C	11	0.00000	1.32435	0.00000	2	5	9	12	0	0	0
C	12	-0.01285	2.83861	0.00000	1	11	13	14	15	0	0
H	13	-0.54333	3.23458	0.88557	5	12	0	0	0	0	0
H	14	-0.54333	3.23458	-0.88557	5	12	0	0	0	0	0
H	15	1.00645	3.25433	0.00000	5	12	0	0	0	0	0

F-Benzene, BLYP/6-31G*, E = -331.36614

12											
F	1	0.00000	0.00000	2.30335	0	2	0	0	0	0	0
C	2	0.00000	0.00000	0.93717	2	1	5	6	0	0	0
C	3	0.00000	0.00000	-1.84974	2	4	9	10	0	0	0
H	4	0.00000	0.00000	-2.94318	5	3	0	0	0	0	0
C	5	0.00000	1.22713	0.26126	2	2	7	9	0	0	0
C	6	0.00000	-1.22713	0.26126	2	2	8	10	0	0	0
H	7	0.00000	2.15779	0.83309	5	5	0	0	0	0	0

H	8	0.00000	-2.15779	0.83309	5	6	0	0	0	0	0
C	9	0.00000	1.21763	-1.14470	2	3	5	11	0	0	0
C	10	0.00000	-1.21763	-1.14470	2	3	6	12	0	0	0
H	11	0.00000	2.16693	-1.68826	5	9	0	0	0	0	0
H	12	0.00000	-2.16693	-1.68826	5	10	0	0	0	0	0

p-F-Phenol, BLYP/6-31G*, E = -406.57400

13											
H	1	-0.85383	3.12505	0.00000	5	2	0	0	0	0	0
O	2	0.06268	2.77652	0.00000	6	1	3	0	0	0	0
C	3	0.00000	1.39345	0.00000	2	2	4	10	0	0	0
C	4	1.22464	0.69340	0.00000	2	3	5	6	0	0	0
H	5	2.15872	1.25974	0.00000	5	4	0	0	0	0	0
C	6	1.23051	-0.70904	0.00000	2	4	7	8	0	0	0
H	7	2.16703	-1.27111	0.00000	5	6	0	0	0	0	0
C	8	0.00973	-1.39846	0.00000	2	6	9	12	0	0	0
F	9	0.01717	-2.76663	0.00000	0	8	0	0	0	0	0
C	10	-1.21772	0.68321	0.00000	2	3	11	12	0	0	0
H	11	-2.16984	1.22567	0.00000	5	10	0	0	0	0	0
C	12	-1.21545	-0.72277	0.00000	2	8	10	13	0	0	0
H	13	-2.14836	-1.29059	0.00000	5	12	0	0	0	0	0

p-F-phenoxy Radical, BLYP/6-31G*, E = -405.95017

12											
F	1	0.00000	0.00000	2.68566	0	2	0	0	0	0	0
C	2	0.00000	0.00000	1.33021	2	1	5	6	0	0	0
C	3	0.00000	0.00000	-1.50005	2	4	9	10	0	0	0
O	4	0.00000	0.00000	-2.76809	6	3	0	0	0	0	0
C	5	0.00000	1.24378	0.65560	2	2	7	9	0	0	0
C	6	0.00000	-1.24378	0.65560	2	2	8	10	0	0	0
H	7	0.00000	2.16452	1.24441	5	5	0	0	0	0	0
H	8	0.00000	-2.16452	1.24441	5	6	0	0	0	0	0
C	9	0.00000	1.24893	-0.73053	2	3	5	11	0	0	0
C	10	0.00000	-1.24893	-0.73053	2	3	6	12	0	0	0
H	11	0.00000	2.18240	-1.29840	5	9	0	0	0	0	0
H	12	0.00000	-2.18240	-1.29840	5	10	0	0	0	0	0

Cl-Benzene, BLYP/6-31G*, E = -691.71812

12											
Cl	1	0.00000	0.00000	2.28671	0	0	0	0	0	0	0
C	2	0.00000	0.00000	0.50317	4	5	6	0	0	0	0
C	3	0.00000	0.00000	-2.29334	2	4	9	10	0	0	0
H	4	0.00000	0.00000	-3.38687	5	3	0	0	0	0	0
C	5	0.00000	1.22575	-0.18182	2	2	7	9	0	0	0
C	6	0.00000	-1.22575	-0.18182	2	2	8	10	0	0	0
H	7	0.00000	2.16495	0.37489	5	5	0	0	0	0	0
H	8	0.00000	-2.16495	0.37489	5	6	0	0	0	0	0
C	9	0.00000	1.21627	-1.58794	2	3	5	11	0	0	0
C	10	0.00000	-1.21627	-1.58794	2	3	6	12	0	0	0
H	11	0.00000	2.16676	-2.12947	5	9	0	0	0	0	0
H	12	0.00000	-2.16676	-2.12947	5	10	0	0	0	0	0

p-Cl-Phenol, BLYP/6-31G*, E = -766.92717

13											
H	1	-0.82767	-3.57771	0.00000	5	2	0	0	0	0	0
O	2	0.08495	-3.21852	0.00000	6	1	3	0	0	0	0
C	3	0.01128	-1.83928	0.00000	2	2	4	10	0	0	0
C	4	1.22961	-1.12926	0.00000	2	3	5	6	0	0	0

H	5	2.16916	-1.68658	0.00000	5	4	0	0	0	0	0
C	6	1.22473	0.27256	0.00000	2	4	7	8	0	0	0
H	7	2.16538	0.82671	0.00000	5	6	0	0	0	0	0
C	8	0.00000	0.96242	0.00000	4	6	12	0	0	0	0
Cl	9	-0.00458	2.74560	0.00000	0	0	0	0	0	0	0
C	10	-1.21100	-1.13731	0.00000	2	3	11	12	0	0	0
H	11	-2.16015	-1.68492	0.00000	5	10	0	0	0	0	0
C	12	-1.21869	0.26781	0.00000	2	8	10	13	0	0	0
H	13	-2.16404	0.81387	0.00000	5	12	0	0	0	0	0

p-Cl-Phenoxy Radical, BLYP/6-31G*, E = -766.30122

Cl	1	0.00000	0.00000	2.66586	0	0	0	0	0	0	0
C	2	0.00000	0.00000	0.90243	4	5	6	0	0	0	0
C	3	0.00000	0.00000	-1.94274	2	4	9	10	0	0	0
O	4	0.00000	0.00000	-3.20968	6	3	0	0	0	0	0
C	5	0.00000	1.24222	0.21374	2	2	7	9	0	0	0
C	6	0.00000	-1.24222	0.21374	2	2	8	10	0	0	0
H	7	0.00000	2.17271	0.78600	5	5	0	0	0	0	0
H	8	0.00000	-2.17271	0.78600	5	6	0	0	0	0	0
C	9	0.00000	1.24704	-1.17191	2	3	5	11	0	0	0
C	10	0.00000	-1.24704	-1.17191	2	3	6	12	0	0	0
H	11	0.00000	2.18233	-1.73716	5	9	0	0	0	0	0
H	12	0.00000	-2.18233	-1.73716	5	10	0	0	0	0	0

p-OH-Phenol, BLYP/6-31G*, E = -382.54878

C	1	0.00000	1.41240	0.00000	2	2	4	6	0	0	0
O	2	0.00000	2.79974	0.00000	6	1	3	0	0	0	0
H	3	0.93359	3.09768	0.00000	5	2	0	0	0	0	0
C	4	1.21130	0.68417	0.00000	2	1	5	13	0	0	0
H	5	2.16614	1.22348	0.00000	5	4	0	0	0	0	0
C	6	-1.22133	0.71957	0.00000	2	1	7	11	0	0	0
H	7	-2.16258	1.27413	0.00000	5	6	0	0	0	0	0
C	8	0.00000	-1.41240	0.00000	2	9	11	13	0	0	0
O	9	0.00000	-2.79974	0.00000	6	8	10	0	0	0	0
H	10	-0.93359	-3.09768	0.00000	5	9	0	0	0	0	0
C	11	-1.21130	-0.68417	0.00000	2	6	8	12	0	0	0
H	12	-2.16614	-1.22348	0.00000	5	11	0	0	0	0	0
C	13	1.22133	-0.71957	0.00000	2	4	8	14	0	0	0
H	14	2.16258	-1.27413	0.00000	5	13	0	0	0	0	0

p-OH-Phenoxy Radical, BLYP/6-31G*, E = -381.93123

H	1	-0.85631	3.06840	0.00000	5	2	0	0	0	0	0
O	2	0.05904	2.71181	0.00000	6	1	3	0	0	0	0
C	3	0.00000	1.34282	0.00000	2	2	4	10	0	0	0
C	4	1.24273	0.64647	0.00000	2	3	5	6	0	0	0
H	5	2.16527	1.23319	0.00000	5	4	0	0	0	0	0
C	6	1.25341	-0.73599	0.00000	2	4	7	8	0	0	0
H	7	2.19154	-1.29664	0.00000	5	6	0	0	0	0	0
C	8	0.01291	-1.51839	0.00000	2	6	9	12	0	0	0
O	9	0.01749	-2.78608	0.00000	6	8	0	0	0	0	0
C	10	-1.23451	0.63426	0.00000	2	3	11	12	0	0	0
H	11	-2.17613	1.19738	0.00000	5	10	0	0	0	0	0
C	12	-1.23576	-0.75071	0.00000	2	8	10	13	0	0	0
H	13	-2.16926	-1.31888	0.00000	5	12	0	0	0	0	0

OMe-Benzene, BLYP/6-31G*, E = -346.62234

16															
C	1	0.00000	0.53110	0.00000	2	2	6	12	0	0	0				
C	2	1.38439	0.24479	0.00000	2	1	3	7	0	0	0				
C	3	1.82202	-1.08519	0.00000	2	2	4	8	0	0	0				
C	4	0.89385	-2.14596	0.00000	2	3	5	9	0	0	0				
C	5	-0.47878	-1.85517	0.00000	2	4	6	10	0	0	0				
C	6	-0.93669	-0.52329	0.00000	2	1	5	11	0	0	0				
H	7	2.09043	1.07914	0.00000	5	2	0	0	0	0	0				
H	8	2.89595	-1.29595	0.00000	5	3	0	0	0	0	0				
H	9	1.23996	-3.18325	0.00000	5	4	0	0	0	0	0				
H	10	-1.21217	-2.66769	0.00000	5	5	0	0	0	0	0				
H	11	-2.00909	-0.32158	0.00000	5	6	0	0	0	0	0				
O	12	-0.32556	1.87426	0.00000	6	1	13	0	0	0	0				
C	13	-1.71637	2.22841	0.00000	1	12	14	15	16	0	0				
H	14	-1.74173	3.32721	0.00000	5	13	0	0	0	0	0				
H	15	-2.23468	1.84999	0.90092	5	13	0	0	0	0	0				
H	16	-2.23468	1.84999	-0.90092	5	13	0	0	0	0	0				

p-OMe-Phenol, BLYP/6-31G*, E = -421.82955

17																
C	1	0.00000	0.97745	0.00000	2	2	6	12	0	0	0					
C	2	1.30850	0.44956	0.00000	2	1	3	7	0	0	0					
C	3	1.51603	-0.93591	0.00000	2	2	4	8	0	0	0					
C	4	0.41558	-1.81864	0.00000	2	3	5	9	0	0	0					
C	5	-0.88910	-1.29587	0.00000	2	4	6	10	0	0	0					
C	6	-1.10060	0.09437	0.00000	2	1	5	11	0	0	0					
H	7	2.15385	1.14217	0.00000	5	2	0	0	0	0	0					
H	8	2.53862	-1.33051	0.00000	5	3	0	0	0	0	0					
O	9	0.55314	-3.19930	0.00000	6	4	17	0	0	0	0					
H	10	-1.73645	-1.98600	0.00000	5	5	0	0	0	0	0					
H	11	-2.12470	0.47137	0.00000	5	6	0	0	0	0	0					
O	12	-0.08734	2.36063	0.00000	6	1	13	0	0	0	0					
C	13	-1.39743	2.94236	0.00000	1	12	14	15	16	0	0					
H	14	-1.23989	4.03024	0.00000	5	13	0	0	0	0	0					
H	15	-1.97326	2.65626	0.90059	5	13	0	0	0	0	0					
H	16	-1.97326	2.65626	-0.90059	5	13	0	0	0	0	0					
H	17	1.51079	-3.41039	0.00000	5	9	0	0	0	0	0					

p-OMe-Phenoxy Radical, BLYP/6-31G*, E = -421.21154

16															
C	1	0.00000	0.91136	0.00000	2	2	6	12	0	0	0				
C	2	1.33650	0.40482	0.00000	2	1	3	7	0	0	0				
C	3	1.56726	-0.95576	0.00000	2	2	4	8	0	0	0				
C	4	0.46310	-1.92083	0.00000	2	3	5	9	0	0	0				
C	5	-0.88578	-1.35196	0.00000	2	4	6	10	0	0	0				
C	6	-1.10922	0.01810	0.00000	2	1	5	11	0	0	0				
H	7	2.15508	1.13013	0.00000	5	2	0	0	0	0	0				
H	8	2.58258	-1.36064	0.00000	5	3	0	0	0	0	0				
O	9	0.66203	-3.17307	0.00000	6	4	0	0	0	0	0				
H	10	-1.71985	-2.05864	0.00000	5	5	0	0	0	0	0				
H	11	-2.13103	0.40356	0.00000	5	6	0	0	0	0	0				
O	12	-0.09749	2.27488	0.00000	6	1	13	0	0	0	0				
C	13	-1.40839	2.87987	0.00000	1	12	14	15	16	0	0				
H	14	-1.22813	3.96290	0.00000	5	13	0	0	0	0	0				
H	15	-1.97789	2.59734	0.90230	5	13	0	0	0	0	0				
H	16	-1.97789	2.59734	-0.90230	5	13	0	0	0	0	0				

SH-Benzene, BLYP/6-31G*, E = -630.30189

13												
H	1	1.25576	2.53831	0.00000	5	2	0	0	0	0	0	0
S	2	-0.08690	2.31313	0.00000	0	1	0	0	0	0	0	0
C	3	0.00000	0.50896	0.00000	4	4	10	0	0	0	0	0
C	4	-1.21833	-0.20488	0.00000	2	3	5	6	0	0	0	0
H	5	-2.16954	0.33543	0.00000	5	4	0	0	0	0	0	0
C	6	-1.20910	-1.60878	0.00000	2	4	7	8	0	0	0	0
H	7	-2.15971	-2.15055	0.00000	5	6	0	0	0	0	0	0
C	8	0.00666	-2.31572	0.00000	2	6	9	12	0	0	0	0
H	9	0.00957	-3.40916	0.00000	5	8	0	0	0	0	0	0
C	10	1.22116	-0.19783	0.00000	2	3	11	12	0	0	0	0
H	11	2.17207	0.34315	0.00000	5	10	0	0	0	0	0	0
C	12	1.21800	-1.60309	0.00000	2	8	10	13	0	0	0	0
H	13	2.17191	-2.13925	0.00000	5	12	0	0	0	0	0	0

p-SH-Phenol, BLYP/6-31G*, E = -705.51053

14													
H	1	1.24171	3.01431	0.00000	5	2	0	0	0	0	0	0	0
S	2	-0.09718	2.77601	0.00000	0	1	0	0	0	0	0	0	0
C	3	0.00000	0.96906	0.00000	4	4	10	0	0	0	0	0	0
C	4	-1.21083	0.24676	0.00000	2	3	5	6	0	0	0	0	0
H	5	-2.16797	0.77636	0.00000	5	4	0	0	0	0	0	0	0
C	6	-1.20258	-1.15676	0.00000	2	4	7	8	0	0	0	0	0
H	7	-2.15130	-1.70569	0.00000	5	6	0	0	0	0	0	0	0
C	8	0.01915	-1.85833	0.00000	2	6	9	12	0	0	0	0	0
O	9	0.09446	-3.24002	0.00000	6	8	14	0	0	0	0	0	0
C	10	1.22033	0.25976	0.00000	2	3	11	12	0	0	0	0	0
H	11	2.17210	0.79875	0.00000	5	10	0	0	0	0	0	0	0
C	12	1.23212	-1.14221	0.00000	2	8	10	13	0	0	0	0	0
H	13	2.17518	-1.69410	0.00000	5	12	0	0	0	0	0	0	0
H	14	-0.81965	-3.59528	0.00000	5	9	0	0	0	0	0	0	0

p-SH-Phenoxy Radical, BLYP/6-31G*, E = -704.88996

13												
H	1	1.24606	2.93237	0.00000	0	2	0	0	0	0	0	0
S	2	-0.09295	2.68940	0.00000	0	1	0	0	0	0	0	0
C	3	0.00000	0.91154	0.00000	4	4	10	0	0	0	0	0
C	4	-1.23562	0.19326	0.00000	2	3	5	6	0	0	0	0
H	5	-2.17879	0.74913	0.00000	5	4	0	0	0	0	0	0
C	6	-1.23873	-1.18909	0.00000	2	4	7	8	0	0	0	0
H	7	-2.17395	-1.75489	0.00000	5	6	0	0	0	0	0	0
C	8	0.00748	-1.96204	0.00000	2	6	9	12	0	0	0	0
O	9	0.01288	-3.22742	0.00000	6	8	0	0	0	0	0	0
C	10	1.23847	0.20193	0.00000	2	3	11	12	0	0	0	0
H	11	2.18062	0.75938	0.00000	5	10	0	0	0	0	0	0
C	12	1.24879	-1.18157	0.00000	2	8	10	13	0	0	0	0
H	13	2.18781	-1.74126	0.00000	5	12	0	0	0	0	0	0

SMe-Benzene, BLYP/6-31G*, E = -669.58977

16															
C	1	0.00000	0.25407	0.00000	4	2	6	0	0	0	0	0	0	0	0
C	2	1.30507	0.80141	0.00000	2	1	3	7	0	0	0	0	0	0	0
C	3	2.42498	-0.04216	0.00000	2	2	4	8	0	0	0	0	0	0	0
C	4	2.26585	-1.44077	0.00000	2	3	5	9	0	0	0	0	0	0	0
C	5	0.97141	-1.98455	0.00000	2	4	6	10	0	0	0	0	0	0	0
C	6	-0.16010	-1.14816	0.00000	2	1	5	11	0	0	0	0	0	0	0

H	7	1.43884	1.88751	0.00000	5	2	0	0	0	0	0
H	8	3.42747	0.39667	0.00000	5	3	0	0	0	0	0
H	9	3.14094	-2.09670	0.00000	5	4	0	0	0	0	0
H	10	0.83205	-3.07016	0.00000	5	5	0	0	0	0	0
H	11	-1.15510	-1.59714	0.00000	5	6	0	0	0	0	0
S	12	-1.36023	1.43798	0.00000	0	0	0	0	0	0	0
C	13	-2.86747	0.37646	0.00000	2	14	15	16	0	0	0
H	14	-3.71659	1.07582	0.00000	5	13	0	0	0	0	0
H	15	-2.92120	-0.25079	0.90277	5	13	0	0	0	0	0
H	16	-2.92120	-0.25079	-0.90277	5	13	0	0	0	0	0

p-SMe-Phenol, BLYP/6-31G*, E = -744.79824

17											
C	1	0.00000	0.63080	0.00000	4	2	6	0	0	0	0
C	2	1.37057	0.28671	0.00000	2	1	3	7	0	0	0
C	3	1.77271	-1.05626	0.00000	2	2	4	8	0	0	0
C	4	0.80864	-2.08490	0.00000	2	3	5	9	0	0	0
C	5	-0.55827	-1.75291	0.00000	2	4	6	10	0	0	0
C	6	-0.95749	-0.40689	0.00000	2	1	5	11	0	0	0
H	7	2.13154	1.07293	0.00000	5	2	0	0	0	0	0
H	8	2.84057	-1.30496	0.00000	5	3	0	0	0	0	0
O	9	1.14267	-3.42876	0.00000	6	4	17	0	0	0	0
H	10	-1.30078	-2.55487	0.00000	5	5	0	0	0	0	0
H	11	-2.02575	-0.18188	0.00000	5	6	0	0	0	0	0
S	12	-0.39369	2.39308	0.00000	0	0	0	0	0	0	0
C	13	-2.23628	2.42210	0.00000	2	14	15	16	0	0	0
H	14	-2.51374	3.48661	0.00000	5	13	0	0	0	0	0
H	15	-2.64722	1.94441	0.90257	5	13	0	0	0	0	0
H	16	-2.64722	1.94441	-0.90257	5	13	0	0	0	0	0
H	17	2.12097	-3.49786	0.00000	5	9	0	0	0	0	0

p-SMe-Phenoxy Radical, BLYP/6-31G*, E = -744.17947

16											
C	1	0.00000	0.57466	0.00000	4	2	6	0	0	0	0
C	2	1.40134	0.27299	0.00000	2	1	3	7	0	0	0
C	3	1.83967	-1.03620	0.00000	2	2	4	8	0	0	0
C	4	0.90047	-2.16211	0.00000	2	3	5	9	0	0	0
C	5	-0.52096	-1.80869	0.00000	2	4	6	10	0	0	0
C	6	-0.94878	-0.49037	0.00000	2	1	5	11	0	0	0
H	7	2.12229	1.09727	0.00000	5	2	0	0	0	0	0
H	8	2.90577	-1.27806	0.00000	5	3	0	0	0	0	0
O	9	1.29219	-3.36613	0.00000	6	4	0	0	0	0	0
H	10	-1.23769	-2.63448	0.00000	5	5	0	0	0	0	0
H	11	-2.01939	-0.27311	0.00000	5	6	0	0	0	0	0
S	12	-0.41829	2.29993	0.00000	0	0	0	0	0	0	0
C	13	-2.26257	2.33402	0.00000	2	14	15	16	0	0	0
H	14	-2.53387	3.39968	0.00000	5	13	0	0	0	0	0
H	15	-2.66851	1.85654	0.90375	5	13	0	0	0	0	0
H	16	-2.66851	1.85654	-0.90375	5	13	0	0	0	0	0

NH2-Benzene, BLYP/6-31G*, E = -387.46683

14											
H	1	-0.00015	-2.98984	0.00000	5	2	0	0	0	0	0
C	2	0.00038	-1.89662	0.00000	2	1	3	11	0	0	0
C	3	0.00073	-1.18000	1.21096	2	2	4	5	0	0	0
H	4	0.00036	-1.71678	2.16514	5	3	0	0	0	0	0
C	5	0.00073	0.22195	1.21938	2	3	6	7	0	0	0
H	6	0.00017	0.76733	2.16954	5	5	0	0	0	0	0

C	7	-0.00001	0.94779	0.00000	2	5	8	13	0	0	0
N	8	-0.00185	2.33654	0.00000	0	7	9	10	0	0	0
H	9	-0.00392	2.86131	0.86738	5	8	0	0	0	0	0
H	10	-0.00392	2.86131	-0.86738	5	8	0	0	0	0	0
C	11	0.00073	-1.18000	-1.21096	2	2	12	13	0	0	0
H	12	0.00036	-1.71678	-2.16514	5	11	0	0	0	0	0
C	13	0.00073	0.22195	-1.21938	2	7	11	14	0	0	0
H	14	0.00017	0.76733	-2.16954	5	13	0	0	0	0	0

p-NH₂-Phenol, BLYP/6-31G*, E = -362.67562

15											
O	1	2.81723	0.09628	0.00926	6	2	15	0	0	0	0
C	2	1.42975	0.01755	0.00115	2	1	3	11	0	0	0
C	3	0.72830	-1.20276	-0.00058	2	2	4	5	0	0	0
H	4	1.27778	-2.15161	0.00511	5	3	0	0	0	0	0
C	5	-0.67629	-1.21438	-0.00446	2	3	6	7	0	0	0
H	6	-1.20706	-2.17239	-0.00972	5	5	0	0	0	0	0
C	7	-1.41136	-0.00779	-0.00741	2	5	8	13	0	0	0
N	8	-2.82833	-0.01633	-0.08686	0	7	9	10	0	0	0
H	9	-3.25204	-0.85313	0.32089	5	8	0	0	0	0	0
H	10	-3.26085	0.81740	0.31796	5	8	0	0	0	0	0
C	11	0.70843	1.22726	-0.00046	2	2	12	13	0	0	0
H	12	1.25726	2.17231	0.00477	5	11	0	0	0	0	0
C	13	-0.69250	1.21188	-0.00467	2	7	11	14	0	0	0
H	14	-1.24125	2.15989	-0.00963	5	13	0	0	0	0	0
H	15	3.16867	-0.81893	0.00320	5	1	0	0	0	0	0

NMe₂-Benzene, BLYP/6-31G*, E = -366.02800

20											
H	1	0.11392	-3.76892	0.00000	5	2	0	0	0	0	0
C	2	0.06727	-2.67653	0.00000	2	1	3	11	0	0	0
C	3	0.03658	-1.95804	1.20747	2	2	4	5	0	0	0
H	4	0.06770	-2.49093	2.16344	5	3	0	0	0	0	0
C	5	-0.02574	-0.55704	1.21737	2	3	6	7	0	0	0
H	6	-0.03885	-0.03947	2.17723	5	5	0	0	0	0	0
C	7	-0.07119	0.18185	0.00000	2	5	8	13	0	0	0
N	8	-0.17198	1.58328	0.00000	0	7	9	10	0	0	0
C	9	0.03658	2.31413	1.25284	1	8	15	16	17	0	0
C	10	0.03658	2.31413	-1.25284	1	8	18	19	20	0	0
C	11	0.03658	-1.95804	-1.20747	2	2	12	13	0	0	0
H	12	0.06770	-2.49093	-2.16344	5	11	0	0	0	0	0
C	13	-0.02574	-0.55704	-1.21737	2	7	11	14	0	0	0
H	14	-0.03885	-0.03947	-2.17723	5	13	0	0	0	0	0
H	15	-0.09386	3.38950	1.06541	5	9	0	0	0	0	0
H	16	-0.70928	2.01736	2.01049	5	9	0	0	0	0	0
H	17	1.04644	2.15624	1.68712	5	9	0	0	0	0	0
H	18	-0.09386	3.38950	-1.06541	5	10	0	0	0	0	0
H	19	-0.70928	2.01736	-2.01049	5	10	0	0	0	0	0
H	20	1.04644	2.15624	-1.68712	5	10	0	0	0	0	0

p-NMe₂-Phenol, BLYP/6-31G*, E = -441.23484

21											
O	1	-3.61381	-0.08934	0.06539	6	2	15	0	0	0	0
C	2	-2.22681	-0.01582	0.01530	2	1	3	11	0	0	0
C	3	-1.51760	1.19782	-0.00407	2	2	4	5	0	0	0
H	4	-2.05971	2.15072	0.02672	5	3	0	0	0	0	0
C	5	-0.11418	1.20846	-0.05208	2	3	6	7	0	0	0
H	6	0.39174	2.17426	-0.05631	5	5	0	0	0	0	0

C	7	0.63273	0.00019	-0.09454	2	5	8	13	0	0	0
N	8	2.04297	0.00503	-0.19187	0	7	9	10	0	0	0
C	9	2.75470	1.25538	0.08637	1	8	16	17	18	0	0
C	10	2.76570	-1.23748	0.09581	1	8	19	20	21	0	0
C	11	-1.50599	-1.22356	-0.00761	2	2	12	13	0	0	0
H	12	-2.05336	-2.16933	0.01976	5	11	0	0	0	0	0
C	13	-0.10615	-1.21647	-0.05638	2	7	11	14	0	0	0
H	14	0.41120	-2.17630	-0.06479	5	13	0	0	0	0	0
H	15	-3.96049	0.82771	0.07505	5	1	0	0	0	0	0
H	16	3.83421	1.08663	-0.03842	5	9	0	0	0	0	0
H	17	2.45950	2.04053	-0.63058	5	9	0	0	0	0	0
H	18	2.57793	1.64517	1.11254	5	9	0	0	0	0	0
H	19	3.84369	-1.05922	-0.02886	5	10	0	0	0	0	0
H	20	2.47932	-2.03009	-0.61617	5	10	0	0	0	0	0
H	21	2.59124	-1.62170	1.12425	5	10	0	0	0	0	0

p-NMe2-Phenoxy Radical, BLYP/6-31G*, E = -440.62362

20

O	1	-0.00087	3.60556	0.00000	6	2	0	0	0	0	0
C	2	-0.00087	2.33772	0.00000	2	1	3	11	0	0	0
C	3	-0.00087	1.55281	1.23481	2	2	4	5	0	0	0
H	4	-0.00247	2.10979	2.17588	5	3	0	0	0	0	0
C	5	0.00036	0.17051	1.23243	2	3	6	7	0	0	0
H	6	0.00065	-0.36367	2.18433	5	5	0	0	0	0	0
C	7	0.00264	-0.57068	0.00000	2	5	8	13	0	0	0
N	8	0.00764	-1.95811	0.00000	0	7	9	10	0	0	0
C	9	-0.00207	-2.70432	1.26574	1	8	15	16	17	0	0
C	10	-0.00207	-2.70432	-1.26574	1	8	18	19	20	0	0
C	11	-0.00087	1.55281	-1.23481	2	2	12	13	0	0	0
H	12	-0.00247	2.10979	-2.17588	5	11	0	0	0	0	0
C	13	0.00036	0.17051	-1.23243	2	7	11	14	0	0	0
H	14	0.00065	-0.36367	-2.18433	5	13	0	0	0	0	0
H	15	0.01282	-3.78026	1.04917	5	9	0	0	0	0	0
H	16	0.88290	-2.46539	1.88311	5	9	0	0	0	0	0
H	17	-0.90699	-2.48445	1.86172	5	9	0	0	0	0	0
H	18	0.01282	-3.78026	-1.04917	5	10	0	0	0	0	0
H	19	0.88290	-2.46539	-1.88311	5	10	0	0	0	0	0
H	20	-0.90699	-2.48445	-1.86172	5	10	0	0	0	0	0

Phenoxy Anion, BLYP/6-31G*, E = -306.76485

12

O	1	0.00000	0.00000	2.37179	6	2	0	0	0	0	0
C	2	0.00000	0.00000	1.09319	2	1	5	6	0	0	0
C	3	0.00000	0.00000	-1.84398	2	4	9	10	0	0	0
H	4	0.00000	0.00000	-2.94090	5	3	0	0	0	0	0
C	5	0.00000	1.22289	0.28741	2	2	7	9	0	0	0
C	6	0.00000	-1.22289	0.28741	2	2	8	10	0	0	0
H	7	0.00000	2.17381	0.83753	5	5	0	0	0	0	0
H	8	0.00000	-2.17381	0.83753	5	6	0	0	0	0	0
C	9	0.00000	1.21128	-1.11142	2	3	5	11	0	0	0
C	10	0.00000	-1.21128	-1.11142	2	3	6	12	0	0	0
H	11	0.00000	2.16838	-1.65780	5	9	0	0	0	0	0
H	12	0.00000	-2.16838	-1.65780	5	10	0	0	0	0	0

p-O-Phenol, BLYP/6-31G*, E = -381.96890

13

H	1	2.28019	2.23580	0.00000	5	2	0	0	0	0	0
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O	2	2.48264	1.27669	0.00000	6	1	3	0	0	0	0
C	3	1.20726	0.63757	0.00000	2	2	4	10	0	0	0
C	4	1.15316	-0.77015	0.00000	2	3	5	6	0	0	0
H	5	2.09698	-1.33263	0.00000	5	4	0	0	0	0	0
C	6	-0.08064	-1.43684	0.00000	2	4	7	8	0	0	0
H	7	-0.10752	-2.53455	0.00000	5	6	0	0	0	0	0
C	8	-1.37271	-0.74919	0.00000	2	6	9	12	0	0	0
O	9	-2.49977	-1.35688	0.00000	6	8	0	0	0	0	0
C	10	0.00000	1.36400	0.00000	2	3	11	12	0	0	0
H	11	0.03903	2.46776	0.00000	5	10	0	0	0	0	0
C	12	-1.24066	0.70695	0.00000	2	8	10	13	0	0	0
H	13	-2.17011	1.29101	0.00000	5	12	0	0	0	0	0

p-O-Phenoxy Radical, BLYP/6-31G*, E = -381.39389

12											
C	1	0.00000	0.00000	1.48376	2	2	3	5	0	0	0
O	2	0.00000	0.00000	2.76409	6	1	0	0	0	0	0
C	3	0.00000	1.23196	0.69184	2	1	4	11	0	0	0
H	4	0.00000	2.17208	1.25968	5	3	0	0	0	0	0
C	5	0.00000	-1.23196	0.69184	2	1	6	9	0	0	0
H	6	0.00000	-2.17208	1.25968	5	5	0	0	0	0	0
C	7	0.00000	0.00000	-1.48376	2	8	9	11	0	0	0
O	8	0.00000	0.00000	-2.76409	6	7	0	0	0	0	0
C	9	0.00000	-1.23196	-0.69184	2	5	7	10	0	0	0
H	10	0.00000	-2.17208	-1.25968	5	9	0	0	0	0	0
C	11	0.00000	1.23196	-0.69184	2	3	7	12	0	0	0
H	12	0.00000	2.17208	-1.25968	5	11	0	0	0	0	0

CHO-Benzene, BLYP/6-31G*, E = -345.44123

14											
H	1	0.82706	-3.23662	0.00000	5	2	0	0	0	0	0
C	2	0.59898	-2.16648	0.00000	2	1	3	8	0	0	0
C	3	-0.74556	-1.73919	0.00000	2	2	4	5	0	0	0
H	4	-1.55196	-2.47856	0.00000	5	3	0	0	0	0	0
C	5	-1.04617	-0.37226	0.00000	2	3	6	7	0	0	0
H	6	-2.07768	-0.01050	0.00000	5	5	0	0	0	0	0
C	7	0.00000	0.58021	0.00000	2	5	10	12	0	0	0
C	8	1.64324	-1.22404	0.00000	2	2	9	10	0	0	0
H	9	2.68425	-1.56025	0.00000	5	8	0	0	0	0	0
C	10	1.34393	0.14713	0.00000	2	7	8	11	0	0	0
H	11	2.14754	0.89148	0.00000	5	10	0	0	0	0	0
C	12	-0.30934	2.03611	0.00000	2	7	13	14	0	0	0
O	13	-1.44193	2.51548	0.00000	6	12	0	0	0	0	0
H	14	0.59574	2.70164	0.00000	5	12	0	0	0	0	0

p-CHO-Phenol, BLYP/6-31G*, E = -420.65386

15											
O	1	0.52123	-3.11699	0.00000	6	2	15	0	0	0	0
C	2	0.30904	-1.75889	0.00000	2	1	3	8	0	0	0
C	3	-0.98770	-1.19061	0.00000	2	2	4	5	0	0	0
H	4	-1.86800	-1.84394	0.00000	5	3	0	0	0	0	0
C	5	-1.13604	0.19744	0.00000	2	3	6	7	0	0	0
H	6	-2.12734	0.65803	0.00000	5	5	0	0	0	0	0
C	7	0.00000	1.04171	0.00000	2	5	10	12	0	0	0
C	8	1.45239	-0.92952	0.00000	2	2	9	10	0	0	0
H	9	2.44217	-1.39175	0.00000	5	8	0	0	0	0	0
C	10	1.28917	0.45838	0.00000	2	7	8	11	0	0	0

H	11	2.17136	1.10785	0.00000	5	10	0	0	0	0	0
C	12	-0.15698	2.51421	0.00000	2	7	13	14	0	0	0
O	13	-1.23391	3.11233	0.00000	6	12	0	0	0	0	0
H	14	0.81376	3.08088	0.00000	5	12	0	0	0	0	0
H	15	-0.34978	-3.56996	0.00000	5	1	0	0	0	0	0

p-CHO-Phenoxy Radical, BLYP/6-31G*, E = -420.02244

O	14	1	0.47727	-3.12037	0.00000	6	2	0	0	0	0	0
C	2	0.32900	-1.86529	0.00000	2	1	3	8	0	0	0	0
C	3	-1.00527	-1.24505	0.00000	2	2	4	5	0	0	0	0
H	4	-1.86370	-1.92173	0.00000	5	3	0	0	0	0	0	0
C	5	-1.15157	0.12703	0.00000	2	3	6	7	0	0	0	0
H	6	-2.13541	0.60384	0.00000	5	5	0	0	0	0	0	0
C	7	0.00000	0.97616	0.00000	2	5	10	12	0	0	0	0
C	8	1.48697	-0.95872	0.00000	2	2	9	10	0	0	0	0
H	9	2.47779	-1.41990	0.00000	5	8	0	0	0	0	0	0
C	10	1.31121	0.41347	0.00000	2	7	8	11	0	0	0	0
H	11	2.17498	1.08780	0.00000	5	10	0	0	0	0	0	0
C	12	-0.16821	2.45057	0.00000	2	7	13	14	0	0	0	0
O	13	-1.25928	3.02390	0.00000	6	12	0	0	0	0	0	0
H	14	0.78968	3.03272	0.00000	5	12	0	0	0	0	0	0

COMe-Benzene, BLYP/6-31G*, E = -384.73532

H	17	1	0.76774	-3.62883	0.00000	5	2	0	0	0	0	0
C	2	0.55933	-2.55460	0.00000	2	1	3	8	0	0	0	0
C	3	1.61486	-1.62208	0.00000	2	2	4	5	0	0	0	0
H	4	2.65222	-1.97005	0.00000	5	3	0	0	0	0	0	0
C	5	1.33684	-0.24905	0.00000	2	3	6	7	0	0	0	0
H	6	2.13775	0.49401	0.00000	5	5	0	0	0	0	0	0
C	7	0.00000	0.21488	0.00000	2	5	10	12	0	0	0	0
C	8	-0.77351	-2.10599	0.00000	2	2	9	10	0	0	0	0
H	9	-1.59553	-2.82797	0.00000	5	8	0	0	0	0	0	0
C	10	-1.05253	-0.72974	0.00000	2	7	8	11	0	0	0	0
H	11	-2.09325	-0.39519	0.00000	5	10	0	0	0	0	0	0
C	12	-0.23851	1.70504	0.00000	2	7	13	14	0	0	0	0
O	13	0.70970	2.49710	0.00000	6	12	0	0	0	0	0	0
C	14	-1.68266	2.22340	0.00000	1	12	15	16	17	0	0	0
H	15	-1.66118	3.32170	0.00000	5	14	0	0	0	0	0	0
H	16	-2.23410	1.86922	0.88862	5	14	0	0	0	0	0	0
H	17	-2.23410	1.86922	-0.88862	5	14	0	0	0	0	0	0

p-COMe-Phenol, BLYP/6-31G*, E = -459.94760

O	18	1	0.13675	-3.53407	0.00000	6	2	15	0	0	0	0
C	2	0.13190	-2.15788	0.00000	2	1	3	8	0	0	0	0
C	3	1.32093	-1.39339	0.00000	2	2	4	5	0	0	0	0
H	4	2.29398	-1.89885	0.00000	5	3	0	0	0	0	0	0
C	5	1.24876	0.00128	0.00000	2	3	6	7	0	0	0	0
H	6	2.15658	0.60909	0.00000	5	5	0	0	0	0	0	0
C	7	0.00000	0.66893	0.00000	2	5	10	12	0	0	0	0
C	8	-1.12324	-1.51309	0.00000	2	2	9	10	0	0	0	0
H	9	-2.03137	-2.12043	0.00000	5	8	0	0	0	0	0	0
C	10	-1.18011	-0.11519	0.00000	2	7	8	11	0	0	0	0
H	11	-2.15991	0.36849	0.00000	5	10	0	0	0	0	0	0
C	12	-0.00629	2.16970	0.00000	2	7	13	14	0	0	0	0
O	13	1.05238	2.81063	0.00000	6	12	0	0	0	0	0	0

C	14	-1.35369	2.90539	0.00000	1	12	16	17	18	0	0
H	15	1.06951	-3.83962	0.00000	5	1	0	0	0	0	0
H	16	-1.16121	3.98691	0.00000	5	14	0	0	0	0	0
H	17	-1.95509	2.64372	0.88864	5	14	0	0	0	0	0
H	18	-1.95509	2.64372	-0.88864	5	14	0	0	0	0	0

p-COMe-Phenoxy Radical, BLYP/6-31G*, E = -459.31705

O	17	1	0.23946	-3.52751	0.00000	6	2	0	0	0	0	0
C	2	0.16726	-2.26440	0.00000	2	1	3	8	0	0	0	0
C	3	1.36998	-1.42235	0.00000	2	2	4	5	0	0	0	0
H	4	2.33460	-1.93671	0.00000	5	3	0	0	0	0	0	0
C	5	1.27552	-0.04502	0.00000	2	3	6	7	0	0	0	0
H	6	2.16388	0.59108	0.00000	5	5	0	0	0	0	0	0
C	7	0.00000	0.60468	0.00000	2	5	10	12	0	0	0	0
C	8	-1.12534	-1.56769	0.00000	2	2	9	10	0	0	0	0
H	9	-2.02434	-2.18937	0.00000	5	8	0	0	0	0	0	0
C	10	-1.19153	-0.18500	0.00000	2	7	8	11	0	0	0	0
H	11	-2.16640	0.30905	0.00000	5	10	0	0	0	0	0	0
C	12	-0.02401	2.11006	0.00000	2	7	13	14	0	0	0	0
O	13	1.03751	2.74649	0.00000	6	12	0	0	0	0	0	0
C	14	-1.37141	2.83764	0.00000	1	12	15	16	17	0	0	0
H	15	-1.18368	3.91977	0.00000	5	14	0	0	0	0	0	0
H	16	-1.97130	2.57344	0.88875	5	14	0	0	0	0	0	0
H	17	-1.97130	2.57344	-0.88875	5	14	0	0	0	0	0	0

SO2Me-Benzene, BLYP/6-31G*, E = -819.96708

H	18	1	-0.10007	4.21350	0.00000	5	2	0	0	0	0	0
C	2	-0.10808	3.11963	0.00000	2	1	3	11	0	0	0	0
C	3	-0.11321	2.41973	1.22072	2	2	4	5	0	0	0	0
H	4	-0.12320	2.96720	2.16752	5	3	0	0	0	0	0	0
C	5	-0.11321	1.01430	1.22759	2	3	6	7	0	0	0	0
H	6	-0.13858	0.45138	2.16337	5	5	0	0	0	0	0	0
C	7	-0.10330	0.32984	0.00000	4	5	13	0	0	0	0	0
S	8	-0.08729	-1.50255	0.00000	0	9	10	0	0	0	0	0
O	9	-0.64866	-1.96581	1.30243	6	8	0	0	0	0	0	0
O	10	-0.64866	-1.96581	-1.30243	6	8	0	0	0	0	0	0
C	11	-0.11321	2.41973	-1.22072	2	2	12	13	0	0	0	0
H	12	-0.12320	2.96720	-2.16752	5	11	0	0	0	0	0	0
C	13	-0.11321	1.01430	-1.22759	2	7	11	14	0	0	0	0
H	14	-0.13858	0.45138	-2.16337	5	13	0	0	0	0	0	0
C	15	1.71045	-1.91003	0.00000	2	16	17	18	0	0	0	0
H	16	1.77539	-3.00801	0.00000	5	15	0	0	0	0	0	0
H	17	2.17302	-1.49699	0.90719	5	15	0	0	0	0	0	0
H	18	2.17302	-1.49699	-0.90719	5	15	0	0	0	0	0	0

p-SO2Me-Phenol, BLYP/6-31G*, E = -895.17845

H	19	1	-4.45255	0.82142	0.09906	5	2	0	0	0	0	0
O	2	-4.08875	-0.08994	0.09015	6	1	3	0	0	0	0	0
C	3	-2.71600	-0.01565	0.03590	2	2	4	16	0	0	0	0
C	4	-2.00904	-1.23810	-0.00203	2	3	5	6	0	0	0	0
H	5	-2.57092	-2.17479	0.00581	5	4	0	0	0	0	0	0
C	6	-0.61119	-1.22854	-0.06531	2	4	7	8	0	0	0	0
H	7	-0.05230	-2.16530	-0.12314	5	6	0	0	0	0	0	0
C	8	0.07862	-0.00031	-0.08293	4	6	18	0	0	0	0	0
S	9	1.89779	0.01098	-0.17316	0	10	15	0	0	0	0	0

O	10	2.33265	-1.26467	-0.81402	6	9	0	0	0	0	0
C	11	2.43022	-0.05649	1.59123	2	12	13	14	0	0	0
H	12	3.52999	-0.05636	1.57764	5	11	0	0	0	0	0
H	13	2.05101	-0.98110	2.04836	5	11	0	0	0	0	0
H	14	2.05128	0.83205	2.11514	5	11	0	0	0	0	0
O	15	2.32089	1.33829	-0.70859	6	9	0	0	0	0	0
C	16	-2.01969	1.21255	0.00785	2	3	17	18	0	0	0
H	17	-2.57450	2.15736	0.02325	5	16	0	0	0	0	0
C	18	-0.61902	1.21981	-0.05399	2	8	16	19	0	0	0
H	19	-0.06846	2.16192	-0.10029	5	18	0	0	0	0	0

p-SO2Me-Phenoxy Radical, BLYP/6-31G*, E = -894.54540

O	1	-0.15527	4.08014	0.00000	6	2	0	0	0	0	0
C	2	-0.15527	2.81248	0.00000	2	1	3	11	0	0	0
C	3	-0.15527	2.04735	1.25146	2	2	4	5	0	0	0
H	4	-0.17661	2.61752	2.18356	5	3	0	0	0	0	0
C	5	-0.12925	0.66034	1.24271	2	3	6	7	0	0	0
H	6	-0.14493	0.08202	2.16979	5	5	0	0	0	0	0
C	7	-0.09723	-0.02396	0.00000	4	5	13	0	0	0	0
S	8	-0.03736	-1.86158	0.00000	0	9	10	0	0	0	0
O	9	-0.59345	-2.32473	1.30345	6	8	0	0	0	0	0
O	10	-0.59345	-2.32473	-1.30345	6	8	0	0	0	0	0
C	11	-0.15527	2.04735	-1.25146	2	2	12	13	0	0	0
H	12	-0.17661	2.61752	-2.18356	5	11	0	0	0	0	0
C	13	-0.12925	0.66034	-1.24271	2	7	11	14	0	0	0
H	14	-0.14493	0.08202	-2.16979	5	13	0	0	0	0	0
C	15	1.76831	-2.22558	0.00000	2	16	17	18	0	0	0
H	16	1.85593	-3.32220	0.00000	5	15	0	0	0	0	0
H	17	2.22069	-1.80339	0.90809	5	15	0	0	0	0	0
H	18	2.22069	-1.80339	-0.90809	5	15	0	0	0	0	0

CN-Benzene, BLYP/6-31G*, E = -324.36567

C	1	0.00000	0.00000	2.05599	4	2	13	0	0	0	0
C	2	0.00000	0.00000	0.61742	2	1	5	6	0	0	0
C	3	0.00000	0.00000	-2.19674	2	4	9	10	0	0	0
H	4	0.00000	0.00000	-3.29049	5	3	0	0	0	0	0
C	5	0.00000	1.22669	-0.09235	2	2	7	9	0	0	0
C	6	0.00000	-1.22669	-0.09235	2	2	8	10	0	0	0
H	7	0.00000	2.16827	0.46153	5	5	0	0	0	0	0
H	8	0.00000	-2.16827	0.46153	5	6	0	0	0	0	0
C	9	0.00000	1.21934	-1.49431	2	3	5	11	0	0	0
C	10	0.00000	-1.21934	-1.49431	2	3	6	12	0	0	0
H	11	0.00000	2.16698	-2.03989	5	9	0	0	0	0	0
H	12	0.00000	-2.16698	-2.03989	5	10	0	0	0	0	0
N	13	0.00000	0.00000	3.23244	0	1	0	0	0	0	0

p-CH-Phenol, BLYP/6-31G*, E = -399.57731

H	1	-0.82547	-3.46401	0.00000	5	2	0	0	0	0	0
O	2	0.08570	-3.09956	0.00000	6	1	3	0	0	0	0
C	3	0.01214	-1.72652	0.00000	2	2	4	10	0	0	0
C	4	1.23386	-1.01775	0.00000	2	3	5	6	0	0	0
H	5	2.17093	-1.57867	0.00000	5	4	0	0	0	0	0
C	6	1.22639	0.37852	0.00000	2	4	7	8	0	0	0
H	7	2.16918	0.93017	0.00000	5	6	0	0	0	0	0
C	8	0.00000	1.09401	0.00000	2	6	9	12	0	0	0

C	9	-0.00561	2.52929	0.00000	4	8	14	0	0	0	0
C	10	-1.21391	-1.02618	0.00000	2	3	11	12	0	0	0
H	11	-2.16040	-1.57778	0.00000	5	10	0	0	0	0	0
C	12	-1.21969	0.37293	0.00000	2	8	10	13	0	0	0
H	13	-2.16743	0.91597	0.00000	5	12	0	0	0	0	0
N	14	-0.01021	3.70643	0.00000	0	9	0	0	0	0	0

p-CN-Phenoxy Radical, BLYP/6-31G*, E = -398.94668

C	1	0.00000	0.00000	-2.45496	4	2	13	0	0	0	0
C	2	0.00000	0.00000	-1.02737	2	1	5	6	0	0	0
C	3	0.00000	0.00000	1.83579	2	4	9	10	0	0	0
O	4	0.00000	0.00000	3.09956	6	3	0	0	0	0	0
C	5	0.00000	1.24447	-0.31491	2	2	7	9	0	0	0
C	6	0.00000	-1.24447	-0.31491	2	2	8	10	0	0	0
H	7	0.00000	2.17738	-0.88421	5	5	0	0	0	0	0
H	8	0.00000	-2.17738	-0.88421	5	6	0	0	0	0	0
C	9	0.00000	1.25123	1.06659	2	3	5	11	0	0	0
C	10	0.00000	-1.25123	1.06659	2	3	6	12	0	0	0
H	11	0.00000	2.18401	1.63561	5	9	0	0	0	0	0
H	12	0.00000	-2.18401	1.63561	5	10	0	0	0	0	0
N	13	0.00000	0.00000	-3.63430	0	1	0	0	0	0	0

NO2-Benzene, BLYP/6-31G*, E = -436.63315

N	1	0.00000	0.00000	1.73337	0	2	13	14	0	0	0
C	2	0.00000	0.00000	0.24360	2	1	5	6	0	0	0
C	3	0.00000	0.00000	-2.53891	2	4	9	10	0	0	0
H	4	0.00000	0.00000	-3.63261	5	3	0	0	0	0	0
C	5	0.00000	1.22962	-0.43466	2	2	7	9	0	0	0
C	6	0.00000	-1.22962	-0.43466	2	2	8	10	0	0	0
H	7	0.00000	2.15734	0.13790	5	5	0	0	0	0	0
H	8	0.00000	-2.15734	0.13790	5	6	0	0	0	0	0
C	9	0.00000	1.22086	-1.83770	2	3	5	11	0	0	0
C	10	0.00000	-1.22086	-1.83770	2	3	6	12	0	0	0
H	11	0.00000	2.16820	-2.38346	5	9	0	0	0	0	0
H	12	0.00000	-2.16820	-2.38346	5	10	0	0	0	0	0
O	13	0.00000	1.10767	2.31439	6	1	0	0	0	0	0
O	14	0.00000	-1.10767	2.31439	6	1	0	0	0	0	0

p-NO2-Phenol, BLYP/6-31G*, E = -511.84549

H	1	0.81755	-3.83257	0.00000	5	2	0	0	0	0	0
O	2	-0.09272	-3.46469	0.00000	6	1	3	0	0	0	0
C	3	-0.01679	-2.09443	0.00000	2	2	4	10	0	0	0
C	4	-1.23979	-1.38423	0.00000	2	3	5	6	0	0	0
H	5	-2.17697	-1.94469	0.00000	5	4	0	0	0	0	0
C	6	-1.23125	0.01178	0.00000	2	4	7	8	0	0	0
H	7	-2.15799	0.58567	0.00000	5	6	0	0	0	0	0
C	8	0.00000	0.69539	0.00000	2	6	9	12	0	0	0
N	9	0.00884	2.17158	0.00000	0	8	14	15	0	0	0
C	10	1.21302	-1.39669	0.00000	2	3	11	12	0	0	0
H	11	2.15798	-1.95049	0.00000	5	10	0	0	0	0	0
C	12	1.22236	0.00186	0.00000	2	8	10	13	0	0	0
H	13	2.15563	0.56510	0.00000	5	12	0	0	0	0	0
O	14	-1.09652	2.76209	0.00000	6	9	0	0	0	0	0
O	15	1.12133	2.74933	0.00000	6	9	0	0	0	0	0

p-NO₂-Phenoxy Radical, BLYP/6-31G*, E = -511.21141

14													
N	1	0.00000	0.00000	-2.11390	0	2	13	14	0	0	0		
C	2	0.00000	0.00000	-0.62905	2	1	5	6	0	0	0		
C	3	0.00000	0.00000	2.20057	2	4	9	10	0	0	0		
O	4	0.00000	0.00000	3.46501	6	3	0	0	0	0	0		
C	5	0.00000	1.24621	0.04930	2	2	7	9	0	0	0		
C	6	0.00000	-1.24621	0.04930	2	2	8	10	0	0	0		
H	7	0.00000	2.16431	-0.53927	5	5	0	0	0	0	0		
H	8	0.00000	-2.16431	-0.53927	5	6	0	0	0	0	0		
C	9	0.00000	1.25321	1.43312	2	3	5	11	0	0	0		
C	10	0.00000	-1.25321	1.43312	2	3	6	12	0	0	0		
H	11	0.00000	2.18562	2.00249	5	9	0	0	0	0	0		
H	12	0.00000	-2.18562	2.00249	5	10	0	0	0	0	0		
O	13	0.00000	1.11059	-2.69171	6	1	0	0	0	0	0		
O	14	0.00000	-1.11059	-2.69171	6	1	0	0	0	0	0		

CF₃-Benzene, BLYP/6-31G*, E = -569.14012

15														
H	1	1.68402	3.57594	0.00000	5	2	0	0	0	0	0			
C	2	1.21475	2.58781	0.00000	2	1	3	7	0	0	0			
C	3	2.01052	1.42681	0.00000	2	2	4	5	0	0	0			
H	4	3.10120	1.50738	0.00000	5	3	0	0	0	0	0			
C	5	1.40596	0.16099	0.00000	2	3	6	11	0	0	0			
H	6	2.01923	-0.74392	0.00000	5	5	0	0	0	0	0			
C	7	-0.18618	2.47896	0.00000	2	2	8	9	0	0	0			
H	8	-0.80707	3.37937	0.00000	5	7	0	0	0	0	0			
C	9	-0.79717	1.21330	0.00000	2	7	10	11	0	0	0			
H	10	-1.88494	1.12284	0.00000	5	9	0	0	0	0	0			
C	11	0.00000	0.05437	0.00000	2	5	9	12	0	0	0			
C	12	-0.62481	-1.32316	0.00000	1	11	13	14	15	0	0			
F	13	-0.24019	-2.05022	1.09955	0	12	0	0	0	0	0			
F	14	-0.24019	-2.05022	-1.09955	0	12	0	0	0	0	0			
F	15	-1.99193	-1.28135	0.00000	0	12	0	0	0	0	0			

p-CF₃-Phenol, BLYP/6-31G*, E = -644.35094

16															
H	1	-0.57330	-4.22391	0.00000	5	2	0	0	0	0	0				
O	2	0.31286	-3.80278	0.00000	6	1	3	0	0	0	0				
C	3	0.16148	-2.43393	0.00000	2	2	4	8	0	0	0				
C	4	-1.10002	-1.79973	0.00000	2	3	5	6	0	0	0				
H	5	-2.01682	-2.39942	0.00000	5	4	0	0	0	0	0				
C	6	-1.17542	-0.40108	0.00000	2	4	7	12	0	0	0				
H	7	-2.15309	0.08770	0.00000	5	6	0	0	0	0	0				
C	8	1.34060	-1.66083	0.00000	2	3	9	10	0	0	0				
H	9	2.30755	-2.16870	0.00000	5	8	0	0	0	0	0				
C	10	1.25503	-0.26366	0.00000	2	8	11	12	0	0	0				
H	11	2.16738	0.33544	0.00000	5	10	0	0	0	0	0				
C	12	0.00000	0.37640	0.00000	2	6	10	13	0	0	0				
C	13	-0.11427	1.88057	0.00000	1	12	14	15	16	0	0				
F	14	-0.80052	2.34034	1.09890	0	13	0	0	0	0	0				
F	15	-0.80052	2.34034	-1.09890	0	13	0	0	0	0	0				
F	16	1.10782	2.49763	0.00000	0	13	0	0	0	0	0				

p-CF₃-Phenoxy Radical, BLYP/6-31G*, E = -643.71962

15														
O	1	0.32623	-3.79233	0.00000	6	2	0	0	0	0	0			
C	2	0.22185	-2.52882	0.00000	2	1	3	7	0	0	0			

C	3	-1.08423	-1.86211	0.00000	2	2	4	5	0	0	0
H	4	-1.97056	-2.50110	0.00000	5	3	0	0	0	0	0
C	5	-1.17958	-0.48140	0.00000	2	3	6	11	0	0	0
H	6	-2.15603	0.01049	0.00000	5	5	0	0	0	0	0
C	7	1.40533	-1.66501	0.00000	2	2	8	9	0	0	0
H	8	2.38068	-2.15769	0.00000	5	7	0	0	0	0	0
C	9	1.28599	-0.28276	0.00000	2	7	10	11	0	0	0
H	10	2.17166	0.35571	0.00000	5	9	0	0	0	0	0
C	11	0.00000	0.31740	0.00000	2	5	9	12	0	0	0
C	12	-0.15555	1.82431	0.00000	1	11	13	14	15	0	0
F	13	-0.85551	2.24576	1.10085	0	12	0	0	0	0	0
F	14	-0.85551	2.24576	-1.10085	0	12	0	0	0	0	0
F	15	1.04454	2.47534	0.00000	0	12	0	0	0	0	0