Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary material

Table S1: Oscillator strength and energies (kcal/mol) of 2HAP-1 singlet excited states

	TD-B3LYP			EOM-CCSD			CAS(13,16)			CASPT2(13,16)	
	f	energy	symmetry	f	energy	symmetry	f	energy	symmetry	energy	symmetry
S1	0.084	90.7	A'	0.105	99.5	A'	0.000	103.5	A"	90.6	A"
S2	0.000	92.2	A"	0.000	99.7	A"	0.187	116.4	A'	91.1	A'
S3	0.159	116.6	A'	0.124	129.3	A'	0.000	138.7	A"	123.4	A'
S4	0.004	131.8	A"	0.003	142.1	A"	0.008	150.3	A"	142.4	A"
S5	0.168	133.7	A'	0.535	150.5	A'	0.335	157.1	A'	146.2	A'
S6	0.000	140.9	A"	0.005	152.4	A"	0.002	158.9	A"	151.3	A"
S7	0.220	141.9	A'	0.223	154.8	A'	0.074	170.2	A'	163.9	A"
S8	0.000	142.6	A"	0.003	156.8	A"	0.014	171.3	A"		
S9	0.003	147.2	A"	0.001	165.8	A"	0.000	177.5	A"		
S10	0.001	150.4	A"	0.037	166.7	A'	0.006	177.9	A'		
S11	0.014	153.8	A'	0.047	167.8	A'	0.114	187.2	A'		

Table S2: Oscillator strength and energies (kcal/mol) of 2HAP-2 singlet excited states

	TD-B3LYP			EOM-CCSD			CAS(13,16)			CASPT2(13,16)	
	f	energy	symmetry	f	energy	symmetry	f	energy	symmetry	energy	symmetry
S1	0.000	82.2	A"	0.000	91.5	A"	0.000	93.8	A"	80.6	A"
S2	0.085	99.9	A'	0.070	107.0	A'	0.095	123.0	A'	97.5	A'
S3	0.000	121.8	A"	0.000	135.8	A"	0.001	133.0	A"	135.1	A"
S4	0.115	122.0	A'	0.111	136.0	A'	0.012	148.0	A"	136.7	A'
S5	0.000	127.8	A"	0.008	149.4	A"	0.002	154.4	A"	142.4	A'
S6	0.022	134.6	A'	0.337	153.7	A'	0.071	160.8	A'	150.8	A"
S7	0.295	137.2	A'	0.408	156.5	A'	0.140	163.5	A'	157.9	A"
S8	0.005	137.5	A"	0.002	157.8	A"	0.000	166.1	A"		
S9	0.015	141.4	A'	0.000	158.0	A"	0.011	166.9	A"		
S10	0.001	141.7	A"	0.293	160.7	A'	0.008	171.4	A'		
S11	0.220	145.1	A'	0.003	161.7	A"	0.000	176.9	A"		
S12	0.000	145.7	A"	0.006	166.8	A"	0.094	178.8	A'		
S13	0.007	148.9	A"	0.021	167.1	A'	0.181	191.9	A'		
S14	0.009	149.9	A'	0.003	170.2	A"	1.053	202.9	A'		

Table S3: Oscillator strength and energies (kcal/mol) of 3HAP-a1 singlet excited states

	TD-B3LYP			EOM-CCSD			CAS(13,16)			CASPT2(13,16)	
	f	energy	symmetry	f	energy	symmetry	f	energy	symmetry	energy	symmetry
S1	0.000	86.6	A"	0.000	94.7	A"	0.105	99.0	A"	85.2	A"
S2	0.050	96.3	A'	0.041	106.9	A'	0.077	125.5	A'	100.8	A'
S3	0.151	116.4	A'	0.185	133.9	A'	0.003	136.4	A"	123.3	A'
S4	0.000	130.3	A"	0.000	138.0	A"	0.012	149.0	A"	138.0	A"
S5	0.000	133.5	A"	0.003	152.0	A"	0.000	153.6	A"	146.7	A'
S6	0.252	135.3	A'	0.496	153.1	A'	0.330	158.8	A'	152.4	A"
S7	0.002	138.4	A"	0.275	160.6	A'	0.008	163.3	A"	159.7	A"
S8	0.058	145.2	A'	0.003	162.0	A"	0.000	171.7	A'		
S9	0.156	146.6	A'	0.080	162.8	A'	0.000	172.1	A"		
S10	0.000	149.6	A"	0.004	165.4	A"	0.157	175.6	A'		
S11	0.011	151.6	A'	0.000	169.5	A"	0.008	182.3	A'		

Table S4: Oscillator strength and energies (kcal/mol) of 3HAP-a2 singlet excited states

	TD-B3LYP			EOM-CCSD			CAS(13,16)			CASPT2(13,16)	
	f	energy	symmetry	f	energy	symmetry	f	energy	symmetry	energy	symmetry
S1	0.000	85.9	A"	0.000	94.1	A"	0.000	97.7	A"	85.3	A"
S2	0.045	96.6	A'	0.039	106.9	A'	0.070	123.0	A'	100.0	A'
S3	0.150	117.9	A'	0.000	135.4	A"	0.004	134.0	A"	126.4	A'
S4	0.000	126.7	A"	0.172	135.6	A'	0.003	154.7	A"	135.4	A"
S5	0.000	131.6	A"	0.004	151.5	A"	0.000	158.8	A"	147.6	A'
S6	0.278	135.9	A'	0.550	153.6	A'	0.226	158.8	A'	152.3	A"
S7	0.003	138.2	A"	0.006	159.2	A"	0.018	172.8	A"	156.2	A"
S8	0.014	143.9	A'	0.250	161.0	A'	0.005	173.2	A'		
S9	0.004	146.1	A"	0.001	161.9	A"	0.001	174.3	A"		
S10	0.194	146.1	A'	0.113	163.3	A'	0.043	182.0	A'		
S11	0.000	148.5	A"	0.001	169.4	A"	0.000	183.6	A"		
S12	0.019	149.2	A'	0.011	169.8	A"	0.175	184.0	A'		
S13	0.001	151.1	A"	0.020	171.7	A'	0.805	193.7	A'		

Table S5: Oscillator strength and energies (kcal/mol) of 4HAP-1 singlet excited states

	TD-B3LYP			EOM-CCSD			CAS(13,16)			CASPT2(13,16)	
	f	energy	symmetry	f	energy	symmetry	f	energy	symmetry	energy	symmetry
S1	0.000	88.5	A"	0.000	96.3	A"	0.000	99.4	A"	86.2	A"
S2	0.278	110.3	A'	0.003	113.0	A'	0.033	125.2	A'	103.8	A'
S3	0.034	111.3	A'	0.380	126.2	A'	0.003	133.3	A"	117.3	A'
S4	0.000	122.1	A"	0.000	136.1	A"	0.001	149.1	A"	136.2	A"
S5	0.000	127.7	A"	0.000	151.9	A"	0.231	153.9	A'	152.3	A"
S6	0.153	131.8	A'	0.288	153.5	A'	0.001	156.7	A"	157.4	A'
S7	0.000	139.8	A"	0.094	160.1	A'	0.000	164.9	A"	159.3	A"
S8	0.022	142.0	A'	0.000	160.3	A"	0.020	167.7	A"		
S9	0.031	145.9	A'	0.000	161.3	A"	0.007	168.4	A'		
S10	0.002	147.6	A"	0.001	163.6	A"	0.001	175.0	A'		
S11	0.282	149.8	A'	0.396	164.6	A'	0.443	183.3	A'		
S12	0.001	151.9	A"	0.004	168.1	A"	0.001	187.1	A"		

Excited State Calculations at TD B3LYP/6-311+G** level

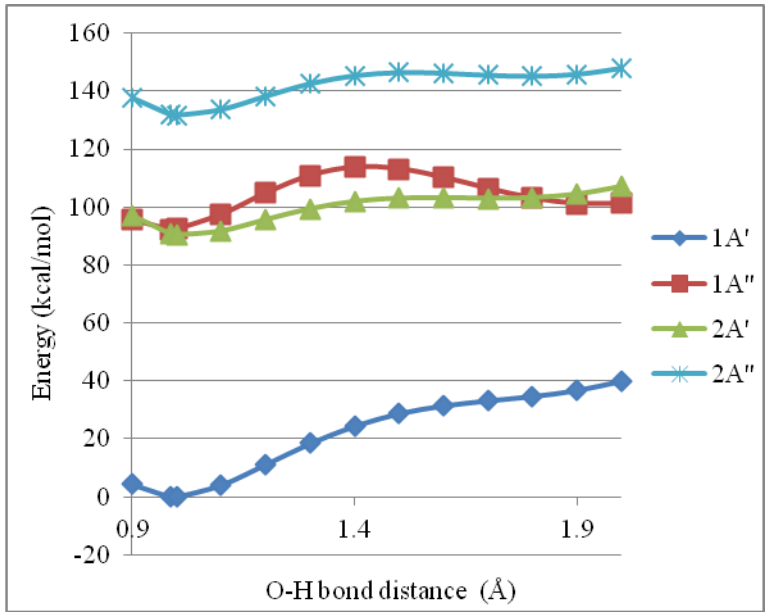

Fig. S1: The potential energies of the ground state and singlet excited states along the O-H bond distance of 2HAP-1 at TD B3LYP/6-311+G** level.

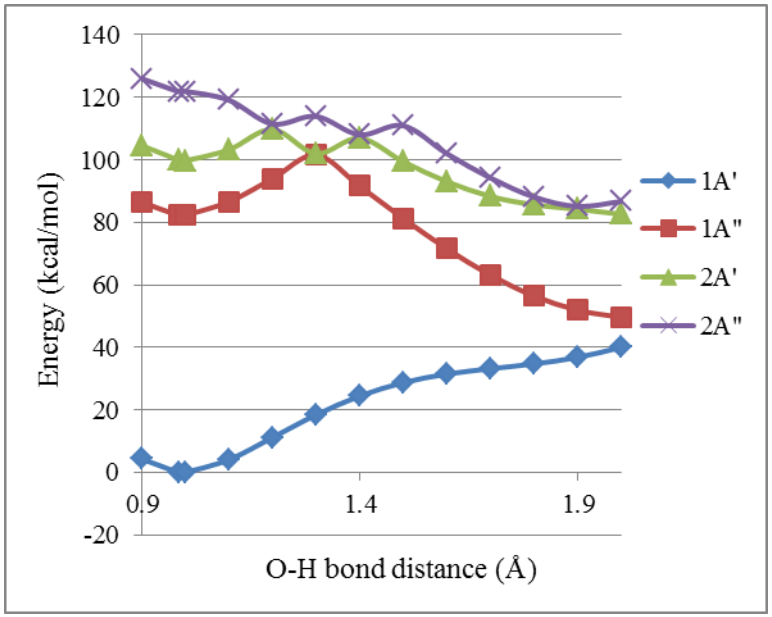

Fig. S2: The potential energies of the ground state and singlet excited states along the O-H bond distance of 2HAP-2 at TD B3LYP/6-311+G** level (non-planar).

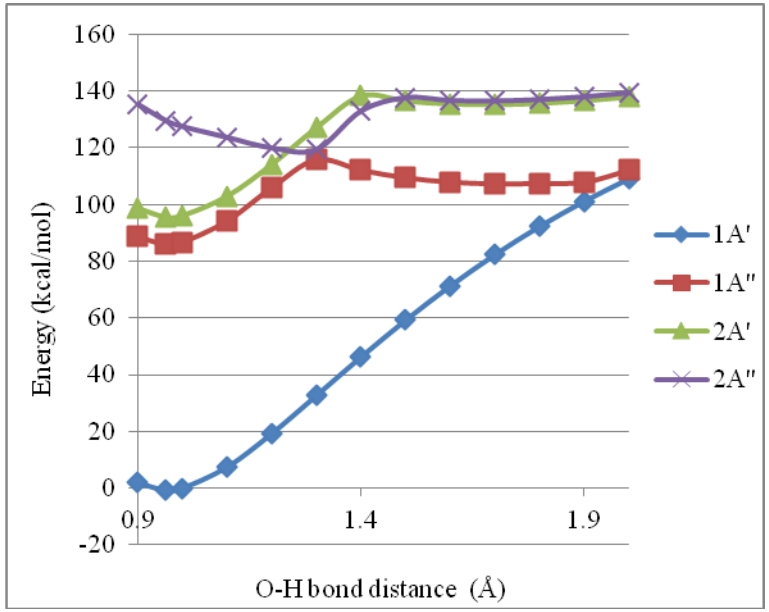

Fig. S3: The potential energies of the ground state and singlet excited states along the O-H bond distance of 3HAP-a1 at TD B3LYP/6-311+G** level.

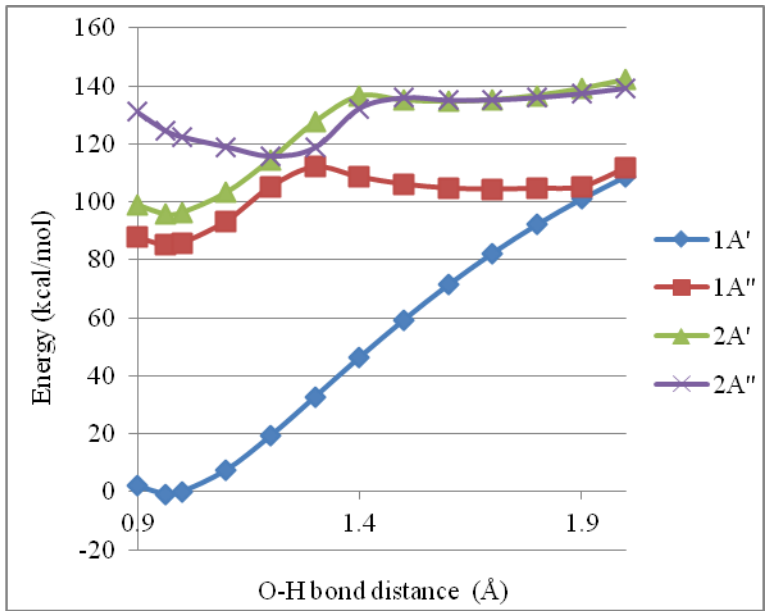

Fig. S4: The potential energies of the ground state and singlet excited states along the O-H bond distance of 3HAP-b1 at TD B3LYP/6-311+G** level.

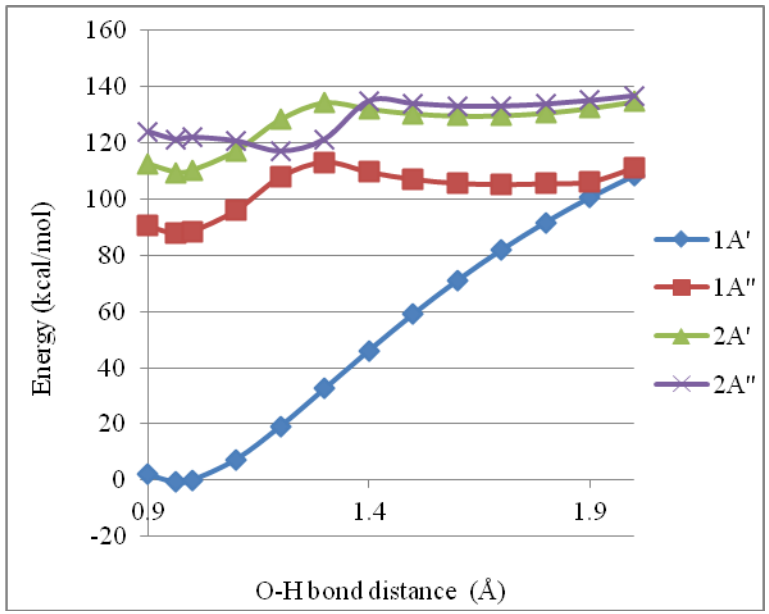

Fig. S5: The potential energies of the ground state and singlet excited states along the O-H bond distance of 4HAP-1 at TD B3LYP/6-311+G** level.

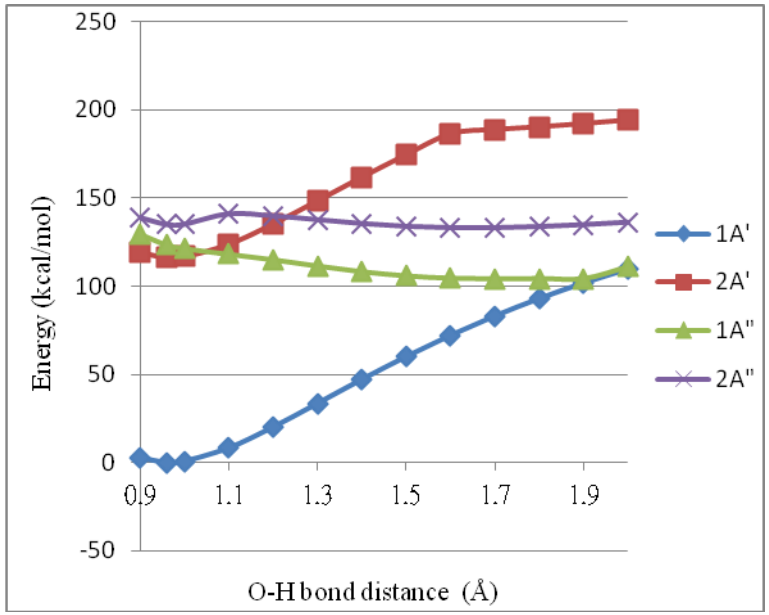

Fig. S6: The potential energies of the ground state and singlet excited states along the O-H bond distance of phenol at TD B3LYP/6-311+G** level.