

Supporting Information

Polarization Effects for Hydrogen-Bonded Complexes of Substituted Phenols with Water and Chloride Ion

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	HF/6-311+G**	MP2/6-311+G**	complex 3	complex 3	complex 4	complex 4
		//HF/6-311+G**	HF	MP2	HF	MP2
PhOH	-305.6398948	-306.6632927	-381.7031394	-382.950224	-381.698935	-382.945302
O ₂ NPhOH	-509.1698046	-510.7640653	-585.2357555	-587.05353	-585.227898	-587.045841
H ₂ NPhOH	-360.6846571	-361.8919039	-436.7473622	-438.178292	-436.744321	-438.174517
NPhOH	-397.3958459	-398.6979011	-473.4613274	-474.987067	-473.454109	-474.979742
H ₃ CPhOH	-344.6849562	-345.8627592	-420.7479083	-422.149451	-420.744218	-422.144996
ClPhOH	-764.5627466	-765.7223036	-840.626995	-842.010201	-840.621461	-842.004454
F ₃ CPhOH	-641.3572507	-643.1211196	-717.4220994	-719.409746	-717.415686	-719.403233
FPhOH	-404.5183477	-405.7388421	-480.5822528	-482.026468	-480.577304	-482.02109
HOPhOH	-380.5193946	-381.7417692	-456.5825477	-458.028654	-456.578883	-458.024465
H ₂ O	-76.0533051	-76.2739687				
Cl ⁻	-459.5654245	-459.7035702				

Energies in a.u.

complex 5	complex 5
HF	MP2
-765.2345464	-766.4066246
-968.7801555	-970.5233004
-820.2771823	-821.6329068
-857.003979	-858.4553969
-804.2784247	-805.6051856
-1224.163494	-1225.471472
-1100.961312	-1102.875345
-864.117137	-865.4864205
-840.1136808	-841.484703