Electrochemical measurements and theoretical studies for understanding the behavior of Catechol, Resorcinol and Hydroquinone on the boron doped diamond surface

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Supplementary material: dates in DFT 6-311 ++ G (d, p)

FIGURE 8: INTERMEDIATE ENERGIES

vacuum

Name	Gibbs/hartree	Relative	Relative/eV
CT1	-382.729575	0	0
CT2	-382.193415	0.53616	14.58944976
CT3	-381.462378	1.267197	34.48169757
CT4	-381.579729	1.149846	31.28845951
CT5	-381.448978	1.280597	34.84632497
CT6	-381.496338	1.233237	33.55761201

HQ1	-382.726222	0	0
HQ2	-382.17265	0.553572	15.06324769
HQ3	-381.473079	1.253143	34.09927417
HQ4	-381.589889	1.136333	30.92075726
HQ5	-381.432294	1.293928	35.20907481
HQ6	-381.50809	1.218132	33.14658985

RS1	-382.72921	0	0
RS2	-382.18222	0.54699	14.88414489
RS3	-381.48468	1.244531	33.86493304
RS4	-381.56870	1.160514	31.57874645
RS5	-381.46427	1.264936	34.4201735
RS6	-382.71126	0.017949	0.488410239

Implicit solvent

Name	Gibbs/hartree	Relative	Relative/eV
CT1	-382.738067	0	0
CT2	-382.279433	0.458634	12.47988977
CT3	-381.78495	0.953117	25.93526669
CT4	-381.67081	1.067257	29.04113023
CT5	-381.465336	1.272731	34.63228324
CT6	-381.509381	1.228686	33.43377475

HQ1	-382.737128	0	0
HQ2	-382.267918	0.46921	12.76767331
HQ3	-381.78193	0.955198	25.99189278
HQ4	-381.674254	1.062874	28.92186441
HQ5	-381.424537	1.312591	35.7169137
HQ6	-382	1.219312	33.17869883

RS1	-382.73965	0	0
RS2	-382.274727	0.464923	12.65101975
RS3	-381.793829	0.945821	25.73673523
RS4	-381.657809	1.081841	29.43797545
RS5	-381.475099	1.264551	34.40969726
RS6	-382.724475	0.015175	0.412926925

Ionization Potential and Electronic Affinity of Table 1

Following the reference: C.G. Zhan, J. A. Nichols, and D. A. Dixon; *J. Phys. Chem. A* 2003, *107,* 4184-4195

The indications for the calculation of Ionization Potential and Electronic Affinity: IP: *E*(M+) - *E*(M) and EA: *E*(M) - *E*(M-)

	Vacuum		Implicit solvent	
Name	**Energy (au)**	**Energy (eV)**	**Energy (au)**	**Energy (eV)**
CT1 (M)	-382,729575	-10414,454	-382,73807	-10414,686
CT1+ (M+)	-382,436772	-10406,487	-382,51904	-10408,726
CT6 (M)	-381,496338	-10380,897	-381,50938	-10381,252
CT6- (M-)	-381,579729	-10383,166	-381,67081	-10385,644
HQ1 (M)	-382,726222	-10414,363	-382,73715	-10414,661
HQ1+ (M+)	-382,44169	-10406,621	-382,52619	-10408,92
HQ6 (M)	-381,50809	-10381,217	-381,51782	-10381,481
HQ6- (M-)	-381,589889	-10383,442	-381,67426	-10385,738
RS1	-382,72921	-10414,445	-382,73966	-10414,729
RS1+ (M+)	-382,43280	-10406,379	-382,51674	-10408,663
RS6 (M)	-382,71126	-10413,956	-382,72448	-10414,316
RS6- (M-)	-382,73467	-10414,593	-382,82153	-10416,957

Vacuum	solvent
IP = E(+) - E	
7,967462433	5,95986206

Vacuum	solvent
EA = E - E(-)	
2,269152501	4,39264452

Vacuum	solvent
IP = E(+) - E	
7,742400252	5,74035093

Vacuum	solvent
EA = E - E(-)	
2,225832589	4,25680721

Vacuum	solvent
IP = E(+) - E	
8,065639721	6,06590333

Vacuum	solvent
EA = E - E(-)	
0,63700951	2,64069149