Supplementary Information:

Study of the BHT Oxidation Mechanism Coupling Theory and Experiment

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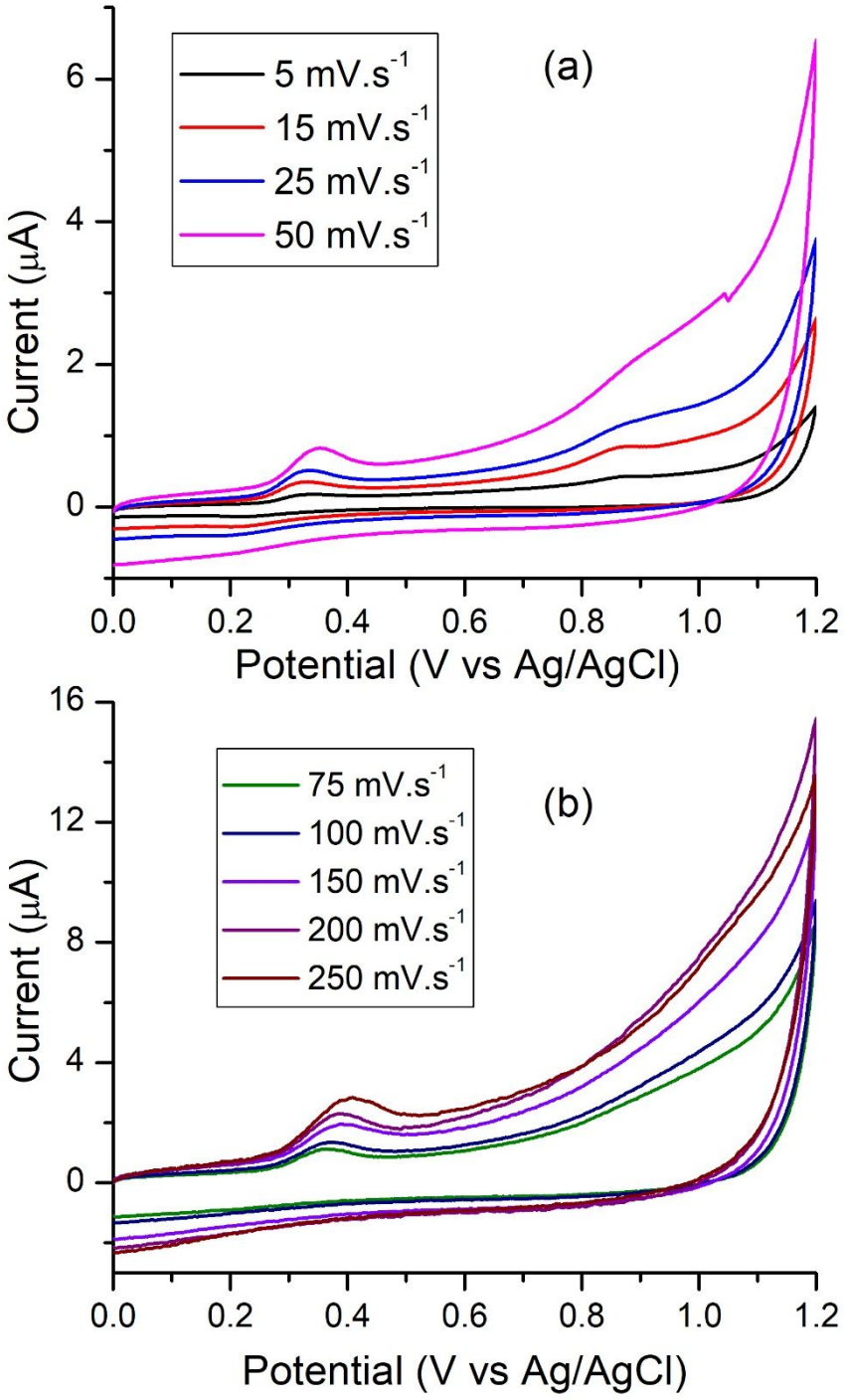

Figure S1. Voltammograms for BHT 33 μM in 10.0 ml of solution containing 20% ACN in Britton-Robinson buffer, pH = 5.54, at different scan rates.

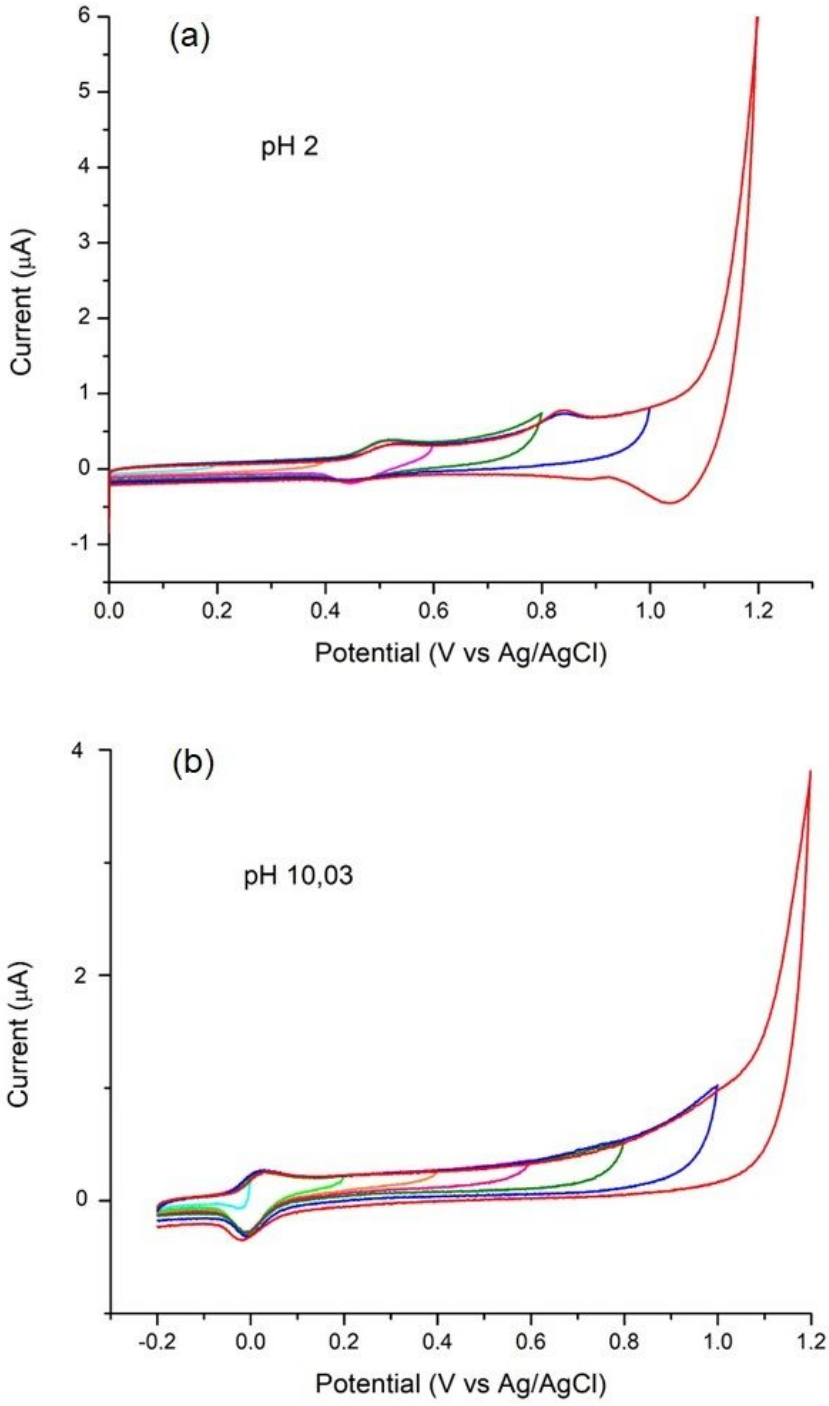

Figure S2. Voltammograms for BHT 33 μM in 10.0 ml of solution containing 20% ACN in Britton-Robinson buffer at pH 2 (a) and pH 10 (b) with different potential windows (0 to 0.6 V in pink line; 0 to 0.8 V in green line; 0 to 1.0 V in blue line; 0 to 1.2 V in red line). Scan rate of 10 mV/s.

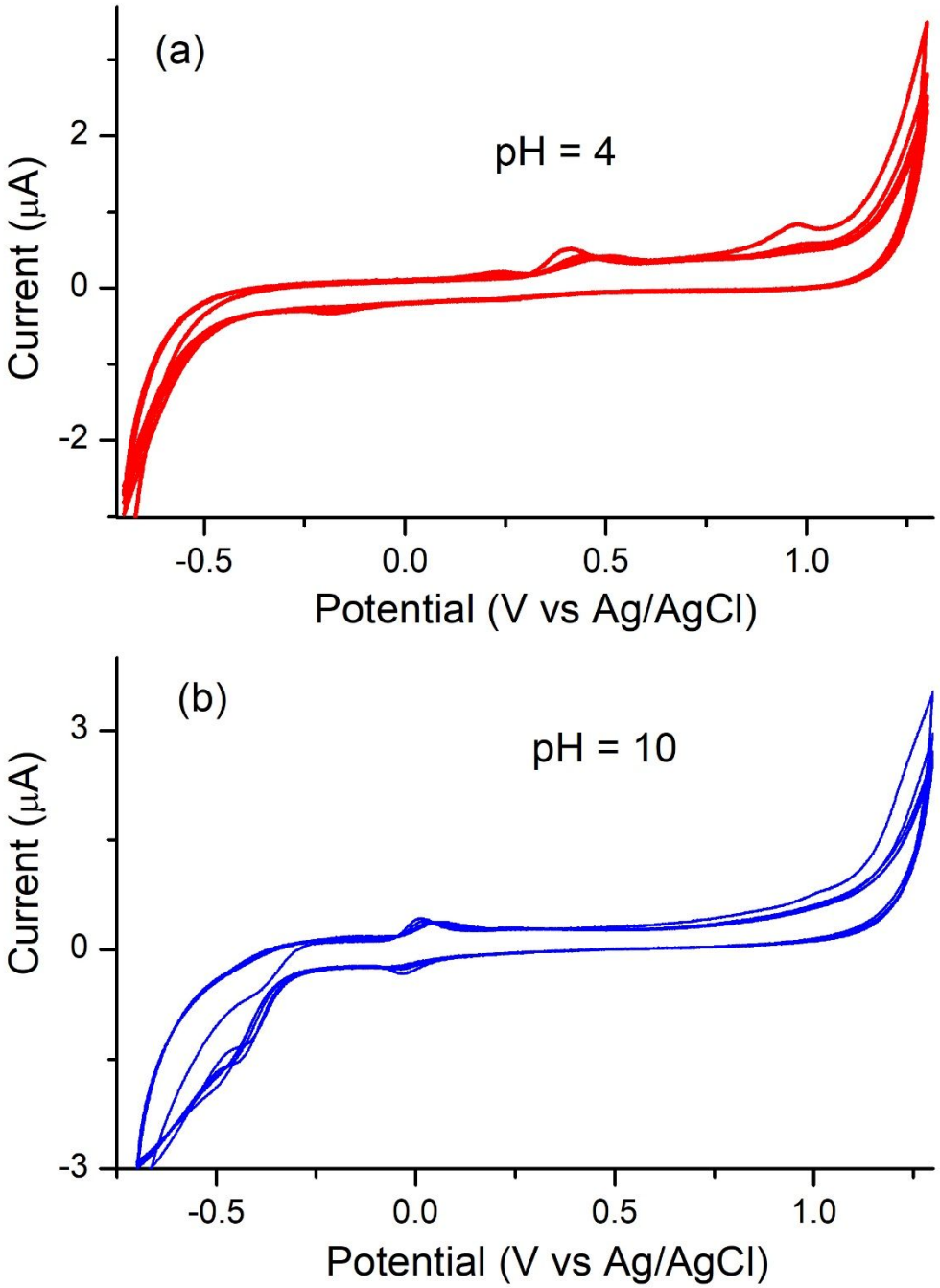

Figure S3. Voltammograms for BHT 33 μM in 10.0 ml of solution containing 20% ACN in Britton-Robinson buffer at different pH 4 (a) and 10 (b). It showed five consecutive scans. Scan rate of 10 mV/s.

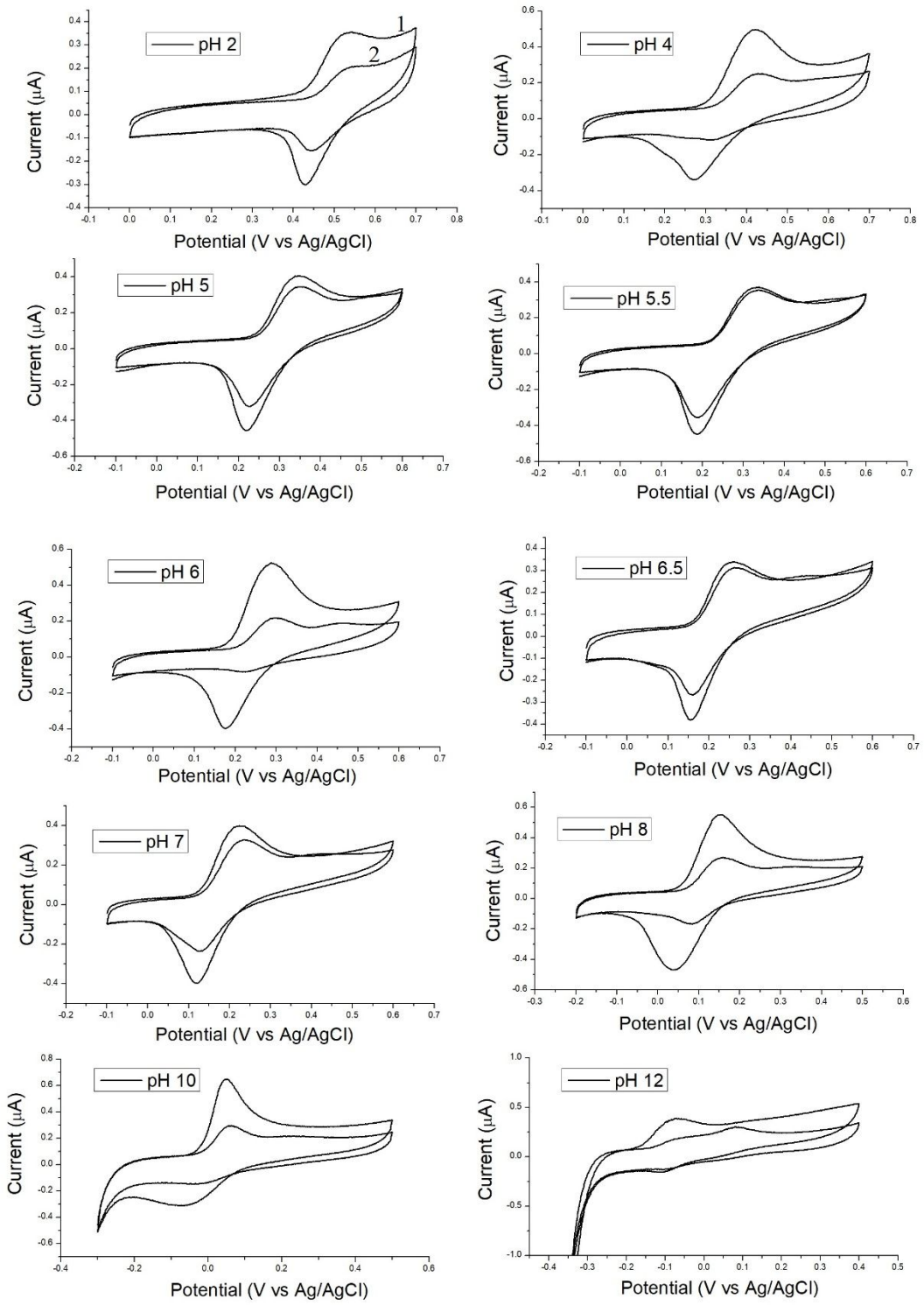

Figure S4. Cyclic voltammograms for BHT 33 μM in 10.0 ml of solution containing 20% ACN in Britton-Robinson buffer at different pH values (2-12). It showed two consecutive scans in the potential window assayed, marked with 1 and 2, respectively. Scan rate of 10 mV/s.

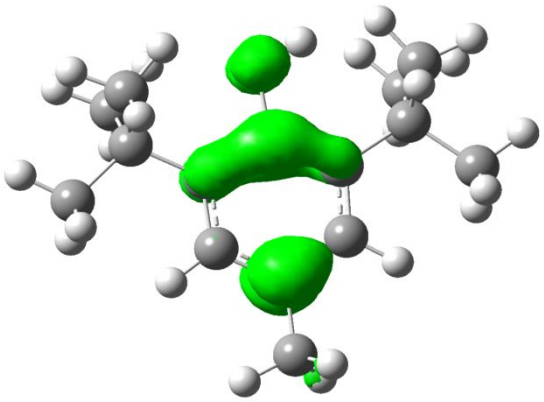

Figure S5. Spin density of **BHT**$^{\cdot+}$. Isovalue 0.02. Density 0.005.

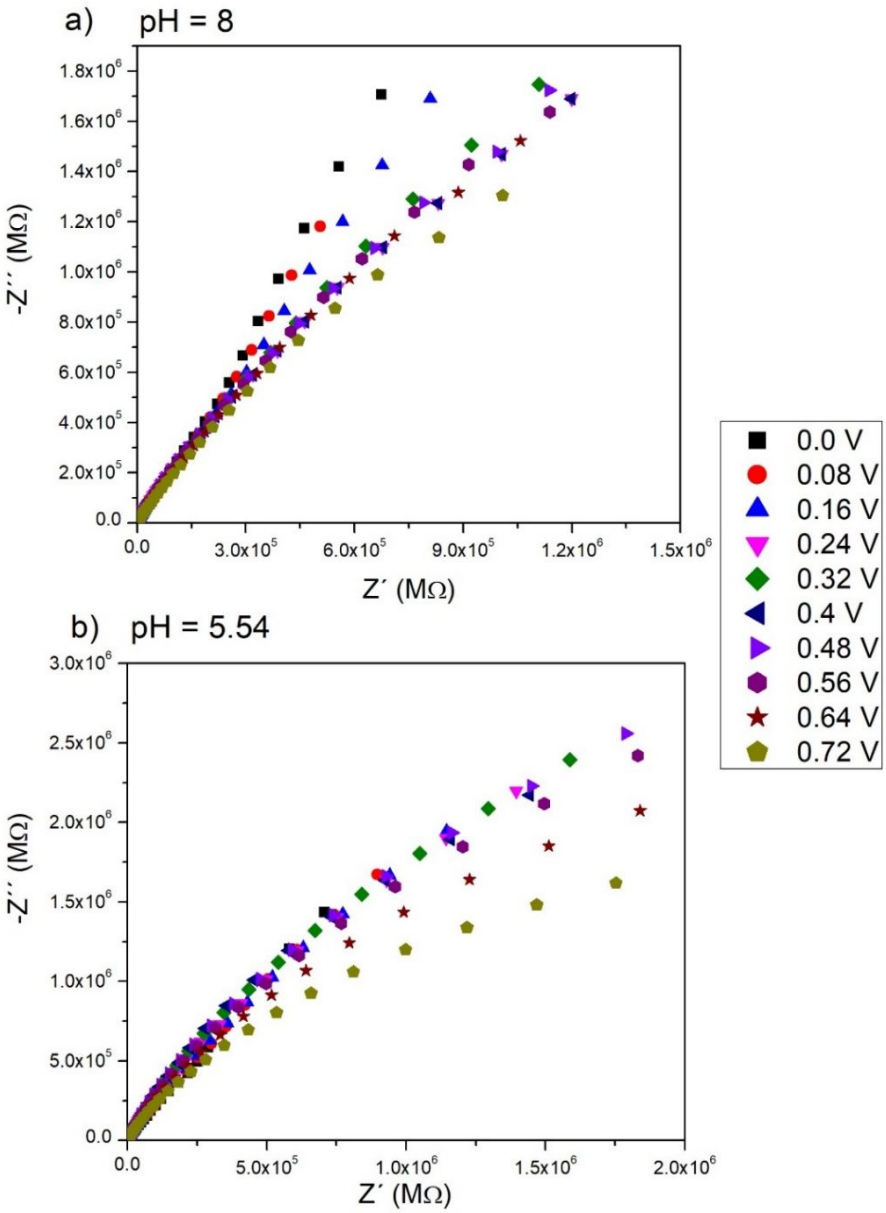

Figure S6. Impedance measurements for pH = 8 (a) and 5.54 (b) for different potential values.

Table S1. Impedance fitting results for pH 5.54.

pH	E/V	Parámetros		Error%
5.54	0.0	R_Ω/Ω	93.38	9.732
		$Y_0/\ \mu F.s^{1-\gamma}$	3.342	4.532
		γ	0.812	1.011
	0.08	R_Ω/Ω	96.63	9.138
		$Y_0/\ \mu F.s^{1-\gamma}$	2.839	4.374
		γ	0.828	0.956
	0.16	R_Ω/Ω	98.40	8.426
		$Y_0/\ \mu F.s^{1-\gamma}$	2.549	4.063
		γ	0.836	0.882
	0.24	R_Ω/Ω	92.15	10.45
		$Y_0/\ \mu F.s^{1-\gamma}$	2.435	4.479
		γ	0.815	0.967
	0.32	R_Ω/Ω	81.35	16.02
		$Y_0/\ \mu F.s^{1-\gamma}$	3.018	6.035
		γ	0.777	1.315
	0.4	R_Ω/Ω	86.80	10.47
		$Y_0/\ \mu F.s^{1-\gamma}$	3.518	4.967
		γ	0.809	1.102
	0.48	R_Ω/Ω	73.41	17.16
		$Y_0/\ \mu F.s^{1-\gamma}$	2.814	5.726
		γ	0.771	1.245
	0.56	R_Ω/Ω	82.56	9.933
		$Y_0/\ \mu F.s^{1-\gamma}$	4.59	4.793
		γ	0.797	1.104
	0.64	R_Ω/Ω	86.40	11.08
		$Y_0/\ \mu F.s^{1-\gamma}$	4.969	5.055
		γ	0.772	1.195
	0.72	R_Ω/Ω	78.05	11.70
		$Y_0/\ \mu F.s^{1-\gamma}$	6.532	5.485
		γ	0.760	1.323

Mean values for pH 5.5: R_Ω = 86.913 Y_0 = 3.6606 $\mu F.s^{1-\gamma}$ γ = 0.7977

Table S2. Impedance fitting results for pH 8.

pH	E/V	Parámetros		Error%
8	0.0	R_Ω/Ω	64.58	10.30
		$Y_0/\ \mu F.s^{1-\gamma}$	2.1250	3.176
		γ	0.803	0.680
	0.08	R_Ω/Ω	67.86	8.379
		$Y_0/\ \mu F.s^{1-\gamma}$	1.878	2.741
		γ	0.818	0.581
	0.16	R_Ω/Ω	69.67	6.797

		Y_0/ μF.s$^{1-\gamma}$	1.632	2.325
		γ	0.834	0.487
	0.24	R_Ω/Ω	74.80	4.968
		Y_0/ μF.s$^{1-\gamma}$	2.441	2.486
		γ	0.875	0.530
	0.32	R_Ω/Ω	65.35	12.13
		Y_0/ μF.s$^{1-\gamma}$	3.442	5.307
		γ	0.813	1.134
	0.4	R_Ω/Ω	63.25	13.42
		Y_0/ μF.s$^{1-\gamma}$	1.711	4.241
		γ	0.818	0.865
	0.48	R_Ω/Ω	69.60	10.81
		Y_0/ μF.s$^{1-\gamma}$	2.499	4.660
		γ	0.833	0.969
	0.56	R_Ω/Ω	64.14	14.40
		Y_0/ μF.s$^{1-\gamma}$	2.738	5.614
		γ	0.809	1.167
	0.64	R_Ω/Ω	63.51	9.063
		Y_0/ μF.s$^{1-\gamma}$	6.724	3.169
		γ	0.720	0.857
	0.72	R_Ω/Ω	55.52	12.91
		Y_0/ μF.s$^{1-\gamma}$	6.674	3.834
		γ	0.713	0.982

Mean values for pH 8: R_Ω = 65.828 Y_0 = 3.1864 μF.s$^{1-\gamma}$ γ = 0.8036

Equations for the electrochemical mechanism of BHT

$$\frac{\partial C_{BHT}}{\partial t} = D_{BHT}\frac{\partial {C_{BHT}}^2}{\partial^2 x} \quad \text{(S1)}$$

$$\frac{\partial C_{BHT^*}}{\partial t} = D_{BHT}\frac{\partial {C_{BHT^*}}^2}{\partial^2 x} - k_{f1}(C_{BHT^*})^2 + k_{b1}C_{dimer} \quad \text{(S2)}$$

$$\frac{\partial \Gamma_{BHT}}{\partial t} = v_{ads,BHT} - v_{des,BHT} - k_{ox,1}^{ads}\Gamma_{BHT} + k_{red,1}^{ads}\Gamma_{BHT^*} \quad \text{(S3)}$$

$$\frac{\partial \Gamma_{BHT^*}}{\partial t} = v_{ads,BHT^*} - v_{des,BHT^*} + k_{ox,1}^{ads}\Gamma_{BHT} - k_{red,1}^{ads}\Gamma_{BHT^*} - k_{ox,2}^{ads}\Gamma_{BHT^*} + k_{red,2}^{ads}\Gamma_{BHT^+} \quad \text{(S4)}$$

$$\frac{\partial \Gamma_{BHT^+}}{\partial t} = v_{ads,BHT^+} - v_{des,BHT^+} + k_{ox,2}^{ads}\Gamma_{BHT^*} - k_{red,2}^{ads}\Gamma_{BHT^+} - k_{f2,ads}\Gamma_{BHT^+} \quad \text{(S5)}$$

where

$$k_{ox,i}^{ads} = k_{i,ads}^{0} e^{(1-\alpha)(E_{act}-{E_i}^0)F/RT} \quad \text{(S6)}$$

$$k_{red,i}^{ads} = k_{i,ads}^{0} e^{-\alpha(E_{act}-{E_i}^0)F/RT} \quad \text{(S7)}$$

according to the Butler-Volmer approach.

Faradaic current:

$$I_f = I_{f1} + I_{f,ads1} + I_{f,ads2} \quad \text{(S8)}$$

$$I_{f1} = AFk_1^0[C_{BHT}e^{(1-\alpha)F(E_{act}-{E_1}^0)/RT} - C_{BHT^*}e^{-\alpha F(E_{act}-{E_1}^0)/RT}] \quad \text{(S9)}$$

$$I_{f,ads1} = AFk_{1,ads}^0\left[\Gamma_{BHT}e^{(1-\alpha)F(E_{act}-E_{1,ads}^0)/RT} - \Gamma_{BHT^*}e^{-\alpha F(E_{act}-E_{1,ads}^0)/RT}\right] \quad \text{(S10)}$$

$$I_{f,ads2} = AFk_{2,ads}^0\left[\Gamma_{BHT^*}e^{(1-\alpha)F(E_{act}-E_{2,ads}^0)/RT} - \Gamma_{BHT+}e^{-\alpha_j F(E_{act}-E_{2,ads}^0)/RT}\right] \quad \text{(S11)}$$

with boundary condition at the electrode surface:

$$D_{BHT}\left(\frac{\partial C_{BHT}}{\partial x}\right)_{x=0} = \frac{I_{f1}}{FA} + v_{ads,BHT} - v_{des,\mathrm{BHT}} \quad \text{(S12)}$$

$$D_{BHT}\left(\frac{\partial C_{BHT^*}}{\partial x}\right)_{x=0} = -\frac{I_{f1}}{FA} + v_{ads,BHT^*} - v_{des,BHT^*} \quad \text{(S13)}$$

Computational information

The main calculation information resulting from the structure optimization using the method DFT B3LYP/6-31+G(d,p)/SMD is summarized above**.** If more information is needed it can be requested to the corresponding author.

BHT

Imaginaries frequencies: 0
Electronic energy: -661.340495 Hartree
Z-matrix
0 1

C	-0.01023300	2.27960100	-0.01744100
C	-1.20901800	1.55879500	-0.00387100
C	-1.25135800	0.15813800	-0.00423500
C	-0.00684300	-0.52308500	-0.01610600
C	1.23523600	0.15812400	-0.01725600
C	1.18722200	1.56295700	-0.02585600
H	-2.13582000	2.12015800	0.00210600
H	2.11143000	2.12753000	-0.03536500
C	-2.60864700	-0.58959100	0.00392200
C	2.60408200	-0.57526000	0.00767400
O	-0.07127300	-1.90786100	-0.01244800
H	0.79573900	-2.28863600	-0.19851500
C	-0.01647100	3.79160700	0.00140300
H	-0.75480600	4.19860500	-0.69847100
H	-0.27029600	4.17865400	0.99670200
H	0.96451500	4.19516300	-0.26775100
C	2.79929400	-1.46199900	-1.25060100
H	2.09958400	-2.30012200	-1.34015400
H	2.70303000	-0.86228300	-2.16190300
H	3.80326600	-1.90004000	-1.23579400
C	2.75103800	-1.41968800	1.30051000
H	3.73393900	-1.90418900	1.31279900
H	2.68036100	-0.77650600	2.18447900
H	1.99886600	-2.20641400	1.40540000

C	3.78548100	0.42018300	0.00666700
H	3.77325300	1.07569500	0.88318600
H	4.72181200	-0.14669000	0.03097100
H	3.79895700	1.04394600	-0.89302700
C	-2.76455100	-1.45697400	-1.26975200
H	-2.71197700	-0.83362500	-2.17006800
H	-1.99714200	-2.22904200	-1.34315000
H	-3.74374000	-1.95043300	-1.26170600
C	-2.73995700	-1.47266800	1.26963900
H	-2.66877300	-0.86049600	2.17634900
H	-3.71954200	-1.96532900	1.27511800
H	-1.97250100	-2.24658400	1.31916400
C	-3.80238500	0.38993800	0.02189500
H	-4.73216600	-0.18871900	0.02904900
H	-3.80290300	1.02636400	0.91330000
H	-3.82222300	1.03540400	-0.86268000

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BHT$^{\cdot+}$

Imaginaries frequencies: 0
Electronic energy: -661.143179 Hartree
Z-matrix
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C	-0.01226200	2.26034600	-0.00984000
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C	-1.29360400	0.17940200	-0.00158000
C	-0.01313200	-0.51782300	-0.01932900
C	1.27209400	0.16384300	-0.01558200
C	1.21460600	1.53877300	-0.01703200
H	-2.14867300	2.14179400	0.01273400
H	2.12495600	2.12341800	-0.02015200
C	-2.63056900	-0.58131800	0.00638700
C	2.62366100	-0.58534800	0.00787200
O	-0.10232300	-1.83357100	-0.04110500
H	0.75785600	-2.28393200	-0.08160700
C	0.01857400	3.75008800	-0.01085600
H	-0.98382100	4.18118900	-0.01067200
H	0.56868300	4.11588900	0.86651700
H	0.56905200	4.11523200	-0.88808800
C	2.77810200	-1.52149000	-1.22202000
H	2.12311400	-2.39962500	-1.22339600
H	2.60163700	-0.97350800	-2.15277600
H	3.80196600	-1.90727400	-1.24017800
C	2.78012400	-1.38007400	1.33292300
H	3.76698400	-1.85379100	1.34530200
H	2.71226400	-0.70682100	2.19326700
H	2.03891600	-2.17350900	1.47121000
C	3.80233200	0.40962000	-0.05310400
H	3.81413100	1.08764800	0.80558600
H	4.73560000	-0.16041100	-0.03681900
H	3.79037900	1.00497200	-0.97176400
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H	-2.70525800	-0.81614600	-2.17276900
H	-2.01573400	-2.22559000	-1.34390800
H	-3.75759400	-1.92017600	-1.27168500

C	-2.73913100	-1.47365700	1.27099300
H	-2.65359700	-0.86861000	2.18015700
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C	-3.82398500	0.39571700	0.03320600
H	-4.74917500	-0.18816300	0.04080900
H	-3.82158800	1.02571500	0.92875800
H	-3.84718000	1.04293100	-0.84959400

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2 3 2.0 7 1.0
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BHT^{2+}

Imaginaries frequencies: 0
Electronic energy: -660.900426 Hartree
Z-matrix
2 1

C	-0.02533200	2.24709800	-0.01768000
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C	-1.34474900	0.19931500	0.00319800
C	-0.01031900	-0.51690600	-0.04439700
C	1.31392900	0.17138800	-0.01047000
C	1.23712900	1.52583900	-0.01125000
H	-2.17315600	2.16508400	0.03849600
H	2.13037000	2.13595800	-0.00804800
C	-2.65208200	-0.57397300	0.01874000
C	2.64925000	-0.58497300	0.01957400
O	-0.11440500	-1.77501100	-0.12136000
H	0.72529100	-2.28326700	-0.16140300
C	0.02439600	3.70131600	-0.03917900
H	-0.95255400	4.17682500	-0.10036900
H	0.56063700	4.03030100	0.87306500
H	0.69724200	4.03553700	-0.84677500
C	2.81143700	-1.49477300	-1.23132400
H	2.15323700	-2.37046900	-1.25689000
H	2.65339600	-0.92591500	-2.15182300
H	3.83359400	-1.88315000	-1.23322100
C	2.77278700	-1.41234000	1.33059100
H	3.76406600	-1.87460000	1.34495000
H	2.67965300	-0.76278100	2.20564200
H	2.03742800	-2.21735400	1.42397500
C	3.82434900	0.41365300	0.00104700
H	3.81740700	1.07289500	0.87437100
H	4.75513300	-0.15870300	0.02469500
H	3.82910100	1.02483300	-0.90698700
C	-2.79885400	-1.41497000	-1.28659500
H	-2.74106700	-0.77117800	-2.16945100
H	-2.04864600	-2.20144500	-1.37073700
H	-3.78788500	-1.88221800	-1.26610800
C	-2.71603600	-1.50555500	1.26680400
H	-2.60642200	-0.92564300	2.18822300
H	-3.70199700	-1.97956200	1.27438500
H	-1.95839600	-2.28940300	1.24785300
C	-3.85048200	0.39128700	0.08913900
H	-4.76706300	-0.20389900	0.10507900
H	-3.83229200	1.00281800	0.99693300
H	-3.89593800	1.05227800	-0.78216300

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2 3 2.0 7 1.0
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BHT·

Imaginaries frequencies: 0
Electronic energy: -660.711516 Hartree
Z-matrix
0 2
C 0.00002200 2.24998500 -0.01365800

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C	-1.27562000	0.15623100	-0.00190100
C	0.00110500	-0.58743600	0.00686000
C	1.27629300	0.15751100	-0.00245900
C	1.22005300	1.53896300	-0.01311900
H	-2.13433500	2.11900500	-0.01921700
H	2.13282700	2.12274000	-0.02172800
C	-2.61761200	-0.59669900	-0.00165800
C	2.61939400	-0.59300000	-0.00162400
O	0.00193700	-1.85241500	0.02079200
C	-0.00745400	3.75063100	0.01378100
H	-0.81664700	4.15619900	-0.60226600
H	-0.17545900	4.11109600	1.03850700
H	0.94482700	4.16425900	-0.32898400
C	2.73923300	-1.48407000	-1.26442700
H	1.96095300	-2.24768200	-1.30289600
H	2.67410200	-0.87704200	-2.17482400
H	3.71423100	-1.98503100	-1.26458900
C	2.74979500	-1.46155700	1.27572200
H	3.72523000	-1.96166000	1.27709200
H	2.69114300	-0.83870800	2.17581000
H	1.97254400	-2.22500700	1.33372000
C	3.81821500	0.37855200	-0.01507700
H	3.83460800	1.02648500	0.86789000
H	4.74467300	-0.20499000	-0.01456700
H	3.82644400	1.01206000	-0.90857600
C	-2.73560400	-1.48727200	-1.26491100
H	-2.67108500	-0.87966900	-2.17498100
H	-1.95611400	-2.24965700	-1.30359000
H	-3.70975200	-1.98989900	-1.26582800
C	-2.74720700	-1.46596700	1.27517300
H	-2.69034300	-0.84336300	2.17555400
H	-3.72162300	-1.96807100	1.27581900
H	-1.96853200	-2.22796000	1.33347000
C	-3.81778000	0.37312600	-0.01519900
H	-4.74348500	-0.21162200	-0.01526800
H	-3.83536700	1.02073800	0.86799200
H	-3.82648400	1.00696500	-0.90847400

1 2 1.5 6 1.5 12 1.0
2 3 2.0 7 1.0
3 4 1.0 9 1.0
4 5 1.0 11 2.0
5 6 2.0 10 1.0
6 8 1.0
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9 28 1.0 32 1.0 36 1.0

10 16 1.0 20 1.0 24 1.0
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12 13 1.0 14 1.0 15 1.0
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16 17 1.0 18 1.0 19 1.0
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20 21 1.0 22 1.0 23 1.0
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24 25 1.0 26 1.0 27 1.0
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28 29 1.0 30 1.0 31 1.0
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32 33 1.0 34 1.0 35 1.0
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36 37 1.0 38 1.0 39 1.0
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BHT^{+}

Imaginaries frequencies: 0
Electronic energy: -660.514451 Hartree
Z-matrix
1 1

C	0.00004500	2.22885800	-0.00907600
C	-1.24998700	1.53525200	-0.01509300
C	-1.32059000	0.17444600	0.00013000
C	0.00038000	-0.58380200	0.04819900
C	1.32136000	0.17550300	0.00038300
C	1.25010100	1.53668100	-0.01446200
H	-2.14527900	2.14316600	-0.03554800
H	2.14502700	2.14502300	-0.03481700
C	-2.63485600	-0.58984200	-0.01809700

C	2.63585500	-0.58775100	-0.01814700
O	0.00112500	-1.80076400	0.14023700
C	-0.00356800	3.70329000	0.02958000
H	-0.89046100	4.12408100	-0.45087400
H	-0.05817100	3.99254400	1.09507300
H	0.91697800	4.13234000	-0.37140300
C	2.68281900	-1.52570800	-1.25713500
H	1.90421700	-2.28890500	-1.22744100
H	2.57863700	-0.95144200	-2.18374500
H	3.65733700	-2.02430500	-1.27447200
C	2.78181100	-1.42146800	1.28669500
H	3.75810900	-1.91669000	1.26865400
H	2.74567600	-0.77292100	2.16821500
H	2.00795200	-2.18405400	1.37942000
C	3.84011500	0.36979600	-0.10204700
H	3.89476700	1.03689400	0.76437200
H	4.75713600	-0.22612000	-0.12180700
H	3.81751100	0.97860600	-1.01190300
C	-2.68149300	-1.52784500	-1.25692100
H	-2.57778400	-0.95359500	-2.18360900
H	-1.90236700	-2.29054400	-1.22736800
H	-3.65562200	-2.02722800	-1.27425200
C	-2.78039900	-1.42334200	1.28676400
H	-2.74479100	-0.77461200	2.16818900
H	-3.75626300	-1.91944700	1.26894700
H	-2.00596000	-2.18533600	1.37980100
C	-3.83953300	0.36717500	-0.10207800
H	-4.75635500	-0.22906900	-0.12168200
H	-3.89440400	1.03441800	0.76422500
H	-3.81724100	0.97586400	-1.01203100

1 2 1.5 6 1.5 12 1.0
2 3 2.0 7 1.0
3 4 1.0 9 1.0
4 5 1.0 11 2.0
5 6 2.0 10 1.0
6 8 1.0
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9 28 1.0 32 1.0 36 1.0
10 16 1.0 20 1.0 24 1.0
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36 37 1.0 38 1.0 39 1.0
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BHTQM

Imaginaries frequencies: 0
Electronic energy: -660.103357 Hartree
Z-matrix
0 1

C	0.00000000	2.31328400	-0.00000100
C	1.24518400	1.56719300	-0.00000200
C	1.29176300	0.20995300	0.00000200
C	0.00000000	-0.54072300	0.00002800
C	-1.29176300	0.20995300	0.00000000
C	-1.24518400	1.56719300	-0.00000200
H	2.15427400	2.15778400	-0.00000800
H	-2.15427400	2.15778300	-0.00000800
C	2.62757500	-0.55932600	0.00000800
C	-2.62757500	-0.55932600	-0.00000900
O	0.00000100	-1.78804700	-0.00001300
C	0.00000000	3.67039400	-0.00000300
H	0.92907000	4.23325700	-0.00000400
H	-0.92907000	4.23325600	-0.00000300
C	-2.74600200	-1.43866500	1.26980400
H	-1.96087800	-2.19449400	1.32276700
H	-2.69328200	-0.82182700	2.17450200
H	-3.71506900	-1.95117300	1.26997300
C	-2.74601300	-1.43861900	-1.26985400

H	-3.71507800	-1.95113200	-1.27002900
H	-2.69330900	-0.82174700	-2.17452900
H	-1.96088600	-2.19444100	-1.32285700
C	-3.83315700	0.40342000	0.00001200
H	-3.84922000	1.04444800	-0.88822400
H	-4.75624100	-0.18550800	0.00001000
H	-3.84920900	1.04442300	0.88826700
C	2.74598500	-1.43865800	1.26982800
H	2.69327000	-0.82181400	2.17452100
H	1.96084900	-2.19447500	1.32279400
H	3.71504400	-1.95118000	1.27000300
C	2.74602900	-1.43862600	-1.26983000
H	2.69332000	-0.82176100	-2.17451000
H	3.71510000	-1.95112700	-1.26999800
H	1.96091200	-2.19445800	-1.32283000
C	3.83315700	0.40342000	0.00004000
H	4.75624200	-0.18550900	0.00005000
H	3.84923100	1.04444500	-0.88819800
H	3.84920000	1.04442500	0.88829300

1 2 1.0 6 1.0 12 2.0
2 3 2.0 7 1.0
3 4 1.0 9 1.0
4 5 1.0 11 2.0
5 6 2.0 10 1.0
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9 27 1.0 31 1.0 35 1.0
10 15 1.0 19 1.0 23 1.0
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