Corrosion Inhibition of Carbon Steel by Anthraquinones Derivatives in 1.0 M HCl: Electrochemical and Quantum Calculations

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The effect of hydroxyl group number of some anthraquinone derivatives 1,2,4-trihydroxyanthraquinone (purpurin) and 1,4-dihydroxyanthraquinone (quinizarin) on their corrosion inhibition efficiency has been reported in order to establish a relationship between inhibitor efficiency and molecular structure. Experimental study is based on the potentiodynamic polarization curves and electrochemical impedance spectroscopy (EIS). On the other hand, the quantum chemistry calculations were performed using B3LYP/6-31G (d) method to determine the electronic and structural parameters of the studied anthraquinone derivatives. The results revealed that the compound containing supplementary group (OH) presents the highest inhibition efficiency (91.5 %) in the case of Purpurin, that value is less than that obtained for Quinizarin (89.0 %). The experimental study indicated that the inhibition efficiency depends on concentration and molecular structure of the investigated compounds. The obtained experimental and theoretical results agree well and confirm that Purpurin, possessing the most number of OH group, is the better inhibitor.

Keywords 1,2,4-trihydroxyanthraquinone, 1,4-dihydroxyanthraquinone, Corrosion inhibitor, EIS, Polarization curves, DFT

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