Application of Newly Quinoline-3-carbonitriles as Corrosion Inhibitors on Mild Steel in 1.0 M HCl: Electrochemical Measurements, HF and DFT/B3LYP Calculations

Nuha Wazzan^{1,*} and Saedah Al-mhyawi¹

¹King Abdulaziz University, Chemistry Department, Faculty of Science, P.O Box 42805 Jeddah 21589, Saudi Arabia

*E-Mail: nwazzan@kau.edu.sa

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In combined experimental and theoretical studies, two new derivatives of quinoline-3-carbonitrile were tested for their anti-corrosive properties for mild steel in a 1.0 M HCl medium. The studied compounds were 4-(4-nitrophenyl)-2-oxo-1,2,5,6-tetrahydrobenzo[*h*]quinoline-3-carbonitrile (NPQC) and 4-(furan-3-yl)-2-oxo-1,2,5,6-tetrahydrobenzo[*h*]quinoline-3-carbonitrile (FQC). The inhibition efficiencies were investigated using electrochemical techniques at different inhibitor's concentrations and temperatures. This study revealed that NPQC and FQC are good inhibitors, and the inhibition efficiency order was NPQC > FQC. The correlation between their molecular reactivity and inhibition efficiency was investigated by two methods (HF and DFT/B3LYP) with two basis sets (6-31+G(d) and 6-311++G(d,p)) in the gas phase and aqueous solution, applying the conductor polarizable continuum model of solvation. The quantum chemical parameters of the neutral and all possible protonated forms of the two inhibitors were evaluated. Very good correlations between the experimental and theoretical data were obtained. Modeling the inhibitor-Fe complexes of the neutral and protonated forms of the inhibitors predicts that N16 is the active site for the adsorption process for both inhibitors. The calculations of the energies of inhibitor-Fe complexes and the N16-Fe bond lengths justify the superior inhibition efficiency of NPQC compared to that of FQC.

Keywords: Anti-corrosive; mild steel; Quinoline-3-carbonitriles; DFT/B3LYP calculations; Quantum chemical parameters.

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