Electrochemical and Quantum Chemical Assessment of Some Thiosemicarbazide Derivatives as Carbon Steel Corrosion Inhibitors in HCl; Continuously Monitoring the Current Change by FFT Voltammetry

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In this study, Firstly, two synthesized thiosemicarbazide derivatives, N-(2-(2-methoxyphenyl)hydrazinecarbonothioyl)benzamide (TSC4) and N-(2-(furan-2-carbonyl)hydrazinecarbonothioyl)benzamide (TSC5), were investigated as carbon steel corrosion inhibitors in 1.0 M HCl by potentiodynamic polarization (PDP), electrochemical impedance spectroscopy (EIS), fast Fourier transform continuous cyclic voltammetry (FFTCCV) and scanning electron microscopy (SEM). PDP results showed the mixed-type inhibition with predominantly anodic effect. EIS experiments showed the increase in polarization resistance and decrease in double layer capacitance by inhibitors adsorption. The maximum IE% values for the solutions containing 1.0×10^{-3} M TSC4 and TSC5 were equal to 94.0% and 94.9%, respectively. FFTCCV results indicated that in addition to inhibition efficiencies, the rate of adsorption for TSC5 is higher than TSC4. In the next step, quantum chemical studies were performed for a five member group of thiosemicarbazide derivatives and revealed that among the calculated electronic parameters, ΔE , the energy gap between HOMO and LUMO, exhibited the maximum correlation ($R^2=0.97$) with %IE. SEM analysis showed improvements of the surface characteristics in the presence of studied inhibitors.

Keywords: Corrosion inhibition; Carbon steel; Quantum chemical calculations, FFT Voltammetry

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