Corrosion Inhibition Behavior of 9-Hydroxyrisperidone as a Green Corrosion Inhibitor for Mild Steel in Hydrochloric Acid: Electrochemical, DFT and MD Simulations Studies

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A green corrosion inhibitor namely, 9-Hydroxyrisperidone (HRD) was investigated for their influence on mild steel corrosion in 1 M HCl using weight loss, Tafel polarization, electrochemical impedance spectroscopy (EIS) and surface morphology techniques. Quantum chemical calculations were also conducted to corroborate experimental findings. The tested compound is mixed type inhibitor following Langmuir adsorption isotherm and involved competitive physisorption and chemisorption mechanisms. The results from electrochemical impedance spectroscopy tests reveal an increase in polarization resistance. Scanning Electron Microscopy (SEM) analyses of steel surfaces in acid-inhibitor solutions showed that tested compound protects mild steel surface effectively. The inhibition property was further elucidated by theoretical approaches; quantum chemical calculation and Molecular Dynamic (MD) simulation.

Keywords: Inhibition, Corrosion, 9-Hydroxyrisperidone, Steel, DFT, Molecular Dynamic.

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