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Inhibitive effect of Clopidogrel as a green corrosion inhibitor for mild steel; statistical modeling and quantum Monte Carlo simulation studies

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Abstract

In this work, response surface method (RSM) is employed to design electrochemical experiments for assessment of a green organic molecule, namely Clopidogrel from cardiovascular drugs class, as a corrosion inhibitor for mild steel in sulfuric acid solution. Mathematical models based on multiple regressions are generated to estimate the influence of the affecting factors like acid concentration, solution temperature and inhibitor concentration on the inhibitive performance of Clopidogrel. The corrosion rates are measured experimentally using potentiodynamic polarization technique. The calculated Langmuir adsorption energy reveals that Clopidogrel adsorbs both physically and chemically onto the mild steel surface and the adsorption type is almost independent of the environmental factors. The adsorption mechanism of Clopidogrel is computed through quantum chemical calculations, confirming that this compound can replace water molecules from the surface upon its adsorption to the metal substrate. The simulation

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