

Effectiveness of Some Novel Heterocyclic Compounds as Corrosion Inhibitors for Carbon Steel

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Abstract

The importance of this work is to introduce new heterocyclic compounds as effective and low-cost corrosion inhibitors. Corrosion of carbon steel is a major problem that destroys the aids of industries and world steel installations; the importance of this work is to introduce new heterocyclic compounds as effective and low-cost corrosion inhibitors. 5-amino-N'-((2-methoxynaphthalen-1-yl)methylene) is one of three carbohydrazide derivatives. 2,4-diamino-N'-((2-methoxy-naphthalene-1-yl)methylene), isoxazole-4-carbohydrazide (H₄) N'-((2-methoxynaphthalen-1-yl)methylene) and pyrimidine-5-carbohydrazide (H₅) The corrosion efficacy of -7,7-dimethyl-2,5-dioxo-4a,5,6,7,8,8a-hexahydro-2H-chromene-3-carbohydrazide (H₆) was investigated. Electrochemical Impedance Spectroscopy (EIS), Potentio Dynamic Polarisation (PDP), Weight Loss measurements (WL), surface morphology analyses by atomic force microscopy (AFM), quantum chemical computations based on density functional theory (DFT), and Molecular Dynamics (MD) simulation were used to detect this corrosion efficacy.

Keywords: *Heterocyclic compound; Corrosion; Polarisation*

Introduction

Carbon steel is used in a variety of applications, including factory structures and petroleum pipelines. These structures may come into contact with a variety of solvents, which might influence their consistency and durability through aggressive action, leading to carbon steel corrosion and disintegration, especially in acidic environments. Because it can be adsorbed on the metal surface through these heteroatoms, heterocyclic organic molecules with numerous bonds and heteroatoms, such as O, N, or S, are good corrosion inhibitors. 2 The adsorption of these chemicals on metal surfaces limits active sites and slows corrosion. Because of the presence of particular functional groups, aromaticity, electronic density, type of corrosive solution, and the structure of the inhibitor, the efficiency of the inhibitor is determined by its physical and chemical properties. Organic corrosion inhibitors are a profitable area of science due to their widespread use in a variety of industries. The most important benefit of corrosion inhibition is the reduction of dangers associated with decreased metal thickness in tanks and pipes, which can lead to material leakage and serious consequences such as fires and explosions. Many studies have shown that heterocyclic chemicals like hydrazide derivatives have a higher inhibitory effect on carbon steel in acidic environments. 10 Hydrazide derivatives have a wide range of uses in medicine and engineering. The anticancer, antibacterial, anti-

inflammatory, analgesic, and antioxidant properties of hydrazides derivatives have been determine. The goal of this study is to see how efficient three newly synthesized hydrazide derivatives are as carbon steel corrosion inhibitors by adding various electron donating atoms like N and O atoms or donating groups like (CH₃) and (OH) to these compounds. The examined compounds have a similar structure in the hydrazide nucleus, but differ in the substituents that alter the inhibitory properties of the compounds. Quantum chemical computations and Monte Carlo simulations were used to further determine the corrosion inhibition of the examined chemicals- (0.0001 g) of each inhibitor was diluted in 3 ml DiMethyl Formamide (DMF), then added to a 100 ml stock solution of 100% ethyl alcohol (99.5%). The stock was then utilized to make the appropriate concentrations. All concentrations less than 1 10⁶ did not provide significant inhibition efficiency; on the other hand, when the inhibitor concentration was raised above 20 10⁶, the inhibition efficiencies did not increase. The corrosion rates of carbon steel were determined using weight loss tests for (H₄ & H₅ & H₆) compounds at 25°C, shows a change in WL in the absence and presence of progressive H₄ concentrations shows the () and inhibition efficacy (percentage of IE). as hydrazide derivative concentrations rise, the percent IE rises, indicating that more hydrazide derivative molecules were adsorbed on the surface, increasing surface coverage. The percentage of inhibition for carbon steel corrosion rises with increasing (H₄ & H₅ & H₆) concentrations, and the percentage of inhibition likewise rises with increasing temperatures, according to the results of all trials. The Temkin isotherm is responsible for the adsorption of chemical molecules on the carbon steel surface. The results of Tafel polarisation show that (H₄ & H₅ & H₆) is a mixed type inhibitor. The inhibition efficiency measured using various approaches are in good agreement. The foundation of a protective layer of (H₄ & H₅ & H₆) on the carbon steel surface was confirmed by FT-IR and XPS analysis. The researched compounds with an inhibition efficacy of greater than 90% are the best inhibitors for any industrial use as carbon steel corrosion inhibitors.