



Experimental and theoretical study on performance of hydrazones as corrosion inhibitors for carbon steel in an acidic media

A thesis submitted to
Chemistry Department
Faculty of Science
Alexandria University

In fulfillment of the requirements for the
Master's degree of Science in Chemistry
2024

Presented by
Hagar Ali Mohamed Ali Abdel Hafez
B.Sc. in Chemistry (2016)
Faculty of Science - Alexandria University

Alexandria University
Faculty of Science
Chemistry Department

Research paper

Article title:

An Exploratory Experimental Analysis Backed by Quantum Mechanical Modeling, Spectroscopic, and Surface Study for C-Steel Surface in the Presence of Hydrazone-Based Schiff Bases to Fix Corrosion Defects in Acidic Media.

Authors: Amira H. E. Moustafa,* Hanaa H. Abdel-Rahman, Assem Barakat, Hagar A. Mohamed, and Ahmed S. El-Kholany

Journal title: American chemical society (ACS Omega)

Journal volume: 9

Article number: <https://doi.org/10.1021/acsomega.4c00199>

Year of publication: 2024

Publisher: American chemical society

Summary

This work focuses on developing corrosion control and protecting the environment by creating affordable, sustainable, environmentally friendly, and efficient corrosion resistance chemicals. That is, through synthesized three hydrazone Schiff bases E-2-(1-hydrazonoethyl)-thiazole (HTZ), 2-((E)-(((Z)-1-(thiazol-2-yl)ethylidene)hydrazono)-methyl)phenol (HTZS), and 2-((E)-(((Z)-1-(pyridin-2-yl)ethylidene)-hydrazono)methyl)phenol (HPYS) and corrosion inhibitors for C-steel in 8 M H_3PO_4 solution that were studied. The chemicals were analyzed by using ^1H NMR and ^{13}C NMR spectroscopy to learn more about them. Predominantly, the hydrazone-based Schiff bases have been considered powerful inhibitors due to their ability to be adsorbed with very low concentrations through their reactive sites (N, O, and S). Maximum surface (θ_{max}) coverage and inhibition efficiency of 83.33% were sufficiently found at 99.00×10^{-3} mol/L concentration of HTZS at 293 K. Galvanostatic experiments demonstrated that raising the concentration of hydrazones improved mass transfer resistance. To study microstructure, scanning, reflectance, and energy-dispersive X-rays were used. Roughness and qualitative adhesion of the adsorbed layer were estimated by an atomic force microscope. After adding 99.00×10^{-3} mol/L of HTZS, the degree of surface brightness and reflectance increases to 137.20, relative to the corroded electrolyte-free solution 27.70. The roughness (R_a) decreased from 0.468 to 0.088 μm by adding HTZS. A surface morphology study confirmed that adding hydrazones to the C-steel dissolution bath greatly improves the surface's look and texture quality. The atomic absorption

spectroscopy technique was used to compare the concentration of the iron ions that remained in the solution after galvanostatic analysis in the absence and presence of the hydrazones under different conditions; it was found that the inhibited solution contained lower concentrations of iron ions as compared to the uninhibited solution. The DFT theoretical analysis verified the observation of hydrazone physical adsorption through bonding electrons that obey kinetic adsorption isotherms. It is based on examining the highest occupied molecular orbital–lowest occupied molecular orbital (HOMO–LUMO), the Fukui functions, and the Mulliken atomic charge. Overall, the results suggest that HTZS is a good corrosion inhibitor with a large surface area due to the presence of S, N, and O atoms, allowing for creating a larger surface due to the large molecular volume of atoms protecting against the corrosion process.