A synthetic coumarin–thiosemicarbazone hybrid as a high-efficiency copper corrosion inhibitor: Adsorption mechanisms and molecular-level insights

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Alwi, Muhammad Ammar Mohamad [a, b]; Ahmad, Mohammad Norazmi [a, c]; Piah, Bijarimi Mat [d]; Pauzi, Hariy [e]; Normaya, Erna [a, c]

[a] Experimental and Theoretical Research Lab, Department of Chemistry, Kulliyyah of Science, International Islamic University of Malaysia, Pahang, Kuantan, 25200, Malaysia

Abstract

A coumarin–thiosemicarbazone (CT) hybrid was synthesized and characterized via FTIR, ^{1}H NMR, and ^{13}C NMR spectroscopy. The compound was obtained via Schiff base condensation of 3-acetyl coumarin and thiosemicarbazide in refluxing ethanol with glacial acetic acid as catalyst. The corrosion inhibition efficiency of CT on copper in hydrochloric acid was optimized using response surface methodology (RSM), achieving 97.15 % under optimal conditions (40.10 °C, 3.10 M HCl, 0.51 mM CT, 15.76 h immersion time). Adsorption studies revealed that CT undergoes spontaneous chemisorption, supported by Langmuir isotherm fitting and a negative Gibbs free energy (ΔG°_ads = −39.95 kJ mol^{-1}). SEM and XPS analyses confirmed the formation of a protective CT film as well as Cu–N/Cu–S interactions. Electrochemical impedance spectroscopy (EIS) and polarization studies

showed increased charge transfer resistance and reduced corrosion current density. Quantum chemical calculations revealed that CT possesses a narrow HOMO–LUMO gap (2.676 eV), high softness (0.748 eV^{-1}), and high electrophilicity (ω = 20.70 eV), indicating strong surface reactivity. Fukui function and XPS analysis showed that nitrogen and sulfur atoms were key adsorption sites. Molecular dynamics simulations supported its adsorption stability, with an interaction energy of −265 kJ/mol. This study demonstrates that CT is a highly efficient, surface-active inhibitor and offers molecular-level insights into its protection mechanism for copper in acidic environments. © 2025

Author keywords

Corrosion resistance; Coumarin; DFT; Electrochemical; RSM optimization; Thiosemicarbazone; XPS

Indexed keywords

Engineering controlled terms

Charge transfer; Chlorine compounds; Copper; Copper compounds; Corrosion inhibitors; Corrosion protection; Electrochemical corrosion; Fourier transform infrared spectroscopy; Gas adsorption; Hydrochloric acid; Molecular dynamics; Nuclear magnetic resonance spectroscopy; Quantum chemistry

Engineering uncontrolled terms

Coumarin; DFT; Electrochemicals; Higher efficiency; Molecular-level insights; Optimisations; Response surface methodology optimization; Response-surface methodology; Thiosemicarbazones; XPS analysis

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Corresponding authors

Corresponding author	E. Normaya
Affiliation	Experimental and Theoretical Research Lab, Department of Chemistry, Kulliyyah of Science, International Islamic University of Malaysia, Pahang, Kuantan, 25200, Malaysia
Email address	ernanormaya@iium.edu.my

Abstract

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