Structural elucidation of a novel dual-substituted thiosemicarbazone scaffold as an efficient copper corrosion inhibitor: Insights from RSM, XPS, and DFT–Fukui analyses

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Abstract

Copper corrosion in acidic environments poses significant challenges in industrial systems, yet limited research has explored dual substitution within thiosemicarbazone scaffolds to enhance adsorption behavior and establish structure–reactivity correlations. This study reports the structural elucidation and inhibition performance of a newly designed dual-substituted thiosemicarbazone inhibitor, pyrazinyl–thiosemicarbazone–aminophenyl (PZTAP), developed for efficient copper protection in hydrochloric acid. The molecule integrates a pyrazinyl ring at N(1) and a 2-aminophenyl group at N(4), forming a conjugated donor–acceptor system that strengthens surface interac

inhibition was evaluated using gravimetric and electrochemical impedance spectroscopy (EIS), with optimization via response surface methodology (RSM). Under optimal conditions (40.95 °C, 2.65 M HCl, 0.63 mM, 12.55 h), PZTAP achieved inhibition efficiencies of 93.78 % (weight loss) and 94.32 % (EIS), with strong agreement between predicted and experimental models (R^2 > 0.99, CV < 2 %). Langmuir isotherm fitting revealed a spontaneous chemisorption mechanism ($\Delta G°ads$ = −40.83 kJ mol^{-1}), supported by Cu–N and Cu–S bonding identified by X-ray photoelectron spectroscopy. Scanning electron microscopy confirmed the formation of a protective surface film. Theoretical results showed a favorable HOMO–LUMO gap (4.04 eV), high HOMO energy (−6.33 eV), and notable global softness (0.4957 eV^{-1}), correlating with efficient electron donation to copper. Molecular electrostatic potential (MEP) and Fukui function analyses identified C = S and C = N groups as dominant nucleophilic adsorption centers. This integrated experimental–theoretical investigation demonstrates that dual substitution significantly enhances donor–acceptor interactions and adsorption strength, establishing PZTAP as a high-efficiency, structure-guided corrosion inhibitor for copper in acidic media. © 2025

Author keywords

Copper corrosion inhibition; density functional theory (DFT–Fukui analysis); Dual-substituted thiosemicarbazone scaffold; Response surface methodology (RSM); Structural elucidation; X-ray photoelectron spectroscopy (XPS)

Indexed keywords

Engineering controlled terms

Adsorption isotherms; Chemisorption; Chlorine compounds; Copper; Corrosion inhibitors; Corrosion protection; Electrochemical corrosion; Hydrochloric acid; Industrial research; Molecules; Scaffolds; Surface properties

Engineering uncontrolled terms

Copper corrosion inhibitions; Density functional theory (DFT–fukui analyze); Density-functional-theory; Dual-substituted thiosemicarbazone scaffold; Response surface methodology; Response-surface methodology; Structural elucidation; Thiosemicarbazones; X-ray photoelectron spectroscopy; X-ray photoelectrons

Engineering main heading

Copper corrosion; Density functional theory; X ray photoelectron spectroscopy

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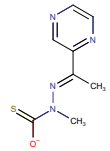
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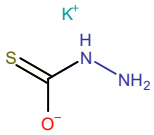
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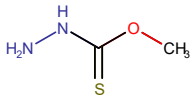
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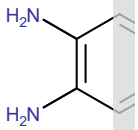
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