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

By

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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 interactions. Corrosion inhibition was evaluated using gravimetric and electrochemical impedance spectroscopy (EIS), with optimization via response surface methodology (RSM). Under optimal conditions (40.95 degrees 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 ($\Delta G_{ads} = -40.83 \text{ kJ mol}^{-1}$), 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.

Keywords

Author Keywords: [Dual-substituted thiosemicarbazone scaffold](#); [Copper corrosion inhibition](#); [Structural elucidation](#); [Response surface methodology \(RSM\)](#); [X-ray photoelectron spectroscopy \(XPS\)](#); [density functional theory \(DFT-Fukui analysis\)](#)

Keywords Plus: [MILD-STEEL](#); [PERFORMANCE](#)

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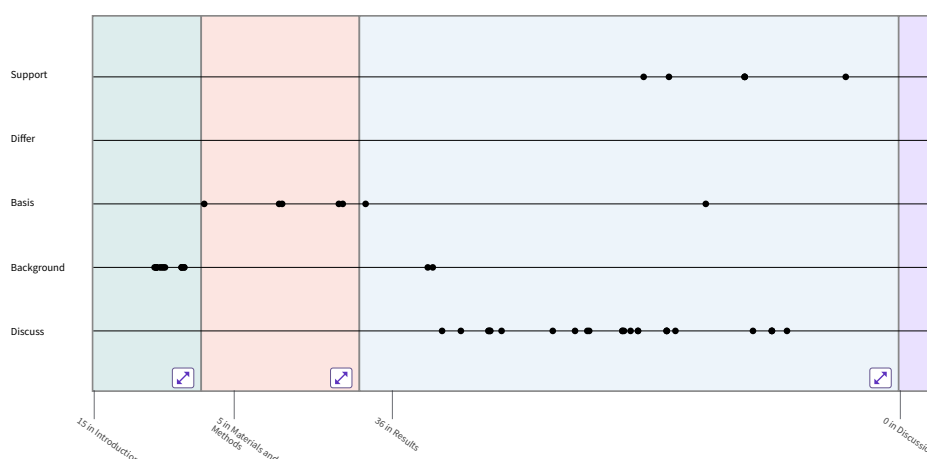
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