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Synthesis, characterization, and evaluation of corrosion inhibition efficiency of 5-((pyridin-3-yloxy) methyl)-1,3,4-oxadiazole-2-thiol (PODT) for Mild Steel in 1 n HCL

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Abstract
A novel heterocyclic compound, 5-((pyridin-3-yloxy) methyl)-1,3,4-oxadiazole-2-thiol (PODT), was synthesized and evaluated as a corrosion inhibitor for mild steel in 1 N HCl. The synthesized compound was characterized by FT-IR, ^1H NMR, elemental analysis, and melting-point determination. Corrosion inhibition performance was assessed using weight-loss and potentiodynamic polarization techniques at different concentrations (100–500 ppm, 300-500 ppm respectively) and temperatures (30–65 °C). The inhibition efficiency increased with concentration, reaching 96.37 % at 500 ppm and 30 °C by weight-loss and 98.1 % by electrochemical analysis. The negative shift in corrosion potential and simultaneous decrease in corrosion current density indicated mixed-type inhibition behavior. The superior performance of PODT is attributed to its multiple donor sites (N, O, S) and π-electron systems that favor adsorption and stable protective film formation on the metal surface. These findings suggest that PODT is an efficient and environmentally promising corrosion inhibitor for industrial applications.

Keywords: Heterocyclic compound, inhibition efficiency, mixed-type inhibition

Introduction

Corrosion of mild steel in acidic environments is a persistent challenge in industrial systems such as acid pickling, descaling, and petroleum refining. The use of organic inhibitors is one of the most effective and economical methods to mitigate this issue. Organic compounds containing heteroatoms (N, O, S) and π-electron systems can adsorb onto metallic surfaces, forming a protective layer that blocks corrosion reactions [1-6].

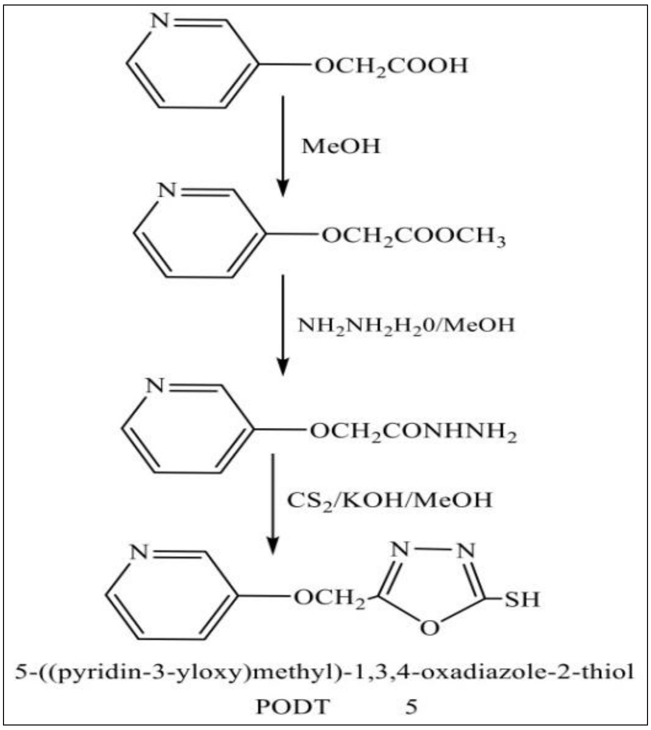
Recent research has focused on designing heterocyclic inhibitors with donor atoms and conjugated systems capable of strong adsorption through chemisorption or physisorption. Among them, oxadiazole-based compounds have received significant attention because of their structural flexibility, aromaticity, and ability to form coordinate bonds with Fe atoms on steel surfaces [7]. The presence of thione (–C=S), hydroxyl, and pyridinyl groups enhances electron density, promoting efficient surface coverage and film stability even at elevated temperatures. These synthesized organic compounds are not only act as a corrosion inhibitor but also useful in other fields like medicine, agriculture, water remediation etc [7-14].

The present work reports the synthesis and evaluation of a new oxadiazole derivative—5-((pyridin-3-yloxy) methyl)-1,3,4-oxadiazole-2-thiol (PODT) as a corrosion inhibitor for mild steel in 1 N HCl. Its inhibition efficiency was investigated through gravimetric and electrochemical technique. The effect of concentration and temperature on inhibition behavior, was analyzed. The study aims to establish the structure–activity correlation of PODT and its potential for sustainable corrosion-control formulations.

Materials and Methods

1. Synthesis of PODT

A mixture of 2-(pyridin-3-yloxy) acetohydrazide (0.1 M), carbon disulfide (7.6 mL, 0.1 M), and potassium hydroxide (5.0 g, 0.1 M) in methanol (50 mL) was refluxed for 6 h (Scheme 1). After solvent removal, the residue was poured into water and acidified slightly with dilute HCl. The solid product was filtered, washed, and recrystallized to obtain PODT (yield 67 %; m.p. 180 °C).



Scheme 1: Synthesis of PODT

2. Characterization of PODT

Chemical formula	M.P.	Molecular Mass	Elemental Analysis Observed (Calculated)
$C_8H_7N_3O_2S$	180 0C	209.22	C= 45.83(45.93); H=3.34 (3.37), N=20.00(20.08); O= 15.21(15.29); S, = 15.31(15.32)

Characteristics I.R. bands (KBr disc):3300cm^{-1}, 3145 cm-1, 2999cm^{-1}, 2830 cm^{-1}, 2725 cm^{-1} (CHstr.), 1679cm^{-1}, 1666 cm^{-1},1610cm^{-1} (C=C, C=N str.)1261 cm^{-1}, 1200cm^{-1}, 1210cm^{-1}, 970cm^{-1}, 729 cm^{-1}.

H^1 NMR: (300 MHz, DMSOd6, TMS, delta, ppm**):**11.5 (SH), 8.01, 7.99, 7.75(Pyridine ring), 5.32 (O-CH2)

3. Corrosion Studies
Mild steel specimens were polished, cleaned, and immersed in 1 N HCl solutions containing varying concentrations of PODT (100–500 ppm). Weight-loss measurements were performed at 30, 40, 50 and 65 °C for 3 h immersion. Electrochemical test PDP were carried out using a three-electrode system: mild steel working electrode, saturated calomel reference, and platinum counter electrode. Polarization curves were recorded from −250 mV to +250 mV vs E_corr at 1 mV s^{-1}.

Results and Discussion
1. Weight-Loss Studies
Table 1 presents the corrosion parameters of mild steel in 1 N HCl with PODT at different concentrations and temperatures. The inhibition efficiency (I.E.) increased with inhibitor concentration and decreased with temperature rise, suggesting predominant physical adsorption.

At 30 °C, PODT achieved 96.37 % I.E. at 500 ppm and 86.61 % at 100 ppm. The corrosion rate decreased drastically from 31.37 mmpy for the blank to 1.13 mmpy at 500 ppm. Even at 65 °C, PODT maintained > 90 % efficiency at high concentration, demonstrating good thermal stability (Fig. 1).

Table 1: Corrosion parameters for mild steel in 1 N HCl with PODT at various temperatures (Immersion = 3 h)

Concentration of Inhibitors (ppm)	Weight Loss (mg)	I.E. (%)	Corrosion Rate (mmpy)
BLANK (1N HCl)	169.45	---	31.37
Compound PODT			
500	6.15	96.37	1.13
400	9.69	94.28	1.79
300	13.59	91.97	2.51
200	17.68	89.56	3.27
100	22.68	86.61	4.19
Corrosion parameters from weight loss studies at 40°C			
BLANK (1N HCl)	172.12	---	31.86
500	8.68	94.95	1.60
400	12.67	92.63	2.34
300	16.78	90.25	3.10
200	21.03	87.78	3.89
100	26.22	84.76	4.85
Corrosion parameters from weight loss studies at 50°C			
BLANK (1N HCl)	174.98	---	32.89
500	12.98	92.58	2.40
400	17.79	89.83	3.29
300	21.97	87.44	4.06
200	25.98	85.15	4.81
100	31.83	81.80	5.89
Corrosion parameters from weight loss studies at 65°C			
BLANK (1N HCl)	178.13	---	32.90
500	15.44	91.33	2.85
400	21.83	87.74	4.04
300	27.01	84.83	5.00
200	33.41	81.24	6.18
100	37.09	79.17	6.86

Fig 1: Variation of inhibition efficiency with temperature for PODT in 1 N HCl

2. Potentiodynamic Polarization
The corrosion current density (Icorr) decreases significantly from 1.2×10^{-3} to 2.3×10^{-5} A/cm², demonstrating strong suppression of corrosion processes. A slight negative shift in Ecorr indicates that PODT behaves as a mixed-type inhibitor, mainly affecting cathodic hydrogen evolution. The small change in βa and βc values indicates that the inhibitor does not alter the corrosion mechanism but reduces both anodic and cathodic reaction rates. The maximum inhibition efficiency of 98.1% at 500 ppm is higher, confirming that PODT offers superior performance at lower concentration. The improvement can be attributed to the presence of additional donor atoms or π-electron systems in PODT, facilitating stronger adsorption and film formation.

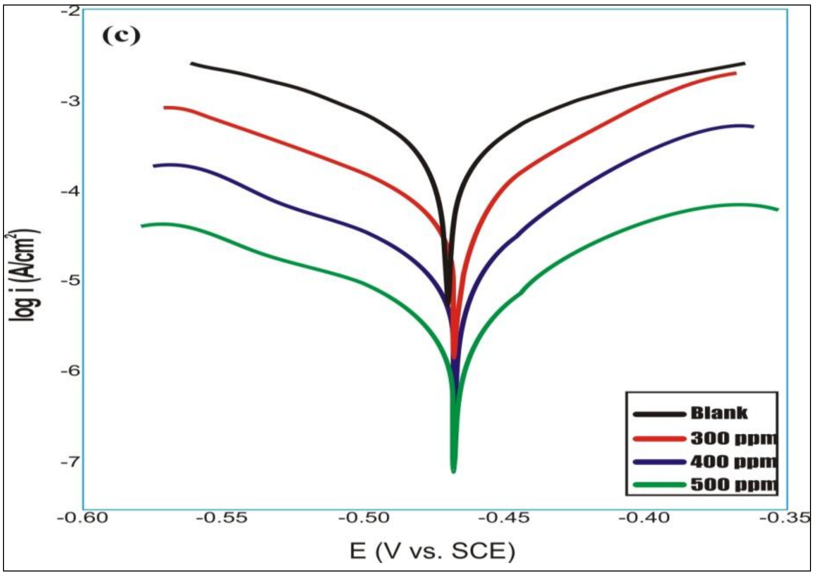


Fig 2: Potentiodynamic Polarization Curves for steel in 1NHCl with different concentrations of PODT

Table 2: Polarization Parameters for Mild Steel in 1 N HCl for Compound 5 (PODT)

Sample	Ecorr (V vs. SCE)	Icorr (A/cm²)	βa (V/dec)	βc (V/dec)	Inhibition Efficiency (%)
Blank	-0.475	1.20×10^{-3}	0.110	0.125	—
300 ppm	-0.472	2.0×10^{-4}	0.104	0.117	83.3
400 ppm	-0.469	6.2×10^{-5}	0.100	0.111	94.8
500 ppm	-0.468	2.3×10^{-5}	0.098	0.108	98.1

Conclusion
The synthesized compound 5-((pyridin-3-yloxy) methyl)-1,3,4-oxadiazole-2-thiol (PODT) was confirmed by spectral and analytical data. Both gravimetric and electrochemical analyses demonstrated that PODT is a highly efficient mixed-type inhibitor for mild steel in 1 N HCl, achieving > 96 % inhibition at 500 ppm. Its efficiency decreased slightly with temperature, indicating predominantly physical adsorption, but remained significant even at 65 °C. The presence of N, O, and S donor atoms and aromatic π-systems facilitated strong adsorption and protective film formation. The compound outperformed related thiadiazole and hydrazone analogues, suggesting its potential as a sustainable corrosion inhibitor for acid cleaning and industrial operations. Future studies will focus on surface adsorption isotherms and quantum chemical modeling to clarify interaction mechanisms at the metal–solution interface.

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