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Applicability of some new pyrimidine derivatives for the corrosion inhibition of mild steel in the acidic environment

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ABSTRACT

The current work targets to discover the potential of two pyrimidine derivatives, ethyl 4-[4-(dimethylamino) phenyl]-6-methyl-2-sulfanylidene-1,2,3,4-tetrahydropyrimidine-5-carboxylate (ESP) and 4-[4-(dimethylamino) phenyl]-6-methyl-*N*-phenyl-2-sulfanylidene-1,2,3,4-tetrahydropyrimidine-5-carboxamide (DSP), for the protection of C1018 steel from acidic corrosion. Electrochemical tests like electrochemical impedance spectroscopy, linear polarization resistance, potentio-dynamic polarization, and electron frequency modulation were employed for assessing the anticorrosive capability of the synthesized ESP and DSP. Both ESP and DSP inhibitors exhibited great inhibition activity, and the inhibition effectiveness attained 88.6 % for ESP and 94.9 % for DSP at saturation concentration.

EIS data for ESP and DSP exposes that inhibition efficacy enhances with an increase in the doses of the two inhibitors by creating a protective film. The finest explanation for the adsorption of the examined molecules on the Fe surface was provided by the Langmuir model. The surface morphology was also evaluated by using SEM and EDX techniques. Computational studies like DFT and MC simulation methods were employed to determine the connection between anticorrosion performance and the inhibitor structure, which agrees with the experimental outcomes.

1. Introduction

Mild steel is largely employed in transportation, construction, medicinal equipment, and other areas, which has an extraordinary impact on social production and human life (Heakal and Elkholy 2017; Bedir et al., 2021a). However, C1018-graded steel is sensitive to corrosion even in mild acidic environments, and after being corroded, which not only threatens people's lives but also produces massive economic losses. Hence, the protection of metal from corrosion is a great deal (Abd El-Lateef et al. 2020; Swathi et al., 2022). Among the various processes, corrosion inhibitor usage is the finest approach for inhibiting metal corrosion in a severe corrosive atmosphere like an acid solution or salt solution via surface adsorption (Rasheeda, Alamri et al., 2022; Rasheeda, Swathi et al., 2022). As mild steel costs are in the moderate range, this process is cheap and simple to carry out.

Countless research has been conducted in the past decade that yields plant extract, inorganic or organic products appropriate for these corrosion systems (Rasheeda et al., 2018). The organic corrosion inhibitors containing hetero atoms (S, O, P or N) play a significant role in achieving corrosion inhibition. Other factors that affect the inhibition of corrosion are the size or shape of the molecule, aromatic rings or delocalized π-electron of the double bond, and the d-orbital of the C1018 steel (Swathi et al., 2023b). So far, so many heterocyclic molecules have been examined by several researchers, including quinoxaline, imidazole,

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