Journal of the Taiwan Institute of Chemical Engineers 000 (2015) 1–14

Contents lists available at ScienceDirect

Journal of the Taiwan Institute of Chemical Engineers

journal homepage: www.elsevier.com/locate/jtice

Thiopyrimidine derivatives as new and effective corrosion inhibitors for mild steel in hydrochloric acid: Electrochemical and quantum chemical studies

Priyanka Singh[a], Ambrish Singh[b], M.A. Quraishi[a,*]

[a] Department of Applied Chemistry, Indian Institute of Technology (Banaras Hindu University), Varanasi 221005, India
[b] Department of Chemistry, Lovely Faculty of Technology and Sciences, Lovely Professional University, Phagwara, India

ARTICLE INFO

Article history:
Received 7 May 2015
Revised 13 October 2015
Accepted 21 October 2015
Available online xxx

Keywords:
Mild steel (MS)
Weight loss
Electrochemical measurements
Scanning electron microscopes (SEM-EDS)
Atomic force microscopy (AFM)
X-ray photoelectron spectroscopy (XPS)

ABSTRACT

The corrosion inhibition properties of thiopyrimidines derivatives *viz.* 5-cyano-6-phenyl-2-thioxo-2,3-dihydropyrimidin-4-one (TP-1), 5-cyano-2-thioxo-6-(p-tolyl)-2,3 dihydropyrimidin-4-one (TP-2), 5-cyano-6-(4-methoxyphenyl)-2-thioxo-2,3-dihydropyrimidin-4-one (TP-3), 6-(4-(dimethylamino)phenyl)-5-cyano-2-thioxo-2,3-dihydropyrimidin-4-one (TP-4) were investigated as corrosion inhibitors by weight loss, electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization methods. Among all thiopyrimidines TP-4 exhibited maximum efficiency of 97% at 200 mg L^{-1}. The results of electrochemical studies revealed that all four TPs were adsorbed on the metal surface by adsorption mechanism and behave as mixed type inhibitors with predominant control on cathodic reaction. The SEM-EDS/AFM/XPS methods were used to corroborate the mechanism of inhibition.

© 2015 Taiwan Institute of Chemical Engineers. Published by Elsevier B.V. All rights reserved.

1. Introduction

Hydrochloric acid solutions are widely used in many industrial processes such as pickling, acidization and cleaning; however, it causes severe corrosion to the metal surface [1–6]. Inhibitors are used to obviate these problems which minimize metal dissolution [7–10].

Several organic compounds have been reported as corrosion inhibitors to prevent metallic corrosion [11–17] but organic compounds containing heteroatoms (O, N, and S) and π bonds are considered as effective corrosion inhibitors because they are readily adsorbed on metal surface through lone pair of electrons and π electrons present in these molecules [18–20].

In the present work we have selected four thiopyrimidines derivatives as corrosion inhibitors for mild steel (MS) in 1 M HCl. The reason of choosing thiopyrimidines as corrosion inhibitors is based on following considerations that both the N and S atoms are present in the same molecule besides the presence of π electrons and lone pair of electrons. It is expected that (a) due to the combined effect of both heteroatoms (N, S) better inhibitive performance could be achieved, and (b) they can be conveniently synthesized from commercially available raw materials. There is only one report on use of thiopyrimidines as corrosion inhibitor [21].

In view of these observations we have synthesized four thiopyrimidines derivatives namely 5-cyano-6-phenyl-2-thioxo-2,3-dihydropyrimidin-4-one (TP-1), 5-cyano-2-thioxo-6-(p-tolyl)-2,3-dihydropyrimidin-4-one (TP-2), 5-cyano-6-(4-methoxyphenyl)-2-thioxo-2,3-dihydropyrimidin-4-one (TP-3), and 6-(4-(dimethylamino)phenyl)-5-cyano-2-thioxo-2,3-dihydropyrimidin-4-one (TP-4) and evaluated their inhibiting performance on corrosion of mild steel by using weight loss, electrochemical impedance spectroscopy (EIS), potentiodynamic polarization techniques. Surface morphology is characterized by SEM-EDS/AFM/XPS analysis.

2 . Experimental

2.1 . Materials and solutions

The composition of the MS coupons is as follows (wt%): C 0.17; Mn 0.46; Si 0.026; Cr 0.050; P 0.012; Cu 0.135; Al 0.023; Ni 0.05; and balance Fe. The MS coupons were mechanically cut into 2.5 cm × 2 cm × 0.025 cm dimensions for weight loss studies and 8 cm × 1 cm × 0.025 cm dimensions for electrochemical study with an exposed area of 1 cm^2.The surfaces of MS coupons were abraded with emery papers (grades ranging from 600 to 1200), washed and degreased with acetone. The test solution of 1 M HCl was prepared by diluting analytical grade 37% HCl with double distilled water.

---

* Corresponding author. Tel. +91 9307025126 (mobile); fax: +91 542 2368428.
E-mail address: maquraishi@rediffmail.com, maquraishi.apc@itbhu.ac.in (M.A. Quraishi).

http://dx.doi.org/10.1016/j.jtice.2015.10.033
1876-1070/© 2015 Taiwan Institute of Chemical Engineers. Published by Elsevier B.V. All rights reserved.

Please cite this article as: P. Singh et al., Thiopyrimidine derivatives as new and effective corrosion inhibitors for mild steel in hydrochloric acid: Electrochemical and quantum chemical studies, Journal of the Taiwan Institute of Chemical Engineers (2015), http://dx.doi.org/10.1016/j.jtice.2015.10.033

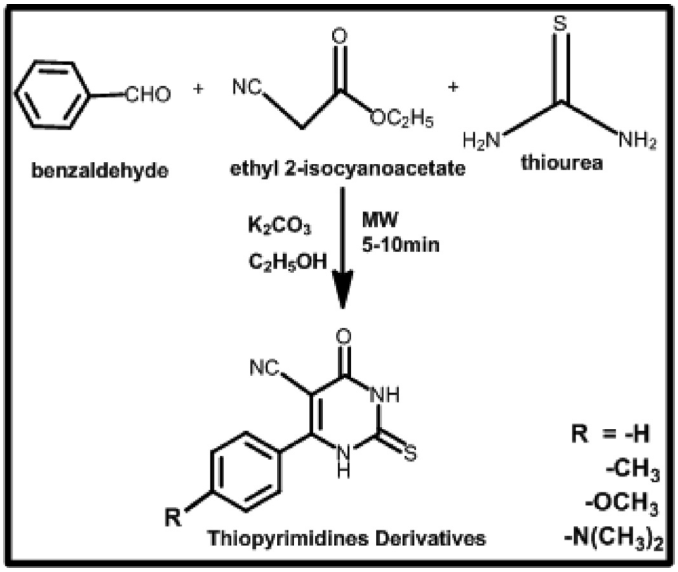


Fig. 1. Synthetic route for the preparation of thiopyrimidines (TPs).

2.2 . Inhibitors

The TPs were synthesized according to previously reported method [22]. The synthetic route is shown in Fig. 1.The compounds were recrystallized from ethanol. The molecular structures of TPs are given in Table 1. IR spectra were recorded on a FTIR (02) [Perkin Elmer, Bruker] spectrophotometer, ^{1}HNMR spectra were recorded on a Bruker DPX-300 instrument at 300 MHz, in DMSO-d_6 relative to tetramethylsilane as an internal reference and UV–vis absorption spectra were recorded using a Perkin-Elmer Lambda-25 spectrophotometer employing a quartz cuvette having optical path length of 1 cm.

2.3 . Weight loss measurements

Weight loss experiments were performed as per reported method [23,24]. The abraded MS coupons were tested in absence and presence of various concentrations (25–250 mg L^{-1}) for 3 h of immersion in 1 M HCl at 308 K.

2.4 . Electrochemical measurements

The electrochemical experiments were performed by using a three electrodes cell, connected to a Potentiostat/Galvanostat G300-45050 (Gamry Instruments Inc., USA). Gamry Echem Analyst 5.50 software package was used for data fitting. This cell assembly contains MS, platinum and saturated calomel electrodes (SCE) as working, auxiliary and reference electrodes, respectively. All experiments were carried out at 308 K temperature.

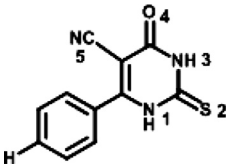
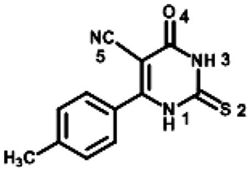
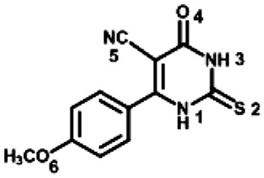
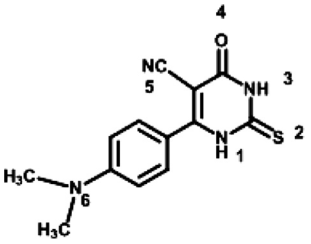
Tafel curves were obtained by changing the electrode potential from −0.25 V to +0.25 V *vs.* open corrosion potential at 1.0 mV s^{-1} of scan rate. EIS were measured in a frequency range from 100 kHz to 0.01 Hz, with amplitude of 10 mV AC signal. The experiments were performed after an immersion period of 30 min in 1 M HCl.

2.5 . Surface characterization

2.5.1 . Scanning electron microscopy (SEM-EDS)

Surface analysis of the MS coupons was carried out in absence and presence of optimum concentration of TPs using a scanning electron

Table 1
Molecular structures of TPs.

Inhibitors	Molecular structures
5-Cyano-6-phenyl-2-thioxo-2,3-dihydropyrimidin-4(1H)-one **(TP-1)**	
5-Cyano-2-thioxo-6-(p-tolyl)-2,3-dihydropyrimidin-4(1H)-one **(TP-2)**	
5-Cyano-6-(4-methoxyphenyl)-2-thioxo-2,3-dihydropyrimidin-4(1H)-one **(TP-3)**	
6-(4-(Dimethylamino)phenyl)-5-cyano-2-thioxo-2,3-dihydropyrimidin-4(1H)-one **(TP-4)**	

Please cite this article as: P. Singh et al., Thiopyrimidine derivatives as new and effective corrosion inhibitors for mild steel in hydrochloric acid: Electrochemical and quantum chemical studies, Journal of the Taiwan Institute of Chemical Engineers (2015), http://dx.doi.org/10.1016/j.jtice.2015.10.033

Download English Version:

https://daneshyari.com/en/article/690508

Download Persian Version:

https://daneshyari.com/article/690508

Daneshyari.com