



Corrosion inhibition performance of chromone-3-acrylic acid derivatives for low alloy steel with theoretical modeling and experimental aspects



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ARTICLE INFO

Article history:

Received 10 June 2017

Received in revised form 7 August 2017

Accepted 11 August 2017

Available online 15 August 2017

Keywords:

Low Alloy Steel

Chromone

Corrosion

Inhibition efficiency, DFT

ABSTRACT

Chromone-3-acrylic acid (CA) and its derivatives viz. 6-hydroxy chromone-3-acrylic acid (6-OH-CA) and 7-methoxy chromone-3-acrylic acid (7-Me-CA) were synthesized and studied for inhibition of Low Alloy Steel corrosion in 1 M H₂SO₄ at different concentration and temperature using Gravimetric, Polarization technique, EIS, AFM, DFT and MD calculations. Mass loss, Potentiodynamic Polarization and EIS results showed that inhibition efficiency increased with gradual increments in concentration of CA compounds. Polarization study revealed that these compounds act as mixed type inhibitors and Langmuir adsorption isotherm is fitted well for adsorption. The order of inhibition efficiency is 7-Me-CA (88.00%) > CA (96.37%) > 6-OH-CA (96.77%). A proposed inhibition mechanism has further been described including the support from all the experimental as well as theoretical techniques.

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1. Introduction

Low Alloy Steel (LAS) is commonly used as construction, storage and engineering material due to its cost affordability, abundance and convenience for fabrication. It also provides material properties that are acceptable for many applications in machinery and industry [1–3]. During oil well acidification as well as in oil recovery techniques in different acidic environments, gas production systems, rather, at every stage of production such as extraction, refining, storage and transportation of oil etc. through pipelines cause deterioration and sometimes, even failure of LAS equipments due to corrosion. Unfortunately, this corrosion of LAS leads to huge economic losses affecting badly any nation's GDP growth [4]. So, it demands crucially to develop some excellent and eco-friendly inhibitors, for, the most efficient and practical method to overcome corrosion is approached by implementing corrosion inhibitors in comparison to other corrosion controlling methods [5–7]. Moreover, the yield efficiency of inorganic corrosion inhibitors was found not so high in addition to their environmental risk [6–7].

The adsorption characteristics LAS of corrosion inhibitors depend upon the chemical moiety of the molecule, type of functional groups and the electron density at the donor atoms. Organic compounds, containing heteroatom's (N, O, S, and P), electronegative functional groups,

π -electrons and aromatic rings as electron density rich centers which are considered as good adsorptive centers [8–9]. These heterocyclic organic inhibitors get adsorb onto the LAS surface or form protective insoluble layer and block corrosion sites, which reduces contact of corroding material with the corrosive medium/LAS [10].

Chromone and its derivatives make a class of naturally occurring heterocyclic compounds and have been isolated or synthesized for biological activities like anti-inflammatory, neuroprotective, anti-HIV, anti-tumor, anti-allergic, and, anti-cancer etc. [11–13]. Chromone class of compounds have not been much explored for corrosion control purposes except Bhkakh and Hadi who have reported corrosion inhibition studies of the Schiff bases of formyl chromones [14]. One of the interesting property of these compounds is their electron donating tendency towards metal ions, which enables them to form strong ligands in coordination compounds [15], thus, these compounds need to be explored in corrosion field also. In present study, we have chosen chromone-3-acrylic acid derivatives with oxygen as heteroatom along with π -electrons which may make them suitable agent for corrosion inhibition of LAS in sulphuric acid.

In view of this, three chromone compounds have been synthesized named as chromone-3-acrylic acid (CA), 6-hydroxy chromone-3-acrylic acid (6-OH-CA) and 7-methoxy chromone-3-acrylic acid (7-Me-CA) and studied their properties as corrosion inhibitors for LAS in 1 M sulphuric acid medium using various experimental techniques and theoretical aspects.

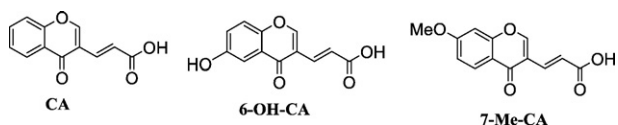
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2. Experimental detail

2.1. Materials and sample preparation

The Low Alloy Steel, a rectangular sheet having composition (wt%); C = 0.14; Si = 0.03; Mn = 0.032; S = 0.05; P = 0.20; Ni = 0.01; Cu = 0.01; Cr = 0.01 and remainder iron (Fe) was used for all the experiments. The surface of LAS was abraded and polished mechanically with 400, 600, 800, 1000 and 2000 grade of emery paper (SiC). The working electrode was thereafter degreased with acetone, rinsed with bi-distilled water and then dried at room temperature before further use. The experiments were carried out at different temperatures (within ± 0.1 °C accuracy) controlled thermostatically by using a water thermostat. The Chromone 3-Acrylic acid derivatives were synthesized as earlier reported [16–19] and the details of the characterization data for the synthesized inhibitors have been given in Supplementary Information. The chemical structures of the three acrylic acids are mentioned below:



The acidic medium of 1 M H₂SO₄ was prepared by dilution analytical grade H₂SO₄ (minimum assay 98.0%, Qualikem, India) of known molarity with bidistilled water.

2.2. Experimental technique

2.2.1. Weight loss measurements

Weight loss experiments were conducted on finely abraded and polished and dried LAS sheets of dimension $3 \times 1.5 \times 0.028$ cm³ and weighing accurately using a digital balance (citizen scale CX 230) with 0.001 mg sensitivity. The Low Alloy Steel specimens were immersed in 1 M H₂SO₄ for 4 h in absence and presence of studied inhibitors at different temperature (303 K, 313 K, and 323 K.) and at different concentration (200, 400, 600, 800 and 1000 ppm). Once the weight loss experiments completed, the all specimens were cleaned with bidistilled water and acetone, dried and weighed again. All weight loss tests were carried out in triplicate with standard deviation of the order 0.01 for sample, not for population. The corrosion rate in mmpy was calculated from the Eq. (1)

$$\text{Corrosion rate (CR)} = \frac{534 \times \Delta W}{DAT} \quad (1)$$

where ΔW is the weight loss of LAS (mg), D is the density of Low Alloy Steel (7.86 g cm⁻³), A is the total area of LAS sheet (cm²), and T is the immersion time in hours. The CR values were used to calculate the inhibition efficiency (η) by the following equation.

$$\eta\% = \frac{CR^0 - CR}{CR^0} \times 100 \quad (2)$$

where CR and CR^0 are the values of corrosion rate of LAS with and without inhibitors, respectively.

2.3. Electrochemical measurements

Electrochemical measurements were conducted using electrochemical workstation PGSTAT204, Autolab, Netherland with FRA32M module controlled by NOVA 1.11 software. The electrochemical measurements were carried out using a three electrode cell assembly. A silver silver chloride electrode, provided with luggin capillary probe, was used as reference electrode along with graphite electrode as a counter electrode. The LAS acted as a working electrode (WE) with an exposed

area of 1 cm², fitted to a specially designed holder and the tip of luggin probe was made in close proximity to working electrode in order to decrease the IR drop.

Before commencing the electrochemical measurements, the working electrode was kept for sufficient time in the corrosive solution which took 60 to 65 min in order to attain a constant value for the open circuit potential (OCP). Then, potentiodynamic polarization curve were recorded in absence and presence of the inhibitors in potential range from -250 to $+250$ mV with a scan rate of 0.001 V/s. Electrochemical parameters including cathodic and anodic Tafel slopes (β_c and β_a), corrosion potential (E_{corr}), corrosion rate (CR) and corrosion current density (i_{corr}) are placed in Table 2 at 303 K. The percentage inhibition efficiency was calculated using the relation:

$$\eta\% = \frac{i_{corr}^0 - i_{corr}}{i_{corr}^0} \times 100 \quad (3)$$

where i_{corr}^0 and i_{corr} are the corrosion current densities of LAS without and with inhibitor, respectively.

The Electrochemical Impedance Spectroscopy (EIS) measurement data were carried out from 100 kHz to 0.01 Hz using ac signal of 5 mV amplitude. EIS parameters include charge transfer resistance (R_{CT}), Constant Phase Element (CPE) and maximum frequency (f_{max}). Based on EIS data, the inhibition efficiency ($\eta\%$), and double layer capacitance (C_{dl}) were calculated by using the following relation:

$$C_{dl} = \frac{1}{2\pi f_{max} R_{CT}} \quad (4)$$

$$\eta\% = \frac{R_{CT} - R_{CT}^0}{R_{CT}^0} \times 100 \quad (5)$$

where R_{CT} and R_{CT}^0 are the values of charge transfer resistance with and without inhibitor, respectively.

2.4. Scanning electron microscopy (SEM)

LAS specimen were immersed in 1 M H₂SO₄ solution with and without inhibitors at 1000 ppm concentration for 4 h at 303 K after polishing and cleaning the LAS specimen by different grade of emery papers. Thereafter, the specimens retrieved, were washed with bidistilled water and dry acetone, dried and then kept in desiccator till they were transferred to SEM chamber for surface morphology. All the SEM images were taken at $\times 500$ magnification.

2.5. Atomic force microscopy (AFM)

First, the samples were rubbed with SiC abrasive paper having range 600–2000 grade, followed by washing with bi-distilled water and acetone. After 4 h immersion in 1 M H₂SO₄ solution with and without inhibitor at room temperature, the specimens were cleaned with doubly distilled water and acetone and thereafter dried.

The topographic changes of the corroded metal surface of each specimen sheet having size 1×1 cm² were examined in standard mode with AFM Instrument (Model: Nanosurf Naio) from Molecular Image (Pico Scan). Micro-fabricated single beam Si₃N₄ having resonance frequency in the range of 13 kHz. The spring constant (0.2 N/m) of the cantilevers was used to calculate the Roughness of Metal Surface (RMS) of the uninhibited and inhibited LAS and Nao program was used to interpret the image.

2.6. Molecular modeling detail

Density functional theory (DFT) method has been exploited for geometry optimizations and all quantum chemical parameters considering the system in water phase. Hybrid functional, B3LYP comprising

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