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Inhibition of mild steel corrosion in hydrochloric using three different 1,2,4-triazole Schiff's bases: A comparative study of electrochemical, theoretical and spectroscopic results

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ABSTRACT

The inhibition properties of three triazole Schiff's bases namely, (4-(4-hydroxybenzylideneamino)-4H-1,2,4-triazole-3,5-diyl)dimethanol (HATD), (4-(4-methoxybenzylideneamino)-4H-1,2,4-triazole-3,5-diyl)dimethanol (MATD) and (4-(3,4-dimethoxybenzylideneamino)-4H-1,2,4-triazole-3,5-diyl)dimethanol (DMATD) for mild steel corrosion in hydrochloric acid have been investigated by weight loss, electrochemical, spectroscopic and computational studies. The results showed that synthesized compounds act as effective inhibitors for mild steel in hydrochloric acid. Inhibition efficiency of these inhibitors increases with inhibitor concentration, but decreases with temperature and acid concentration. The inhibition efficiencies obtained from experimental studies are in good agreement with theoretically calculated values and results of spectroscopic studies.

1. Introduction

The use of inhibitors is one of the most significant and practical methods for the protection of metals against acid corrosion. Recently, many nitrogen containing organic compounds such as triazines [1–3], triazoles [4–6], imidazolines [7–9] etc. have been identified as corrosion inhibitors for mild steel in acid medium.It is also reported that Schiff's base of these heterocyclic compounds exhibit better inhibition efficiency than the corresponding aldehydes and amines. The mechanism of inhibition is explained in terms of formation of protective film on metal surface through adsorption. The adsorption process depends on nature and chemical structure of inhibitor and charge on metal surface [10].

Electronic properties are important in determining the inhibition efficiency of organic molecules. It has been reported that, molecules with low band gap energies are highly reactive and are efficient inhibitors. As an easy and accurate experimental technique, UV–Visible spectroscopy is used to estimate band gap energies of organic π conjugated molecules. From UV–Visible spectroscopy, the band gap energy can be calculated using the wavelength derived from low energy absorption band of the spectrum [11–13].Quantum chemical calculations are also very powerful theoretical tools in determining molecular structure and electronic properties of the molecules. The electronic properties such as the Frontier orbital energies, energy gap, dipole moment etc. correlate the inhibition effect and molecular structure of inhibitors [14–18]. The aim of the present investigation is to synthesize and screen the corrosion inhibition efficiency of 1,2,4-triazole Schiff's bases namely, (4-(4-hydroxy benzylideneamino)-4H-1,2,4-triazole-3,5-diyl)dimethanol (HATD), (4-(4-methoxybenzylideneamino)-4H-1,2,4-triazole-3,5-diyl)dimethanol (MATD) and (4-(3,4-dimethoxybenzylideneamino)-4H-1,2,4-triazole-3,5-diyl)dimethanol (DMATD) for the corrosion of mild steel in HCl solution. The corrosion inhibition efficiencies of these molecules were compared with electronic properties obtained from experimental observations and theoretical calculations.

2. Experimental

2.1. Material and medium

Mild steel samples of composition (in wt%): C (0.2%), Mn (1%), P (0.03%), S (0.02%) and Fe (98.75%) were used for electrochemical and weight loss studies. Prior to the experiment, samples were polished with emery paper of different grades as recommended by ASTM and then degreased by washing with dilute HCl and acetone followed by distilled water. The medium for the study was prepared as aqueous solutions of analytical grade HCl (Merck).

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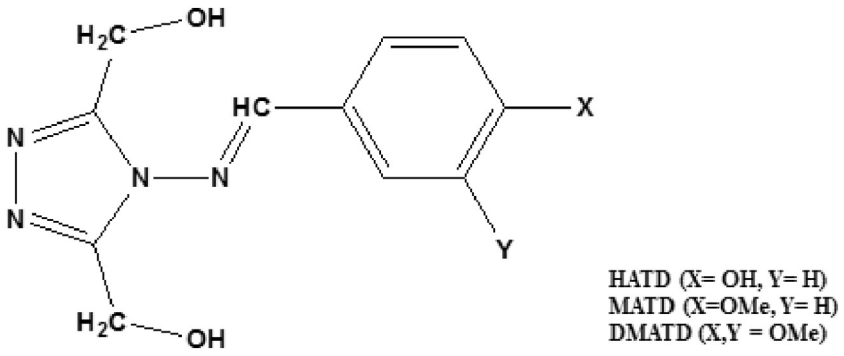

Fig. 1. Structures of inhibitor molecule.

The inhibitors were synthesized by the condensation of (4-Amino-4H-1,2,4-triazole-3,5-diyl)dimethanol (ATD) with 4-hydroxybenzaldehyde (HATD), 4-methoxybenzaldehyde (MATD) and 3,4-dimethoxybenzaldehyde (DMATD) in ethanol (Fig. 1). The triazole precursor ATD was synthesized by the reaction of hydrazine hydrate and glycolic acid [19]. The purified and recrystallized compounds are then characterized by physico-chemical methods and various concentrations of these compounds are used in the present study.

2.2. UV–Visible spectroscopy

Prior to corrosion investigations, UV–Visible spectra of the synthesized inhibitors in hydrochloric acid medium were measured with JASCO-V-550 spectrophotometer.

2.3. Weight loss studies

Weight loss analysis was carried out to examine the effect of inhibitor concentration and acid concentration on inhibition efficiency of the inhibitors. Pre-weighed mild steel samples of 1.8 × 2.1 cm^2 area were immersed in 0.5, 1 and 1.5 N HCl solutions in the absence and presence of different concentrations of HATD, MATD and DMATD. After 24 h, the specimens were taken out, washed initially under running tape water and finally cleaned with 15–20% HCl followed by acetone and then accurately weighed. From the Weight loss data in each experiment, the corrosion rate (C.R) and inhibition efficiency, η (%) were calculated using the following relations [20–23],

$$C.R\left(\mathrm{mgcm^{-2}h^{-1}}\right) = \frac{W}{At} \quad (1)$$

where W is the weight loss of mild steel (mg), A is the area of specimen (cm^2) and t is the immersion time (h).

$$\eta\,(\%) = \frac{W0 - W}{W0} \times 100 \quad (2)$$

where W_0 and W are the weight loss for mild steel in HCl solutions in the absence and presence of inhibitor.

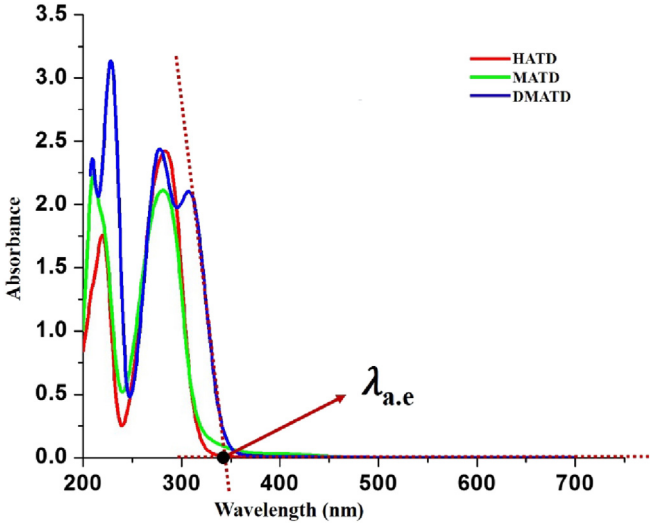

Fig. 2. UV–Visible spectrum of the inhibitor molecules.

2.4. Electrochemical studies

Electrochemical studies were carried out in Gill AC computer controlled electrochemical work station (ACM, U.K model no: 1475) using a conventional three electrode cell with saturated calomel as reference electrode, platinum rod as auxiliary electrode and mild steel samples of 1 cm^2 area as working electrode. Prior to each set of experiments, the samples were immersed in test solution for 1 h to establish steady state open circuit potential (E_{ocp}). Polarization curves were obtained between −250 mV to +250 mV potential range with a sweep rate of 60 mV/min. The values of corrosion potential (E_{corr}), corrosion rate (C.R) and corrosion current density (i_{corr}) were obtained from the curve. The inhibition efficiency, η (%), was calculated from the values of corrosion current density as follows [24],

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

where i_{corr} and i_{corr*} are the corrosion current density in the absence and presence of inhibitor respectively. Electrochemical impedance spectroscopic measurements were conducted at OCP in the frequency range of 0.1 Hz to 10 kHz by applying an alternating potential of 10 mV peak to peak voltage excitation. Values of charge transfer resistance (R_{ct}) and corrosion rate were obtained and inhibition efficiency was calculated in terms of charge transfer resistance as follows,

$$\eta\,(\%) = \frac{R_{ct}^{*} - R_{ct}}{R_{ct}^{*}} \times 100 \quad (4)$$