Experimental studies on corrosion inhibition performance of acetylthiophene thiosemicarbazone for mild steel in HCl complemented with DFT investigation

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Abstract

The University of Technology in Baghdad addresses problems related to the corrosion of metals. In the present investigation, a thiophene derivative, namely, 2-acetylthiophene thiosemicarbazone (2-AT), was synthesized and examined as a corrosion inhibitor for mild steel in a 1-M hydrochloric acid environment by using weight loss and scanning electron microscopic techniques. The inhibition efficiency of this inhibitor increases with increase in concentration, which offered an inhibition efficiency up to 96%. It was found that the inhibition efficiency decreases with long immersion time. The temperature effect on the inhibition performance was studied at various immersion times and revealed that the inhibition efficiency decreases with increasing temperature. The adsorption of the inhibitor on the surface of mild steel in the corrosive environment followed the Langmuir isotherm. The results of scanning electron microscopy (SEM) reveal that the 2-AT molecules confirmed the presence of a protective layer on the surface of a mild steel sample. The density-functional theory as a quantum modeling technique which is used to study the electronic structure reveals that the obtained findings were found to be consistent with the experimental results.

Keywords: mild steel; inhibition; thiophene; weight loss; HOMO;

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1. INTRODUCTION

Corrosion inhibitors are added to the corrosive (acidic and basic) solutions to reduce corrosion on the surface of metals [1, 2].

Hydrochloric acid is widely utilized in industries such as pickling, cleaning, descaling, and oil-well acidizing [3, 4]. Corrosion inhibitors used in acidic solutions are mostly aliphatic or aromatic organic compounds, and most of them are molecules with heteroatoms such as phosphorous, nitrogen, sulfur, and oxygen and are absorbed on the surface of the metals. In corrosion studies, the formation of a metal complex between inhibitor molecules as electron donor and metal surface atoms as electron acceptor due to unoccupied d-orbital of iron atoms was proposed [5–13]. The molecules of organic inhibitors which adsorbed on the metal/solution interface execute through H₂O molecule replacement by organic molecules as in equation (1):

\[
\text{Org}_{(\text{sol})} + \text{H}_2\text{O} \rightarrow \text{Org}_{(\text{ads})} + \text{H}_2\text{O} \tag{1}
\]

where Org(sol) is organic molecules in the solution, Org(ads) is organic molecules adsorbed on the surface of metal, and x is H₂O molecules which are replaced by the inhibitor molecules. The Schiff base molecules reveal better inhibition performance than their aldehydes and/or amines [14]. Thiosemicarbazide and its derivatives were used as corrosion inhibitors, as the molecule...
has three chelating sites suitable for bonding with the iron atoms of the mild steel surface which are the two nitrogen atoms, thione and imine groups with unshared pairs of electrons [15–24]. Thiophenes adsorb on the surface of mild steel and control or block corrosion [25]. Substituted imines control the corrosion through forming metal complexes on the metal surface [26]. The seeking for significant corrosion inhibitors was performed for the development of thiosemicarbazides [27]. Complementing our previous researches in the field of synthesis of new corrosion inhibitors [28–35], herein we synthesized a new corrosion inhibitor, namely, 2-AT, and its inhibitive performance on mild steel corrosion in corrosive solution was examined using gravimetric and SEM techniques. The effects of concentrations (0.1–0.5 mM), temperature (303–333 K), and immersion (1–24 h) on the corrosion attitude of mild steel in 1 M hydrochloric acid solution was investigated. The novelty of this work was to use an organic compound as a possible corrosion inhibitor for mild steel in HCl solution.

2. MATERIALS AND METHODS

2.1. Materials

Corrosion investigations have been done on mild steel specimens having the following composition (wt. %): carbon, 0.210; manganese 0.050; silicon 0.380; aluminum 0.010; sulfur 0.050; phosphorus 0.090; and iron balance. Mild steel specimen with an active surface area 4.5 cm$^2$ was cut and polished by emery paper of various grades for gravimetric techniques. Previous to the experiments, mild steel specimen was rinsed with double-distilled water, degreased in acetone, and dried with a desiccator.

2.2. Test solutions

The measurements were conducted in aerated, non-stirred analytical reagent-grade hydrochloric acid solution which was freshly prepared using double-distilled water to obtain 1 M of HCl solution. ‘1 M HCl solution have been prepared in the laboratory by diluting the appropriate volume of analytical grade 37% hydrochloric acid with double distilled water.’ The newly synthesized inhibitor concentration ranged from 0.1 to 0.5 mM, for 1, 5, 10 and 24 h of immersion time, and the solution temperature varied from 303 to 333 K and the solution volume was 250 mL. Each experiment was repeated three times, and the mean was reported to verify the reproducibility of the measurements. One molar of HCl solution was prepared in the laboratory by diluting the appropriate volume of analytical-grade 37% hydrochloric acid with double-distilled water.

2.3. Synthesis of corrosion inhibitor

2-Acetylthiophene thiosemicarbazone (2-AT) as a new corrosion inhibitor was synthesized by condensing hydrazinecarbothioamide (0.01 mol) with 1-(thiophen-2-yl)ethenone (0.01 mol) in methanol (70 mL) with drops of glacial acetic acid for 14 h (Scheme 1). The purity of the new corrosion inhibitor was confirmed by thin-layer chromatography (TLC) and filtered, washed with alcohol, and dried, yielding 73%, M.P. 136°C. The yellow product was characterized by spectroscopic (FT-IR, $^1$H-NMR, and $^{13}$C-NMR) and CHN elemental analysis techniques. FT-IR (cm$^{-1}$): 3396.68, 3221.99 and 3144.71 for N–H. 1592.09 for C=N and 954.88 for C=S. $^1$H NMR, DMSOd$_6$, δ: 2.01 ppm (3H, s, CH$_3$), 6.99–7.10 ppm (m, thiophene ring), 7.11 ppm (2H, d, NH) and 7.23 ppm (1H, d, NH). $^{13}$C-NMR, DMSOd$_6$, δ: 14.98(CH3); 125.43, 126.77 and 128.68 (carbon of thiophene ring), 150.42 (H–C=N–N) and 179.02 (C=S).

2.4. Weight loss method

Gravimetric techniques were used to examine the inhibitive performance of 2-AT to control or reduce the corrosion of mild steel surface in 250 mL of 1 M hydrochloric acid solution at 303 K by immersing mild-steel specimens in the absence and presence of 0.1–0.5 mM of 2-AT. The period of immersion times 1, 2, 5, 10 and 24 h were utilized for gravimetric techniques. The examined specimens were then removed from the corrosive solution, washed, dried and weighed. The corrosion rate (CR), inhibition efficiency (IE%) and surface coverage ($\theta$) were evaluated according to equations (2–4).

$$C_R (mmy^{-1}) = \frac{87.6W}{atd}$$

(2)

where $W$ is the weight loss, $a$ is the exposed specimen area (cm$^2$), $t$ is the exposure time (h) and $d$ is the specimen density (g/cm).

$$\theta = \frac{C_{R0} - C_{Ri}}{C_{R0}}$$

(3)

$$IE (%) = \frac{C_{R0} - C_{Ri}}{C_{R0}} \times 100$$

(4)

where $C_{R0}$ is the corrosion rate in the absence of 2-acetyltiothiophene thiosemicarbazone and $C_{Ri}$ is the corrosion rate in the presence of 2-AT. These measurements were repeated at various temperatures of 303, 313, 323 and 333 K through utilizing the water thermostat to determine the solution temperature.

2.5. Scanning electron microscopic analysis

SEM (scanning electron microscopy, TM1000 Hitachi Tabletop Microscope) was utilized to investigate the mild steel surface for the examined specimens in the absence and presence of 2-acetyltiothiophene thiosemicarbazone with a concentration of
molecules in the acid solution. Surface of the metal and the heterogeneous atoms of the inhibitor over, the current inhibitor molecules form a protective layer on the surface of mild steel, as a result of the bonding between the adsorbed molecules and the metal surface. This bonding leads to a decrease in the corrosion rate of mild steel in the presence of the inhibitor.

2.6. Quantum chemical study
A computational quantum mechanical modeling method was performed through utilizing density-functional theory (DFT) to study the electronic structures of 2-AT molecules in order to calculate the physical properties of 2-acetylthiophene thiosemicarbazone molecules. The geometry optimization of 2-AT molecules was obtained through utilization of DFT/B3LYP with a 6-31G basis set. Theoretical parameters such as the highest occupied molecular orbital energy, lowest unoccupied molecular orbital energy, energy gap, dipole moment, hardness, softness and fraction of electrons transferred have been determined.

3. RESULTS AND DISCUSSIONS

3.1. Synthesis of corrosion inhibitor
2-Acetylthiophene thiosemicarbazone was synthesized by condensing thiosemicarbazide with 2-acetylthiophene under reflux to give 2-acetylthiophene thiosemicarbazone (Scheme 1). The purity of 2-AT was confirmed by TLC. The chemical structure of the synthesized compound was characterized by FT-IR and NMR techniques and CHN elemental analysis. 2-AT showed the C=N group band at 592 cm⁻¹, which indicates the formation of the Schiff base compound. In the ¹³C-NMR spectrum of 2-AT, a signal of δ 150 showed the presence of the C–SH H–C=N–N carbon and the C=S signal appeared at 179 ppm. The structure of 2-AT is shown in Scheme 1.

3.2. Weight loss measurements: concentration effect
The corrosion rate and inhibition efficiency offered by 2-AT were evaluated by weight loss method after a period of 1, 5, 10 and 24 h of immersion at 303 K, shown in Figure 1. From Figure 1, it is clear that the corrosion rate of mild steel in 1 M hydrochloric acid is found to decrease with increasing exposure time duration and concentration of the tested inhibitor. From Figure 1, it is obvious that inhibitive performance increases with inhibitor concentration increase. This result could be imputed to the increase in the number of inhibitor molecules adsorbed on the mild steel surface, which isolates the metal surface from the corrosive environment, conducting impediment of mild steel dissolution [36]. To compare the inhibition ability of some organic inhibitors [37, 38] and the corrosion inhibitor in this study as a possible inhibitor of metal in 1 M hydrochloric acid, the current inhibitor showed a higher inhibition efficiency compared to other inhibitors. Moreover, the current inhibitor molecules form a protective layer on the surface of mild steel, as a result of the bonding between the surface of the metal and the heterogeneous atoms of the inhibitor molecules in the acid solution.

3.3. Weight loss measurements: time effect
Time is a significant parameter when describing the corrosion inhibitor. To evaluate the stability of the adsorption rate of the tested inhibitor molecules, exposure time investigations were conducted in 1 M hydrochloric acid solution. The immersion time range was 1, 5, 10 and 24 h. The results demonstrated in Figure 1 indicate the influence of exposure time on inhibition efficiency of 2-AT as a new corrosion inhibitor. The highest inhibitive efficiency was achieved at 5–10 h as the early times of exposure. This result was because of prompt adsorption of 2-acetylthiophene thiosemicarbazone molecules on the surface of mild steel due to the highest number of inhibitor molecules that block the surface of metal from the corrosive solution. After 10 h of exposure, the inhibition efficiency decreased. The decrease in inhibitive efficiency was imputed to desorption of the 2-AT molecules on the surface of mild steel. In addition, the corrosion rate was increased with immersion time increase. This fact can be explained according to adsorption theory. When 2-AT molecules on to the surface of mild steel was desorbed, a mild steel was exposed to hydrochloric acid solution, thereby increasing the contact of a mild steel surface/corrosive environment, which results in the dissolution of metal. Furthermore, the corrosion rate increases with increasing exposure time, which was imputed to a low number of 2-AT molecules in a corrosive environment to control or reduce the dissolution of metal; it is obvious that after 2-AT molecules were desorbed, they turned inefficient and thus did not participate in the inhibitive approach.

3.4. Weight loss measurements: temperature effect
Corrosion inhibition experiments were executed at various temperatures (303, 313, 323 and 333 K). The corrosion rate and inhibition efficiency of metal in 1 M hydrochloric acid solution in the absence and presence 2-AT as a corrosion inhibitor at various temperatures, obtained from gravimetric techniques, are demonstrated in Figure 2. The corrosion rate in the presence of the tested inhibitor increased with increases in the solution temperature from 303 to 333 K. From Figure 2, it is obvious that the highest inhibition efficiency of 96% was obtained for the 0.5 mM concentration of 2-AT at 303 K. The inhibition efficiency decrease with increasing temperature indicates the fact that the 2-AT molecule layer formed on the mild steel surface is lower protective at 323 and 333 K.

3.5. Adsorption isotherm
Chemisorption is the formation of chemical bonds. The problem of distinguishing between chemisorption and physisorption is basically the same as that of distinguishing between chemical and physical interactions in general. The chemical nature of the adsorptive may vary through dissociation of the surface. Chemisorption energy may be endothermic or exothermic. Since the adsorbed molecules are bonded to the surface through valence bonds, they will occupy certain adsorption sites on the surface and only one layer of chemisorbed molecules is formed. Physisorption
of intermolecular forces does not involve a significant change in the electronic orbital patterns. The elementary step in physical adsorption does not involve an activation energy. The interaction between the chemical compounds and the metal depended on different adsorption isotherms. In general, those usually utilized were the Langmuir adsorption isotherm, Temkin adsorption isotherm and Frumkin adsorption isotherm. The surface coverage for various inhibitor concentrations in 1 M HCl solution was examined to determine an appropriate adsorption isotherm. Fitting \( C_{inh}/\theta \) vs \( C_{inh} \) produces a straight line as demonstrated by the graphs. 

Figure 1. Effect of exposure time on corrosion rate and inhibition efficiency of mild steel in 1 M HCl in the presence of different concentrations (0.1–0.5 mM) of 2-AT.

Figure 2. Effect of temperature on corrosion rate and inhibition efficiency of mild steel in 1 M HCl in the presence of different concentrations of 2-AT.
where which followed equation (5). Inhibitor molecules obey the Langmuir adsorption isotherm at 303.0 K. This elucidates that the adsorption of the tested inhibitor molecules was of chemisorption type [39].

![Figure 3. Langmuir plots of C_{inh}/θ vs C_{inh} for 2-AT.](image)

in Figure 3, with correlation coefficient \( r^2 \) values 0.998 for 2-AT at 303.0 K. This elucidates that the adsorption of the tested inhibitor molecules obeys the Langmuir adsorption isotherm which followed equation (5).

\[
\frac{C_{inh}}{\theta} = \frac{1}{K_{ads}} + C_{inh}
\]  

(5)

where \( C_{inh} \) is the concentration of the tested inhibitor and \( K_{ads} \) is the equilibrium constant.

The slope value for the tested inhibitor was determined and found to be near unity, confirming the Langmuir isotherm. From Figure 3, the intercept values of \( K_{ads} \) were evaluated. \( K_{ads} \) having large values for the investigated inhibitor suggests further effective adsorption and hence best inhibition performance. The utilization of the \( K_{ads} \) value can calculate the free energy (\( \Delta G^o \)) value through following equation (6).

\[
\Delta G^o_{ads} = -RT \ln (55.5 \ K_{ads})
\]  

(6)

where \( R \) is the gas constant and \( T \) is the temperature. The concentration of water is 55.5 mol/L.

It is obvious that the value of \( \Delta G^o_{ads} \) is \(-41.9 \) kJ/mol. In general, the value of \( \Delta G^o_{ads} \) is around 20 kJ/mol, the adsorption type was regarded as physical adsorption and the inhibition performance was because of the electrostatic interactions between the charged inhibitor species and the charged surface of the mild steel, while if the value of \( \Delta G^o_{ads} \) above \(-40 \) kJ/mol was chemisorption, that is because of the reaction between un-shared electron pairs of inhibitor molecules and un-occupied d-orbitals of the iron atoms of the surface of mild steel. The pairs of electron transfer from the inhibitor species to the mild steel surface to form a coordination bond. The \( \Delta G^o_{ads} \) Value of the synthesized corrosion inhibitor in 1 M HCl solution suggested that the adsorption of synthesized inhibitor molecules was of chemisorption type [39].

3.6. Scanning electron microscopy

The mild steel surface was tested with SEM in 1 M hydrochloric acid solution in the absence and presence of 0.5 mM of the new tested inhibitor. The immersion time was 5 h. Figure 4a and b demonstrate the morphology surface of mild steel, and it is obvious that mild steel specimen in the absence of inhibitor (Figure 5a) is badly damaged. Figure 4b shows that the mild steel surface in the presence of the synthesized inhibitor is smooth. It was concluded that 2-AT can reduce the dissolution of the metal surface in a corrosive environment; this is because the 2-AT inhibitor was effective in reducing the corrosion rate of the metal surface. This enhancement in surface morphology is due to the formation of a protective film of 2-AT molecules on the metal surface which reduces the corrosion rate.

3.7. Theoretical calculation

In order to investigate the influence of structure of the inhibitor molecule on the inhibitive performance, theoretical studies were carried out with density functional theory (DFT) and all the computations were performed by using geometry optimization. Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO), energy gap (\( \Delta G \)), dipole moment (\( \mu \)), absolute electronegativity (\( \chi \)), global hardness (\( \eta \)) and softness (\( \sigma \)), number of transferred electrons (\( N \)) and molecular structure are demonstrated in Figure 5. The HOMO and LUMO energies are important factors for the chemical species reactivity prediction. Generally, HOMO energy is related with the ability of donating electrons of a molecule. The inhibitive performance increases with the increase in the energy value of HOMO. Energy of Highest Occupied Molecular Orbital with a high value for a molecule refers to the ability of this molecule to donate electrons to low energy of un-occupied d-orbitals. A low energy value of Lowest Unoccupied Molecular Orbital of ELUMO for a molecule indicates that this molecule has the tendency to accept electrons from the donor molecules [40]. Previous studies indicate that energy gap and dipole moment with low and high values respectively are responsible for the excellent inhibition
moment value [43, 44], and others reported that the inhibition efficiency increased with decrease in the dipole moment value.

My point of view regarding the factor of dipole moment and its relationship to the efficiency of corrosion inhibition is relative, meaning that in certain cases it is better to have a dipole moment that is low so that the efficiency of inhibition is high and in other cases it is better to have a high dipole moment and the inhibition efficiency becomes high. Thus, positive and negative dipole moments are dependent on two factors: one is major and the other is minor. The main factor relates to the structure of the molecule, so if the molecule has a steric hindrance, the effect of the dipole moment on the inhibitory efficacy is positive and, by the high value of dipole moment, comes with good inhibition performance. The minor factor is the band gap energy. The value of an energy gap is negative with the value of the dipole moment.

If the value of the energy gap is high (coming with a low value of ELUMO) and the value of the dipole moment is small, then the inhibition efficiency is good. The value of the dipole moment in the current research is low (−1.3144) and the energy gap value is high (ELUMO is −0.203 eV), so we expect an excellent inhibition efficiency, and this is proven by experimental results. The HOMO and LUMO molecular orbital density distributions of the 2-AT molecule are displayed in Figure 5. As shown from Figure 5, the HOMO and LUMO distributions were mainly around the whole structure of the studied molecule. In general, it is obvious from Figure 5 that the distribution of HOMO was all over the inhibitor molecule due to containing nitrogen and sulfur atoms in addition to pi-bonds. Thus, the areas having N and S atoms and pi-bonds were possibly the major coupling sites. The inhibition efficiency was increased with EHOMO, and electron density increased. The iron atoms for mild steel specimen have un-occupied d-orbitals. N and S atoms and pi-bonds have pairs of electrons that are remarkable for coupling with iron d-orbitals and determining the adsorption of the inhibitor molecules on the mild steel surface.

Table 1. Electronic properties of 2-AT molecules calculated by DFT.

| I  | A  | ΔE  | ΔN | μ  |
|----|----|-----|----|----|
| 9.018 | 0.203 | 7.744 | 4.61 | 3.87 | 0.258 | 0.71 | 1.314 |

χFe iron electronegativity has a theoretical value of 7.0 eV, χinh 2-AT electronegativity, and ηFe iron hardness has the theoretical value 0. Finally, ηinh is the 2-AT hardness.

The value of EHOMO was −9.018 eV. The high value of HOMO indicates that the new synthesized inhibitor molecules have excellent ability to retard and control the corrosion. An energy gap value (−7.7442 eV) was found for the new synthesized inhibitor. According to the energy gap value, it can be confirmed that the 2-AT molecule has high ability to be adsorbed on the surface of tested mild steel specimen. Previous studies about dipole moment and its relation with inhibition performance were confusing. Some of the researchers reported that the relation was positive and the inhibition efficiency increased with increase in the dipole moment value [41, 42]. For the quantum factors, equations (7–12) have been applied [42].

\[ I = -E_{HOMO} \]  
\[ A = -E_{LUMO} \]  
\[ \chi = \frac{I + A}{2} \]  
\[ \eta = \frac{I - A}{2} \]  
\[ \sigma = \frac{1}{\eta} \]  
\[ \Delta N = \frac{\chi_{Fe} - \chi_{inh}}{2(\eta_{Fe} + \eta_{inh})} \]

Figure 6. Schematic of the proposed mechanism of 2-AT molecules on the mild steel surface.
The excellent inhibitive performance for the examined inhibitor led to an increase in the HOMO energy and electron density distribution in the molecule. The electronegativity is an important factor which shows the tendency of the synthesized inhibitor to attract electrons. The electronegativity value of the 2-AT molecule is demonstrated in Table 1. The low value of electronegativity comes with good adsorption of the 2-AT molecule on the surface of the metal. The excellent corrosion inhibitor may have softness with high value and hardness with high value. Table 1 indicates that the 2-AT molecule has significant values of softness and hardness which indicate excellent inhibition efficiency.

3.8. Suggested mechanism
The adsorption of 2-AT molecules on the metal surface can be demonstrated through chemisorption processes. The specific corrosion inhibition mechanism of 2-AT molecules to the metal surface is clearly obeyed, as shown in equations (13–15):

\[
Fe + (2 - AT) \rightarrow Fe(2 - AT)_{\text{ads}} \quad (13)
\]

\[
Fe + (2 - AT)_{\text{ads}} \rightarrow Fe^{+2}(2 - AT)_{\text{ads}} + ne^- \quad (14)
\]

\[
(2 - AT)_{\text{aq}} + H_2O_{\text{ads}} \rightarrow (2 - AT)_{\text{ads}} + H_2O_{\text{aq}} \quad (15)
\]

The chemisorption of 2-AT molecules on the coupon surface is indicated by the interactions of donor–acceptor between the unshared heteroatom of 2-AT molecules with the d-orbitals of iron atoms on the coupon surface. DFT calculations and experimental findings reveal that the 2-AT molecules have excellent inhibitive performance; it imputed to bindings between 2-AT molecules and the surface of mild steel. The 2-AT molecules could be adsorbed onto the metal surface through coordination bonds, forming a stable layer which has the ability to protect the mild steel surface and improve the inhibitive performance. Therefore, it increases the number of heteroatoms and the molecular weight of the parent molecules (hydrazinecarbothioamide and 1-(thiopen-2-yl)ethenone) and produces the new molecule 2-AT, which was an efficient technique to increase the inhibition efficiency. The corrosion inhibition mechanism of 2-AT molecules is hereby proposed from the complexation theory demonstrated in Figure 6. Functional groups such as imine, amines, C=S and –S– in the 2-AT molecules donate the pairs of electrons to the unoccupied d-orbital of iron and form coordination bonds which block the active sites exposed to a hydrochloric acid environment, decreasing the corrosion rate (Figure 6).

4. CONCLUSION
The inhibitive performance of a new synthesized inhibitor, namely 2-acetylthiophene thiosemicarbazone (2-AT), has been assessed in this investigation through utilizing the weight loss techniques and surface analyses. 2-AT exhibits excellent inhibition efficiency for mild steel in a 1-M hydrochloric acid environment due to the presence of four nitrogen atoms and two sulfur atoms in addition to four pi-bonds and one heterocyclic ring according to the 1H-NMR, 13C-NMR and FT-IR spectroscopically techniques. The inhibition efficiency increased with increasing inhibitor concentration and decreased with rising temperature. The new synthesized inhibitor has an inhibition efficiency of 96.6% at 303.0 K after 5 h at the concentration of 0.5 mM. The SEM analysis demonstrated that the tested inhibitor molecules adsorb on the mild steel surface and form a protective layer. The adsorption of the tested inhibitor molecule film was found to obey the Langmuir adsorption isotherm. The value of Gibbs free energy suggested that the adsorption mechanism of the tested inhibitor molecules on the mild steel surface is chemisorption.

CONFLICTS OF INTEREST
The authors declare no conflict of interest.

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REFERENCES
[1] Yilgor E, Yilgor IG, Guler TC et al. 2004. Reviews on Corrosion Inhibitor Science and Technology. Berlin: Springer.
[2] Salman TA, Zinad DS, Jaber SH et al. Effect of 1,3,4 thiadiazole scaffold on the corrosion inhibition of mild steel in acidic medium: an experimental and computational study. Int. J. BioTrubo-Corrosion 2019;5:1–11. doi: 10.1007/s40735-019-0243-7.
[3] Habeeb HJ, Luabli HM, Dakhil RM et al. Development of new corrosion inhibitor tested on mild steel supported by electrochemical study. Results Phys. 2018;8:1260–7. doi: 10.1016/j.rinp.2018.02.015.
[4] Al-Amiery A, Kadhum A, Mohamad A et al. Electrochemical study on newly synthesized chlorocurcumin as an inhibitor for mild steel corrosion in hydrochloric acid. Materials 2013;6:5466–77. doi: 10.3390/ma6125466.
[5] A. Ali, M. T. Saeed, and S. U. Rahman. “The isoxazolidines: a new class of corrosion inhibitors of mild steel in acidic medium,” Corros Sci, 2003;45:253–266.
[6] Junaudi S, Kadhum A, Al-Amiery A et al. Synthesis and characterization of novel corrosion inhibitor derived from oleic acid: 2-amino5-oleyl1,3,4-thiadiazol (AOT). Int. J. Electrochem Sci. 2012;7:3543–54.
[7] Kadhim A, Al-Okbi A, Jamil DM et al. Experimental and theoretical studies of benzoazines corrosion inhibitors. Results Phys. 2017;7:4013–9. doi: 10.1016/j.rinp.2017.10.027.
[8] Al-Azawi KP, Mohammed IM, Al-Baghdadi SB et al. Experimental and quantum chemical simulations on the corrosion inhibition of mild steel by 3-((5-(3,5-dinitrophenyl)-1,3,4-thiadiazol-2-yl)amino)indolin-2-one. Results Phys. 2018;9:278–83. doi: 10.1016/j.rinp.2018.02.055.
[9] Al-Baghdadi SB, Hashim FG, Salam AQ et al. Synthesis and corrosion inhibition application of NATN on mild steel surface in acidic media complemented with DFT studies. Results Phys. 2018;8:1178–84. doi: 10.1016/j.rinp.2018.02.007.
[10] Al-Obaidy AHMJ, Kadhum A, Al-Baghdadi SB et al. Eco-friendly corrosion inhibitor: experimental studies on the corrosion inhibition performance of creatinine for mild steel in HCl complemented with quantum chemical calculations. Int. J. Electrochem Sci. 2015;10:3961–72.

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