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Experimental and quantum chemical simulations on the corrosion inhibition of mild steel by 3-((5-(3,5-dinitrophenyl)-1,3,4-thiadiazol-2-yl)imino)indolin-2-one

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ABSTRACT

Iraq has been one of the most extensive oil and natural gas industries in the world. The corrosion of mild steel is costly and insufficiency process. It is responsible for great loss in manufacture and environment. Natural and organic inhibitors have been utilized for a long time to inhibit the corrosion. Selected thiadiazol derivative, namely 3-((5-(3,5-dinitrophenyl)-1,3,4-thiadiazol-2-yl)imino)indolin-2-one (TDIO) was investigated for it inhibitive impacts in 1 M HCl medium on corrosion of mild steel using weight loss and scanning electron microscope techniques. The maximum inhibition efficiency up to 90.7% at the maximum inhibitor concentration 0.5 mM. Surface morphology of results demonstrated that TDIO formed adsorbed film on surface of mild steel in hydrochloric acid solution. Give molecular based clarifications to the inhibitive impacts of the studied. The interactions between mild steel surface and the inhibitor molecules have been undertaken to further corroborate the methodological results.

Introduction

Thiadiazoles continue to be of a major attention to a enormous number of investigators due to their considerable medicinal and industrial importance. Alloys such as mild steel were much of the time utilized as a development material in various manufactures because of their minimal effort and high mechanical quality. Be that as it may, it is inclined to erosion in fluid condition, especially acidic solutions, which were typically engaged with mechanical activities, for example, corrosive pickling, modern corrosive cleaning, corrosive descaling and oil well acidizing processes [1,2]. Heterocyclic molecules have been accounted for as successful erosion inhibitors since they can without much of a stretch adsorb on metallic surface by means of their π-and non-holding electrons, benzene rings and polar substituents groups, which go about as adsorption centers [3–8]. A considerable lot of these heterocyclic molecules can be prepared via different easy, low cost approaches [9]. Deferent approaches utilized in the investigations of corrosion inhibitions in corrosive solution that were electrochemical [10–12], theoretical chemical calculations [13–16] and surface morphology [17]. Then again, weight reduction methods [18,19], electrochemical technique [20–22] and surface investigations strategies [23] have as of late been connected in MIC thinks about. Different natural and synthetic organic molecules, particularly those that contain N, O, S, and P heteroatoms and in addition π-electron frameworks have been utilized as corrosion inhibitors for metals in watery arrangements [24–26].

The present examination in this manner researches was study the adsorption of new hetrocyclic compound on mild steel in corrosive solution by 3-((5-(3,5-dinitrophenyl)-1,3,4-thiadiazol-2-yl) imino)indolin-2-one researched and it corrosion inhibition performance for the surface of mild steel [27] in 1 M HCl environment was investigated. Weight loss technique have been utilized to quantify the protection performance of TDIO for mild steel. Surface morphology examination utilizing of the SEM (the scanning electron microscope) was conducted to prove that the TDIO protect

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the surface of the studied alloy versus the corrosive media. Theoretical studies and simulations employee DFT technique were performed to support the abilities of TDIO as superior corrosion inhibitor with inhibition efficiency 90.7%. The synthesized inhibitor that was employee in this study was shown in Fig. 1.

Materials and methods

Corrosion inhibitor synthesis

Solvents and starting materials were obtained from Sigma-Aldrich Malaysia. FTIR spectra were recorded via Shimadzu 8300 spectrometer. CHN analysis were obtained through Carlo Erba 5500 CHN elemental analyzer. The spectra of NMR were recorded via Bruker Spectrospin instrument equipped with 300 MHz UltraShield employing DMSO-d6 as a solvent and TMS internal standard. An equimolar of satin and 5-(3,5-dinitrophenyl)-1,3,4-thiadiazol-2-amine have been dissolved in appropriate quantity of absolute ethanol have relaxed for one hour than added dropwise to the reaction mixture few drops of glacial acetic acid and continuous reflation for another 12 h. Cool and recrystallized with ethanol. Yield, 66.8%; mp 280–283 °C. FT-IRcm-1; 3429.7 (N—H amine), 3064.8 (C—H aromatic), 1681.7 (carbonyl), 1617.3 (C=N Schiff base), 1588.4 (C=N intra ring). Proton NMR in DMSO-d6; δ: 8.28 ppm (s, 1H, NH), 7.28–7.83 (m, H-Ar). Carbon-NMR in DMSO-d6: 116.9, 118.7, 121.4, 125.4, 128.7, 129.3, 131.6, 133.2, 137.3, 139.2, 141.3, 151.6, 152.1, 164.9, 172.6. CHN Analysis for $C_{16}H_8N_6O_5S$; Found (Calculated): C, 50.07% (48.49); H, 1.97% (2.03); N, 21.68% (21.20).

Samples preparation

The mild steel spaceman were a structure of C (0.21%), Si (0.38%), Mn (0.05%), P (0.09%), Al (0.01%), and Fe (99.21%) have been slices mechanically to little coupons for weight loss examination. Going before to all methodological methodologies, the coupons were cleaned according to the standard procedure to be specific ASTM G1-03 [18]. The acidic solution 1.0 M HCl has been worker for every one of the tests. The examining solution was utilizing 1.0 M HCl arrangement with various concentrations of TDIO: 0.1, 0.2, 0.3, 0.4 and 0.5 mM. The solution without TDIO was considered as clear for correlation. The sum total of what tests have been done at 303, 313, 323 and 333 K by methods for indoor regulator water bath.

Weight loss measurements

The cleaned and weighed mild steel samples were drenched in HCl solution with/without different concentrations of TDIO for f h at 303 K, individually. In addition, the coupons of mild steel were inundated in destructive medium with and without off TDIO at the grouping of concentration in mM for 5 h at various degrees of temperatures that were 303, 313, 323 and 333 K, individually. By then, the mild steel samples were launching, scoured with a brush, cleaned by water and acetone; by then drying and weighing through scientific adjust.

The estimations of corrosion performance (%*IE*) was figured through representative the Eq. (1).

$$IE\% = \frac{W_o - W_1}{W_o} \times 100 \tag{1}$$

where wo (weight loss in absence of TDIO) and w1 (weight loss in presence of TDIO).

Corrosion rates was represents as in Eq. (2) [19,20].

$$C_R = \frac{\text{mg}}{\text{cm}^2 h^1} \tag{2}$$

The characterization of the mild steel surface

The surface of mild steel spacemen beforehand, at that point after the immersed in HCl solution in nonappearance and nearness 0.5 mM TDIO for 5 h at 303 K were portray by checking SEM (scanning electron microscope).

Computation methods

Quantum estimations for tested inhibitor the optimization of inhibitor molecules was finished using the density function theory (DFT)/B3LYP supplemented with basis set 6-31G. The quantum method was utilized to elucidate quantum parameters, for instance, EHOMO and ELUMO (Energy of highest occupied molecular orbital and Energy of lowest unoccupied molecular orbital) and μ (dipole moment) that were essential to discover the corrosion mechanism for the inhibitor TDIO. Quantum parameters have been computed to Figuring E HOMO, E LUMO, ΔE as in condition 3, chemical hardness (η) as in Eq. (4), hemical softness (σ) as in Eq. (5), global electronic chemical potential (μ) as in Eq. (6) and Electrophilicity index (ω) as in Eq. (7) [21].

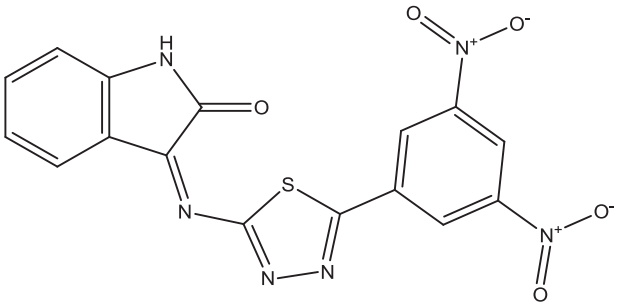
$$\Delta E = E_{LUMO} - E_{HOMO} \tag{3}$$

$$\eta = \frac{1}{2}(E_{HOMO} - E_{LUMO}) \tag{4}$$

$$\sigma = \frac{1}{\eta} \tag{5}$$

$$\mu = \frac{1}{2}(E_{HOMO} + E_{LUMO}) \tag{6}$$

$$\omega = \frac{\mu^2}{2\eta} \tag{7}$$



3-((5-(3,5-dinitrophenyl)-1,3,4-thiadiazol-2-yl)imino)indolin-2-one

Fig. 1. Chemical structures of the corrosion inhibitor.

Results and discussion

Weight loss corrosion screening were done on the surface of mild steel in 1 M hydrochloric acid solution without and with the synthesized corrosion inhibitor namely TDIO over a 5 h as reaction time. Fig. 2 and represents corrosion rates and the inhibition performance respectively for various concentrations of TDIO at 303, 313, 323, 333, and 343 K, respectively. The inhibition efficiencies were calculated based on Eq. (1).

Fig. 2 demonstrates the plot of the CR of TDIO versus the concentrations at deferent temperatures degree. The CR diminished from 0.89 $mg{\cdot}cm^{-2}{\cdot}h^{-1}$ at the inhibitor concentration of 0.1 mM

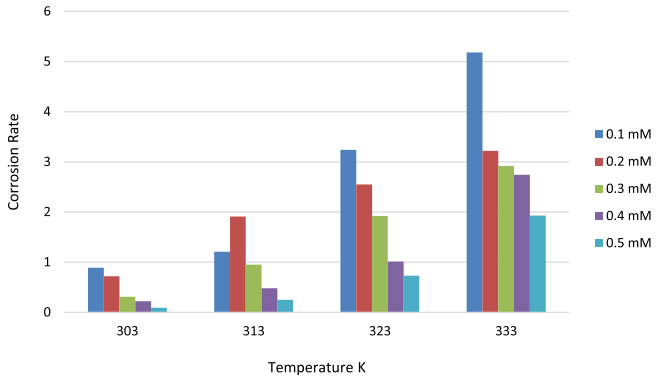


Fig. 2. Impact of concentration of TDIO on corrosion rate at various temperature degrees.

to 0.09 mg·cm^{-2}·h^{-1} at the inhibitor concentration of 0.1 mM in hydrochloric acid solution. CR diminished slightly with increasing concentration at the 313 K to reach 0.25 mg·cm^{-2}·h^{-1} at a concentration of 0.5 mM. At 323 K and 333 as in Fig. 2, the curves demonstrated to have similar shapes as the curves at 303 K and 313 K.

Fig. 3 demonstrate the plot of the inhibition percent vs the concentration of the inhibitor at the temperature degrees of 303, 313, 323 and 333 K respectively. It can be seen that the inhibition performance was not sufficiently affect by the raising of temperature degree from 303 K to 313, especially at the inhibitor concentrations 0.2 mM, 0.3 mM and 0.4 mM; whereas at 0.5 mM concentrations the inhibitor extremely increased the percent inhibition. At the temperature degree 333 K, it has been observe that the concentration of inhibitor has no big impact on inhibition process and this may be due to the denaturation of inhibitor.

Assessment of the results shows that inhibition performance of the investigated inhibitor increased with increasing of concentration. The inhibition efficiencies increased with increasing of inhibitor concentration and this could explained on the basis of amount of adsorption with surfactant coverage molecules, increases with increasing concentrations. The inhibition performance increased parallel regarding to concentration inhibitor increased, that suggests the retardation of surface of mild steel corrosion in inhibited solution compared to uninhibited environment.

It is credited due to increasing in the dynamic surface efficiency (IE%/100). The highest value of inhibition performance, of 90.7% was acquired at 0.5 mM concentration for TDIO. Furthermore, increases in the concentration of inhibitor above the ideal concentration in this study 0.5 mM do not issue any considerable change in the restraint effectiveness. The Arrhenius equation have applied effectively to demonstrate the effect of temperature degrees on the inhibition performance of TDIO as studied compound. It is clarifying via the following equation [28,29].

$$lnC_R = \frac{-E_a}{RT} + lnA \tag{8}$$

where, A, E_a, R and T, represents Arrhenius factor, activation energy, gas constant and absolute temperature respectively.

The values of energy in the without and with TDIO were calculated based on Arrhenius plots that represented in Fig. 4 as in Eq. (9)

$$Slope = -\frac{\Delta E_a}{2.303R} \tag{9}$$

The values of E_a was 90 kJ mol^{-1} for TDIO. The results indicate that the value of E_a in presence of TDIO was higher than that without of TDIO that indicate the presence of TDIO become additional barrier were carried out for mild steel corrosion due to forming protective film that decrease CR [28].

Adsorption isotherm

The adsorption of the TDIO. On surface of mild steel is a considerable process which was related to inhibition efficiency. In this investigation, among many study isotherms, the Langmuir isotherm donate the better proper. The excellent adsorption isotherm in this case was election based on the value of regression coefficient for each studied isotherm. It could be seen that though the values of regression coefficient was more close to ident for Langmuir adsorption isotherm parallel to Temkin and Freundlich adsorption isotherms, however the Langmuir isotherm was not strictly followed as the slope value of are significantly deviated from unit. The Langmuir isotherm can be represented as follows [21–24].

$$K_{ads}C = \frac{\theta}{1-\theta} \tag{10}$$

where Kads, C and θ are desorption constant, concentration of TDIO and surface coverage (θ = IE%/100) respectively.

Kads value of studied inhibitor compound at various temperature degrees was acquired with Langmuir isotherm as shown in Fig. 5. The value standard free energy (ΔG^o_{ads}) to be based on Kads value according to the Eq. (11).

$$\Delta G^o_{ads} = -RTln(55.5K_{ads}) \tag{11}$$

Eq. (11), the value 55.5 represent the water concentration in acidic solution. The values of (ΔG^o_{ads}) give facts about interaction between for TDIO and mild steel surface. Generally, (ΔG^o_{ads}) value

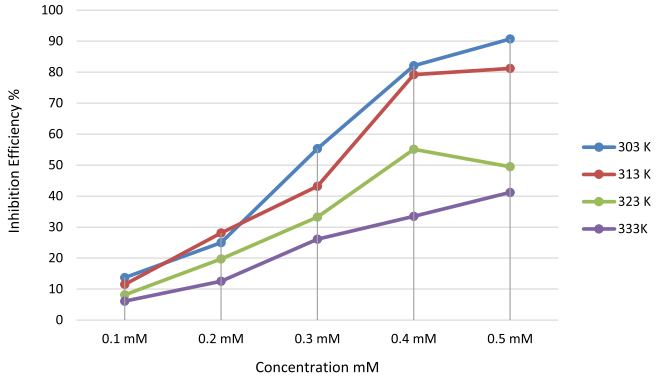


Fig. 3. Impact of concentration of TDIO on inhibition efficiencies at various temperature degrees.

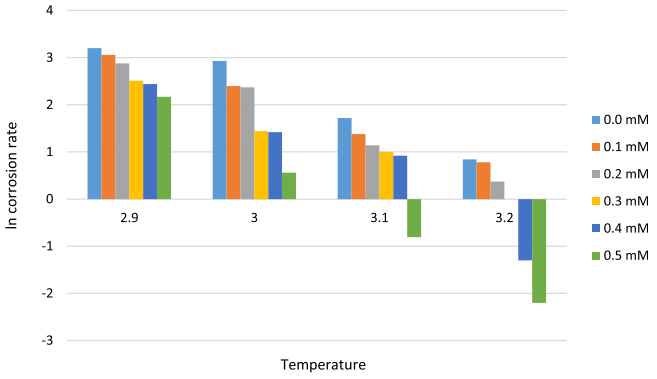


Fig. 4. Arrhenius plot of impact of temperature on the corrosion rate of mild steel in 1 M HCl solution with and without the presence of various conc. of TDIO.

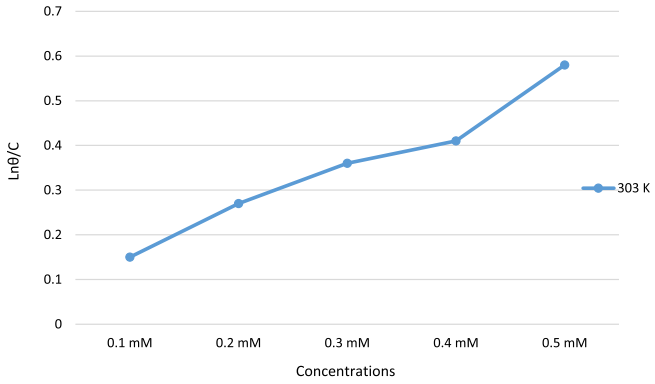


Fig. 5. Langmuir adsorption isotherm for TDIO on surface of mild steel in 1 M HCl at 303 K temperature.

if equal or around to −20 kJ mol^{-1} is lead to physisorption interaction between appositively charged for TDIO molecules and mild steel surface, whereas if (ΔG^{o}_{ads}) equel or around to −40 kJ mol^{-1} related with chemisorption between for TDIO and surface of mild steel. From our results it may be shown that value of (ΔG^{o}_{ads}) in this case was 29.7 kJ mol^{-1} signalize that for TDIO molecules react with the surface of mild steel through physisorption and chemisorption modes [30–33].

Surface morphology studies

Fig. 6a and b elucidate the SEM images of the of mild steel surface coupons that was immersed in acidic solution for 5 h, in presence and absence of TDIO as corrosion inhibitor. The Fig. 6a, imply that SEM image of coupon 1 M of hydrochloric acid as corrosive solution in the absence of TDIO as corrosion inhibitor, that explain a serious damaged in surface of coupon. Moreover 0.5 mM of TDIO as corrosion inhibitor added to the hydrochloric acid solution the surface image as in Fig. 7b was distinguished through effectively protective film, that indicate that the inhibitor TDIO adsorbed on the coupon surface and block it from acidic impact.

Quantum chemical calculations

The studied compound TDIO various from other compounds by the five oxygen atoms and six nitrogen atoms with the two substituted nitro groups in addition to the resonance effect between aryl and 2-imine-1,3,4-thiadiazole groups that linked together to produce molecule with unique and significant properties due to inductive and resonance effects. From the optimized geometrical structure for TDIO, the molecular structure is planar due to the aromaticity of the molecule. The electronic structure of the TDIO was

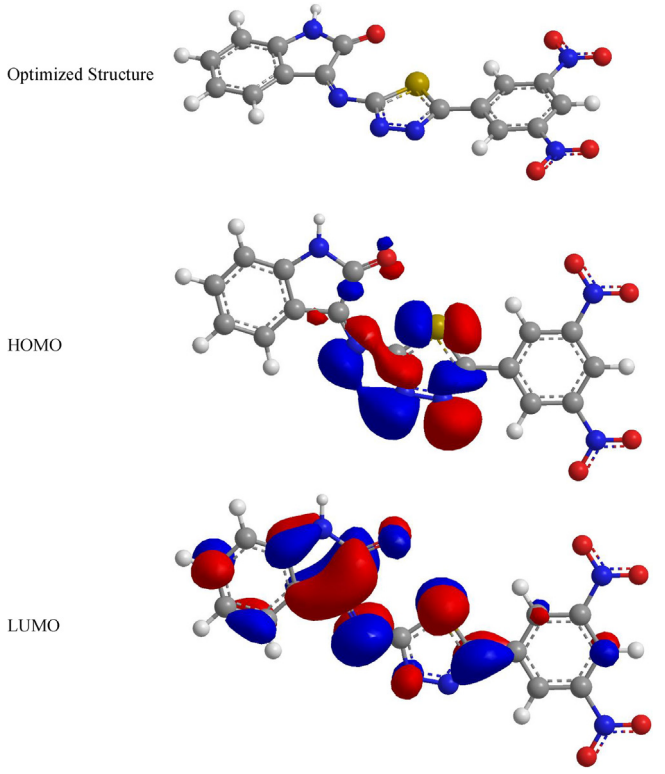


Fig. 7. Optimized structure and the HOMO and LUMO orbitals for TDIO molecule.

elucidate using the DFT/B3LYP with the basic set 6–311G. HOMO and LUMO (highest occupied molecular orbital and lowest unoccupied molecular orbital) studied for TDIO and showed in Fig. 7. The parameters, energy gap (ΔE = ELUMO – EHOMO), dipole moment (μ) and electronegativity (χ) were shown in Table 1. EHOMO showed electron giving ability of the TDIO, and has more electron giving susceptibility compare to other studied inhibitors [34,35]. The electron releasing groups that were aryl and thiadiazole gathering in TDIO increase the electron donating capacity of TDIO molecules as they were demonstrated in above. HOMO and LUMO energies can be characterize as the measure of affinity for electron of TDIO molecules. The energies of LUMO were not offer any orderly patterns. Furthermore, ΔE is second huge parameter that depict the connection of molecules and the coupon surface. The ΔE of TDIO was comprised with reactivity and related with higher inhibition performance contrasting with inhibitors molecules that with high estimation of ΔE. The researched TDIO has variations of energy gap and that was of 2.096 eV as shown in Fig. 7. The relative

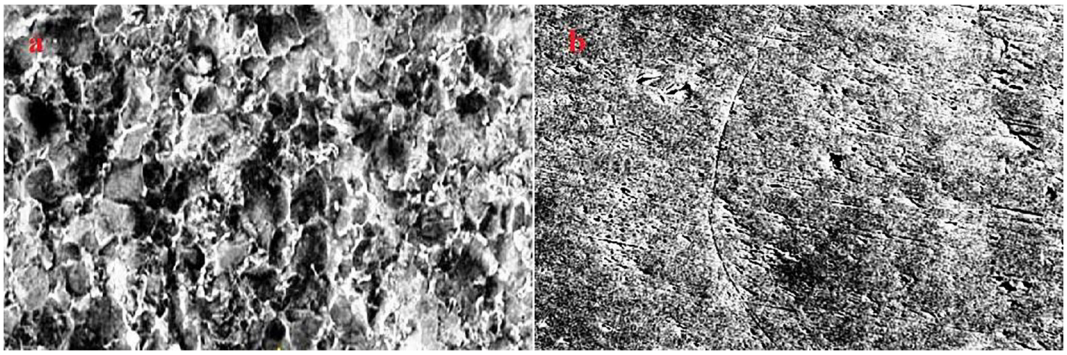


Fig. 6. The SEM images of coupons surface in 1 M of hydrochloric acid in the absence (a) and presence (b) of 0.5 mM of TDIO.

Table 1
Electronic and structural parameters for TDIO molecule.

Parameters	Inhibitor
HOMO [eV]	−7.531
LUMO [eV]	−5.435
ΔE = ELUMO − EHOMO [eV]	2.096
Dipole moment [D]	6.521
Electron affinity (A)	7.531
Ionization potential (I)	5.435
Electronegativity χ $\left[\chi = \frac{I+A}{2}\right]$	6.553
Global hardness $\left[\eta = \frac{I-A}{2}\right]$	1.048
Chemical softness $\left[S = \frac{1}{\eta}\right]$	0.9541

electron giving ability of TDIO could be upheld by the electronegativity (χ). Largely, the molecules with least χ are connected with higher electron giving propensity showed higher restraint proficiency contrasting with molecules with higher estimation of (χ). In this examination, the estimations of (χ) completely support our approach results. The dipole moment is a critical character that could be used to connect the relative collaboration of inhibitor molecules with the alloy surface. Generally, molecules for the inhibitors that have dipole moment with high value are connected with polarizability having high value and excellent effective surface area and hence should be excellent corrosion inhibitors as comparing with other inhibitor with having dipole moment with low values. Regarding to our work, the value of dipole moment of TDIO was 6.521 that imply NANT has perfect inhibition performance surface area and has excellent inhibition performance. Furthermore, from Table 1 it could be concluded that the dipole moment of TDIO has higher value comparing to that of water and this indicating TDIO molecules have higher efficiency to react either physically or chemically with the coupon surface. From above, TDIO molecules mat be adsorbed on the surface of coupon through substituent of water molecules [36–38]. HOMO and LUMO results which computed for TDIO, shown that the HOMO orbital are created via similar active center. The LUMO orbital of TDIO was shifted to dinitrobenzene ring. The LUMO orbital of the TDIO molecule were located at the part of molecule that was aryl ring.

Softness with hardness have been named universal reactivity descriptor that were computationally calculated by DFT [39]. They were used to evaluate the stability and reactivity of molecule. Hardness explain the impedance towards the polarization of the electron of molecule under little interruption of chemical reaction. Hard molecule has great energy gap and soft molecule has good energy gap [34]. In this work, the TDIO has hardness value 1.048 and it was proved that the corrosion inhibitor molecules that have the hardness with minimum value was predictable to be an excellent inhibitor. Transfer of electron in easy way need maximum value chemical softness [35]. TDIO has with the chemical softness value of 0.9541 eV so, it has the maximum inhibition efficiency.

Conclusion

The inhibition impact of new synthesized compound namely TDIO on mild steel corrosion in 1 M HCl were studied utilizing of weight loss and scanning electron microscopy techniques. Theoretical quantum chemical calculations have been utilized to corroborate experimental findings. The weight loss results demonstrate that TDIO inhibit the acid induced corrosion and the inhibition efficiency increase with increase in concentration. The highest inhibition efficiency was 90% that showed the highest protection performance against corrosive solution. TDIO molecules inhibit mild steel corrosion in 1 M HCl by adsorbing on the steel surface and form protective film through chemisorption and physisorption. SEM images revealed that TDIO adsorbed on mild steel surface and form protective film that shield the surface from direct impact of corrosion in corrosive solution. Molecular quantum chemical calculations demonstrate that the reactive sites in the TDIO molecules are the oxygen and nitrogen atoms with pi-electron.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.rinp.2018.02.055.

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