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Synthesis and corrosion inhibition application of NATN on mild steel surface in acidic media complemented with DFT studies

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ABSTRACT

The corrosion inhibition effectiveness of thiosemicarbazide compound, namely 3-nitro-5-(2-amino-1,3,4-thiadiazolyl)nitrobenzene (NATN), on mild steel in 1 M hydrochloric acid media has been investigated by weight loss technique. The results exhibit that the corrosion ratio of mild steel was reduced regarding to adding NATN. The corrosion inhibition rate for the NATN was 92.3% at the highest investigated NATN concentration. From the weight loss results it could be concluded that NATN with sulfur, nitrogen and oxygen atoms has clarified best corrosion inhibition achievement comparing to 3,5-dinitrobenzoic acid. Regarding to theoretical studies, DFT was employee to figured geometrical structure and electronic characteristics on NATN. The investigation have been extensive to the HOMO and LUMO analysis to evaluate the energy gap, Ionization potential, Electron Affinity, Global Hardness, Chemical Potential, Electrophilicity, Electronegativity and Polarizability.

Introduction

Alloys are exceedingly applied in manufacture processing applications, and might be undergo to various acidic mediums. Acids were aggressive on the metal surface and progress to serious corrosion issues. Corrosion have been controlled by employing natural or synthetic inhibitors. Most of the utilizing inhibitors were from organic molecules with hetro-atoms such as nitrogen, sulphur, phosphorus and oxygen in addition to double bonds or aromatic rings in their structure, that adsorbed on the surface of the metals [1]. Corrosion inhibitors usually have the ability to control the corrosion through forming different kinds of films in various route, such as adsorption through formation of precipitates or through forming of inactive layer on the surface of the metal. Several organic inhibitors impeded the corrosion process by forming invisible thin film on the metal surface [2]. The equipment's naphtha industries are usually synthetic from steel. Ordinarily fifteen-percentage acid was pumped due to etching the rocks, that were integrated into the conducted tubes. This operation improves the permeability of the petrol reservoir, that in turn rise the recovery efficiency of petrol. Without the corrosion inhibitor, there would be spoilage of industrial equipment's, and hence the corrosion inhibitors would be efficient route to diminish the corrosion. Usually utilization of corrosion inhibitors in corrosive solutions were compounds with heteroatoms in addition to double bonds, aromatic ring in the structure of these compounds [3]. Corrosive media are exceedingly employees in industries for various approaches such as pickling, cleaning, descaling and acidizing. Through the past era, considerable methods were utilized to diminish the corrosion happed by corrosive media. One of these methods for minimizing corrosion is the employee of inhibitors [4]. The employment of organic coating was the most classical technique to protect alloys in the acidic and basic solutions. However, decay process progress to damage the protective coating [5]. The inhibitor may then combine with freshly generated Fe^{2+} ions on the steel surface, forming metal inhibitor complexes [6–10]. To extend our previous work on designing novel inhibitor molecules [11–17], the 3-nitro-5-(2-amino-1,3,4-thiadiazolyl)nitrobenzene (NATN), was synthesized. The molecular structure of this inhibitor is determined by CHN analysis, FTIR spectroscopy, and NMR spectroscopy. The abilities of this molecules to inhibit MS corrosion in an acidic solution are determined by the weight loss method and scanning electron microscopy (SEM). The corrosion inhibitor was synthesized and employee in this investigation were shown in Fig. 1.

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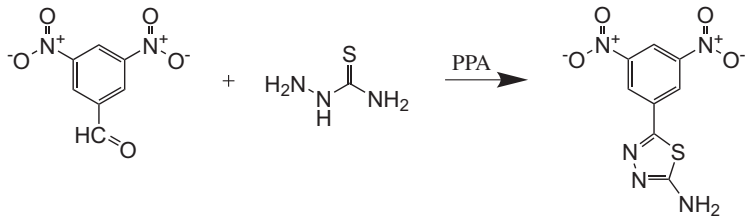

Fig. 1. Chemical structures of the investigated inhibitor, NANT.

Materials and methods

Inhibitor synthesis

All chemicals have been obtaining from Sigma-Aldrich Malaysia. Shimadzu FTIR-8300 spectrometer was employed to record FTIR spectra. Carlo Erba 5500 CHN elemental analyzer was utilized to figuration the CHN. Bruker Spectrospin instrument equipped with 300 MHz UltraShield magnets was performed to record the spectra of the synthesized compounds and the utilized solvent and internal standard were DMSO d_6 and TMS respectively.

Synthetic procedures 3-nitro-5-(2-amino-1,3,4-thiadiazolyl) nitrobenzene

Mixture of equimolar of (0.1 mol) 3-nitrobenzoic acid and thiosemicarbazide has been was poured to polyphosphoric acid and stirred at 90 °C for 4 h. Cooled then added ice to the mixture. Alkalized by ammonium hydroxide then filtered and dried [18]. Yield, 57%; mp 244 °C. FT-IR; 3451.3 (amino group), 3072.6 (C—H aromatic), 16599.3 (C=N azomethane), 1459.2 (C—N nitro group). 1H NMR; δ: 6.61 (s, NH2); 7.71–7.84 (m, Ar-H); 8.95 (d, 1H, Ar-H). 13C NMR: 168.3.6, 155.8, 135.2, 127.9 and 121.8. CHN: C, 35.11 (35.96); H, 1.94 (1.89); N, 26.35 (26.21).

Spaceman preparation

The mild steel samples were a composition of C (0.21%), Si (0.38%), Mn (0.05%), P (0.09%), Al (0.01%), and Fe (99.21%) have been cuts mechanically to small coupons for weight loss investigation. Preceding to all methodological approaches, the coupons were cleaned regarding to the standard technique namely ASTM G1-03 [19]. The corrosive solution 1.0 M hydrochloric acid has been prepared and employee for all the experiments. The testing solution was prepared using 1.0 M HCl solution with different concentrations of NANT: 0.1, 0.2, 0.3, 0.4 and 0.5 mM. The solution in absence of NANT was considered as blank for comparison. All experiments have been done at 303 ± 1 K by means of thermostat water bath.

Weight loss measurements

The mild steel coupons (cleaned and weighed) in triplicate were immersed in HCl medium with/without various concentrations of NANT for 1, 2, 5 and 10 h at 303 K, respectively. Moreover, the coupons of mild steel were immersed in corrosive medium with and without of NANT at the concentration of 5 mM for 1, 2, 5 and 10 h at deferent temperatures degrees that were 303, 313, 323 and 333 K, respectively. At that point, the coupons were ejecting, scoured with a brush, cleaned by water and acetone, at that point drying and weighing through analytical balance.

The values of inhibition efficiencies (*%IE*) have been calculated through employee the Eq. (1).

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

where w_o (weight loss in absence of NANT) and w_1 (weight loss in presence of NANT).

The CR (corrosion rates) has been specified through employee the Eq. (2) [20,21].

$$C_R = \frac{87.6w}{atp} \tag{2}$$

Surface characterization

Morphology of the surface of mild steel coupons previously, then after the inundated in corrosive medium in absence and presence 0.5 mM NANT for 5 h at 303 K were describe by scanning electron microscope, SEM.

Calculation methods

Quantum chemical calculations the optimization of synthesized molecule has been done utilizing the density function theory (DFT)/B3LYP complemented with basis set 6-31G. The quantum approach was used to figure some quantum parameters, for example, E LUMO (lowest unoccupied molecular orbital energy) and μ (dipole moment) that were important to find out the mechanism of inhibition. Quantum parameters have been calculated to Figuring E_{HOMO}, E_{LUMO}, ΔE as in Eq. (3), chemical hardness (η) as in Eq. (4), chemical softness (σ) as in Eq. (5), global electronic chemical potential (μ) *as in* Eq. (6) and Electrophilicity index (ω) as in Eq. (7) [22].

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

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

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

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

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

Results and discussion

As seen from Fig. 2 that corrosion rates decrease while the inhibition efficiencies 3, increase with incremental concentration of

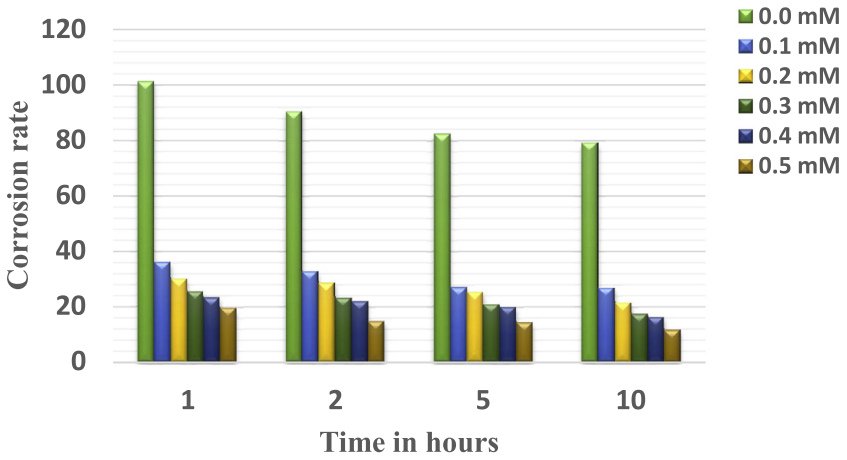

Fig. 2. The corrosion rate curves for mild steel in absence and presence of different concentrations of NANT.

inhibitor. However, inhibition efficiencies of inhibitor suggesting a better inhibitive capacity towards corrosion. It is discovered that the maximum efficiency reaches 92.3%. Assessment of the results demonstrate that inhibition effectiveness of the investigated compound increments with expanding of concentrations. It is credited because of increment in the dynamic surface efficiency (IE%/100). The highest value of inhibition efficiency, of 92.3% was acquired at 0.5 mM concentration for NANT. Further, increases in the inhibitor concentration do not issue any considerable change in the restraint effectiveness showing that 0.5 mM is ideal inhibitor concentration. The inhibition efficiency of NANT as investigated molecule could be can be clarified impute to presence of the 2-amino-1,3,4-thiadiazole attached to the dinitrobenzene moiety. The best inhibition achievement of the NANT was impute to presence of electron withdrawing for two nitro groups attached to the phenyl at benzene moiety. These electron groups in NANT molecules increase the resonance capability of NANT molecules toward conjugations owing to presence of unshared electron pairs on the nitrogen, sulfur and oxygen atoms and thus increase the inhibition performance (Fig. 3.).

Effect of temperature

The weight loss methodology was also performed at various temperature continue from 308 to 338 K to consideration the impact of temperature on the inhibition effectiveness of the NANT molecules and to figuration the kinetic parameters in addition thermodynamic parameters. The results are pictorial in the Fig. 4, signalize that inhibition efficiency of the NANT molecules diminution with rising temperatures.

The diminution inhibition performance on rising temperature of the solution may be imputing to increasing in NANT molecules mobility that in turn reduction the interactions between mild steel surface and NANT molecules [26]. Furthermore, quick scratching and desorption of the adsorbed NANT molecules at higher temperature degree might be diminution the inhibition performance. The Arrhenius equation may be applied effectively to demonstrate the impact of temperature on the inhibition efficiency of NANT as investigated molecules. It is clarify through following equation [23,26].

$$lnC_R = \frac{-E_a}{RT} + lnA \tag{5}$$

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

The values of energy in the absence and presence of NANT molecules were computed regarding to Eq. (6), from Arrhenius plots that represented in Fig. 5.

$$Slope = -\frac{\Delta E_a}{2.303R} \tag{6}$$

The values of E_a was 92 kJmol^{-1} for NANT. It clears from the obtained results that value of E_a in presence of NANT molecules as corrosion inhibitor was higher than that in absence of NANT molecules which obviously signalize that in presence of NANT

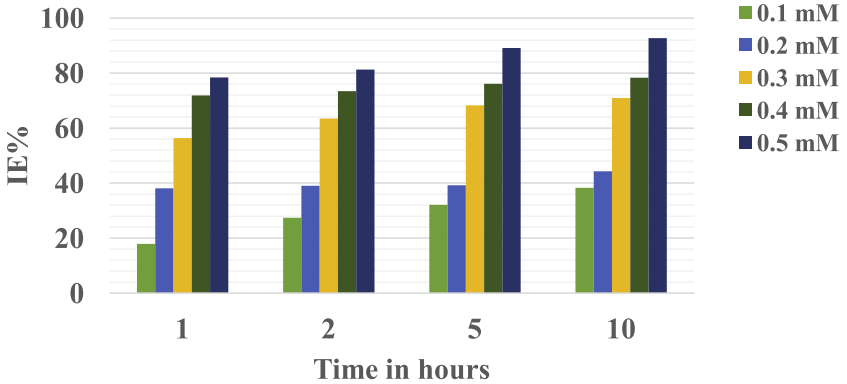

Fig. 3. The inhibition efficiencies for mild steel in absence and presence of different concentrations of NANT at 303 K.

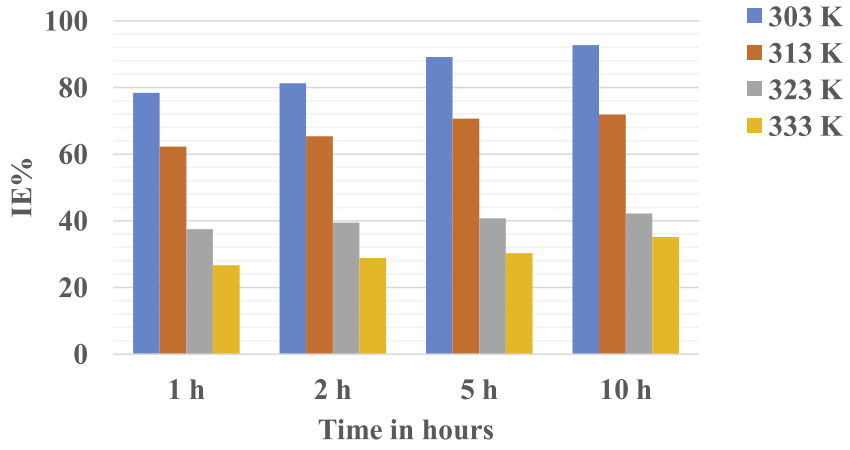

Fig. 4. The inhibition efficiencies for mild steel at different temperatures and deferent times.

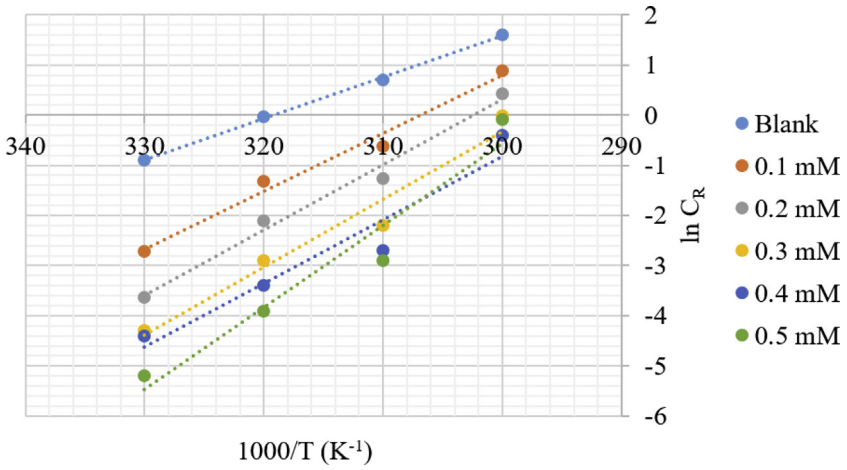

Fig. 5. Arrhenius plots for NANT at various temperatures.

molecules additional energy barrier were carried out for mild steel corrosion due to forming protective film that diminution the corrosion rate [27].

Adsorption isotherm

The adsorption of the NANT molecules as corrosion inhibitor on the mild steel surface is a significant approach that is related with inhibition performance. Based on the quality of adsorbent and/or adsorbate, adsorption might be chemically or physically. Various adsorption isotherms were proposed to characterize the adsorption approaches. In this study, among several investigated isotherms, the Langmuir isotherm donate the better proper. The superior adsorption isotherm in this case was election based on the value of regression coefficient (R_2) for each investigated isotherm. It could be seen that though the values of R_2 were more close to unity for Langmuir adsorption isotherm parallel to Temkin and Freundlich adsorption isotherms, whilst the Langmuir isotherm was not severely followed as the values of slopes are significantly deviated from unity. The Langmuir isotherm can be represented as follows [22–25]:

$$K_{ads}C = \frac{\theta}{1-\theta} \tag{6}$$

where K_{ads}, C and θ are adsorption-desorption constant, concentration of NANT and surface coverage ($\theta = IE\%/100$) respectively.

K_{ads} values of investigated inhibitor molecules at various temperatures were acquired with Langmuir isotherm plot demonstrate in Fig. 5. The standard free energy value (ΔG^o_{ads}) to be based on K_{ads} value regarding to the Eq. (7) (Fig. 6):

$$\Delta G^o_{ads} = -RTln(55.5K_{ads}) \tag{7}$$

Eq. (7), the value 55.5 symbolize the water concentration in corrosive medium. The values of (ΔG^o_{ads}) and K_{ads} were demonstrated in Table 1.ΔG^o_{ads} values of give facts concerning interaction between NANT molecules as corrosion inhibitor and surface of mild steel. Usually, the value of ΔG^o_{ads} that equal or around to $-20\,kJmol^{-1}$ is linked with physisorption interaction between appositively charged NANT molecules and surface of mild steel, while the value of ΔG^o_{ads} $-40\,kJmol^{-1}$ around related with chemisorption between NANT molecules and surface of mild steel. From the results pictorial in Table 1 it could be shown that value of (G^o_{ads}) in this case was $32.85\,kJmol^{-1}$ signalize that NANT molecules react with the surface of mild steel through together physisorption and chemisorption modes [28–31].

Surface morphology studies

Fig. 7a and b respectively demonstrate the SEM pictures of the surface of mild steel specimen that was exposure to the corrosive solution for 5 h, in presence and absence of NANT as corrosion inhibitor. The surface of mild steel was analyzed and demonstrated

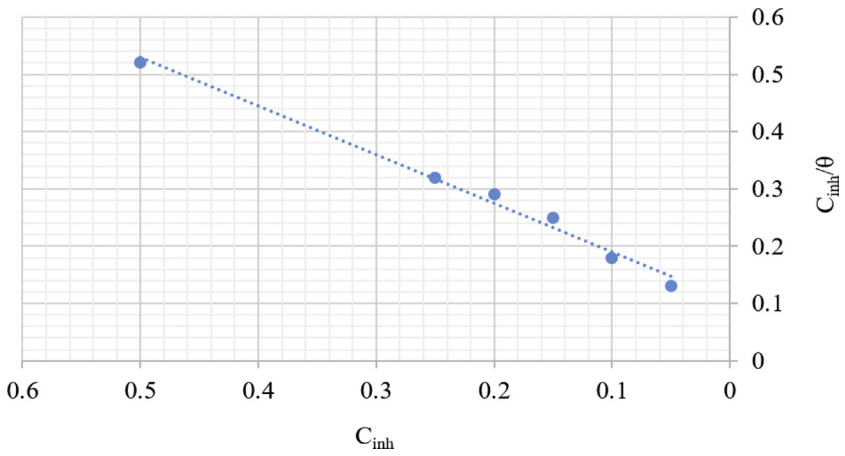

Fig. 6. Langmuir adsorption isotherm for NANT on surface of mild steel in 1 M HCl at 303 K temperature.

Table 1
Electronic and structural parameters for NANT molecule employing DFT approach.

Parameters	NANT
HOMO [eV]	−7.564
LUMO [eV]	−3.861
ΔE = ELUMO − EHOMO [eV]	3.763
Charge/Charge	2.1680
Dipole moment [D]	10.3259
Charge/Dipole	−24.5384
Electron affinity (A)	7.564
Ionization potential (I)	3.861
Electronegativity χ [$\chi = \frac{I+A}{2}$]	5.7125
Global hardness [$\eta = \frac{I-A}{2}$]	1.8515
Chemical softness [$S = \frac{1}{\eta}$]	0.5401

significant surface after exposing to the corrosive media. Fig. 7b, imply that SEM picture of surface of mild steel in 1 M of hydrochloric acid as corrosive solution in the absence of NANT as corrosion inhibitor, that obviously demonstrates a major damaged surface Fig. 7b. In the other hand 0.5 mM of NANT as corrosion inhibitor added to the corrosive solution the surface picture (Fig. 7a) was distinguished through effectively protective film, that indicate that the investigated NANT adsorbed on the surface of mild steel and block it from corrosive solution.

Quantum chemical calculations

The investigated compound NANT deferent from other compounds by the number of oxygen and nitrogen atoms in addition to the two substituted nitro groups in addition to the resonance effect between aryl and amine-1,3,4-thiadiazole groups that linked together to produce molecule with unique and significant properties due to inductive and resonance impacts. From the optimized geometrical structure, it can be say that the studied molecular structure is planar due to the aromaticity of the molecule. The electronic qualities of the molecules changes because of nitro groups. The electronic qualities of the NANT was figured utilizing the strategy DFT/B3LYP with the premise set 6-311G. HOMO and LUMO highest occupied molecular orbital and lowest unoccupied molecular orbital) examined for NANT as inhibitor compound and were appeared in Fig. 8. The studied parameters that were named energy of frontier molecular electrons, energy gap (ΔE = ELUMO − EHOMO), dipole moment (μ) and electronegativity (χ) were appeared in Table 1. EHOMO demonstrates electron-giving capacity of the corrosion inhibitor compound, and in this study. It clearly demonstrates that NANT compound has more electron giving susceptibility compare to other studied inhibitors. The inclination of estimations of EHOMO spotted for explored inhibitor compound very help the test consequences of inhibition performance. The electron releasing groups that were aryl and thiadiazole gathering in NANT increment the electron donating susceptibility of NANT molecules as they were appeared in above. In disparity to HOMO energies, energies estimation of LUMO can be characterize as the measure of affinity for electron of NANT molecules. In this examination the estimations of energies of LUMO were not offer any orderly patterns. Furthermore, ΔE is second huge parameter that depict the connection of particles and the surface of the metal. For the most part, the lower esteem ΔE of inhibitors are comprised with reactivity and related with higher inhibition performance contrasting with inhibitors molecules that with high estimation of ΔE. The researched compound NANT has little variations of energy gap and that was of 3.763 eV as shown in Fig. 8. The relative electron giving ability of the researched inhibitor NANT could be

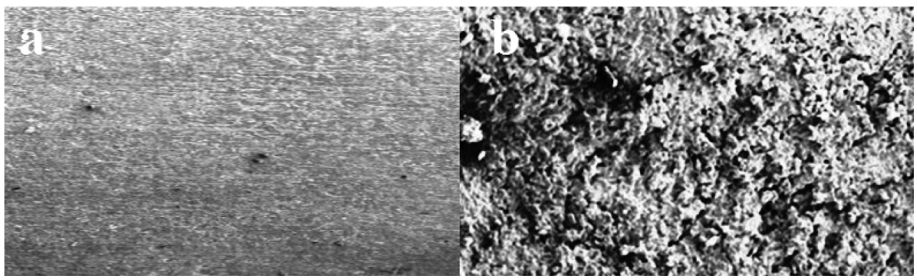

Fig. 7. The SEM picture of surface of mild steel in 1 M of hydrochloric acid as corrosive solution in the presence (Fig. 7a) and absence (7b) of 0.5 mM of NANT as corrosion inhibitor.

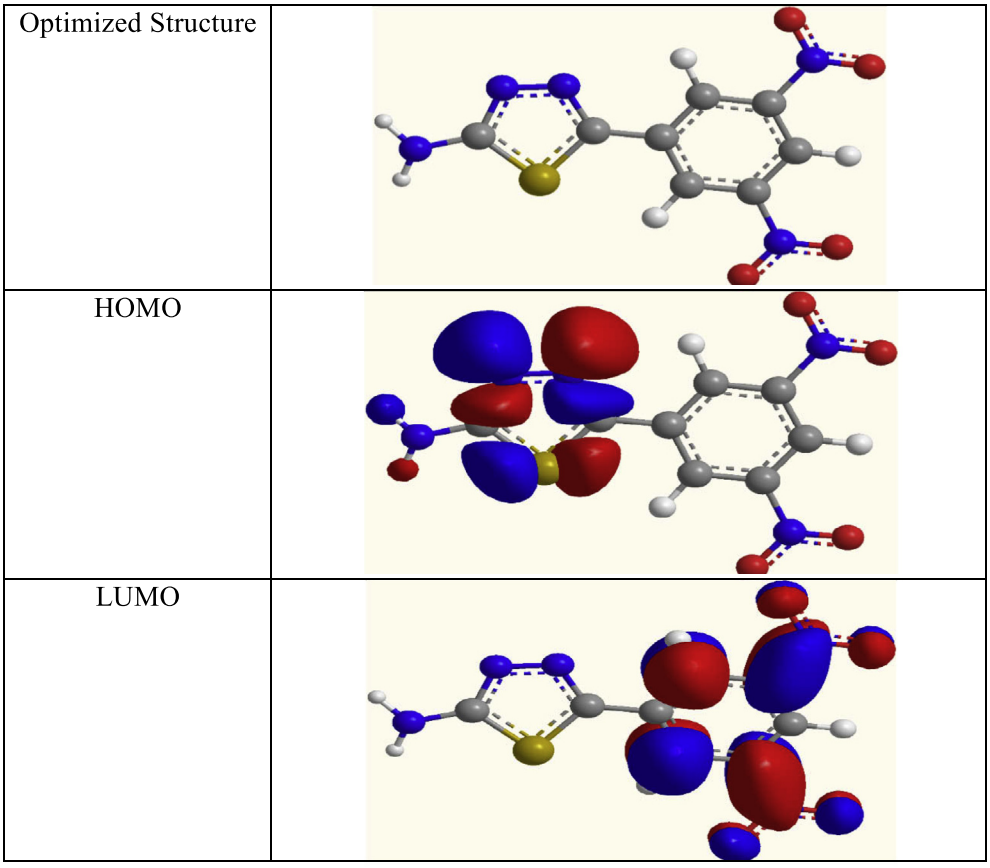

Fig. 8. Optimized structure and the HOMO and LUMO orbitals for NANT molecule in employing DFT approach.

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 NANT inhibitor molecule was 10.3259 that imply NANT has perfect inhibition performance surface area and has excellent corrosion inhibition. Furthermore, from Table 1 it could be concluded that the dipole moment of NANT as examined corrosion inhibitor has higher value comparing to that of water and this indicating NANT molecule has higher activity to react either physically or chemically with the alloy surface. From above, NANT molecules could be adsorbed on the mild steel surface via substituent of water molecules [32–34]. HOMO and LUMO results which computed theoretically for the examined compound NANT, shown that the HOMO orbital are created via similar active center. The LUMO orbital of NANT was shifted to dinitrobenzene ring. The LUMO orbital of the NANT molecule were located at the part of molecule that was aryl ring.

Chemical softness with hardness were the essential chemical characteristics, named universal reactivity descriptor which were computationally justified via the field of DFT [35]. These were the critical qualities to assess the stability with the reactivity of the studies molecule. Unmistakably the hardness for the most part demonstrates 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 [36]. In this work, the NANT has hardness value 1.8515 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 [37]. NANT has with the chemical softness value of 0.5401 eV so; it has the maximum inhibition efficiency.

Conclusion

The inhibitive effects of five carbazole derivatives (CZs) on mild steel corrosion and bio-corrosion in 1 M HCl and microbial environments were investigated using electrochemical techniques, weight loss measurements, scanning electron microscopy (SEM) and energy dispersive X-ray (EDX) techniques. Theoretical quantum chemical calculations and molecular dynamic simulation studies were used to corroborate experimental findings. The following conclusions can be drawn from the results:

1. Potentiodynamic polarization measurements revealed that the studied CZs are mixed-type corrosion inhibitors with predominantly cathodic inhibitive effects.
2. Both electrochemical and weight loss results showed that all the compounds inhibit both the acid (1 M HCl) induced corrosion and microbial corrosion and their inhibition efficiencies increase with increase in concentration.

3. The highest inhibition efficiencies were recorded for THCZ and EHCZDCZ in 1 M HCl, while CZ showed the highest protection efficiency against MIC.
4. The studied inhibitor molecules inhibit mild steel corrosion in 1 M HCl by adsorbing on the steel surface and form protective film. Their adsorption obeys Langmuir isotherm and occur mainly via physisorption.
5. SEM images and EDX analyses also revealed that the studied compounds adsorbed on mild steel surface and form protective film that shield the surface from direct effect of corrosion in acidic and SRB media.
6. Molecular quantum chemical calculations showed that the reactive sites in the inhibitor molecules are mainly the N-atom of the carbazole ring, the pi-electron centres, and the other substituent heteroatoms (Br in DBCZ, O—H in HCZ, and C═O in EHCZDCA).
7. Molecular dynamic simulations revealed that the studied molecules have strong interactions with Fe surface.

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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.2018.02.007.

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