

Comprehensive evaluation of 1-(2,5-dihydroxyphenyl) ethanone thiosemicarbazone as a corrosion inhibitor for mild steel in HCl: integrating weight loss measurements and quantum chemical calculations

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Abstract

This research article investigates the corrosion inhibitory properties of 1-(2,5-dihydroxyphenyl) ethanone thiosemicarbazone (DETSC) on mild steel in HCl. Experimental results reveal that a 0.5 mM concentration of DETSC exhibits an impressive inhibition efficiency of 94.2% at 303 K. The adsorption of DETSC molecules onto the mild steel surface adheres to the Langmuir model, resulting in a robust and dense protective film. The effect of concentration on inhibition efficiency was examined across various DETSC concentrations (0.1, 0.2, 0.3, 0.4, 0.5, and 1 mM) at 303 K and different immersion periods (1, 5, 10, 24, and 48 hours). Findings indicate that inhibition efficiency increases with concentration, though there is a slight decrease after 24 hours of immersion. Temperature-dependent corrosion inhibition was also studied at 303, 313, 323, and 333 K, using an optimum immersion time of five hours and varying inhibitor concentrations. Results demonstrate that an increase in temperature leads to a decrease in inhibition efficiency. The experimental approach was complemented with theoretical calculations based on Density Functional Theory (DFT) to gain a comprehensive understanding of the anticorrosive performance and inhibition mechanism. The integrated approach provides precise insights into the corrosion inhibiting efficiency of DETSC under varying physical and chemical conditions of the mild steel surface. These findings offer novel strategies for developing and enhancing practical corrosion inhibitors.

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1. Introduction

The problem of corrosion is still relevant in many industries because metal instruments, especially made of mild steel, predominate there [1, 2]. Corrosion can lead to a number of negative repercussions, the outcome often being both financial loss and damage or loss of life. Besides, the danger of corrosion increases because of the constant use of hydrochloric acid in industrial environments [3]. The increasing use of mild steel in a variety of industrial applications makes comprehending the development of effective corrosion improvement methods an urgent task. One of the most promising ways to do so is to make use of organic corrosion inhibitors [4–6]. Being based on organic compounds, these inhibitors possess truly powerful features essential for reducing corrosion due to the fact that they develop protecting covers on metal surfaces. These functions limit the intensity of corrosive actions. The use of heteroatoms including nitrogen, oxygen, and sulfur in organic inhibitors has gained significance [7, 8]. They increase the effect of the inhibitors by promoting their interaction with metals due to the formation of strong bonds. It is possible to assume that organic inhibitors containing heteroatoms can be viewed as more reliable since such elements contribute to the ingestion of stable protective films on the surface of metals [9]. It is extremely important to disrupt the process of corrosion due to nitrogen, sulfur, and oxygen-containing organic inhibitors coordinate with metal ions to minimize the concentration of aggressive and oxidative species [10]. Moreover, being widely used in various industrial processes from cleaning to surface treatment, hydrochloric acid application makes necessary to develop an effective way of corrosion control [11]. The properties of HCl make it an aggressive acid necessitating proactivity in any search for inhibitors that can work effectively under such conditions [12]. As such, 1-(2,5-dihydroxyphenyl) ethanone thiosemicarbazone (DETSC), is an interesting agent that may be used with HCl as it is rich in sulfur and oxygen groups. As such, its inhibitive properties should be considered to progress the development of efficient methods of protection against corrosion, especially such ones, which include heteroatoms. In this project a combination of Density Functional Theory calculations, which is a highly effective tool in corrosion inhibition research, will be used to investigate molecular interactions between DETSC and metal surfaces [13–15]. This is done to elucidate once and for all the secrets of the anti-corrosion potential of the inhibitor and to make an informed contribution to the study of the role heteroatoms play in increasing efficiency of organic inhibitors in a broader sense. Hence, it can be hoped that one of the outcomes of the proposed study will be that it may not only be used by the academics to better understand how it operates, but it may also be used by the Industry to develop and improve organic inhibitors that can be used to prevent corrosion in chemical environments.

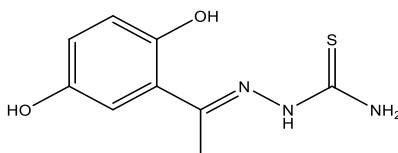


Figure 1. The molecular structure of DETSC.

2. Experimental part

2.1. Composition of material samples

The mild steel coupons utilized in this investigation had a rectangular shape, measuring 2.0 cm×2.5 cm×0.1 cm. The material composition, comprising 0.21 wt.% carbon, 0.09 wt.% phosphorus, 0.05 wt.% manganese, 0.038 wt.% silicon, 0.01 wt.% aluminum, 0.050 wt.% sulfur, and iron (balance), closely mirrors the typical composition of mild steel. Before experimentation, the specimen surfaces underwent meticulous mechanical polishing using various emery papers. Subsequently, the samples were cleansed with double-distilled water, degreased with acetone, and subjected to drying within a desiccator. The hydrochloric acid solution (1 M) used in the experiments was freshly prepared by diluting 37% analytical grade hydrochloric acid with distilled water.

2.2. Weight loss measurements

The weight loss experiments were carried out using a freshly prepared 1 M hydrochloric acid solution as the corrosive environment. Gravimetric weight loss techniques were approved by evaluating the weight loss in the presence and absence of DETSC as a corrosion inhibitor in the corrosive medium. Various concentrations of DETSC electrolytes to the gravimetric experiments (0.1, 0.2, 0.3, 0.4, 0.5, and 1.0 mM) [16, 17]. Gravimetric weight loss experiments were selected for different immersion times, namely, 1 hour, 2 hours, 5 hours, 10 hours, and 24 hours. In all the experiments, the temperatures of the electrolytes were maintained at constant values by the assistance of a water bath, and the controlling was achieved using a thermostatically regulated water bath. Corrosion coupons were immersed in the electrolytes at different applicable temperatures of 303 K, 313 K, 323 K, and 333 K, respectively, for a fixed time period of five hours. This experiment was carried out as a triplicate experiment to improve precision, and the average values of weight loss were calculated. The corrosion rate (C_R) was recorded, the surface coverage (θ) and the inhibition efficiency (IE) were calculated from the gravimetric weight loss data using ASTM method by using Equations 1–3 [18, 19].

$$C_R = \frac{87.6W}{dat} \quad (1)$$

W is the weight loss, d is the density, a is the surface area and t is the immersion time

$$IE\% = \frac{C_{R(\text{in absence of inhibitor})} - C_{R(\text{in presence of inhibitor})}}{C_{R(\text{in absence of inhibitor})}} \cdot 100 \quad (2)$$

$$\theta = \frac{C_{R(\text{in absence of inhibitor})} - C_{R(\text{in presence of inhibitor})}}{C_{R(\text{in absence of inhibitor})}} \quad (3)$$

Equation 3 assumes a blocking mechanism of action, where the inhibitor molecules adsorb onto the metal surface, thereby blocking active sites and hindering electrochemical reactions. This assumption is supported by the observed adsorption behavior and the formation of a protective monolayer.

2.3. Computational study

Using the density functional theory, the electronic structure of the DETSC molecule was studied computationally through a quantum chemical modeling. The aforementioned calculations were performed usually by the B3LYP functional method with a 6-31G basis set and then the geometry optimization of the DETSC molecule was done. The HOMO – Highest Occupied Molecular Orbital and LUMO – Lowest Unoccupied Molecular Orbital were determined to be frontier molecular orbitals. These orbitals were used in determining crucial parameters, including energy gap (ΔE), global hardness (η), softness (σ), absolute electronegativity (χ) and number of transferred electrons (ΔN) by using Equations 4–8 below [20, 21].

$$\Delta E = E_{\text{HOMO}} - E_{\text{LUMO}} \quad (4)$$

$$\eta = -\frac{E_{\text{HOMO}} - E_{\text{LUMO}}}{2} \quad (5)$$

$$\sigma = \frac{1}{\eta} \quad (6)$$

$$\chi = -\frac{E_{\text{HOMO}} + E_{\text{LUMO}}}{2} \quad (7)$$

$$\Delta N = \frac{7 - \chi}{2\eta} \quad (8)$$

3. Results and Discussion

3.1. Weight loss measurements

Corrosion rate (CR) of mild steel in HCl at 1 M was evaluated using weight loss measurement at 303, 313, 323, and 333 K in the presence of DETSC. Figure 2 shows that the increase in DETSC concentration at 303 K enhanced the inhibition efficiency remarkably. At 0 mM inhibitor concentration, the C_R of the mild steel was $4.31 \text{ mg} \cdot \text{cm}^{-2} \cdot \text{h}^{-1}$. However, at the optimum concentration $0.32 C_R$, the corrosion rate decreased markedly. The reduction in weight loss with increasing concentration of the inhibitor revealed the corrosion inhibition effect of DETSC on mild steel in HCl [22]. DETSC was highly effective with the inhibition efficiency reaching 94.2% at 0.05 mM concentration after 5 h of immersion. The interaction between mild steel and DETSC was controlled by the presence of nitrogen and sulfur heteroatoms. DETSC underwent a chemical reaction with the mild steel surface

leading to inhibition efficiency. The resonance effect and higher reactivity of the compound due to its stability also enhanced the inhibition of mild steel corrosion in hydrochloric acid [23].

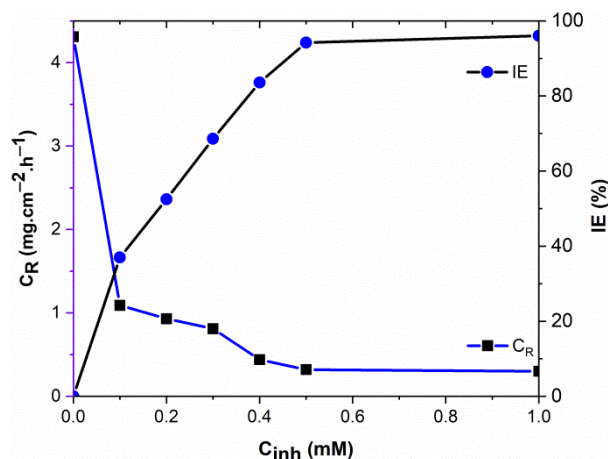


Figure 2. Variation of C_R and IE% with different concentration of DETSC for 5 hours as immersion time at 303 K for mild steel in 1 M HCl.

3.2. Effect of immersion time

Time-dependent investigations in the field of the effects of corrosion inhibitors are essential for the codependency of the interaction between corrosion and inhibitors. The stability of the protective film based on DETSC and its adsorption rate was investigated within the 1 hour, 5 hours, 10 hours, 24 hours, and 48 hours of immersion in Figure 3. The results were presented in the form of a graph that displays the corrosion rate and the inhibitor efficiency depending on the immersion time. The data showcases a compelling relationship between immersion time, corrosion rate, and inhibition efficiency [24]. The corrosion rate decreases with increasing immersion time up to a certain point, emphasizing the effectiveness of DETSC in mitigating corrosion over short to moderate exposure durations. However, a nuanced trend emerges as the immersion time extends to 24 hours. Inhibition efficiency tends to decrease at longer immersion periods, indicating a diminishing protective effect. This decline is attributed to the desorption of DETSC molecules from the coupon surface, suggesting a temporary nature of the inhibitor's film. In summary, the numerical results underscore the time-sensitive nature of DETSC's corrosion inhibition mechanism [25]. A compelling connection between the immersion time, corrosion rate and inhibition effect is revealed in the data. The corrosion rate decreases with increase in immersion time, meaning that for short to medium term exposure periods, DETSC is quite successful in reducing corrosion. However, as immersion time approaches 24 hours, there is a more subtle trend and it can be seen that like bond strength, shutdown appears earlier and earlier. Inhibition efficiency tends to decline as immersion time increases longer, suggesting a deteriorating protective effect. This is due to DETSC molecules desorbing from the surface of the coupon, indicating that inhibitor's films have only a temporary. The numerical results prove that

DETSC's protection against corrosion begins to decline by a considerable amount upwards of 24 hours of exposure time.

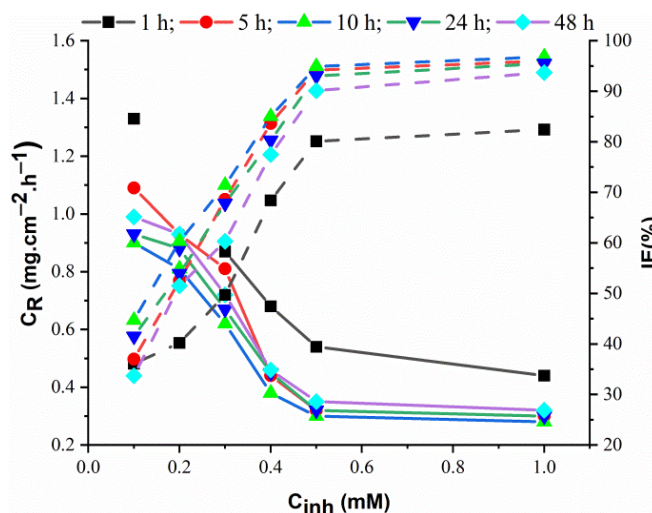


Figure 3. Variation of C_R and $IE\%$ with different concentration of DETSC for various immersion time at 303 K for mild steel in 1 M HCl.

3.3. Effect of temperature

The effect of temperature on the corrosion rate, as well as the inhibitive performance of DETSC, was studied systematically. The addition of DETSC produced a significant decrease in the corrosion rate; this is ascribed to the interaction between the DETSC molecules and the coupon's surface [26]. Furthermore, the weight loss data indicate the corrosion rate in the solution which is at 303, 313, 323 and 333 K, respectively. Figure 4 is the Arrhenius plot of the corrosion rate as a function of temperature which is calculated as follows [27]:

$$C_R = Ae^{-\frac{E_a}{RT}} \quad (9)$$

Here, A represents the pre-exponential factor, E_a is the activation energy, R is the gas constant, and T is the absolute temperature. The determination of the activation energy value shows that the inhibitor molecules were adsorbed onto the coupon surface by a chemisorption mechanism in the presence of DETSC [28]. Figure 5 shows the variation of corrosion rate and inhibition efficiency with different DETSC concentrations at different temperatures. DETSC exhibited a high inhibition efficiency of 94.2% at 303 K, which increased to 80.1% at 333 K. The process of heating the tested solution indicates an exothermic mechanism. From the temperature-dependent performance of DETSC more details about what should occur for the testing could be determined [29]. While the DETSC displayed good inhibition efficiency for the tested solutions of the hydrochloric acid of room temperature is inhibited, the efficiency was reduced when the temperature increased. Such temperature sensitivity indicates that the inhibitive mechanism of DETSC is activated by the energy changes accompanying the corrosion process. Thus, a deep insight into temperature

effects is required to design effective inhibitors for corrosion under different environmental conditions. The detailed investigation of the influence of temperature on the inhibition efficiency of DETSC gives reasonable information for the further application of this compound in the real corrosion prevention processes [30].

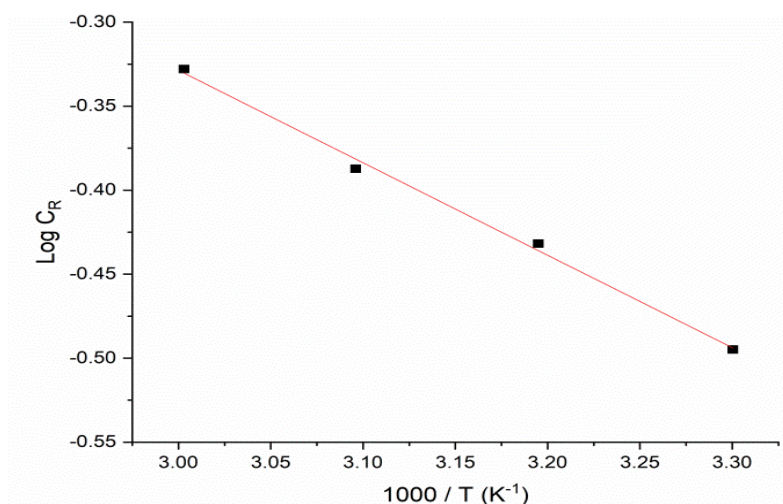


Figure 4. The Arrhenius plot for mild steel corrosion in acidic solution in the presence of DETSC (0.5 mM) at various temperatures.

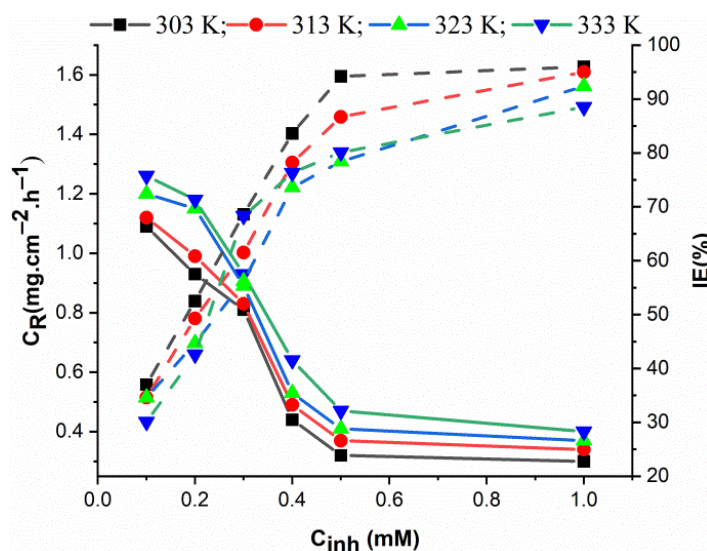


Figure 5. Variation of C_R and $IE\%$ with a different concentration of DETSC for various temperature in 1 M HCl.

3.4. Adsorption isotherms

As far as the field of acid corrosion is concerned, it is generally assumed that inhibitor molecules act on the metal surface by adsorption. The latter process is believed to cause a modification of the structure of the charged double layer of the specific defects, which decreases the rate of the partial electrochemical reactions. Adsorption generally takes place

on the active centers of the metal surface, thus causing a decrease in the effect of metal reactivity during the dissolving process [31]. In addition, if the adsorption and the reduction in the inhibitor molecule concentration happen on the dot, it is possible to develop a solid protective film. For that reason, adsorption behavior of the molecules of the inhibitor is fundamental to consider to comprehend the mechanism of their activity. Adsorption isotherms explain how the coverage of the interface by the adsorbate films relates to the concentration of the material of the solution [32]. The weight loss technique was used to determine the surface coverage (θ) of DETSC and also evaluate the adsorption isotherm model. The adsorption isotherms are important since they provide insight into understanding the intricate processes and phenomena involving adsorption of inhibitor molecules on a mild steel surface. This adsorption can occur through either physical or chemical mechanisms and can be explained with the help of various isotherms like the Langmuir, Temkin and Freundlich [33]. Figure 6 enables the fitting of data into well-established adsorption isotherms and understanding the adsorbent nature of the inhibitor performance. Perhaps unexpectedly, the adsorption of the DETSC molecules on the mild steel is in line with the Langmuir isothermal model, as supported by the high value of the regression coefficient ($R^2=0.9792$). The linear plot of the Langmuir model which shows the relationship between C/θ and C indicated the linearity of the adsorption process. The slope and the intercept of the Langmuir model are 0.835 and 0.175 respectively. Evaluated K_{ads} using Equation 10 also allows more information about the adsorption process. Using Equation 11, the determination of free energy (ΔG_{ads}^0) allows the critical parameter to understand the nature of the interaction of DETSC molecules on the coupon surface [34].

$$\frac{C_{\text{inh}}}{\theta} = \frac{1}{K_{\text{ads}}} + C_{\text{inh}} \quad (10)$$

$$\Delta G_{\text{ads}}^0 = -RT \ln(55.5 K_{\text{ads}}) \quad (11)$$

where 55.5 is the water concentration, R is the gas constant, and T is the absolute temperature.

The calculated value of ΔG_{ads}^0 for 1-(2,5-dihydroxyphenyl) ethanone thiosemicarbazone is $-33.75 \text{ kJ}\cdot\text{mol}^{-1}$. According to well-established literature, ΔG_{ads} values below $-20 \text{ kJ}\cdot\text{mol}^{-1}$ are characteristic of physisorption, while values above $-40 \text{ kJ}\cdot\text{mol}^{-1}$ point to chemisorption. Therefore, with a value of ΔG_{ads}^0 of $-33.75 \text{ kJ}\cdot\text{mol}^{-1}$, the interaction model of the inhibitor molecules with the surface of the tested coupon involves mixed physical and chemical adsorption. This understanding of the adsorption mechanism contributes to a thorough knowledge of the inhibition process.

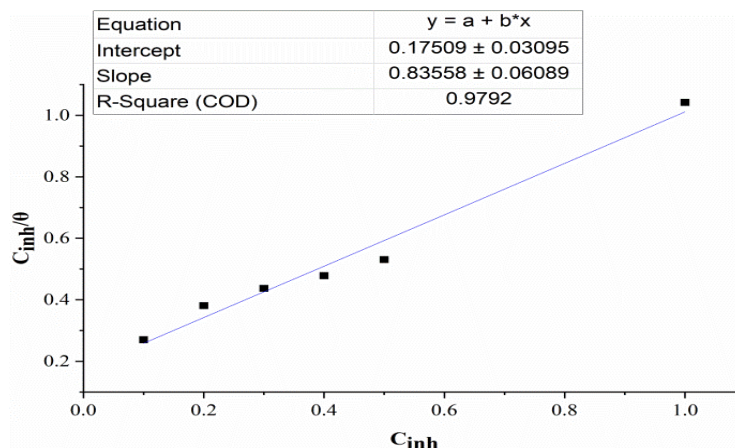


Figure 6. Langmuir adsorption model of DETSC.

3.5. Density functional theory analysis

Density functional theory (DFT) parameters were employed to understand quantitatively the inhibitory performance and the inhibition mechanism of the DETSC molecule. Quantum chemical parameters such as frontier molecular orbitals HOMO and LUMO, energy gap (ΔE), electronegativity (χ), global hardness (η), softness (σ), a fraction of transferred electrons (ΔN) and atomic charges are essential factors to determine molecular interactions and stability [37]. The optimized molecular structure of DETSC is illustrated in Figure 7 which is obtained by using DFT studies. As can be seen that the HOMO value of the compound is -8.327 eV which states that the molecule can donate the electrons to the vacant d -orbitals of iron. The LUMO value is -0.962 eV which denotes the power of the inhibitor molecule to accept the electrons from iron. The high value of HOMO indicates the DETSC molecule can give the electrons to vacant d -orbitals of iron. Most importantly, the obtained value correlates with the experimental result. A small value of LUMO suggests that DETSC can obtain electrons on back donation from iron [38]. The energy gap (ΔE) is an important parameter, the DETSC has the numerical value of -7.365 eV which signified substantial inhibitive efficiency. The electronegativity (χ) value of 4.645 eV added quantitative information on molecular stability and reactivity. The global hardness (η) and softness (σ) values were also important in the understanding of molecular stability and reactivity high [39]. A high ΔE combined with low softness ($\sigma = 0.271$ eV $^{-1}$) and high global hardness ($\eta = 3.6825$ eV), provides further quantitative insights into the substantial inhibitive efficiency. The high energy gap of DETSC together with its complex molecular structure supports the revealed performances of their inhibited action [40]. According to DFT analysis, a molecule with a high value of softness and low global hardness has relatively high efficiency. The σ calculated value of 0.293 eV $^{-1}$ also suggested that DETSC could be rapidly absorbed on the coupon surface, hence matching its experimental inhibition result. The large negative atomic charges especially in the nitrogen, and sulfur atoms of DETSC ($\Delta N = 0.320$) enhance the molecule adsorption on the coupon surface forming strong coordination bonds with mild steel [41]. The relationship between experimental findings and numerical quantum

parameters, and atomic charges have assisted in a better understanding of DETSC inhibition mechanism. The concurrence of the adsorption of DETSC on the mild steel surface, reasoned by the very high inhibition efficiency 94.2%, is also assisted by the quantitative DFT-based molecular attributes. Hence, this integrated approach, combining numerical and experimental insights, not only the expansion of the complete view of DETSC's inhibition features but also provides the opportunity to start to develop and enhance a corrosion inhibitor on a quantitative base [42].

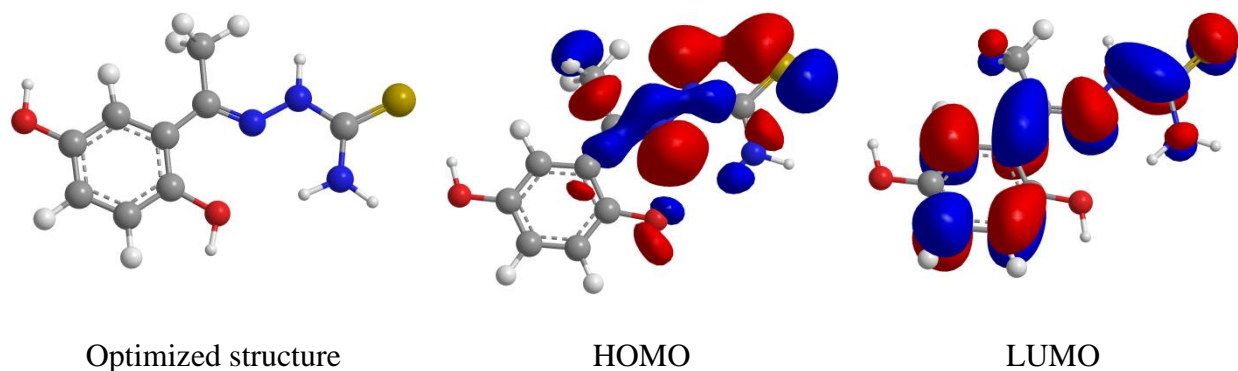


Figure 7. Optimized structure, Highest Occupied MO, and Lowest Unoccupied MO of DETSC molecules.

Atomic charges assignment suggestions essential understanding of the DETSC molecule chemical reactivity and potential interactions with the mild steel surface. Numeric information of atomic charges was gained by programs of DFT and provides quantitative explanation of the electron distribution within a molecule.

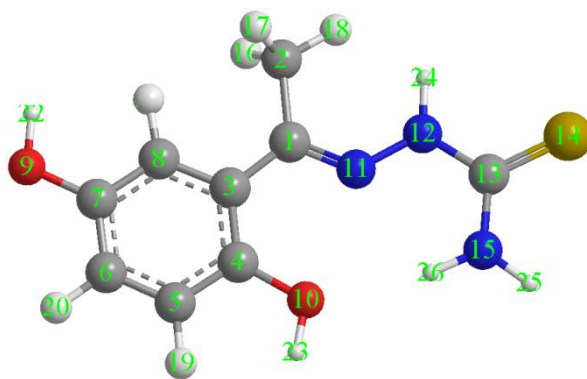


Figure 8. Optimized structure with atomic numbers.

For all atomic charges for carbon atoms in discrete variable: $C_1=0.0197755$, $C_2=-0.199739$, $C_3=-0.0146879$, $C_4=0.17903$; $C_5=-0.105403$; $C_6=0.211933$; $C_7=0.211933$; $C_8=-0.162995$. Thus, it is worthy to state that the obtained data proved variability for the eight carbon atoms of the same type and to the potential distinct roles within the molecule. Moreover, the positive charges for C_1 , C_4 , C_7 , and C_{13} with these locations indicate electron-donating capability. Correspondingly, the changes in C_2 , C_3 , C_5 ,

C₆, and C₈ with their location bear negative charges, which, accordingly, defines that the defined carbon atoms accept atoms. Therefore, the defined behavior and predicted atoms and all possible directions have to be justified. The negative charge for oxygen atoms are O₉ = -0.278969, O₁₀ = 0.211933, they consider accepting atoms and propose some changes with the formation of coordination bonds with metal surface. Compelling into consideration the charge of the nitrogen atoms, one can see the broad spectrum of charges being evaluated: N₁₁ = -0.129695; N₁₅ = -0.0225437. The positive charge on N₁₂ allows one to consider that it donates electrons. The negative charge on N₁₁ and N₁₅ confirmations that these atoms are capable of accepting electrons. Moreover, a rather big negative charge on the Sulphur atom suggests that this atom accepts electrons. On the other hand, one may suggest that this atom is the one capable of being adsorbed on a metal surface. The essential distribution of atomic charges provided vital foresight of polarity and reactivity of the DETSC molecule's various atoms; thus, it was a key determinant of its behavior towards the mild steel surface. Additionally, it can be noted that atoms with higher amounts of negative charges, specifically oxygen, nitrogen, and sulfur, will most likely coordinate the bond with metal surfaces; therefore, the distribution lends an explanation for DETSC's experimental correlation inhibition study [43,44].

3.6. Proposed inhibition mechanism

Determining the inhibition mechanism is necessary for understanding how the DETSC molecule reduces the rate of corrosion on the surface of a mild steel substrate. A review on the results of the experiments combined with the insights provided by the Density Functional Theory indicates a likely way that the inhibition process may take place [45].

a. Adsorption onto mild steel surface

It is expected that the DETSC strictly attaches to the surface of mild steel. The different isotherms all show that it adsorbed on the surface. Langmuir isotherm had high regression coefficient values, indicating it is the best model to show cover the whole surface, and hence there is monolayer adsorption. The calculated adsorption free energy ΔG_{ads}^0 , proving that the adsorption process is dominated by chemisorption [46].

b. Electron transfer and coordination bonds

Due to the high energy gap, DETSC molecule is characterized by the definite charge on certain atoms and it is capable of donation of electrons to certain carbon atoms, oxygen and nitrogen. Besides, electron accepting is demonstrated by the reaction on this way originating at the other carbon atoms. The formation of the coordination bonds with the atoms, concentrating a higher charge of electron-negative atoms such as oxygen, nitrogen and sulfur takes place. Moreover, attracting a large space charge on sulfur atom is an important condition [47].

c. Protective film formation

Molecules of the organic inhibitor, 1-(2,5-dihydroxyphenyl) ethanone thiosemicarbazone, are adsorbed onto the surface of mild steel, resulting in the formation of a quasi-monolayer that acts as a protective barrier. This quasi-monolayer, as supported by density functional theory calculations, impedes the progress of electrochemical reactions on the metal surface. The adsorption follows the Langmuir model, indicating a compact and uniform layer of inhibitor molecules [48].

d. Time-dependent inhibition behavior

Regarding time-dependent studies, it is demonstrated that DETSC is primarily an effective inhibitor over short to moderate immersion times. An obvious retrieval with extended exposure, however, results in inhibition efficiency decreasing parallel to an increase, suggesting that the inhibitor film is temporary, and the DETSC molecules desorb from the mild steel's surface [49].

e. Temperature influence on inhibition

Temperature-dependent studies indicate that inhibition efficiency of DETSC decreases as temperature rises. Such a tendency is characteristic, meaning that temperature and inhibition efficiency are uncompromising. Thus, a good corrosion inhibitor should be capable of providing a much thorough comprehension of its effects as a function of temperature [50].

This mechanism of inhibition has been proven to be a suggestion contained in the right. DETSC molecules are adsorbed onto the mild steel surface and take on the role of transferring electrons as well as forming coordination connections between atoms to form compounds. Furthermore, they also cause formation of a shielding film that preserves corrosive reactions from occurring any longer. Thus DETSC should be considered as an effective corrosion inhibitor for mild steel in HCl solutions, but all these factors need further study and discussion.

4. Conclusion

Corrosion is an electrochemical reaction, in the attempt to obtain a suitable corrosion inhibitor for mild steel exposed to hydrochloric acid solution, research on the inhibitory ability of 1-(2,5-dihydroxyphenyl) ethanone thiosemicarbazone (DETSC) has been of great value. The comprehensive study, combining techniques of experimentation and theory based on Density Functional Theory (DFT), suggests a nuanced understanding of DETSC's corrosion inhibition potential. It was established by experiments that DETSC has a very good inhibitor performance at the concentration of 0.5 mM being 94.2% measured from the weight loss of at 303 K. According to the adsorption isothermal, the product film layer on the mild steel is compact which follows the Langmuir law. The presence of the thiazole ring on DETSC plays an important role in protective of the mild steel. The DFT investigation supports the experimental results, and a quantitative clarification of the molecular basis that

governs the inhibition behavior of DETSC. The high energy gap (ΔE), global hardness (η) and small softness (σ), indicating that it has good inhibitive efficacy. From the calculated atomic charges, it can determine that the molecule is strongly level to the formation of the coordination bonds with the surface of mild steel; it may account for the increased adsorption capacity of the inhibitor under consideration.

In the proposed mechanism, DETSC is adsorbed on the mild steel surface, assisting electron transfer and the formation of coordination bonds. Subsequent, the formation of a protective film that inhibits corrosive reactions. However, the nature of this film is not permanent since the time-dependent studies establishes that inhibition efficiency decreases with increasing time. Therefore, duration of the immersion is a critical consideration. It is interesting that the inhibition effect of the corrosion inhibitor decreases slightly with increasing temperature. A more developed description of the process in which the inhibition effect and inhibition performance are enhanced was obtained through the integration of theoretical calculations and experimental methods in accordance with the theory of practical density. The conventional method allows the evaluation of the performance of DETSC as a corrosion inhibitor and reveals its chemical and physical absorption on the soft steel surface. This type of effective research provides knowledge and enables the development of corrosion inhibitors for industry. The cooperation of experimental and theoretical approaches to obtain useful information has been successful and useful to understanding the potential of DETSC as a corrosion inhibitor. The data imply that the results found during the experiments could be applicable not only for the understanding of the fundamentals of corrosion inhibition but also for the industry where mild steel is applied in corrosive media. Overall, the research indicates that DETSC may be a great start for future work on corrosion inhibition.

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