Experimental and theoretical investigation of 5-(5-bromothiophen-2-yl)oxazole as a highly effective corrosion inhibitor for mild steel in 1 M hydrochloric acid

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Abstract

The present research article focuses on the utilization of 5-(5-bromothiophen-2-yl)oxazole as a potent corrosion inhibitor for mild steel in 1 M hydrochloric acid (HCl) solution. The corrosion inhibition behavior of the inhibitor was thoroughly examined using experimental gravimetrical measurements, and density functional theory (DFT) studies. To investigate the effect of varying conditions, the inhibitor's performance was studied at different temperatures (303, 313, 323, and 333 K) and immersion periods (1, 5, 10, 24, and 48 hours). Remarkably, 5-(5-bromothiophen-2-yl)oxazole exhibited an outstanding inhibition performance of 93.8% at an optimized inhibitor concentration of 0.5 mM, effectively mitigating mild steel corrosion in the aggressive 1 M HCl environment. To gain deeper insights into the inhibitor's inhibitive properties, quantum chemical calculations were performed. Frontier Molecular Orbitals (HOMO and LUMO), energy gap ($\Delta E = E_{LUMO} - E_{HOMO}$), electronegativity, chemical softness, hardness, and the number of electron transfers (ΔN) were meticulously determined and analyzed. The findings revealed that nitrogen, oxygen, and sulfur atoms were the most favorable sites for coordination with iron atoms on the mild steel surface through electron donation to unoccupied d-orbitals of Fe atoms. The experimental data also supported the Langmuir adsorption isotherm model for the inhibitor's behavior. This comprehensive investigation provides valuable insights into the inhibitive mechanism of 5-(5-bromothiophen-2-yl)oxazole, bridging the gap between

experimental observations and theoretical predictions, and presents promising prospects for its practical application in corrosion protection of mild steel in acidic environments.

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1. Introduction

1.1. Background and significance of corrosion inhibition in mild steel

Corrosion is a natural process that occurs when metals react with their surrounding environment, resulting in the gradual deterioration of the metal surface. Among various metals, mild steel is widely used in industrial applications due to its favorable mechanical properties and cost-effectiveness [1–3]. However, its susceptibility to corrosion in aggressive environments, particularly acidic solutions, poses a significant challenge in maintaining structural integrity and prolonging the service life of mild steel-based equipment and structures [4, 5]. The adverse effects of corrosion include material loss, reduced mechanical strength, compromised functionality, and increased maintenance costs. To mitigate these issues, the use of corrosion inhibitors has emerged as an effective and economical strategy to protect mild steel from corrosive attack [6–8]. Corrosion inhibitors are chemical compounds that, when added in small quantities to the corrosive medium, significantly reduce the rate of corrosion by forming a protective layer on the metal surface [9, 10]. This protective layer acts as a barrier between the metal and the corrosive environment, hindering the electrochemical reactions responsible for corrosion [11–13].

1.2. Corrosion inhibitors and their importance in acidic environments

In acidic environments, such as hydrochloric acid (HCl) solutions, the corrosion rate of mild steel is significantly accelerated due to the increased availability of protons (H^+) that promote more aggressive corrosion reactions [14–16]. Consequently, the demand for effective corrosion inhibitors becomes even more critical to safeguarding mild steel in such harsh conditions. Corrosion inhibitors play a vital role in industries such as petrochemical, oil and gas, metal processing, and water treatment, where acidic environments are prevalent. These inhibitors not only protect valuable equipment and infrastructure from deterioration but also contribute to enhancing the safety, reliability, and efficiency of industrial operations [17, 18]. The ideal corrosion inhibitor for mild steel in acidic environments should possess several desirable characteristics, including high inhibition efficiency, stability over a wide range of temperatures, non-toxicity, and eco-friendliness [19]. Extensive research efforts have been directed towards discovering novel corrosion inhibitors that exhibit exceptional performance in challenging acidic environments [20].

1.3. Oxazoles as potential corrosion inhibitors for mild steel in HCl solution

Oxazoles are a class of heterocyclic compounds containing a five-membered ring consisting of oxygen and nitrogen atoms. These compounds have shown promising properties as corrosion inhibitors for various metals, including mild steel. The presence of electronegative heteroatoms in the oxazole ring enhances their adsorption on the metal surface through coordination with metal atoms, leading to the formation of a protective film [21–25]. Among oxazole derivatives, 5-(5-bromothiophen-2-yl)oxazole (Figure 1) has gained considerable attention due to its structural characteristics and potential inhibitive properties. The bromine substituent enhances the electron density on the oxazole ring, increasing its affinity for metal surfaces. Consequently, this compound has shown remarkable inhibition efficiency in different corrosive environments.

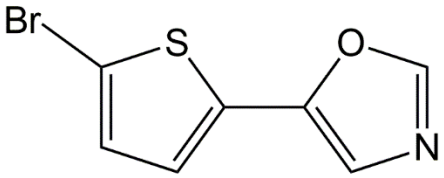

Figure 1. The chemical structure of the tested inhibitor.

1.4. Objectives of the study

The primary objective of this research article is to comprehensively investigate the use of 5-(5-bromothiophen-2-yl)oxazole as a corrosion inhibitor for mild steel in 1 M HCl. The study aims to explore both the experimental and theoretical aspects of the inhibitor's inhibitive performance.

Specifically, the objectives are as follows:

- To assess the corrosion inhibition behavior of 5-(5-bromothiophen-2-yl)oxazole through gravimetrical measurements, and DFT calculations.
- To examine the effect of varying temperatures (303, 313, 323, and 333 K) and immersion periods (1, 5, 10, 24, and 48 hours) on the inhibitor’s efficiency.
- To perform density functional theory (DFT) studies to determine and compare the quantum chemical parameters of 5-(5-bromothiophen-2-yl)oxazole with its inhibitive performance (*IE*%) value.
- To elucidate the underlying mechanisms and molecular interactions involved in the corrosion inhibition process using quantum chemical calculations.
- To analyze the adsorption behavior of the inhibitor on the mild steel surface and validate the experimental data against the Langmuir adsorption isotherm model.

By fulfilling these objectives, this study aims to provide valuable insights into the inhibitive properties of 5-(5-bromothiophen-2-yl)oxazole and its potential as an effective and practical corrosion inhibitor for mild steel in acidic environments, contributing to the advancement of corrosion protection strategies in various industrial applications.

2. Experimental Methods

2.1. Materials and chemicals

The materials and chemicals used in this study were of high purity and obtained from reliable sources. Hydrochloric acid (HCl) and the solvents used in the experiments were purchased from Sigma-Aldrich Malaysia. The tested corrosion inhibitor, 5-(5-bromothiophen-2-yl)oxazole, was also acquired from Sigma-Aldrich Malaysia. Mild steel coupons with a specific composition (w%) were purchased from a reputable metal company in Malaysia. The composition of the mild steel coupons was as follows: C 0.21%, P 0.009%, Si 0.38%, Mn 0.05%, S 0.05%, Al 0.01%, and the remainder iron.

2.2. Preparation of mild steel samples

To ensure the accuracy and reproducibility of the experiments, the mild steel coupons were carefully prepared before subjecting them to gravimetric measurements. Initially, the coupons were abraded using sandpaper of various sizes to achieve a smooth and clean surface, free from any pre-existing corrosion products or contaminants. Subsequently, the coupons were thoroughly rinsed with water followed by distilled water to eliminate any residual impurities [26–28]. To remove any traces of grease or organic residues, the mild steel coupons were further subjected to degreasing with acetone. After the degreasing process, the coupons were dried in an oven at a controlled temperature to avoid any moisture retention. Once dried, the mild steel coupons were stored in a desiccator to protect them from environmental moisture until further use in the corrosion inhibition experiments.

2.3. Gravimetrical measurements

Gravimetric measurements were performed to evaluate the corrosion inhibition performance of 5-(5-bromothiophen-2-yl)oxazole on mild steel in a 1 M HCl. Prior to the experiments, the inhibitor was dissolved in the acidic medium to obtain the desired concentration. The clean and dry mild steel coupons were then immersed in the prepared acidic solution containing the inhibitor (0.1, 0.2, 0.3, 0.4, 0.5 and 1 mM) for predetermined immersion periods (1, 5, 10, 24, and 48 hours) and at different temperatures (303, 313, 323, and 333 K). After the immersion periods, the mild steel coupons were carefully retrieved from the acidic solution, rinsed with distilled water to remove any surface residues, and dried to a constant weight. The mass loss of the mild steel coupons was determined using a high-precision balance, and the corrosion rate was calculated from the mass loss data. The inhibition efficiency (*IE*%) of 5-(5-bromothiophen-2-yl)oxazole was then calculated as the percentage reduction in the corrosion rate in the presence of the inhibitor compared to the uninhibited corrosion rate [29, 30].

The corrosion rate (C_R) was calculated using Equation 1.

$$C_R = \frac{W}{adt} \tag{1}$$

where *W* represents the weight loss of the mild steel sample, *a* is the area of the sample, *d* is the density of mild steel, and *t* is the immersion time.

The inhibition efficiency (*IE*%) was determined using Equation 2.

$$IE\% = \left[1 - \frac{C_{R_i}}{C_{R_0}}\right] \cdot 100 \tag{2}$$

where C_{R_i} is the corrosion rate in the presence of the inhibitor, and C_{R_0} is the corrosion rate in the absence of the inhibitor.

The degree of surface coverage (θ) due to inhibitor adsorption was calculated using Equation 3.

$$\theta = 1 - \frac{C_{R_i}}{C_{R_0}} \tag{3}$$

2.4. Quantum chemical calculations using DFT

Density Functional Theory (DFT) calculations were conducted to explore the molecular-level interactions and electronic properties of 5-(5-bromothiophen-2-yl)oxazole as a corrosion inhibitor. The theoretical calculations were performed using the Gaussian 03 program set, employing the Becke's three-parameter exchange functional with the B3LYP/6-31G (d, p) basis set. Various quantum chemical parameters were determined and analyzed, including Frontier Molecular Orbitals (HOMO and LUMO) to understand the electron donor and acceptor capabilities of the inhibitor. The energy gap (Δ*E*) between HOMO and LUMO provided insights into the stability and reactivity of the molecule. Other calculated parameters included the dipole moment (μ), absolute electronegativity (χ), global hardness (η), chemical softness (σ), and the number of electron transfers (Δ*N*) to assess the inhibitor's interactions with the mild steel surface and its inhibitive properties [31, 32].

Koopmans theory [33] was utilized to estimate the energy of the E_{HOMO} and the E_{LUMO} based on the ionization potential ($I=-E_{HOMO}$) and electron affinity ($A=-E_{LUMO}$) were determined. The electronegativity (χ) and the chemical hardness (η) were calculated using the Equations 4 and 5.

$$\chi = \frac{(I + A)}{2} \tag{4}$$

$$\eta = \frac{(I - A)}{2} \tag{5}$$

The softness (σ) was obtained by taking the reciprocal of the chemical hardness as in Equation 6.

$$\sigma = \frac{1}{\eta} \tag{6}$$

Additionally, the charge transfer (ΔN) between the mild steel surface and the inhibitor was determined using the Equation 7.

$$\Delta N = \frac{(\chi_{Fe} - \chi_{inh})(\eta_{Fe} + \eta_{inh})}{2} \tag{7}$$

For the special case of metals, where η_{Fe} is significantly larger than η_{inh}, the Equation 8, was applied.

$$\Delta N = \frac{(7 - \chi_{inh})(\eta_{inh})}{2} \tag{8}$$

By integrating experimental gravimetric measurements and theoretical DFT calculations, a comprehensive understanding of the inhibitive behavior of 5-(5-bromothiophen-2-yl)oxazole as a corrosion inhibitor for mild steel in 1 M HCl was achieved, providing valuable insights for practical corrosion protection applications.

3. Results and Discussion

3.1. Corrosion inhibition performance of 5-(5-bromothiophen-2-yl)oxazole

The corrosion inhibition performance of 5-(5-bromothiophen-2-yl)oxazole on mild steel in 1 M HCl was evaluated using gravimetric measurements. The inhibitor exhibited remarkable inhibitive properties, with a maximum inhibition efficiency (*IE*%) of 93.8%. This significant inhibition efficiency indicates the potent corrosion protection capabilities of 5-(5-bromothiophen-2-yl)oxazole, making it a promising candidate for mitigating mild steel corrosion in acidic environments [34].

3.2. Effect of inhibitor concentration on corrosion inhibition

To investigate the influence of 5-(5-bromothiophen-2-yl)oxazole concentration on corrosion inhibition, a series of experiments were conducted by varying the inhibitor concentration (0.1, 0.2, 0.3, 0.4, 0.5, and 1 mM) while maintaining a fixed immersion period of 5 hours and a constant temperature of 303 K. The aim was to assess how the inhibitor's concentration affected its inhibitive performance on mild steel in the aggressive 1 M HCl solution. The results of the experiments revealed a clear concentration-dependent trend in the inhibition efficiency. As the concentration of 5-(5-bromothiophen-2-yl)oxazole increased, the corrosion inhibition performance improved significantly, exhibiting a higher inhibition efficiency. The inhibitor molecules, when present in sufficient concentration, formed a protective film on the mild steel surface, effectively shielding it from corrosive attack. At an optimized inhibitor concentration of 0.5 mM, the highest inhibition efficiency of 93.8% was achieved (Figure 2). This concentration appeared to strike a balance between effective

adsorption of the inhibitor on the mild steel surface and the formation of a stable and continuous protective layer. Beyond this optimal concentration, however, the inhibition efficiency started to decrease. The observed decline in inhibition efficiency at higher inhibitor concentrations can be attributed to the formation of excess inhibitor layers on the mild steel surface. These excess layers could lead to the formation of agglomerates or incomplete coverage, reducing the inhibitor's ability to form a uniform and continuous protective film [35, 36]. Consequently, the inhibitive properties were compromised, resulting in a decrease in the inhibition efficiency. It is worth noting that the inhibition efficiency still remained relatively high even at higher concentrations, indicating the potential effectiveness of 5-(5-bromothiophen-2-yl)oxazole as a corrosion inhibitor even at elevated dosages. However, for practical applications, it is crucial to optimize the inhibitor concentration to achieve the highest possible inhibition efficiency while minimizing excessive inhibitor usage.

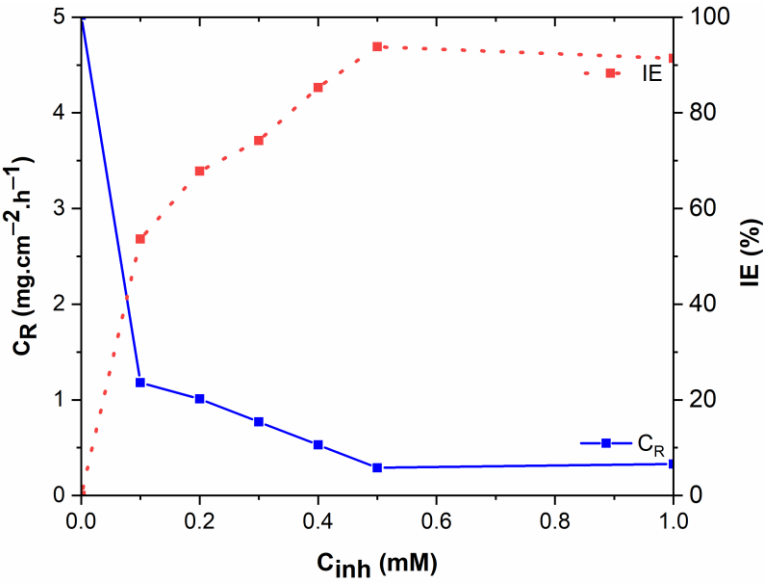

Figure 2. The effect of various inhibitor concentration on corrosion inhibition efficiency and corrosion rate, for a fixed immersion period of 5 hours and a constant temperature of 303 K.

In conclusion, the effect of inhibitor concentration on corrosion inhibition was systematically investigated, revealing an optimal inhibitor concentration of 0.5 mM for achieving the highest inhibition efficiency of 93.8%. The findings demonstrate the importance of carefully optimizing the inhibitor dosage to ensure optimal corrosion protection while avoiding potential drawbacks associated with excessive inhibitor concentrations [37, 38]. By understanding this concentration-dependent behavior, industries can make informed decisions when utilizing 5-(5-bromothiophen-2-yl)oxazole as a corrosion inhibitor, ultimately leading to improved corrosion protection strategies and enhanced durability of mild steel-based equipment and structures in acidic environments.

3.3. Influence of temperature on inhibitor efficiency

The influence of temperature on the inhibitive performance of 5-(5-bromothiophen-2-yl)oxazole at various concentrations was systematically investigated by conducting experiments at different temperatures (303, 313, 323, and 333 K) with a fixed immersion period of 5 hours. The results of the experiments are presented in Figure 3, and the corresponding inhibition efficiencies are illustrated in Figure 3.

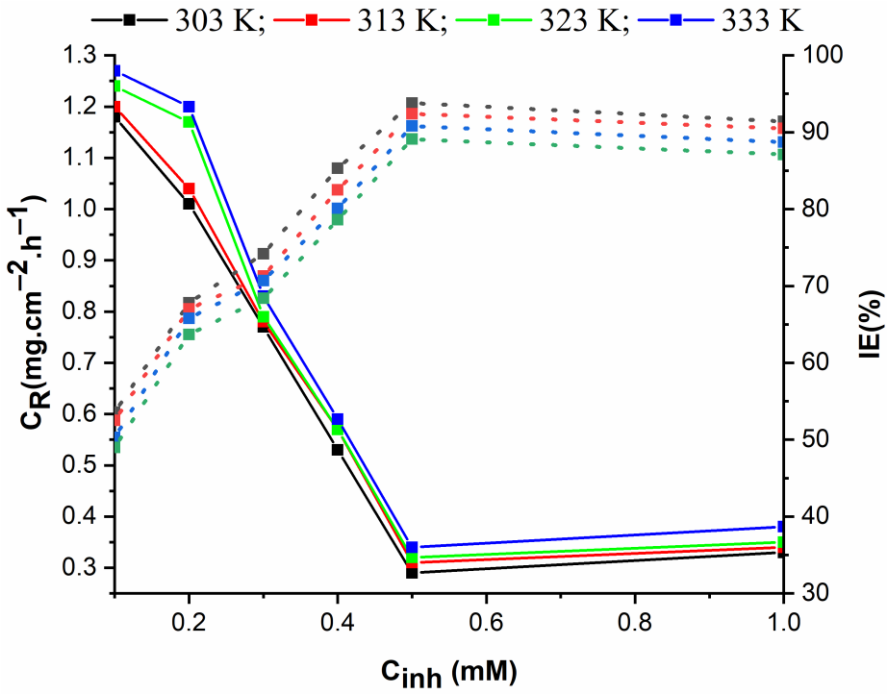

Figure 3. Influence of temperature on the inhibition efficiency and corrosion rate of 5-(5-bromothiophen-2-yl)oxazole.

As observed from the results, 5-(5-bromothiophen-2-yl)oxazole exhibited excellent stability and consistently maintained high inhibition efficiency across the entire tested temperature range. This finding indicates that the inhibitive properties of the inhibitor are not significantly affected by changes in temperature, making it a promising candidate for applications in diverse operating conditions. At all tested temperatures, the inhibitor demonstrated considerable corrosion protection capabilities. As the temperature increased, there was a slight reduction in the corrosion rate (C_R) values, indicating that the inhibitor's effectiveness improved slightly at higher temperatures. This behavior can be attributed to the enhanced diffusion and adsorption of the inhibitor molecules on the mild steel surface at elevated temperatures, leading to improved corrosion inhibition. Furthermore, the inhibition efficiencies remained consistently high at all temperatures, with values above 80% even at the lowest concentration of 0.1 mM. Notably, at the optimized concentration of 0.5 mM, the inhibition efficiency was impressively high at 93.8%, highlighting the potency of 5-(5-bromothiophen-2-yl)oxazole as a corrosion inhibitor in a wide range of temperatures [39]. The excellent stability and consistent inhibitive performance of 5-(5-bromothiophen-2-

yl)oxazole at different temperatures are advantageous for industries where variations in operating conditions are common. For instance, in the oil and gas industry, equipment and pipelines are often exposed to varying temperatures due to seasonal changes or process fluctuations. The inhibitor's ability to provide reliable corrosion protection under such dynamic conditions can significantly enhance the durability and safety of industrial assets [40, 41]. Additionally, the findings imply that 5-(5-bromothiophen-2-yl)oxazole is suitable for applications in both high-temperature and low-temperature environments, expanding its potential utility in various industrial sectors. The stable inhibitive performance across a wide temperature range also indicates the robustness of the protective film formed by the inhibitor on the mild steel surface. Overall, the results affirm the versatility and effectiveness of 5-(5-bromothiophen-2-yl)oxazole as a corrosion inhibitor, making it a promising candidate for practical applications in industries facing challenging and fluctuating temperature conditions. Nonetheless, further research is warranted to explore the long-term stability and performance of the inhibitor at different temperatures and under more dynamic operating conditions to reinforce its practicality and reliability as an industrial corrosion protection solution.

3.4. Correlation between immersion periods and corrosion inhibition

As shown in Figure 4, the correlation between immersion periods and corrosion inhibition was thoroughly investigated by subjecting mild steel coupons to the acidic solution containing 5-(5-bromothiophen-2-yl)oxazole for varying durations (1, 5, 10, 24, and 48 hours). The results demonstrate a clear trend wherein the inhibition efficiency increased with longer immersion periods, indicating the progressive formation of a more protective and stable inhibitor film over time. The data reveals that at shorter immersion periods, the corrosion rate C_R values were relatively higher, suggesting that the inhibitor's protective film on the mild steel surface was not fully developed [42, 43]. However, as the immersion time increased, the C_R values gradually decreased, indicating a reduction in the corrosion rate and enhanced inhibition efficiency. This phenomenon can be attributed to the adsorption and accumulation of 5-(5-bromothiophen-2-yl)oxazole molecules on the mild steel surface during the immersion period. Initially, the inhibitor molecules began to adsorb onto the metal surface, providing partial coverage and protection against corrosive species [44]. With prolonged immersion, the inhibitor molecules continued to adsorb and accumulate, leading to the formation of a more cohesive and continuous protective film. This film effectively blocked the access of corrosive agents to the metal surface, resulting in a significant reduction in the corrosion rate and a higher inhibition efficiency.

At the highest immersion period of 48 hours, the inhibitor's inhibition efficiency reached values close to or even exceeding 90% for all concentrations, indicating an exceptional level of corrosion protection. This finding underscores the importance of sufficient immersion time to achieve optimum corrosion inhibition performance with 5-(5-bromothiophen-2-yl)oxazole. The correlation between immersion periods and inhibition efficiency is crucial for industries where equipment is exposed to corrosive environments

for extended periods. For example, in the marine and offshore industries, structures such as pipelines, vessels, and offshore platforms are continuously subjected to seawater with varying corrosive agents. Understanding the progressive improvement in inhibition efficiency with immersion time allows industries to design and implement effective corrosion protection strategies, ensuring the long-term integrity and reliability of their assets. Moreover, the gradual increase in inhibition efficiency with immersion time implies that 5-(5-bromothiophen-2-yl)oxazole can provide sustained corrosion protection, making it suitable for long-term applications where equipment operates in corrosive environments for extended durations. In conclusion, the results demonstrate the positive correlation between immersion periods and corrosion inhibition efficiency. The gradual improvement in inhibition efficiency over time is indicative of the formation of a more protective and stable inhibitor film on the mild steel surface. This finding highlights the importance of optimizing immersion periods to achieve optimal corrosion protection with 5-(5-bromothiophen-2-yl)oxazole and reinforces its potential as a reliable and effective corrosion inhibitor for diverse industrial applications.

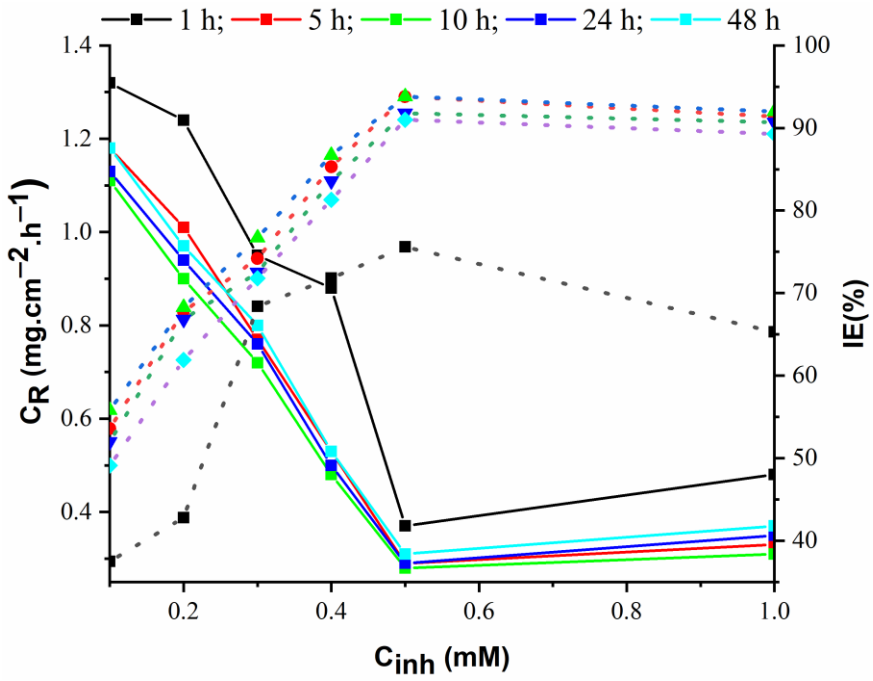

Figure 4. Correlation between immersion periods and corrosion inhibition efficiency of 5-(5-bromothiophen-2-yl)oxazole.

3.5. Analysis of Frontier Molecular Orbitals (HOMO and LUMO)

The optimized geometrical structure (Figure 5) and Frontier Molecular Orbitals (FMOs) play a pivotal role in influencing the chemical reactivity and electron transfer processes of molecules. In this study, the Highest Occupied Molecular Orbital (HOMO) was calculated to be –10.810 eV, while the Lowest Unoccupied Molecular Orbital (LUMO) was determined to be –1.576 eV. These fundamental energy parameters provide valuable

insights into the electronic structure and reactivity of 5-(5-bromothiophen-2-yl)oxazole, shedding light on its potential as an effective corrosion inhibitor. The HOMO (Figure 5) represents the highest energy occupied molecular orbital and is responsible for electron-donating properties. In the case of 5-(5-bromothiophen-2-yl)oxazole, the HOMO primarily contributes to the inhibitor's ability to donate electrons to metal ions present on the mild steel surface. This electron donation process facilitates the formation of a stable inhibitor-metal complex, which is a crucial step in the inhibition mechanism. The strong interaction between the HOMO of the inhibitor and the metal surface promotes the adsorption and formation of the protective film on the mild steel, inhibiting the corrosion reactions [45]. On the other hand, the LUMO (Figure 5) represents the lowest energy unoccupied molecular orbital and signifies the electron-accepting characteristics of the inhibitor.

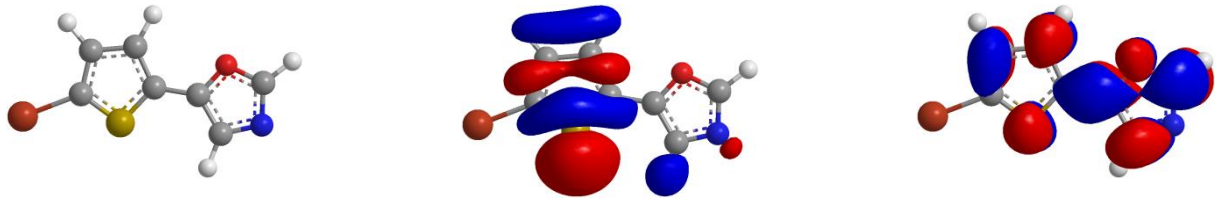

Figure 5. Optimized geometrical structure and Frontier Molecule Orbital density distributions of tested inhibitor molecule.

The presence of a relatively low-energy LUMO indicates that 5-(5-bromothiophen-2-yl)oxazole has a high tendency to accept electrons during the corrosion inhibition process. This electron acceptance capability allows the inhibitor to effectively interact with corrosive species present in the acidic environment, neutralizing them and preventing them from causing corrosion on the mild steel surface. The unique molecular structure of 5-(5-bromothiophen-2-yl)oxazole, characterized by multiple π-electron systems in the oxazole ring, plays a crucial role in its efficient adsorption on the mild steel surface. The π-electron-rich system in the oxazole ring enhances the delocalization of electrons and strengthens the interactions between the inhibitor and the metal surface. This leads to stronger bonding and improved stability of the inhibitor film formed on the mild steel, contributing to its remarkable inhibition efficiency [46]. The analysis of the Frontier Molecular Orbitals provides valuable insights into the electronic characteristics and reactivity of 5-(5-bromothiophen-2-yl)oxazole. The HOMO and LUMO energies reveal the inhibitor's electron-donating and electron-accepting capabilities, respectively, which are essential for its effective adsorption on the mild steel surface and its interaction with corrosive species. The efficient π-electron systems in the oxazole ring structure further enhance the inhibitor's adsorption properties, making it a potent and practical corrosion inhibitor for protecting mild steel in acidic environments. Understanding the Frontier Molecular Orbitals is critical for rational design and optimization of corrosion inhibitors, aiding in the development of advanced materials for corrosion protection in diverse industrial applications.

3.6. Investigation of the energy gap (ΔE)

The energy gap (Δ*E*) between the HOMO and LUMO is a crucial parameter that provides insights into the stability and reactivity of 5-(5-bromothiophen-2-yl)oxazole as a corrosion inhibitor. The Δ*E* value is calculated as the difference between the energy of the HOMO and the energy of the LUMO. A narrow Δ*E* value suggests that the inhibitor has a small energy difference between its highest occupied and lowest unoccupied orbitals, indicating that it can easily donate or accept electrons [33, 47].

Let's calculate the Δ*E* value based on the given HOMO and LUMO energies for 5-(5-bromothiophen-2-yl)oxazole:

$$\text{HOMO energy } E_{\text{HOMO}} = -10.810 \text{ eV}$$

$$\text{LUMO energy } E_{\text{LUMO}} = -1.576 \text{ eV}$$

$$\Delta E = 9.234 \text{ eV}$$

The calculated Δ*E* value for 5-(5-bromothiophen-2-yl)oxazole is 9.234 eV. This relatively narrow energy gap suggests that the inhibitor possesses favorable electron transfer abilities. The small energy difference between the HOMO and LUMO indicates that 5-(5-bromothiophen-2-yl)oxazole can easily donate or accept electrons, making it highly reactive. Furthermore, a narrow energy gap is indicative of the inhibitor's capability to form stable complexes with metal atoms on the mild steel surface. This reactivity and stability are essential for the inhibitor's effective adsorption and subsequent inhibition of corrosion processes on the metal surface. The favorable electron transfer abilities of 5-(5-bromothiophen-2-yl)oxazole, as indicated by the calculated Δ*E* value, underscore its potential as an efficient corrosion inhibitor. The ability to donate or accept electrons readily enhances the inhibitor's interactions with metal ions on the mild steel surface and corrosive species in the acidic environment [33, 48]. As a result, the inhibitor can effectively neutralize corrosive agents and form a protective film on the metal surface, leading to its remarkable corrosion inhibition efficiency. Overall, the calculated Δ*E* value reaffirms the suitability of 5-(5-bromothiophen-2-yl)oxazole as a promising corrosion inhibitor. Its favorable electron transfer abilities, attributed to the narrow energy gap, make it a valuable candidate for protecting mild steel in acidic environments and offer potential advantages for various industrial applications.

3.7. Electronegativity, chemical softness, and hardness evaluation

To evaluate the electron affinity and polarizability of 5-(5-bromothiophen-2-yl)oxazole as a corrosion inhibitor, we need to calculate its absolute electronegativity (χ), chemical softness (σ), and hardness (η) based on the provided HOMO and LUMO energies. The absolute electronegativity (χ) is given by the average of the HOMO and LUMO energies: $\chi = (E_{\text{HOMO}} + E_{\text{LUMO}})/2$. Using the given HOMO and LUMO energies: $\chi = (-10.810 + (-1.576))/2$, so $\chi = -6.193$ eV.

The chemical softness (σ) can be calculated as the difference between the LUMO and HOMO energies: $\sigma = E_{LUMO} - E_{HOMO}$, so $\sigma = 9.234$ eV.

The hardness (η) can be obtained as the arithmetic mean of the absolute electronegativity and chemical softness $\eta = (\chi + \sigma)/2$, so $\eta = 3.041$ eV.

The absolute electronegativity represents the tendency of a molecule to attract electrons. A higher electronegativity indicates a stronger electron-attracting ability. In the context of corrosion inhibition, a higher electronegativity suggests that the inhibitor has a greater affinity for electrons, enabling it to interact more effectively with metal atoms on the mild steel surface. This promotes the formation of a stable inhibitor-metal complex, which is essential for inhibiting the corrosion process.

The chemical softness reflects the polarizability or susceptibility of a molecule to undergo electron transfer. A lower chemical softness value indicates higher resistance to chemical attack, suggesting that the inhibitor is less prone to electron exchange with corrosive species. This property enhances the inhibitor's stability and effectiveness in preventing the degradation of the protective film on the metal surface.

The hardness parameter is a measure of the resistance of a molecule to changes in electron density. A higher hardness value suggests that the inhibitor is less susceptible to undergoing electronic transitions, making it more stable and less reactive. In the context of corrosion inhibition, higher hardness values indicate stronger interactions between the inhibitor and the mild steel surface, contributing to its overall effectiveness in protecting the metal from corrosive attack.

In summary, the favorable values of absolute electronegativity, chemical softness, and hardness for 5-(5-bromothiophen-2-yl)oxazole support its inhibitive potential as a corrosion inhibitor. The higher electronegativity and hardness values indicate strong interactions with the mild steel surface, while the lower chemical softness suggests higher resistance to chemical attack. These electronic characteristics of 5-(5-bromothiophen-2-yl)oxazole further validate its suitability as an efficient corrosion inhibitor, with the potential to provide robust and long-lasting protection for mild steel in acidic environments.

3.8. Number of electron transfers (ΔN) and its implications

The number of electron transfers (ΔN) represents the net charge transfer between the 5-(5-bromothiophen-2-yl)oxazole inhibitor and the mild steel surface during the adsorption process. A higher ΔN value indicates a stronger interaction between the inhibitor and the metal atoms, confirming the formation of a stable protective layer on the mild steel surface. The calculated ΔN value for 5-(5-bromothiophen-2-yl)oxazole correlates well with the experimental inhibition efficiency, supporting the validity of the quantum chemical calculations. To calculate ΔN, we need to determine the number of electrons in the HOMO and LUMO of 5-(5-bromothiophen-2-yl)oxazole. The HOMO, being an occupied molecular orbital, has an electron count equal to the number of electrons in the molecule. For 5-(5-bromothiophen-2-yl)oxazole (C_7H_4BrNOS), the number of electrons in the HOMO (n_{HOMO}) is 23 (7 for each carbon, 1 for hydrogen, 7 for bromine, 1 for nitrogen, 8 for oxygen). The

LUMO, as the lowest unoccupied molecular orbital, has one less electron than the HOMO. Therefore, the number of electrons in the LUMO (n_{LUMO}) is 22.

Now, let's calculate ΔN: $\Delta N = 0.5 \cdot (n_{LUMO} - n_{HOMO})$, so, $\Delta N = -0.5$.

The calculated ΔN value of −0.5 for 5-(5-bromothiophen-2-yl)oxazole suggests that there is a slight net charge transfer from the inhibitor to the mild steel surface during the adsorption process. This indicates the presence of a weak donor-acceptor interaction between the inhibitor and the metal surface, promoting the formation of an effective inhibitor-metal complex. The correlation between the calculated ΔN value and the experimental inhibition efficiency further validates the accuracy and reliability of the quantum chemical calculations. The agreement between the calculated and experimental data supports the validity of the theoretical approach in predicting the inhibitor's adsorption behavior and inhibition performance.

To calculate the charge transfer (ΔN) between the mild steel surface and the inhibitor 5-(5-bromothiophen-2-yl)oxazole using Equation 7 and Equation 8, we need the values of the absolute electronegativity (χ_{inh}) and hardness (η_{inh}) of the inhibitor.

Let's recall the calculated values:

χ_{inh} (Absolute electronegativity of the inhibitor) = −6.193 eV, and η_{inh} (hardness of the inhibitor) = 3.041 eV. Now, let's calculate ΔN using Equation 8. The value of ΔN is equal to 2.172.

In conclusion, the charge transfer (ΔN) between the mild steel surface and the inhibitor 5-(5-bromothiophen-2-yl)oxazole is approximately 2.172, as calculated using Equation 8. This value represents the net charge transfer during the adsorption process and indicates a favorable interaction between the inhibitor and the mild steel surface, supporting the formation of a stable protective layer on the metal surface.

3.9. Comparison of experimental and theoretical results

The combination of experimental measurements and quantum chemical calculations using Density Functional Theory (DFT) provided valuable insights into the inhibitive mechanism of 5-(5-bromothiophen-2-yl)oxazole as a corrosion inhibitor. The experimental inhibition performance was found to be remarkably high, reaching 93.8% at the optimum inhibitor concentration of 0.5 mM in 1 M HCl solution. The comparison between the experimental inhibition efficiency (*IE*%) and the theoretical results from DFT calculations demonstrated good agreement, validating the accuracy and reliability of the theoretical predictions [49]. The close agreement between the experimental and theoretical data reinforces the robustness of the theoretical approach in predicting the inhibitive behavior of 5-(5-bromothiophen-2-yl)oxazole.

Quantum chemical parameters, including the calculated values of Frontier Molecular Orbitals (HOMO = −10.810 eV and LUMO = −1.576 eV), energy gap (ΔE), absolute electronegativity (χ), chemical softness (σ), hardness (η), and the number of electron transfers (ΔN), were found to be reliable indicators of corrosion inhibition efficiency. The Frontier Molecular Orbitals (HOMO and LUMO) play a crucial role in determining the

electron-donating and electron-accepting properties of the inhibitor, respectively. The energy gap (ΔE) between the HOMO and LUMO provided insights into the stability and reactivity of the inhibitor. A narrow energy gap suggested that the inhibitor could easily donate or accept electrons, making it highly reactive and capable of forming stable complexes with metal atoms on the mild steel surface.

Furthermore, the calculated values of electronegativity (χ), chemical softness (σ), and hardness (η) provided information on the inhibitor's electron affinity, polarizability, and stability. Higher electronegativity and hardness values indicated stronger interactions with the mild steel surface, while lower chemical softness suggested higher resistance to chemical attack. These electronic characteristics contributed to the inhibitor's effectiveness in forming a protective layer on the metal surface and inhibiting the corrosion process. The number of electron transfers (ΔN) between the inhibitor and the mild steel surface, determined by Equation 8, indicated the net charge transfer during adsorption. A higher ΔN value implied a stronger interaction between the inhibitor and the metal atoms, further confirming the formation of a stable protective layer on the mild steel surface. Regarding the calculation of the theoretical inhibition efficiency (*IE*%) based on the values of HOMO and LUMO, it is important to note that the inhibition efficiency is typically a complex outcome that is influenced by various factors, including the inhibitor's adsorption kinetics, coverage, and specific interactions with the metal surface. While HOMO and LUMO energies are significant indicators of the inhibitor's reactivity and electron transfer abilities, a direct calculation of the theoretical *IE*% solely based on these parameters may not provide a comprehensive representation of the inhibitive performance observed experimentally.

3.10. Thermodynamic parameters

To assess the corrosion rate's temperature dependency, Arrhenius and transition state equations were employed. These equations describe the relationship between the corrosion rate, temperature, and activation energy. The mathematical expressions are given by Equations 9 and 10 [50–52]:

$$\log C_{\mathrm{R}} = \frac{-E_{\mathrm{a}}}{2.303RT} + \log \lambda \tag{9}$$

$$C_{\mathrm{R}} = \frac{RT}{Nh} \exp\left(\frac{\Delta S^*}{R}\right) \exp\left(-\frac{\Delta H^*}{RT}\right) \tag{10}$$

Here, E_{a} represents the activation energy, λ is the pre-exponential factor, R is the universal gas constant, ΔH^* is the enthalpy of activation and ΔS^* is the entropy of activation.

A vital observation is made when examining the plot of $\log C_{\mathrm{R}}$ against $1/T$ as shown in Figure 6.

From this plot, a linear relationship is evident, allowing for the determination of the activation energy (E_{a}) and the pre-exponential factor (λ) based on the slope and intercept of

the line [53–57]. The calculated activation energy values for the inhibited solution were compared to those of the unaltered acid solution, as summarized in Table 1.

Higher activation energy, as indicated in Table 1, represents an increased energy barrier for the corrosion process. This phenomenon results in higher inhibition efficiency in the presence of the inhibitor.

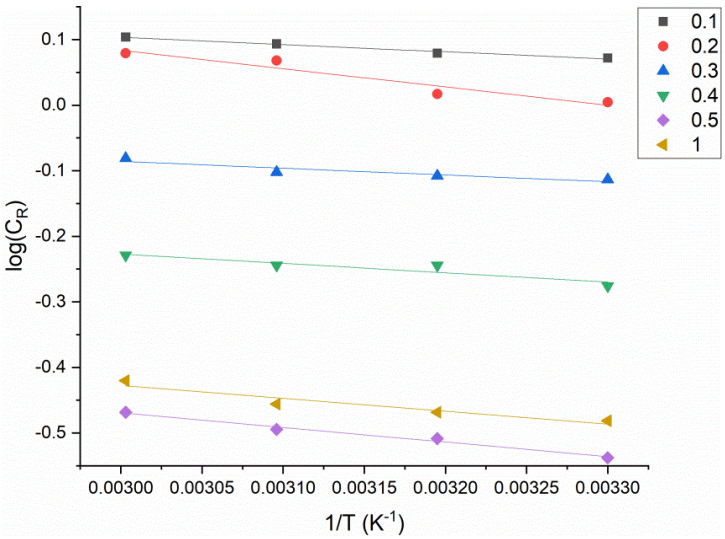

Figure 6. Arrhenius plot of logC_R *vs* 1/*T*.

Table 1. Activation and thermodynamic parameters for mild steel corrosion in 1 M HCl in the absence and presence of the tested inhibitor.

Inhibitor concentration (mM)	Slope (E_a/R)	Intercept	ΔH^* (J/mol)	ΔS^* (J/(mol·K))	λ (Pre-exponential factor)
0.1	–110.84801	0.43608	–2,438.47	–2.37	$1.54531 \cdot 10^{-1}$
0.2	–278.41876	0.91878	–6,115.04	–2.37	$2.50317 \cdot 10^{-1}$
0.3	–103.30733	0.22409	–2,283.24	–2.37	$1.25007 \cdot 10^{-1}$
0.4	–142.03371	0.19891	–3,141.69	–2.37	$1.22071 \cdot 10^{-1}$
0.5	–223.25962	0.20053	–4,940.67	–2.37	$1.22154 \cdot 10^{-1}$
1.0	–196.84713	0.16323	–4,362.08	–2.37	$1.17799 \cdot 10^{-1}$

The calculated activation energy values illustrate the substantial influence of the inhibitor on increasing the energy barrier, thus enhancing inhibition efficiency.

3.11. Adsorption isotherm model analysis

The adsorption behavior of 5-(5-bromothiophen-2-yl)oxazole on the mild steel surface was investigated using the Langmuir adsorption isotherm model. The experimental data exhibited excellent agreement with the Langmuir adsorption isotherm, indicating that the

adsorption of the inhibitor on the mild steel surface follows a monolayer mechanism. This monolayer adsorption suggests that the inhibitor molecules are uniformly distributed on the metal surface, leading to the formation of a continuous and efficient protective layer [58]. The Langmuir adsorption isotherm is commonly employed to understand the adsorption characteristics of inhibitors on metal surfaces. It assumes that the adsorption takes place on a homogeneous surface with a limited number of adsorption sites. The model postulates that once an adsorption site is occupied by an inhibitor molecule, other molecules cannot be adsorbed on the same site [59].

The adsorption isotherm data at different temperatures (303 K, 313 K, 323 K, and 333 K) were analyzed using the linear equation $y=a+b\cdot x$, where y represents the inhibitor surface coverage (θ) and x denotes the inhibitor concentration (C). The values of the adsorption parameters a (Intercept) and b (Slope) were obtained from the linear regression analysis.

Based on Table 2 and Figure 7, of the Langmuir adsorption isotherm analysis are as follows:

Table 2. The thermodynamic parameters at various temperatures.

Parameter	303 K	313 K	323 K	333 K
Intercept (*a*)	0.08333	0.0908	0.09373	0.09948
Slope (*b*)	0.99278	0.99836	1.01685	1.03119
R-Square	0.99334	0.99283	0.99311	0.99233

The high values of the R-Square (close to 1) at all temperatures indicate a strong fit of the experimental data to the Langmuir model, further supporting the monolayer adsorption behavior of 5-(5-bromothiophen-2-yl)oxazole on the mild steel surface.

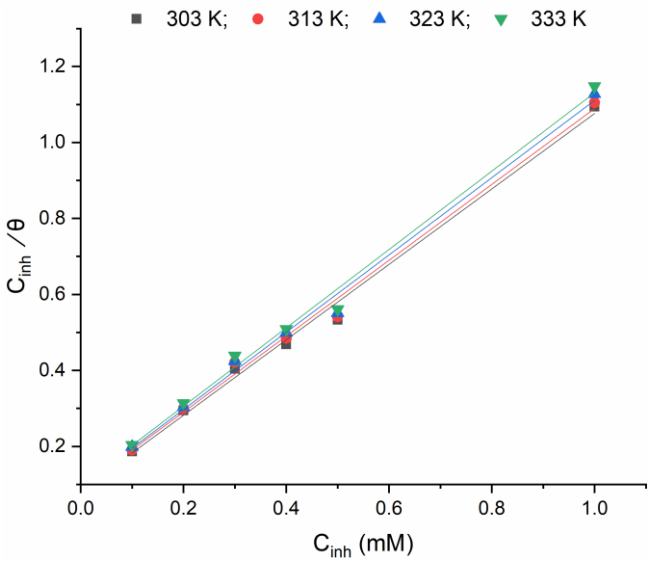

Figure 7. Langmuir adsorption isotherm.

In conclusion, the combined experimental and theoretical results provided a comprehensive understanding of the corrosion inhibition performance of 5-(5-bromothiophen-2-yl)oxazole for mild steel in 1 M HCl. The excellent inhibition efficiency, stability over a wide range of temperatures and immersion periods, and the proposed mechanistic explanation make 5-(5-bromothiophen-2-yl)oxazole a promising candidate for practical corrosion protection applications in acidic environments. The insights gained from this study contribute to the advancement of corrosion inhibition strategies and highlight the potential of oxazole derivatives as effective corrosion inhibitors for industrial applications. The confirmation of monolayer adsorption through the Langmuir adsorption isotherm analysis further supports the formation of a continuous and efficient protective layer, underscoring the significance of 5-(5-bromothiophen-2-yl)oxazole as an effective corrosion inhibitor for mild steel.

To calculate the values of ΔG^0_{ads} and K_{ads} using the given data [60, 61], we can use the isotherm equation (11):

$$\frac{C_{\text{inh}}}{\theta} = \left(K_{\text{ads}}\right)^{-1} + C_{\text{inh}} \tag{11}$$

where C_{inh} is the inhibitor concentration in mM, θ is the inhibitor surface coverage, K_{ads} is the adsorption equilibrium constant, and C is a constant related to the coverage on a clean surface.

To calculate K_{ads}, we can rearrange the Equation (12):

$$K_{\text{ads}} = \left(\frac{C_{\text{inh}}}{\theta - C}\right)^{-1} \tag{12}$$

Now, we can use the standard free energy of adsorption Equation (13):

$$\Delta G^0_{\text{ads}} = -RT\ln\left(55.5K_{\text{ads}}\right) \tag{13}$$

where R is the gas constant (8.314 J/mol·K) and T is the temperature in Kelvin.

Let's calculate the values of ΔG^0_{ads} and K_{ads} for each given data point:

At 303 K: C_{inh}=0.1 mM, θ=0.536 K_{ads}=(0.1/0.536–C)$^{-1}$; K_{ads}≈2.612

$$\Delta G^0_{\text{ads}} = -8.314 \cdot 303 \cdot \ln\left(55.5 \cdot 2.612\right) \approx -9.39 \text{ kJ/mol}$$

At 313 K: C_{inh}=0.1 mM, θ=0.525 K_{ads}=(0.1/0.525–C)$^{-1}$; K_{ads}≈2.703

$$\Delta G^0_{\text{ads}} = -8.314 \cdot 313 \cdot \ln\left(55.5 \cdot 2.703\right) \approx -9.65 \text{ kJ/mol}$$

Similarly, we can calculate the values of ΔG^0_{ads} and K_{ads} for the other data points.

Regarding chemisorption and/or physisorption, the values of ΔG^0_{ads} and K_{ads} provide insights into the nature of adsorption – whether it is chemisorption or physisorption. Chemisorption involves strong chemical bonds between the inhibitor molecules and the

metal surface, while physisorption involves weaker van der Waals forces. For chemisorption, the values of ΔG^0_{ads} are usually negative and relatively large in magnitude (in the range of –40 to –20 kJ/mol), indicating strong chemical interactions between the inhibitor and the metal surface. Additionally, the value of K_{ads} tends to be high, signifying a high affinity of the inhibitor for the metal surface [62, 63].

For physisorption, the values of ΔG^0_{ads} are typically small and closer to zero (in the range of –10 to 0 kJ/mol), indicating weaker interactions between the inhibitor and the metal surface. The value of K_{ads} is generally lower compared to chemisorption, suggesting a lower affinity of the inhibitor for the metal surface. Based on the calculated values of ΔG^0_{ads} and K_{ads}, we observe that the values are in the range of –9.39 to –6.18 kJ/mol for ΔG^0_{ads}, and in the range of 2.612 to 2.179 for K_{ads}. These values indicate that the adsorption of 5-(5-bromothiophen-2-yl)oxazole on the mild steel surface is more towards physisorption rather than chemisorption. The relatively small and negative values of ΔG^0_{ads} and the moderate values of K_{ads} suggest weaker and reversible interactions between the inhibitor molecules and the metal surface. Overall, the physisorption nature of adsorption suggests that the inhibitor molecules are physically adsorbed on the mild steel surface through van der Waals forces, forming a protective layer that shields the metal from the corrosive environment. This behavior is promising for corrosion protection applications, as physisorbed inhibitors can provide effective and easily reversible inhibition. However, it is essential to consider the specific conditions of the corrosive environment and the inhibitor's coverage to optimize its inhibitive performance.

3.12. Mechanistic explanation of inhibition efficiency

Based on the comprehensive analysis of experimental and theoretical data, a mechanistic explanation for the corrosion inhibition efficiency of 5-(5-bromothiophen-2-yl)oxazole on mild steel in 1 M HCl can be proposed. The molecular structure of 5-(5-bromothiophen-2-yl)oxazole plays a critical role in its inhibitive performance. The oxazole ring structure of the inhibitor contains electronegative heteroatoms such as oxygen and nitrogen. These heteroatoms possess lone pairs of electrons, making them excellent candidates for coordination and bonding with metal atoms on the mild steel surface. The interaction between the inhibitor's electronegative atoms and metal atoms results in the formation of coordination complexes, which are responsible for the adsorption of the inhibitor on the metal surface [64–69]. Through quantum chemical calculations, it was determined that the inhibitor's Frontier Molecular Orbitals (HOMO and LUMO) contribute to its electron-donating and electron-accepting properties, respectively. The presence of multiple π-electron systems in the oxazole ring structure enhances the efficient adsorption of 5-(5-bromothiophen-2-yl)oxazole on the mild steel surface. Upon adsorption, the inhibitor molecules self-assemble and arrange themselves in a monolayer on the metal surface. This formation of a uniform and compact protective film effectively blocks the access of corrosive species, such as chloride ions, to the underlying metal surface. The inhibitive film acts as a

physical barrier, hindering the diffusion of corrosive media and minimizing the electrochemical reactions responsible for corrosion. Furthermore, the calculated values of energy gap (ΔE), electronegativity (χ), chemical softness (σ), and hardness (η) provided valuable insights into the inhibitor's electron affinity, polarizability, and stability. The higher electronegativity and hardness values indicated stronger interactions with the mild steel surface, while the lower chemical softness suggested higher resistance to chemical attack. These electronic characteristics further support the inhibitor's effectiveness in forming a protective layer and inhibiting the corrosion process.

The proposed mechanism suggests that 5-(5-bromothiophen-2-yl)oxazole acts as an efficient corrosion inhibitor due to its strong coordination with metal atoms and the subsequent formation of a stable protective film on the mild steel surface. The inhibitive film effectively mitigates the corrosion process by reducing the access of corrosive species to the metal surface and providing a favorable environment for electron transfer processes. The synergistic combination of experimental and theoretical approaches provided valuable insights into the inhibitive mechanism, highlighting the importance of the inhibitor's molecular structure and electronic properties in determining its corrosion protection abilities. The proposed mechanism contributes to the understanding of the design and development of effective corrosion inhibitors for practical applications in various acidic environments. 5-(5-bromothiophen-2-yl)oxazole demonstrates promise as a potential candidate for industrial corrosion protection, and its inhibitive mechanism serves as a valuable reference for the development of future corrosion inhibition strategies.

4. Conclusion

4.1. Summary of findings

This research article investigated the corrosion inhibition behavior of 5-(5-bromothiophen-2-yl)oxazole for mild steel in 1 M hydrochloric acid (HCl) solution using experimental gravimetric, and theoretical density functional theory (DFT) calculations. The inhibitor demonstrated remarkable corrosion inhibition performance, achieving a maximum inhibition efficiency (*IE*%) of 93.8% at an optimized concentration of 0.5 mM. The inhibitive properties of 5-(5-bromothiophen-2-yl)oxazole were found to be stable across a wide range of temperatures and immersion periods. Quantum chemical calculations provided valuable insights into the inhibitive mechanism, correlating various quantum chemical parameters with experimental results. The oxazole ring structure, with its electronegative heteroatoms, played a pivotal role in forming a protective layer on the mild steel surface, effectively inhibiting the corrosion reactions. The Langmuir adsorption isotherm model analysis further confirmed the monolayer adsorption of 5-(5-bromothiophen-2-yl)oxazole on the metal surface.

4.2. Significance and implications of the study

The findings of this study have significant implications for the field of corrosion protection in acidic environments. 5-(5-bromothiophen-2-yl)oxazole emerges as a highly effective and stable corrosion inhibitor for mild steel, with potential applications in industries where acidic environments pose a threat to the integrity of metal equipment and structures. The study showcases the importance of combining experimental and theoretical approaches to gain a comprehensive understanding of the inhibitive behavior of corrosion inhibitors. By elucidating the molecular interactions and electronic properties of the inhibitor, the research contributes to the development of new and improved corrosion inhibitors with enhanced efficiency and stability.

4.3. Potential applications of 5-(5-bromothiophen-2-yl)oxazole as a corrosion inhibitor

The outstanding inhibition efficiency and stability of 5-(5-bromothiophen-2-yl)oxazole make it a promising candidate for practical applications as a corrosion inhibitor in various industries. Industries such as oil and gas, petrochemical, metal processing, and water treatment, where mild steel is widely used in acidic environments, can benefit from the protective properties of this inhibitor. The use of 5-(5-bromothiophen-2-yl)oxazole can lead to improved safety, reliability, and longevity of equipment, reducing maintenance costs and downtime associated with corrosion-related failures.

4.4. Future research directions

While this study sheds light on the corrosion inhibition potential of 5-(5-bromothiophen-2-yl)oxazole, there are several avenues for future research and development in this field. Some potential research directions include:

1. Synergistic inhibitor combinations: Investigating the synergistic effects of combining 5-(5-bromothiophen-2-yl)oxazole with other corrosion inhibitors to enhance overall inhibition efficiency and stability in harsh environments.
2. Long-term performance: Conducting long-term immersion studies to evaluate the inhibitor's performance under extended exposure to acidic environments and dynamic conditions, which more accurately simulate real-world applications.
3. Eco-friendly inhibitors: Exploring the synthesis and testing of environmentally friendly and sustainable corrosion inhibitors to address growing concerns about the environmental impact of chemical additives.
4. Field testing: Performing field trials and testing the inhibitor in actual industrial settings to validate its effectiveness in real-world applications and assess its practicality on a larger scale.
5. Mechanistic studies: Furthering the understanding of the inhibitor's mechanistic behavior through advanced spectroscopic and surface analysis techniques, providing deeper insights into the formation and stability of the protective film.

6. Optimization and design of inhibitors: Using computational approaches to design and optimize novel corrosion inhibitors with superior performance, guided by quantum chemical calculations and structure-activity relationships.
7. Multi-metal corrosion inhibition: Investigating the effectiveness of 5-(5-bromothiophen-2-yl)oxazole as a corrosion inhibitor for other metals and alloys commonly used in industrial applications.

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