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Exploring the Corrosion Inhibition Potential of 2-(2-Aminopropyl)thiazole for Mild Steel in Acidic Environment: Methodological and Theoretical investigation

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ABSTRACT

Mild steel (MS) corrosion in acidic environments presents significant challenges due to the limitations of conventional inhibitors, including concerns related to toxicity and environmental impact. This research explores the potential of 2-(2-Aminopropyl)thiazole (APT) as an inhibitor for corrosion of MS in 1 M HCl environment through methodological and DFT combination study. The inhibitory performance of APT reached an impressive efficiency of 88.2 % under optimized conditions (0.5 mM inhibitor concentration, 303 K), demonstrating its promise as an environmentally friendly alternative. Analysis based on Langmuir adsorption isotherm indicated strong and specific interactions between APT molecules and the steel surface, suggesting the formation of a protective film over time. The correlation between inhibition efficiency, immersion time, and temperature revealed a gradual enhancement of the protective effect, with temperature positively influencing the inhibitor's effectiveness, indicative of a thermally activated adsorption process. Calculations of Density Functional Theory (DFT) supported experimental findings and provide insights into molecular interaction at the interface. Just in these case, the calculated theory of electron transfer suggested that the interaction between APT and the atoms of iron was more favorable what shifted the inhibition process in a good direction. This work not only provide important information about the role of corrosion inhibiting but also relies on a reliable methodology that can be genralised to the analysis of eco-friendly corrosive preventing substances. Moreover, the research results provide a basis for the future development of APT for industrial application, which will deal with the real-world problems in the world. Prog. Color Colorants Coat. 18 (2025), 129-144© Institute for Color Science and Technology.

1. Introduction

It is in the fact that mild steel, although widely used in different industries, has a special set of characteristics, such as low cost and versatility [1]. In general, the impact indicator exhibits a good stability, despite the corrosion risk that becomes evident under severe

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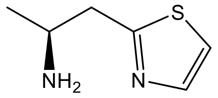
conditions. It could be noticed that in this case when a 1 M HCl was used, there is a constant competition between chemical and electrochemical processes, bringing about faster destruction of steel; the chance of critical infrastructures and security assets could be ruined [2, 3]. Corrosion inhibition in acidic environments is one of the key issues due to the fact that acidic conditions are found in many industrial and natural settings. Metals suffer from especially intense corrosion in acidic environments which might lead to material structural degradation, loss of integrity, and some safety concerns [3]. Acid can be formed from different sources, industrial processes, acid rain from natural environment factors, or even acidic soils and groundwater natural. In industries, acidic environments are often found in the fields like manufacturing, chemical processing and mining. For instance, hydrochloric acid is broadly reused in industrial processes for cleaning, pickling and etching metals and sulfuric acid is particularly popular in battery manufacture, metal extraction and chemical synthesis. These fields, the acid presence lead to electrochemical reactions that causes oxidation - degradation and thereby accelerates the failure of equipment, augment maintenance cost and increase pollution [4, 5]. Besides, in natural settings, acidic conditions can happen in soils, marine environment and even in the atmosphere. Acidic ores, being a consequence among acid rain, organic matter decomposition, and mining activities, can cause pipes, foundations and adjacent fuel reserves corrode underground. In marine region acidic seawater and microbe activity can be accelerators of structure like ships corrosion and unplanned disruption of offshore plants. Along with this, other atmospheric pollutants like sulfur dioxide (SO_2) and nitrogen oxides (NOx) can also be responsible for the formation of acid rain which, in turn, will make the corrosion problem in the urban and industrialized areas more severe [6]. The fact that acidic environments are everywhere and they cause metal infrastructure to corrode makes corrosion inhibition an important function in reducing the corrosion damage and in prolonging the life of the material. The inhibitors, in this case, are layers of protection formed on the metal surfaces that are so active in forming new metal ions, inhibiting the breakdown reaction, and thereby reducing the rate of metal dissolution. They can improve safety and reliability, reduce environmental pollution, and decrease maintenance cost of their products by using strong inhibition techniques like inhibitors which will in turn contribute to sustainability and economic efficiency [7, 8]. The ramifications of steel corrosion extend beyond visual deterioration, encompassing profound economic and environmental consequences [9]. The annual global cost of corrosion, estimated at $2.5 trillion, places a significant burden on industries such as construction, transportation, energy, and manufacturing, impacting both government budgets and private investments [6, 7, 10]. Moreover, corrosion jeopardizes public safety and environmental quality, with deteriorating structures compromising structural integrity and leaking pipes polluting soils and waterways [11]. The imperative to address corrosion challenges has spurred considerable interest in corrosion inhibitors, which serve to either form protective coatings on metal surfaces or modify the corrosive properties of the environment [12]. However, traditional inhibitors often exhibit drawbacks, including toxicity, limited reliability, and high costs, underscoring the need for environmentally friendly alternatives [13-15]. The emergence of bio-based corrosion inhibitors presents a promising solution, offering effectiveness in corrosion prevention while mitigating environmental and toxicity concerns [16, 17]. Among these inhibitors, 2-(2-Aminopropyl)thiazole (APT), with its molecular structure akin to Figure 1 and promising preliminary tests, holds potential as a significant inhibitor for the corrosion of MS in 1 M HCl environments [18-20]. This study adopts a dual experimental and theoretical approach to investigate the inhibition mechanism of APT and assess its viability as an environmentally sustainable corrosion protection solution [21-23]. By elucidating the molecular interactions of APT with steel surfaces and conducting comprehensive evaluations under varying conditions, the current study aims to contribute to the development of environmental friendly and cost efficient strategies for corrosion prevention. Through this endeavor, we endeavor to pave the way for enhanced protection of high-value steel assets in corrosive environments, thereby promoting sustainability and resilience in infrastructure management.



(*S*)-1-(thiazol-2-yl)propan-2-amine

Figure 1: APT molecular structure.

Protection from corrosion in acidic waters has been a challenge for some time and was successfully sustained using conventional inhibitors, each being beneficial and yet with a limitation. Though inorganic finishes are cost effective and readily available alternative, chromates, or phosphates may be contained within them, which raises the question of their toxicity as well as how safe they are for the environment, eventually leading to tighter regulations [26, 27]. Organic inhibitors [28], which add structural diversity and can form protective films, are susceptible [29, 30] to harsh conditions and are not always effective in the same way because of their structure and the composition of the medium [31-33]. Inhibitors based on surfactants, having good adsorption and spread, very often combine combinatorially with other inhibitors [34]. But still, efficiency of these methods can be affected by pH ranges; this may lead to undesired properties of product and even to environment problems [35]. The above flaws become more pronounced when the broader effects are taken into account, such as the toxicity of some compounds which poses a threat to human health and environment [36], the high costs which restrict the widespread adoption of some inhibitors, and the limited effectiveness of certain inhibitors in specific environments or under varying conditions thus reducing the versatility [37]. There has been an increased demand for such inhibitors as cost-effectiveness and broad applicability have been the plus side in most cases [40, 41]. Afterward comes the search for mainly natural sources via sustainable means(techniques) which have championed most solutions [42].

The quest for the best and longest-lasting corrosion inhibition solutions is what leads to the innovation in the inhibitor development. 2-(2-Aminopropyl)thiazole (APT), with its distinctive structure and the remoteness of any applications at this level, denotes one example of the existing ways. Studying the possibility of using APT as an MS corrosion inhibitor in 1C H, corresponds to the change in the society which is calling for environmentally friendly and effective corrosion shielding. This research will be aimed at APT's performance evaluation using a combined experimental and theoretical approach, attempting to determine its inhibition efficiency in different concentrations, immersion periods, and temperatures. Moreover, this research integrates the sorption kinetics of APT on the steel substratum and constructs the corresponding model of APT-metal interaction on the theoretical base of DFT calculations. This effort will be the insignia of a new era of intake preventers, so consequently we will not be far from a place where the security and affordability of infrastructure are two sides of the same coin.

2. Comparison with similar articles

This research we did is based on those early ones focusing on corrosion inhibition and, simultaneously, aims to compare our current finding to the studies carried out before. Several studies have been done to find out the most effective corrosion inhibitors for mild steel in acidic environments, like thiazole derivatives. In contrast to other published articles on the same subject, our analysis gives original observations on the corrosion barrier created by APT and its ability to stop it practically. In comparison with other inhibitors effective in past research, our study not only employs experimental and theoretical strategies but also shows the efficiency of this inhibitor in a reliable manner. In this case, we will analyze the performance of 2-(2-Aminopropyl)thiazole (APT) in comparison with other corrosion inhibitors that are widely used for mild steel in 1 M HCl solution, in terms of the environment, the cost, the synergistic effects and the inhibition efficiency.

2.1. Environmental impact

- APT: Think about APT (apoptosis-inducing peptide) biodegradability and ecotoxicity compared other to inhibitors. Investigate the possible effects of the new technology on the wastewater treatment and disposal needs. Reports suggest that thiazoles could belong among those goods that biodegrade well [40]. However, or should I say, there is no better way to go, but move for the specific evaluation for APT.
- Other Inhibitors: Contrast the effect of widely used inhibitors like mercaptobenzothiazole (MBT) or quaternary ammonium salts (QAS) on the environment. MBT might raise the problem regarding its unknown nature and lack of known endocrine disrupting effect [41]. Investigate the environmental footprint by their manufacturing process and dumping processes.

2.2. Cost

- APT: Find out the cost of making or getting APT as opposed to other inhibitors. Take into account issues such as the supply of raw materials as well as how easy or difficult it is to produce.
- Other Inhibitors: Analyze the cost for of the most typical ones. The price of some organic inhibitors can be higher as they require a very complicated synthesis process.

2.3. Synergistic Effects

- APT: Look into a complementary impact of API in combination with other corrosion inhibitors. Study whether these mixtures like single inhibitors HCl solution status are studied and compare their effectiveness with each of them.
- Other Inhibitors: Review the findings of previous studies that have explored the synergistic effects of joint usage of various inhibitors. One example may be studying the synergistic potential of combining thiazoles with inorganic inhibitors especially for augmented protection [42].

2.4. Inhibition efficiency

- APT: Compare the achieved inhibition efficiency (IE) of APT with those reported for other inhibitors at different concentrations and temperatures. This comparison will highlight the relative strength of APT's protective abilities. Reference relevant studies that explore the IE of various inhibitors for mild steel in HCl solution [43].
- Other Inhibitors: Analyze the IE of commonly used inhibitors like inorganic phosphates or organic molecules. Consider factors like inhibitor concentration, exposure time, and temperature when comparing IE values.

In many sulfur- and nitrogen-containing compounds, thiazole derivatives are highly appreciated for their metal corrosion inhibition ability. Gong et al. prepared and studied the mild steel corrosion inhibition ability of 2-Amino-4-(4-methoxyphenyl)-thiazole in 1.0 M HCl solution by using electrochemical frequency modulation. The results showed that the inhibition performance of this compound was 91 % at the concentration of 2.5 m M [44]. One other study of Alamiery et al. concluded that 2-Amino-4-phenyl-N-benzylidene-5-(1,2,4-triazol-1-yl)thiazole (APNT) is a good corrosion inhibitor for steel in HCl solution. With the concentration of 500 ppm, the inhibition efficiency of APNT is larger than 98 % [45]. Corrosion inhibition of 2-amino-5-mercapto-1,3,4-thiadiazole (2A5MT) was also investigated in 1 M H_2SO_4 solution with different techniques by Döner and others [46]. The result of potentiostatic polarization measurement demonstrated that this compound acts as a mixed-type inhibitor with an efficiency of 97.1 % with a concentration of 10.0 mM. A novel eco-friendly corrosion inhibitor, namely, 4-(pyridin-4-yl)thiazol-2-amine (PTA), was synthesized and evaluated as a corrosion inhibitor for mild steel in 1 M HCl solution. Its inhibition effect against mild steel corrosion was investigated *via* weight loss methods. The experimental results showed that PTA is an effective corrosion inhibitor for mild steel in an acid medium, and the maximum inhibition efficiency reached 96.06% at 0.2 mM concentration [47]. Corrosion inhibition of carbon steel in normal hydrochloric acid solution by 4-(1-hexadecyl-1H-benzo[d]imidazol-2-yl)thiazole has been studied by a weight loss measurments. The experimental results have showed that this organic compound revealed a good corrosion inhibition and that the inhibition efficiency is increased with the inhibitor concentration and the inhibition efficiency was 94.5% at 0.001 M [48]. Besides steel, thazole derivatives are used to inhibit many other metals such as aluminum, copper, zinc, and so on.

3. Experimental

3.1. Reagents and materials

HCl (37 %) with high-quality was diluted with water (double-distilled) to prepare a 1 M HCl solution. The APT inhibitor, sourced from Sigma Aldrich Malaysia, was diluted in this 1 M HCl solution to obtained ranging of concentrations 0.1 to 1.0 mM.

3.2. Sample preparation

MS samples underwent X-ray fluorescence spectrometry analysis to determine their chemical composition: element-content (wt. %); C- 0.21; S- 0.05; Mn - 0.05; Si- 0.38; P - 0.09; Al - 0.01; Fe - (balance) 99.21 (calculated by subtracting the sum of all other elements from 100 %). Following ASTM G1-03 protocols, these samples were prepared and achieved a polished finish with silicon carbide grits in a progression of 120, 600, and 1200 grit. Before immersion, the MS samples underwent meticulous cleaning with acetone, and water (double-distilled) followed by drying in an oven [49, 50].

3.3. Weight loss techniques

Samples were immersed in 400 mL of 1 M HCl solution containing varying concentrations of APT (0.1-1 mM) within 500 mL glass beakers. The experiments were conducted at a constant temperature of 303 K, maintained using a water bath setup in accordance with the NACE TM0169/G31 protocol. The exposure times included one hour, five hours, ten hours, twenty-four hours, and forty-eight hours to capture the corrosion behavior over different time intervals. After each exposure period, the corrosion products were meticulously removed from the surface of the samples. Subsequently, the coupons were dried and weighed to determine the weight loss (ΔW). The surface area (a) of the exposed metal samples, measured in square centimeters (cm²), was also recorded using equation 1 [50, 51]:

$$C_R\ (mg.cm^{-2}h^{-1}) = \Delta W / (at) \quad (1)$$

where C_R is rate of corrosion, ΔW is the specimen weight loss before and after immersion (mg), a refers to the surface area of the exposed metal sample (cm²), and t represents the immersion period (h).

The rates of corrosion without and with the APT, represented as C_{R0} and C_{Ri}, respectively, were utilized to estimate the inhibitive performance (IE) according to equation 2.

$$IE\ (\%) = [(CR_0 - CR_i) / CR_0] \times 100 \quad (2)$$

Surface coverage (θ) without and with the APT was calculated according to equation 3.

$$\theta = 1 - (CR_i / CR_0) \quad (3)$$

To investigate the temperature dependence of corrosion inhibition, coupons were immersed in inhibitor solutions at varying temperatures ranging from 303 to 333 K. Triplicate measurements were conducted for each temperature condition, and the average corrosion rate was calculated to analyze the effect of temperature on the corrosion behavior. To ensure the reliability of our results, each experiment was repeated three times under identical conditions. The data obtained from these replicates were averaged to minimize variability and enhance the accuracy of our findings.

3.4. Adsorption isotherm studies

Langmuir, Temkin, and Frumkin isotherms (equations 4-6) were employed to assess the inhibitor extent coverage on the MS surface. Weight loss techniques were done at various inhibitor concentrations to determine the surface coverage [52-54].

$$\theta = K_{ads} * C / (1 + K_{ads} * C) \quad (4)$$

$$\theta = a * \exp(b * \ln(K_{ads} * C)) \quad (5)$$

$$\theta = K_{ads} * C * \exp(-\alpha * \theta) \quad (6)$$

Where θ is the surface coverage fraction (0 ≤ θ ≤ 1), Kads is the adsorption equilibrium constant (L/mol), C is the inhibitor concentration in the bulk solution (mol/L), a is the pre-exponential factor, b is the constant related to the heat of adsorption, and α represents the interaction parameter.

3.6. DFT Calculations

Quantum mechanics calculations were carried out with the aid of ChemOffice software. Gaussian 09 Revision C.01 software was employed for DFT calculations, utilizing the B3LYP method and the 6-31G++(d,p) basis set. The inhibitor structure was optimized in its neutral form. Koopmans theory, along with equations 7 and 8, was used to determine the electron affinity (A) and ionization energy (I) [55-57].

$$I\ (eV) = -E_{HOMO} \quad (7)$$

$$A\ (eV) = -E_{LUMO} \quad (8)$$

Equations 9-11 were utilized to compute the electronegativity (χ), hardness (η), and softness (σ):

$$\chi = (I + A) / 2 \quad (9)$$

$$\eta = (I - A) / 2 \quad (10)$$

$$\sigma = 1 / 2\eta \quad (11)$$

The electron transfer (ΔN) was evaluated using equation 12, considering the Fe electronegativity of 7 eV and a hardness of 0 eV:

$$\Delta N = (\chi_{Fe} - \chi_{inhibitor}) / 2(\eta_{Fe} + \eta_{inhibitor} \quad (12)$$

4. Results and Discussion

The 2-(2-Aminopropyl)thiazole (APT) having enormous practical applications as the corrosion inhibitor since they have been designed with myriad of functions. The fact that APT has shown its capacity to suppress corrosion of mild steel under acidic conditions brings with it possibilities for the fields of numerous industries and real life sectors. For example, in the construction industry, where steel structures are in direct contact with the environment, APT can be used to extend the lifespan of infrastructure like bridges, pipelines, and buildings. In auto and aerospace fields APT may be used to combat corrosion on vital parts to guarantee protection, for that reason the safety and performance may be improved. Also, in oil and gas sector which is sensitive to corrosion, in which case cut off support of pipelines and equipment can be evaded by employing the Anionic Polymer Technology (APT) thus the need for very expensive repair operations narrowed. In conclusion, the universality and effectiveness of APT make it a must-have tool in fighting corrosion and keeping metal structures in good condition in different real-world scenarios.

4.1. Effect of inhibitor concentration

The study examined how the corrosion rate MS in a 5-minute immersion period was affected when using different inhibitor concentrations, with the particular attention put towards the 5-hour immersion duration. At first, in the absence of an inhibitor, the corrosion rate was high, which indicated the aggressive nature of the environment. However, upon introduction of the inhibitor, a noticeable reduction in the corrosion rate was observed, underscoring its efficacy in inhibiting corrosion. Figure 2 illustrates the impact of various concentrations of APT on the weight loss of MS following a 5-hour immersion in a 1.0 M HCl solution at 303 K. This dataset vividly portrays the corrosion inhibitory effects of APT under these specific conditions [58, 59]. It is evident from the figure that there exists an inverse relationship between inhibitor concentration and the corrosion rate of MS. Lower concentrations (0-0.4 mM) demonstrate a gradual reduction in corrosion rate, attributed to enhanced adsorption of inhibitor molecules on the MS surface, leading to improved surface coverage [60, 61]. As the inhibitor concentration surpasses 0.5 mM, a more pronounced decline in the corrosion rate becomes evident, coupled with a notable increase in inhibitive efficiency. At concentrations of 0.5 and 1.0 mM, the corrosion rate is substantially suppressed, reaching values of 0.37 mg.cm^{-2}h^{-1} and 0.34 mg.cm^{-2}h^{-1}, respectively. This observed trend aligns with the anticipated behavior of corrosion inhibitors, wherein higher concentrations facilitate greater adsorption and the formation of a protective layer on the metal surface. The substantial increase in inhibition efficacy, reaching 88.2 and 91.2 % at 0.5 and 1.0 mM concentrations, respectively, confirms the remarkable efficiencies of the tested inhibitor in mitigating corrosion of MS in HCl. These findings corroborate existing literature on the corrosion inhibition mechanisms and highlight the potential of APT as an efficient corrosive inhibitor for MS in corrosive media [62].

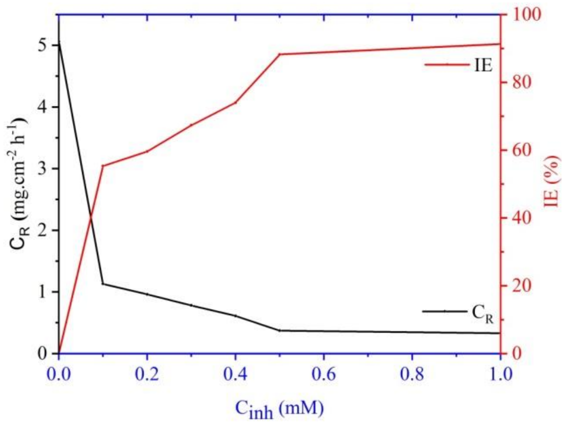


Figure 2: Effects of APT concentrations on MS for the corrosion rate and inhibition efficacy in a 1.0 M HCl solution after 5-h as exposure period time at 303 K.

4.2. Effects of immersion time

This study examined how immersion time affects how MS corrodes in 1.0 M HCl. It also assessed weight loss inhibition and surface coating effectiveness [63, 64]. Figure 3 offers a graphical representation of changes in mass loss over different exposure periods, elucidating the dynamic nature of the corrosion process [65, 66]. Examining immersion times ranging from 1 to 48 hours provided a comprehensive view of corrosion development on MS when exposed to the APT inhibitor. As depicted in Figure 3, there is a consistent decrease in the corrosion rate with longer exposure times, indicating a sustained effect of the inhibitor in reducing the metal's exposure to corrosion over extended periods. Inhibited samples exhibited reduced weight loss compared to uninhibited ones, underscoring the protective role of APT. The inhibitory effectiveness, expressed as a percentage reduction in the corrosion rate, exhibited a direct relationship with immersion time [67, 68]. Although there was a slight increase in inhibitory effectiveness with longer exposure times across all inhibitor concentrations, it is noteworthy that prolonged exposure can lead to gradual depletion or desorption of inhibitor molecules due to complex interactions with the MS surface [69, 70]. At the optimal inhibitor concentration of 5 mM, the inhibition efficiency reached 88.2 % after 5 hours of immersion. The highest inhibition activity of 95.7 % was observed after 48 hours of immersion with a 1.0 mM APT concentration. Beyond a concentration of 1.0 mM, there was no significant difference in inhibition activity within the tested range, suggesting a possible saturation effect [71]. This trend indicates that APT exhibits sustained inhibitive performance over prolonged exposure periods, rendering it a promising corrosion inhibitor for MS in aggressive acidic environments [72, 73]. Overall, the study underscores the crucial role of inhibitor concentration in determining inhibitory ability and highlights the potential of APT as a prospective corrosion inhibitor for MS in acidic planetary environments [74, 75].

4.3. Effect of temperature

This study aimed to investigate the temperature influence on rate of corrosion and the efficacy of inhibitor on MS in a corrosive solution. Figure 4 illustrates the findings, delineating the distinct trajectories of the corrosion process under varying temperature conditions. Analysis of the temperature's impact on corrosion behavior reveals an intriguing trend: as temperature decreases, the corrosion rate accelerates, as depicted in Figure 4. This phenomenon can be attributed to increased chemical interactions and enhanced oxygen absorption capacity at higher temperatures, facilitating a more favorable environment for corrosion reactions [76, 77]. However, this effect also affects the efficiency of inhibition, as higher temperatures exhibit a negative correlation with inhibition efficiency. With rising temperatures, the dynamic energy for inhibitors increases, potentially impacting the formation of protective layers on the MS surface and compromising its protective properties. Consequently, the process of inhibition becomes intricate, as the temperature and energy landscape exert a significant influence on inhibitor efficacy [78, 79]. Nevertheless, despite the complex interplay, inhibition efficiency generally shows a gradual increase overall. An arresting observation comes up concerning how water affects the pigeons after 10 h of surviving completely underwater at 1.0 mM inhibitor concentration: at 333 K, the degree of inhibition achieves 93 percent. From that enormous number (91 %) only a ridiculously low 6 % just immaterial. Rearranging the Vmax/Km confirms the trend of decrease in the reaction rate at 303K, revealing the sensitive relationship between temperature and inhibition effect.

To conclude, HCl solution interferes with MS corrosion mechanisms by different modes. Changes in temperature not only significantly affect the activation of chemicals with the surroundings but also modulate the pace at which actively inhibitors work. This evidence underscores the significance of meticulously assessing temperature conditions in corrosion resistance evaluations, as it can influence the dispersion of various corrosion processes, among other factors.

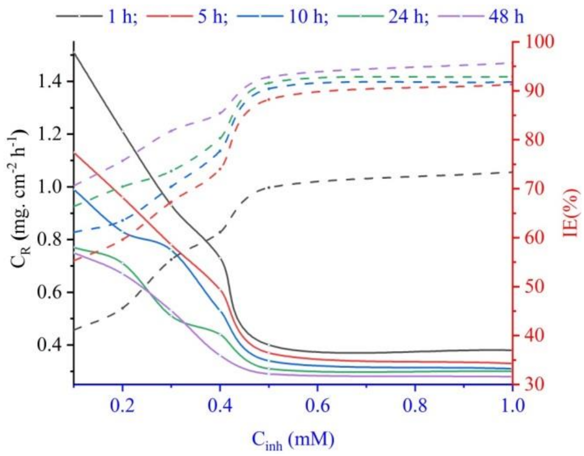


Figure 3: Influence of APT variations on corrosion rate and inhibition efficiency of MS in 1.0 M HCl at different exposure times (constant temperature 303 K).

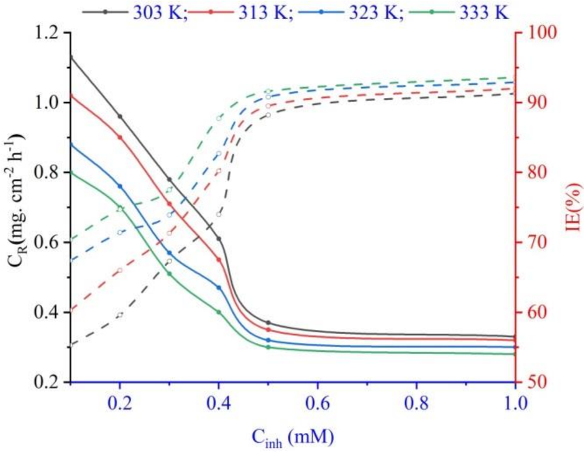


Figure 4: The study of APT concentration in the rates of corrosion and efficiency of inhibition of mild iron in 1M HCl solution at different temperatures with 5-hour immersion time.

4.4. Adsorption isotherm investigations

The observed linear relationship in the plot of C_{inh}/θ against C_{inh} at 303 K validates the suitability of Langmuir isotherm for describing the adsorption process [80]. The high linear regression coefficient further affirms the adequacy of Langmuir compared to alternative isotherm models. The intercept of the straight line in Figure 5 yields the adsorption equilibrium constant (K_{ads}), indicating the strength of interaction between the adsorbate and adsorbent. A higher K_{ads} value signifies more effective adsorption, correlating with higher inhibition efficiency [81, 82].

Adsorption free energy (ΔG_{ads}), as defined in equation 13, serves as a crucial indicator of adsorption interactions. A ΔGoads value less than or equal to -20 kJ/mol suggests physisorption, indicating a weaker interaction where inhibitor molecules adhere to the surface through physical forces [83, 84]. Conversely, an extremely negative ΔG_{ads} value exceeding -40 kJ/mol implies chemisorption, involving the formation of coordination bonds between iron atoms on the coupon surface and the inhibitor molecules [85].

$$\Delta G_{ads} = -RT \ln (55.5K_{ads}) \qquad (13)$$

The calculated value of ΔG_{ads} as -32.14 kJ/mol suggests a mixed interaction type involving both chemisorption and physisorption. This underscores the diverse nature of interactions between the inhibitor and the metal surface, contributing to a comprehensive understanding of the inhibition mechanism. In conclusion, adsorption isotherm studies confirm the effectiveness of Langmuir isotherm in characterizing the adsorption behavior of APT on MS in hydrochloric acid. The mixed reaction type involving both chemisorption and physical adsorption enriches the understanding of the inhibition mechanism, demonstrating the potential of APT as a corrosion inhibitor with versatile reaction modes.

4.5. Computational studies

Experimental findings, complemented by computational analysis, offer valuable insights into the corrosion inhibition mechanism of APT on MS [86]. The computed values for Table 1 provide additional support to the experimental observations. The low values of ΔE (energy gap) and hardness, coupled with high softness, suggest a physical adsorption mechanism consistent with experimental observations [87]. The high HOMO energy correlates with high inhibition efficiency, in line with the adsorption isotherm data (ΔG_{ads}). Furthermore, molecular structure influences adsorption, as indicated by the electron density of active sites, especially sulfur and nitrogen atoms, which are susceptible to electrostatic attacks. Electronegativity plays a crucial role in predicting inhibitory efficacy, with electron transfer values decreasing as inhibitory electronegativity increases [88]. Positive ΔN values confirm the electron donation potential of the inhibitor, further validating the EHOMO trends (Figure 6).

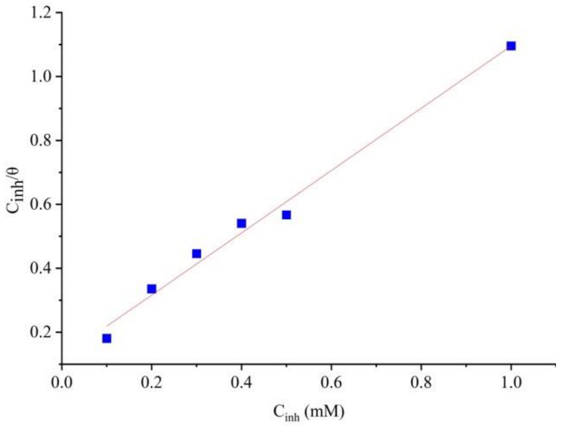
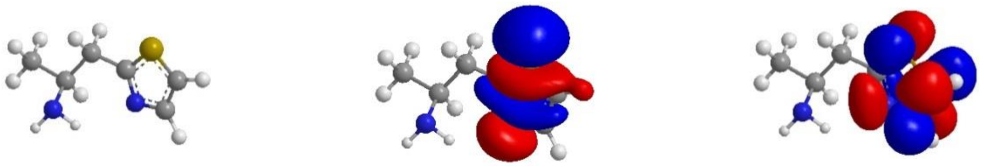


Figure 5: APT Langmuir Isotherm for the surface of MS in a 1.0 M HCl solution at 303 K.



Optimum Structure **HOMO** **LUMO**

Figure 6: Molecular orbitals of APT.

Table 1: Quantum chemical calculations for APT molecule.

Parameter	Value
HOMO Energy (eV)	-8.605
LUMO Energy (eV)	9.145
Energy Gap (ΔE) (eV)	-17.75
Hardness (eV)	8.875
Softness (eV)	0.0565
Electronegativity	-8.875
ΔN (Electron Transfer)	0.27
Dipole moment (µ) (debye)	-0.591

The negative dipole moment of APT indicates its polar nature, suggesting the direction of charge distribution along a specific axis. This polarity, likely influenced by the orientation of functional groups within the molecule, enhances electrostatic interactions with the MS surface, facilitating adsorption and the formation of a protective layer. Analysis of the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) populations around the thiazole ring, nitrogen, and sulfur atoms, reveals significant electron donation capability. This alignment with physisorption mechanisms also verifies the experimental evidence and shows that the molecular structure of APT is responsible for its performance as a corrosion inhibitor [89].

4.6. The limitations and challenges faced are as follows

While conducting the experimental and theoretical investigations, several limitations and challenges were encountered, which warrant discussion: While conducting the experimental and theoretical investigations, several limitations and challenges were encountered, which warrant discussion:

1. Solubility of APT: The top problem caused by the experience we were having was the APT's (2-(2-Aminopropyl)thiazole) solubility in acidic medium. Limited solubility can be a cause of the non-uniform distribution of the inhibitor in the solution, which may lead to variability in the inhibition effectiveness at different concentrations.
2. Data Variability: The triumph of laboratory researchers to establish standardized conditions of experiment, however, does not guarantee the precise and identical results. Small changes in experimental variables, including temperature, pH, and stirring, can influence on the reproducibility of findings during the experiments. Such heterogeneity not only demands further objective and statistical research but also represents the need for an adequate data interpretation taking into account such inconsistencies.
3. Complexity of Corrosion Mechanisms: The corrosive processes in acidic environments are complex and can include several electrochemical reactions, adsorption phenomena and surface interactions. Theoretical models of corrosion inhibition, which pursue the corrosion inhibition mechanism at depth, require advanced theoretical modeling and experimental techniques, which may be a bottleneck in the interpretation of the data and validation.
4. Limited Toxicity Data: The toxicological properties of APT and its ecological influence are to be taken into account when APT is imagined as a practical substitute. Nevertheless, the data on the toxicity of APT may be incomplete in the literature and thus, it is difficult to determine its environmental safety and regulatory compliance accurately.
5. Absence of Electrochemical Methods: The investigation using the electrochemical methods such as potentiodynamic polarization and electrochemical

impedance spectroscopy is restricted by their absence in the experimental study, which leads to a crucial gap in the comprehensive understanding of corrosion inhibition mechanisms. Using these methods as well would be an extra source of knowledge in the area of what drives corrosion processes and its kinetics and thermodynamics.

6. Theoretical Assumptions: Through the use of Density Functional Theory (DFT) in theoretical studies, some simplifications and approximations are done to model the molecular interactions between APT and the metal surface correctly. Such aforementioned erroneous assumptions might indeed cause certain degree(s) of uncertainty and limits in the prediction of adsorption performance and APT inactivation.

By addressing such limitations and challenges, using control experiments with theory input, and thorough data analysis, the accuracy and conclusion of the study can be much improved. Furthermore, future efforts in research are aimed at overcoming the above mentioned challenges to narrow the understanding of corrosion inhibition mechanisms and at the same time to develop testing more effective inhibitors for acidic surroundings.

4.7. Suggested mechanism

The corrosion inhibition mechanism of APT on MS in 1 M HCl solution involves a combination of adsorption processes, which are physical and chemical in character and are coupled with the formation of a protective layer on the metal surface [90]. This layer of protection serves as a barrier that prevents the corrosive elements from reaching the object, thereby decreasing the corrosion rate. As is shown in the Figure 7 the suggested mechanism is shown. APTs molecule sticks to the metal-support matrix (MSM) according to a number of ways, on which the most essential are: van der Waals, hydrogen bonding and electrostatic interactions [91]. This absorption process is the result of the presence of the active sites on the metal surface, such as iron atoms, where APT molecules can be bound. The APT surface monolayer built through adsorption results in direct coverage of the metal, which then prevents it from being exposed to corrosive environment [92, 93]. Physisorption is a nonspecific adsorption mechanism. The APT molecules interact with the metal surface by slightly weaker interactions e.g. van der Waals forces and hydrogen bonding. This method involves the physical adsorption of APT molecules onto the metal surface without any chemical interaction. The adsorption by physisorption of APTs develops a protective film on the surface of the metal which slows down corrosion by keeping away the corrosive species from directly interacting with the metal in a solution [94, 95]. In chemisorption, formation of chemical bonds between adsorbate molecules (APT) and the surface metal takes place. The process of transfering electrons between the APT molecules and the active sites on the metal surface is called electron transfer [96, 97]. The stronger attachment of APT molecules due to the chemisorption rather than the physisorption of molecules is hence forwarded by the feature that it promotes the generation of a stable layer of inhibitors that contributes to a superior protective layer [98-100].

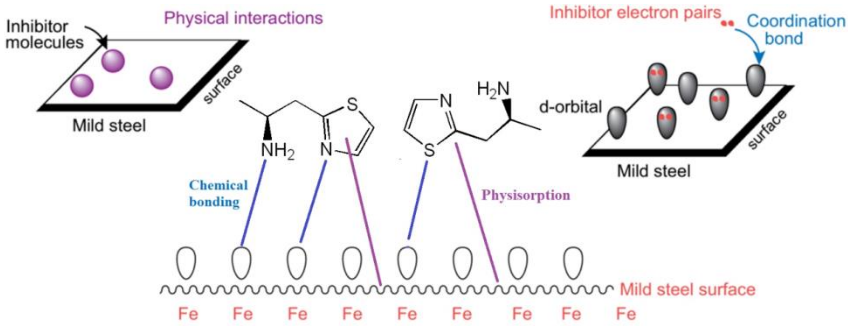


Figure 7: Postulated mechanism of APT molecules adsorption on steel surface.

5. Conclusion

In this study, we determined the ability of 2-(2-Aminopropyl)thiazole (APT) to function as a protective inhibitor of corrosion in 1 M HCl dissolution medium, applying a combination of experimental and theoretical techniques. Our results are important because they show the mechanism of the corrosion inhibition of APT and the possibility of its application in the mitigation of corrosion in acidic environments. A hollow cathode spectroscopy technique was employed to determine that APT displayed remarkable corrosion inhibition performance, as reflected by significantly decreased corrosion rates and a particularly remarkable effect when APT was used at optimal concentration. The experimental data confirmed the fact about the concentration-dependence of corrosion inhibition that involved an increase in APT concentration would lead to more inhibition efficiency. Moreover, the immersion time studies showed that the APT remained effective for a long time even after a prolonged exposure, which implies that it can be used for long-term protection against corrosion. On the other hand, the DFT calculations that were employed in the theoretical investigations shed light on the molecular interactions between the two molecular structures, APT, and mild steel. Computer-proofed data in this model indicates that APT works through physical sorption scheme, just as findings from the APT experiments suggest. In addition, quantum chemical parameters showed that APT had the ability to donate electrons and this supported the fact that it was an efficient inhibitor. In conclusion, our results point out that APT can be a useful corrosion inhibitor for steels in normal environment conditions in the presence of HCl. The advanced mechanism involving adsorption, physisorption, and chemisorption processes explains the built barrier that lays on the mild steel upper surface, protecting it from corrosion. These outcomes are crucial to the development of green corrosion inhibitors and the insights for further research in the field of corrosion inhibition strategies.

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