PROGRESS IN COLOR, COLORANTS AND COATINGS

available online @ www.pccc.icrc.ac.ir

Progress in Color Colorants Coating 17 (2024), 85-96

Ministry of Science, Research and Technology
Institute for Color Science & Technology

Unlocking the Power of 4-Acetamidoantipyrine: A Promising Corrosion Inhibitor for Preserving Mild Steel in Harsh Hydrochloric Acid Environments

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ARTICLE INFO

Article history:
Received: 29 May 2023
Final Revised: 23 July 2023
Accepted: 24 July 2023
Available online: 04 Nov 2023

Keywords:
Corrosion conqueror
High-performing inhibitor
Mild steel savior
Hydrochloric acid defender
Revolutionary breakthrough

ABSTRACT

Corrosion, the relentless foe plaguing industries exposed to hydrochloric acid solutions, threatens material integrity and equipment longevity. To triumph over this formidable adversary, the development of effective corrosion inhibitors is paramount. In this groundbreaking research, we delve into the untapped potential of 4-Acetamidoantipyrine as a corrosion inhibitor for safeguarding mild steel in hydrochloric acid solutions. Through rigorous experimentation, employing weight loss measurements, adsorption studies, and state-of-the-art computational analysis, we unlock the secrets of this remarkable inhibitor's inhibitory mechanisms. The results astoundingly reveal a pronounced decline in the corrosion rate of mild steel as the concentration of 4-acetamidoantipyrine intensifies. At an impressive concentration of 500 ppm, the inhibitor unleashes its full might, exhibiting an awe-inspiring maximum inhibition efficiency of 91.1 %. Further investigation uncovers the formation of a robust monolayer on the surface of mild steel, meticulously adhering to the revered Langmuir adsorption isotherm. Illuminating the binding mechanism, computational analysis highlights the intricate interaction between the inhibitor's nitrogen and oxygen atoms from the pyrazole and amide groups with the metal surface. These revelatory findings underscore the immense potential of 4-Acetamidoantipyrine as an unparalleled corrosion inhibitor, championing the protection of mild steel in the most aggressive hydrochloric acid environments. Moreover, they provide invaluable insights into the enigmatic inhibitory mechanisms employed by this remarkable compound. By shedding light on the captivating interactions and absorption behavior of 4-acetamidoantipyrine, this seminal study pioneers the advancement of corrosion inhibitors, paving the way for continued exploration and transformative breakthroughs in this captivating field. Prog. Color Colorants Coat. 17 (2024), 85-96© Institute for Color Science and Technology.

1. Introduction

Mild steel is widely utilized in various industries, including construction, food processing, and transportation, owing to its advantageous properties such as mechanical strength, ductility, ease of production, and cost-effectiveness [1, 2]. However, the susceptibility of

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Doi: 10.30509/pccc.2023.167147.1223

mild steel to corrosion poses a significant challenge, leading to surface cracking, financial losses, and safety hazards [1, 2]. Hence, it is imperative to prevent corrosion and protect the integrity of mild steel. In recent years, multiple anti-corrosion strategies have been developed, encompassing corrosion inhibitors, coating isolation, alloying, and metal surface modification. Among these approaches, the utilization of corrosion inhibitors has emerged as a cost-effective and straightforward method [2, 3]. Corrosion inhibitors are chemical compounds that form a protective layer on the metal surface, impeding corrosion while preserving the material's original properties. The addition of a small quantity of corrosion inhibitor can significantly reduce the corrosion rate of mild steel under diverse environmental conditions [4, 5]. Extensive research has been conducted on corrosion inhibitors in various industries to effectively reduce the corrosion rate of metal surfaces exposed to aggressive environments. Hydrochloric acid and other acidic solutions find wide application in industrial processes such as acid pickling, industrial cleaning, acid rescaling, oil-well acidification, and petrochemical operations. Inhibitors are commonly employed in acidic solutions to prevent metal dissolution and acid consumption, establishing them as practical means of corrosion protection [6, 7]. Organic inhibitors have demonstrated their effectiveness in mitigating corrosion, and numerous scientific studies have investigated the use of corrosion inhibitors for mild steel in acidic media. In general, inhibitors containing heteroatoms exhibit varying degrees of effectiveness, with the order of preference being oxygen (O) < nitrogen (N) < sulfur (S) < phosphorus (P) [8-15]. Organic molecules can alter the electrochemical behavior of acidic media, thereby reducing their aggressiveness [16-18]. Antipyrine derivatives, which contain oxygen and nitrogen heteroatoms, are frequently employed as corrosion inhibitors. Among them, a specific derivative, namely 4-acetamidoantipyrine (Figure 1), has been investigated as a potential corrosion inhibitor for mild steel in acidic environments. The multifunctional protective properties of this inhibitor position it as a promising novel corrosion inhibitor. The inhibition efficiency of 4-acetamidoantipyrine was evaluated using weight loss techniques, and the experimental results were further correlated with quantum chemical calculations employing density functional theory (DFT) to elucidate the coordination between the inhibitor and the mild-steel surface. Corrosion poses a significant challenge in industries that are exposed to hydrochloric acid solutions, as it threatens the integrity and longevity of materials and equipment. The aggressive nature of hydrochloric acid environments necessitates the development of effective corrosion inhibitors to mitigate the destructive effects. However, identifying suitable corrosion inhibitors that can effectively protect mild steel in such harsh conditions remains a pressing problem. This problem statement underscores the need for novel and efficient corrosion inhibitors that can preserve mild steel in hydrochloric acid environments, prompting the exploration of the untapped potential of 4-Acetamidoantipyrine as a promising solution. The aim of this research is to explore and unlock the potential of 4-acetamidoantipyrine as a corrosion inhibitor for preserving mild steel in harsh hydrochloric acid environments. The study aims to investigate the inhibitory properties and mechanisms of 4-Acetamidoantipyrine through experimental approaches, including weight loss measurements, adsorption studies, and computational analysis.

The objective of this research is to assess the effectiveness of 4-Acetamidoantipyrine as a corrosion inhibitor for mild steel in hydrochloric acid solutions. The specific objectives include:

1. Determine the corrosion rate of mild steel in the presence of varying concentrations of 4-acetamidoantipyrine.
2. Investigate the inhibition efficiency of 4-acetamidoantipyrine at different concentrations, with a focus on achieving maximum efficiency.
3. Study the adsorption behavior of 4-acetamidoantipyrine on the surface of mild steel and analyze its adherence to the Langmuir adsorption isotherm.
4. Utilize computational analysis to explore the interaction between the inhibitor's nitrogen and oxygen atoms and the metal surface, providing insights into the binding mechanism.
5. Highlight the significance of 4-acetamidoantipyrine as a corrosion inhibitor and its potential for safeguarding mild steel in aggressive hydrochloric acid environments.

6.

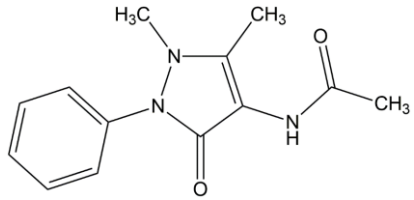

Figure 1: The chemical structure of acetamidoantipyrine.

2. Experimental

2.1. Weight loss measurements

The mild steel samples utilized in this study were provided by The Metal Samples Company and possessed the following composition (wt. %): carbon (0.210), manganese (0.050), silicon (0.380), aluminum (0.010), sulfur (0.050), phosphorus (0.090), and iron. To assess the corrosion behavior of the samples, weight loss measurements and electrochemical techniques were employed. Prior to testing, the mild steel samples underwent preparation steps, including grinding with emery paper, washing with double-distilled water, degreasing with ethanol, and subsequent drying at room temperature. For the creation of the corrosive solution, a 1 M hydrochloric acid solution was prepared by diluting 37 % analytical grade HCl (Merck-Malaysia) with double-distilled water. Varying amounts of acetamidoantipyrine were added to adjust the concentration. The samples were then immersed in the solution for a specified duration and evaluated for any indications of corrosion or degradation. The corrosion rate (CR), inhibition efficiency (IE %), and surface coverage (θ) were calculated according to the NACE standard. The experiments were conducted at different concentrations of acetamidoantipyrine, temperatures, and immersion times to comprehensively assess its effectiveness as a corrosion inhibitor in acidic media. Equations 1–3 [19, 20] were used to calculate the corrosion parameters.

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

$$IE\% = [1 - \frac{C_{R(i)}}{C_{R_o}}] \times 100 \quad (2)$$

$$\theta = 1 - \frac{C_{R(i)}}{C_{R_o}} \quad (3)$$

2.2. Adsorption isotherms

Analyzing the adsorption isotherm type provides valuable information about the characteristics of the compounds under investigation. To evaluate the surface coverage (θ) of the inhibitors, different adsorption isotherms, such as Langmuir, Frum-kin, and Temkin, can be employed. In this study, weight loss measurements were employed to determine the surface coverage (θ) values for various inhibitor concentrations in acidic media. The test samples had dimensions of 1.0 × 1.0 × 0.1 cm, and weight loss measurements were conducted using a scale with a sensitivity of 0.001 g.

2.3. DFT calculations

Quantum chemistry calculations were performed using the Gaussian 09 software [21]. To optimize the inhibitor's structure in the gas phase, the B3LYP method with a 6-31G^{++}(d,p) basis set was employed. The ionization potential (I) and electron affinity (A) were determined as E_{HOMO} and E_{LUMO}, respectively, following Koopman's theorem [22, 23]. Equations 4 and 5 were utilized to calculate the values.

$$I = -E_{HOMO} \quad (4)$$

$$A = -E_{LOMO} \quad (5)$$

Equations 6–9 were employed to calculate quantum chemical parameters including electronegativity (χ), hardness (η), softness (σ), and transferred electrons fractional number (ΔN) [24, 25].

$$\chi = \frac{I+A}{2} \quad (6)$$

$$\eta = \frac{I-A}{2} \quad (7)$$

$$\sigma = \eta^{-1} \quad (8)$$

$$\Delta N = \frac{7-\chi_{inh}}{2(\eta_{inh})} \quad (9)$$

The inhibitor's electronegativity and hardness can be denoted as χ_inh and η_inh, respectively (with Fe as a reference, where χFe = 7 eV and ηFe = 0 eV). Equations 6 and 7 were used to calculate these values.

3. Results and Discussion

3.1. Effects of inhibitor concentrations, immersion periods and Temperatures

In this study, the potential of 4-acetamidoantipyrine as a corrosion inhibitor for mild steel in a hydrochloric acid solution was investigated. The efficacy of the inhibitor was evaluated using weight loss experiments, adsorption studies, and computational analysis techniques [26]. The experimental results demonstrated that the corrosion rate of mild steel decreased as the concentration of 4-acetamidoantipyrine increased, with a maximum inhibition efficiency of 91.1 % observed at a concentration of 500 ppm. The adsorption behavior of the inhibitor on the mild steel surface followed the Langmuir adsorption isotherm, indicating the

formation of a monolayer [27]. Through computational analysis, it was revealed that the inhibitor molecule interacted with the metal surface through the nitrogen and oxygen atoms of the pyrazole and amide groups. These findings highlight the potential of 4-acetamidoantipyrine as an effective corrosion inhibitor for mild steel in a hydrochloric acid solution.

To evaluate the corrosion inhibition characteristics of acetamidoantipyrine, mild steel samples were subjected to immersion in a 1 M hydrochloric acid (HCl) solution containing varying inhibitor concentrations (ranging from 100 to 1000 ppm) for different immersion durations (ranging from 1 to 48 hours) at a temperature of 303 K [28]. The study findings, depicted in Figure 3, illustrate the influence of acetamidoantipyrine concentrations on the corrosion rate and inhibition efficiency of the metal samples at different immersion periods [29].

The experimental findings, as illustrated in Figure 4, demonstrated a significant reduction in the corrosion rate as the concentration of acetamidoantipyrine increased. Notably, the highest inhibition efficiency was achieved at a concentration of 1000 ppm, resulting in a reduction of approximately 70 % compared to the 100 ppm concentration [30]. Furthermore, the inhibitory efficacy was found to be influenced by the immersion period, with longer immersion times leading to greater inhibitory effects. For instance, at a concentration of 1000 ppm acetamidoantipyrine, the corrosion rate was observed to be lowest after 48 hours of immersion, exhibiting an 80 % decrease compared to the 1-hour immersion period [31]. The inhibitory efficiency of acetamidoantipyrine on metal substrates showed a rapid increase during the initial 10 hours of immersion, followed by a stable inhibitory effect between 10 and 24 hours. However, after 24 hours, a gradual decline in inhibitory efficacy was observed, possibly due to the depletion of acetamidoantipyrine molecules resulting from their reaction with the metal surface [32]. The adsorption of acetamidoantipyrine molecules onto the metal substrate plays a crucial role in enhancing the inhibitory effect by forming a uniform coating, acting as a protective barrier against corrosion. Nevertheless, extended immersion periods exceeding 24 hours led to a decrease in inhibitory efficacy.

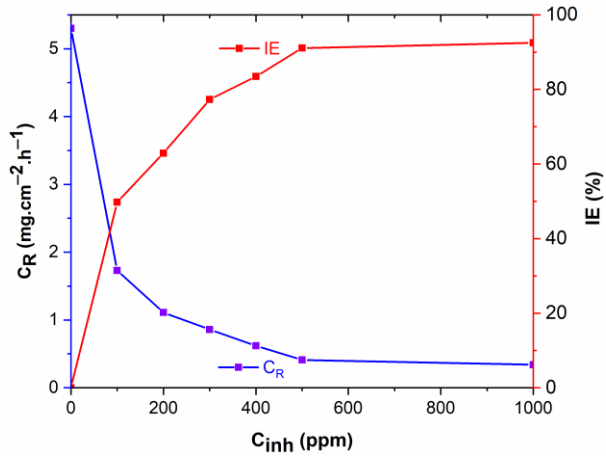

Figure 2: C_R and IE % of mild steel after immersion in a HCl for 5 hours at 303 K, with various concentrations of acetamidoantipyrine.

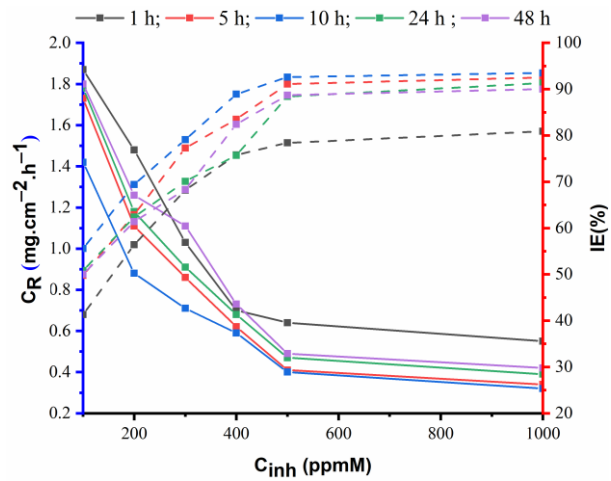

Figure 3: C_R and IE % of mild steel exposed to a corrosive environment for different immersion times at 303 K with various concentrations of acetamidoantipyrine.

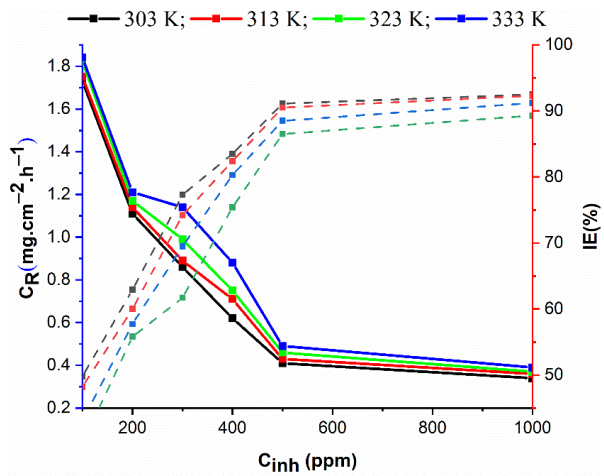

Figure 4: acetamidoantipyrine concentrations effect on the rate of corrosion and inhibitory efficiency of metallic coupons in 1 M HCl at different temperatures for 5 h.

The effectiveness of acetamidoantipyrine as a corrosion inhibitor on metallic substrates was further investigated at various concentrations (ranging from 100 ppm to 1000 ppm) and temperatures (ranging from 303 to 333 K) using mass reduction techniques after a 5-hour immersion period. The results revealed that higher temperatures were associated with increased corrosion rates and decreased inhibition efficiency of acetamidoantipyrine. This could be attributed to the heightened activity of corrosive species in the solution and the thermodynamic instability of the inhibitor at elevated temperatures. Additionally, the rate of reaction between the inhibitor and metallic substrate may contribute to the decline in its inhibition efficiency [34]. The high adsorption density of acetamidoantipyrine on the metal substrate plays a crucial role in its stability and efficacy as a corrosion inhibitor. The formation of a uniform coating prevents the access of corrosive agents to the metal surface, thereby offering effective protection. These findings collectively suggest that acetamidoantipyrine holds promise as an alternative corrosion inhibitor for safeguarding metal surfaces [35]. The study investigated the inhibitory potency of acetamidoantipyrine at different concentration levels on mild steel corrosion at varying temperatures. Results showed that as temperature increased, the inhibitory potency of acetamidoantipyrine decreased at all concentration levels, indicating physisorption. Inhibition efficiencies were further evaluated at temperatures ranging from 303 to 333 K, and at a concentration of 500 ppm, acetamidoantipyrine exhibited considerable inhibitive performance. However, the inhibition efficiency slightly decreased as temperature increased, particularly at the highest concentration level of 1000 ppm, which could be due to both physical and chemical adsorption mechanisms. These findings suggest that the effectiveness of acetamidoantipyrine as a corrosion inhibitor depends primarily on the temperature of the environment and can be used to optimize its use on mild steel surfaces. The present study aimed to explore the inhibitory effectiveness of acetamidoantipyrine at different concentrations on the corrosion of mild steel under varying temperatures. The results revealed a decrease in the inhibitory potency of acetamidoantipyrine with increasing temperature, irrespective of the concentration levels, indicating a physisorption mechanism. Further evaluation of inhibition efficiencies was performed within the temperature range of 303 to 333 K, with a particular focus on a concentration of 500 ppm acetamidoantipyrine. At this concentration, acetamidoantipyrine exhibited notable inhibitive performance. However, as the temperature increased, a slight decrease in inhibition efficiency was observed, especially at the highest concentration level of 1000 ppm. This phenomenon can be attributed to the combined influence of physical and chemical adsorption mechanisms.

Based on these findings, it can be inferred that the effectiveness of acetamidoantipyrine as a corrosion inhibitor is primarily dependent on the temperature of the surrounding environment. These insights are crucial in optimizing the application of acetamidoantipyrine for protecting mild steel surfaces against corrosion.

3.2. Adsorption isotherm

The aim of this investigation was to analyze the interaction between acetamidoantipyrine particles and the metallic substrate by studying the adsorption isotherm. To understand the adsorption mechanism, surface coverage values were obtained through gravimetric tests, and three different isotherm models, namely Temkin, Freundlich, and Langmuir, were employed. The analysis revealed that the Langmuir isotherm model provided the best fit for describing the adsorption process, indicating a monolayer adsorption with a fixed maximum capacity. The Temkin isotherm model suggested that the heat of adsorption governed the adsorption process, while the Freundlich isotherm model proposed that the surface heterogeneity of the adsorbent controlled the process, implying a multi-layer adsorption process. The utilization of the Langmuir isotherm model can assist in determining the maximum adsorption capacity of the adsorbent and the uptake of metal ions under different conditions. Meanwhile, the Temkin and Freundlich isotherms provide valuable insights into the nature of the adsorption process, including the role of heat and surface heterogeneity, respectively [36-38]. These findings have significant implications in the design and optimization of adsorption processes for the removal of metal ions from aqueous solutions. The Langmuir adsorption isotherms exhibited a good fit to the data, with a high regression coefficient (R^2) of 0.995 for acetamidoantipyrine. Thermodynamic parameters are presented in Table 1.

Table 1: Thermodynamic parameters of acetamidoantipyrine at the Temperature rang (303-333 K.

Parameter	303 K	313 K	323 K	333 K
R^2	0.995	0.994	0.993	0.988
Slop	0.0096 ± 3.1994E-4	0.0095 ± 3.615E-4	0.00943 ± 3.834E-4	0.0094 ± 5.032E-4
Intercept	1.0048 ± 0.16262	1.13654 ± 0.18377	1.3531 ± 0.1949	1.6228 ± 0.255

Table 2: The quantum chemical parameters of the acetamidoantipyrine molecule.

$I\ (eV)$	$A\ (eV)$	$E_{HOMO}\ (eV)$	$E_{LUMO}\ (eV)$	$\Delta E\ (eV)$	$\chi\ (eV)$	$\eta\ (eV)$	$\sigma\ (eV^{-1})$	$\Delta N\ (eV)$
7.783	1.08	-7.783	-1.08	6.703	4.431	3.351	0.298	0.383

The Langmuir adsorption isotherm plot in Figure 5 displays the relationship between C_{inh}/θ and C_{inh}. By utilizing equation 12, it is possible to calculate the adsorption parameters.

$$C_{inh}/\theta=(K_{ads})^{-1}+C \quad (12)$$

In this study, the concentration of acetamidoantipyrine is referred to as Cinh, while the surface area is denoted by θ, and the equilibrium constant is represented by K_{ads}. To determine the adsorption parameters (ΔG^o_{ads} and K_{ads}), the researchers analyzed the plot of C/θ versus C using equation 13.

$$\Delta G^o_{ads}=-RT\ \ln(55.5K_{ads}) \quad (13)$$

The expression used to calculate the adsorption parameters includes the molar concentration of water (55.5), as well as the universal gas constant (R) and absolute temperature (T).

Previous studies [39, 40] have established that the ΔG^o_{ads}value can provide insights into the adsorption mechanism. A ΔG^o_{ads} value close to -40 kJmol^{-1} indicates chemisorption, whereas a value near -20 kJmol^{-1} suggests physisorption. In the case of acetamidoantipyrine, the calculated ΔG^o_{ads}value was determined to be -35.87 kJmol^{-1}, indicating a combination of both chemisorption and physisorption mechanisms. The negative value signifies an exothermic and spontaneous adsorption process. The dominance of the chemisorption mechanism implies the formation of strong chemical bonds and irreversible adsorption. However, the proximity to -20 kJmol^{-1} suggests that physical interactions also play a role in the adsorption process, which is commonly observed in real-world systems exhibiting a mixture of chemical and physical interactions [41-43].

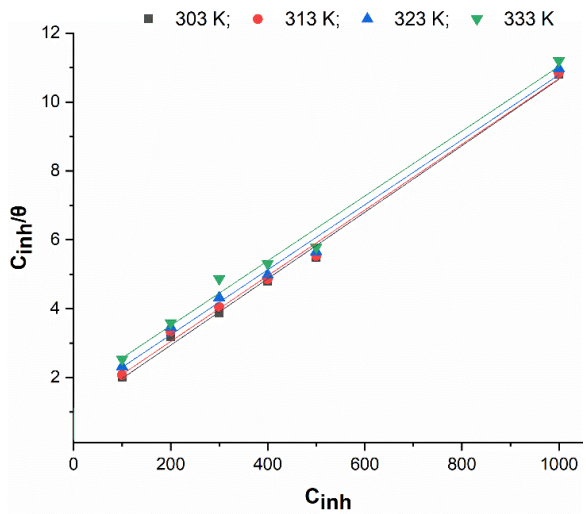

Figure 5: The Langmuir model for a metallic sample in a 1 M HCl solution that has been treated by acetamidoantipyrine with different concentrations.

3.3. DFT

To analyze the reactivity and interactions between the inhibitor molecule and the metal surface, the researchers employed the frontier molecular orbital (FMO) theory and Mullikan charges [44]. According to FMO theory, the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels of a species determine its chemical reactivity. Figure 6 illustrates the optimized geometry, HOMO, and LUMO of the acetamidoantipyrine molecule, while Table 2 provides various quantum chemical parameters [84]. The HOMO density primarily concentrates over the aniline ring, whereas the LUMO is situated over the aniline and oxazole rings. A higher EHOMO value indicates enhanced corrosion inhibition efficiency, as it suggests that the species can donate electrons and form coordinate bonds with the empty d orbitals of metal atoms [45-49].

The ELUMO value indicates the favorable conditions for accepting electrons through back donation from iron atoms, while the EHOMO value suggests the molecule's ability to donate electrons to metal atoms [50]. In the case of acetamidoantipyrine, it exhibits a relatively high EHOMO value and a reasonably low ELUMO value, making it an effective corrosion inhibitor. The energy gap (ΔE = ELUMO - EHOMO) serves as a measure of corrosion inhibition, where a lower ΔE indicates lower kinetic stability of the molecule, making it more polarizable and easier to adsorb on the metal surface [51, 52]. To determine the molecule's point of approach to the metal surface, Mullikan charges were conducted and are depicted in Figure 7. The atoms with the highest negative charges, such as nitrogen and oxygen, act as the most reactive centers for adsorption and can donate electrons to the metal surface through donor-acceptor type interactions.

3.4. Suggestion inhibition mechanism

The prevention of corrosion in a solution is primarily attributed to the adsorption of the inhibitor onto the metal surface, which is influenced by various factors including the aggressive media type, nature and charge of the metal, and charge and dipole moment of the inhibitor [53]. However, predicting the adsorption mechanism is challenging due to the complex nature of corrosion and adsorption processes. In the case of mild steel in acidic media, the surface carries a positive charge in the absence and presence of inhibitors, as revealed by zero charge potential analysis [54]. In an acidic solution, chloride ions tend to adsorb first, resulting in an excess of negative charges near the mild steel surface [55, 56]. Some studies suggest that the protonated form of the inhibitor may interact with the negatively charged metal/solution interface, forming a protective film that hinders the metal's contact with the aggressive medium (physisorption) [57]. Alternatively, the inhibitor may establish coordinate bonds with the d-orbitals of iron atoms and the lone pair of sp2 electrons in heteroatoms, as well as the pi electrons in

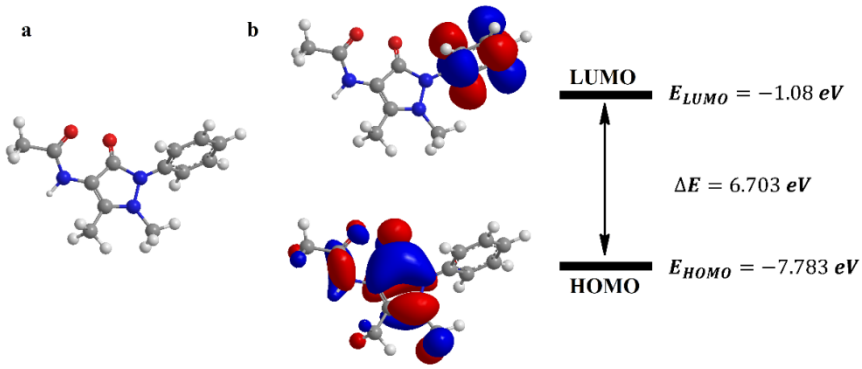

Figure 6: (a) Acetamidoantipyrine optimized chemical structure and (b) acetamidoantipyrine molecule energy gap diagram.

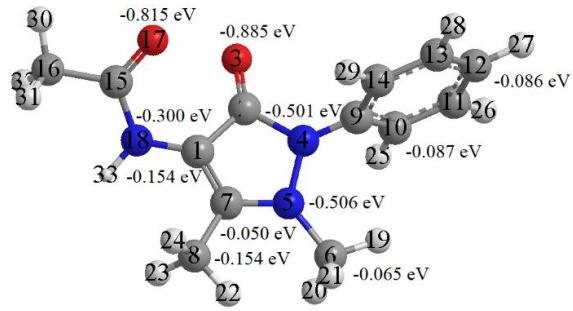

Figure 7: Acetamidoantipyrine molecule atomic charges.

the benzene ring (chemisorption). Hence, both adsorption models can explain the effective corrosion inhibition properties of acetamidoantipyrine. To gain a deeper understanding of how organic compounds prevent corrosion, it is crucial to investigate their attachment to the metal surface. The ability of most organic corrosion inhibitors to hinder corrosion is related to their affinity for the metal/solution interface. Adsorption isotherms can be utilized to study this phenomenon and provide insights into the adsorption mechanism and the types of interactions between the inhibitors and the metal surface. Corrosion inhibitors can adsorb at the interface through physical adsorption, involving weak interactions arising from electrostatic forces between charged molecules and the metal surface, or through chemical adsorption, involving electron sharing between inhibitors and the d-orbitals of iron surface atoms. The inhibitory activity of these chemicals follows the trend O < N < S < P. Figure 8 depicts the detailed interaction between acetamidoantipyrine molecules and the mild steel surface. The inhibitor molecule attaches to the surface through two adsorption routes. The first route involves the interaction between unpaired electrons and the vacant d-orbitals of Fe atoms. The second route involves donor-acceptor interactions between the lone pairs of electrons in oxygen and nitrogen heteroatoms and the unoccupied d-orbitals of iron surface atoms. In these interactions, the active electrons are shared with the d-orbitals of the Fe atom.

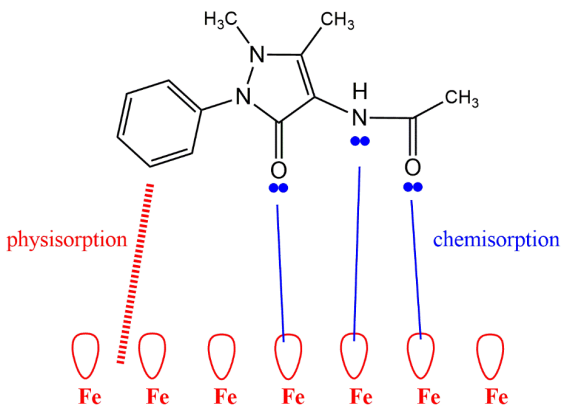

Figure 8: Suggestion mechanism for corrosion inhibition reaction of metallic substrate in inhibited corrosive solution.

3.5. Comparative evaluation of 4-Acetamido-antipyrine and existing corrosion inhibitors for mild steel in hydrochloric acid environments

Previous research has explored a variety of organic and inorganic inhibitors, such as benzotriazole, imidazoline derivatives, and organic salts, for protecting mild steel against corrosion in hydrochloric acid environments. These studies have reported varying degrees of corrosion inhibition, with some achieving impressive inhibition efficiencies. By comparing our results with these published studies, we can evaluate the potential of 4-acetamidoantipyrine as a corrosion inhibitor in relation to existing inhibitors. This comparison allows us to determine whether 4-acetamidoantipyrine exhibits superior inhibitory performance, demonstrating its viability as a promising candidate for corrosion protection in hydrochloric acid environments [59-67].

Furthermore, examining the mechanisms of action and adsorption behaviors of different inhibitors can provide valuable insights into the underlying processes governing corrosion inhibition. This comparative analysis aids in understanding the unique features and advantages of 4-acetamidoantipyrine as a corrosion inhibitor, highlighting its potential contributions to the field. Overall, the inclusion of comparison studies with other published research enhances the comprehensiveness and scientific rigor of our investigation. It allows us to position our findings within the existing body of knowledge, providing a comprehensive assessment of the inhibitory capabilities of 4-acetamidoantipyrine and its potential for practical applications in corrosion protection.

4. Conclusion

In this study, the potential of acetamidoantipyrine as a corrosion inhibitor for mild steel in a hydrochloric acid solution was investigated. The results demonstrated that acetamidoantipyrine had excellent corrosion inhibition properties, with a protection efficiency of 91.1 % at 500 ppm concentration. The inhibition efficiency increased with higher inhibitor concentration but decreased with increasing temperature. The Langmuir adsorption isotherm was employed to analyze the adsorption mechanism, which indicated the formation of a protective adsorption layer on the mild-steel surface that inhibited the corrosion rate. Density functional theory (DFT) was also utilized to understand the correlation between inhibition activity and

molecular structure, revealing that acetamidoantipyrine had high adsorption-inhibition activity. Both experimental and theoretical analyses provided consistent results, suggesting that acetamidoantipyrine could be a promising candidate for use as a corrosion inhibitor for mild steel in acidic conditions. This study provides important insights into the underlying inhibitory mechanisms and paves the way for future research in this area.

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How to cite this article:
Abtan NS, Al-Hamid MAI, Kadhim LA, Sayyid FA, Noori FTM, Kadum A, Alamiery A, Al-Azzawi WK. Unlocking the Power of 4-Acetamidoantipyrine: A Promising Corrosion Inhibitor for Preserving Mild Steel in Harsh Hydrochloric Acid Environments. Prog Color Colorants Coat. 2024;17(1):85-96. Doi: 10.30509/pccc.2023.167147.1223