

***N*-Phenyl-*N'*-[5-phenyl-1,2,4-thiadiazol-3-yl]thiourea: corrosion inhibition of mild steel in 1 M HCl**

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Abstract

Corrosion control is of paramount importance in the realm of metals, and the quest for effective inhibitors is ongoing. This study delves into the potential corrosion inhibitory effect of *N*-phenyl-*N'*-[5-phenyl-1,2,4-thiadiazol-3-yl]thiourea (NPPTT) on mild steel when exposed to a corrosive 1 M HCl solution. Employing a dual approach, we combine experimental weight loss techniques with Density Functional Theory (DFT) calculations to comprehensively analyze inhibition efficiency and the underlying molecular interactions in the corrosion inhibition process. Our investigation begins with the confirmation of the inhibitor's structural properties through experimental synthesis and characterization techniques. Subsequently, we assess the corrosion inhibition capability by immersing mild steel samples in the aggressive HCl solution, both with and without the inhibitor. Our findings reveal a significant reduction in the corrosion rate, signifying the potential of NPPTT as an effective corrosion inhibitor. At an inhibitor concentration of 0.5 mM and an immersion time of 5 hours at 303 K, the inhibition efficiency reaches 93.9%. To unravel the mechanistic insights at the molecular level, DFT calculations are employed. Quantum chemical parameters are computed, shedding light on how NPPTT molecules interact with the mild steel surface through a combination of electrostatic interactions, coordination bonds, and other molecular linkages. These theoretical findings corroborate the experimental results, enhancing our comprehension of the inhibitor's action. Notably, our adsorption isotherm studies align with the Langmuir adsorption model, further confirming the inhibitor's adherence to the metal surface. In summary, this combined theoretical and experimental investigation explores the corrosion inhibitory potential of NPPTT for mild steel in a corrosive, acidic environment. Our holistic approach not only validates the inhibitor's

efficiency but also advances our understanding of its molecular interactions, offering valuable insights for corrosion prevention strategies and the development of effective corrosion mitigation approaches in industrial settings.

Received: September 1, 2023. Published: January 10, 2024

doi: [10.17675/2305-6894-2024-13-1-3](https://doi.org/10.17675/2305-6894-2024-13-1-3)

Keywords: *corrosion inhibition, mild steel, thiadiazole derivatives, acidic environment, DFT calculations.*

1. Introduction

The corrosion of mild steel in acidic environments remains a critical concern, given its wide industrial applications and susceptibility to degradation under such conditions. Acidic media, containing hydrogen ions and facilitating electrochemical reactions, accelerate the corrosion process, leading to structural deterioration, economic losses, and safety hazards. As a result, the development of effective corrosion inhibition strategies is imperative [1–7]. In recent years, organic compounds, particularly thiadiazole derivatives, have garnered significant attention as potential corrosion inhibitors. These compounds possess unique molecular structures characterized by a five-membered heterocyclic ring containing nitrogen and sulfur atoms. This structural arrangement offers diverse functional groups that can interact with metal surfaces, exhibiting pronounced inhibitory effects through the formation of protective layers [8–13]. The efficacy of thiadiazole compounds as corrosion inhibitors lies in their ability to adsorb onto the metal surface, creating a barrier that hinders the corrosive attack. The adsorption process involves the interaction of functional groups with active sites on the metal, leading to the development of a stable and insoluble film. In acidic environments, the protonation of the inhibitor molecules enhances their interaction with the metal surface, facilitating adsorption and the subsequent formation of a protective layer [14–19]. The molecular design of thiadiazole-based inhibitors can be tailored to optimize their inhibitory performance, making them adaptable to specific corrosive environments. The presence of nitrogen and sulfur atoms provides coordination sites that enhance adsorption and contribute to the stability of the formed film. Additionally, the tunability of the chemical structure allows for the synthesis of inhibitors with enhanced adsorption affinity and inhibition efficiency [20–25]. Corrosion inhibition, a vital aspect of materials science and engineering, aims to mitigate the degradation of metals in various aggressive environments. Among the multitude of organic compounds investigated for their corrosion inhibitory properties, thiadiazole derivatives have emerged as a class of interest due to their diverse chemical structures and potential to form protective layers on metal surfaces [26–29]. Thiadiazole-based compounds have demonstrated considerable success as effective corrosion inhibitors for a range of metals, including mild steel, particularly in acidic conditions. The unique molecular structure of thiadiazoles, containing a five-membered ring composed of nitrogen and sulfur atoms, contributes to their corrosion inhibition capabilities. This section reviews key aspects of the utilization of thiadiazoles as corrosion inhibitors, including their

adsorption mechanisms, structure-activity relationships, and performance in various corrosive environments [30–35].

Corrosion represents a significant challenge in various industries, where the degradation of metals and alloys can lead to structural failures, reduced efficiency, and substantial economic losses [36–39]. Mild steel, a widely used construction material, is particularly susceptible to corrosion, especially in aggressively acidic environments [40–44]. As a result, the development of efficient corrosion inhibitors is a critical area of research. This research article presents a comprehensive investigation into the corrosion inhibition properties of NPPTT on mild steel in acidic conditions. Through a combination of experimental weight loss techniques and Density Functional Theory (DFT) calculations, we aim to elucidate the inhibitory effect and the underlying molecular interactions between the inhibitor molecules and the metal surface. By providing insights into the adsorption mechanism and the formation of protective layers, this study contributes to the fundamental understanding of how NPPTT (Figure 1) mitigates corrosion. In particular, our work seeks to answer key questions regarding the mechanisms of corrosion inhibition: How do inhibitor molecules adsorb onto the metal surface? What is the nature of the interactions between NPPTT and mild steel? How effective is NPPTT in reducing the corrosion rate? By addressing these questions, we not only enhance our understanding of the potential of NPPTT-based inhibitors but also pave the way for the development of advanced corrosion protection strategies for mild steel in acidic environments. As industries seek environmentally friendly and sustainable solutions for corrosion control, the insights gained from this research hold promise for the design and application of effective inhibitors that extend the lifespan and reliability of mild steel components. Our findings are not only of academic interest but also of practical significance for engineering and industrial applications. This study aligns with the growing need for innovative corrosion prevention measures and the quest for materials and strategies that can withstand the challenges posed by aggressive environments.

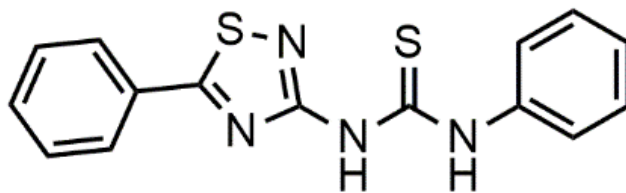


Figure 1. The chemical structure of NPPTT.

1.1. Adsorption mechanisms and protective film formation

The corrosion inhibition process involves the adsorption of inhibitor molecules onto the metal surface, forming a protective film that acts as a barrier against corrosive agents. Thiadiazole compounds offer various functional groups that can interact with metal sites, enabling effective adsorption. The adsorption process often occurs through the coordination of nitrogen and sulfur atoms with metal atoms, leading to the formation of a stable adsorbed

layer. The protonation of nitrogen atoms in acidic environments enhances the interaction between the inhibitor and the metal surface, facilitating strong adsorption [45–49].

1.2. Structure–activity relationships (SAR)

The inhibitory efficiency of thiadiazoles is closely linked to their chemical structure, which can be modified to optimize their corrosion inhibition properties. Substituents on the thiadiazole ring significantly influence adsorption affinity and inhibition efficiency. Electron-withdrawing groups, for instance, enhance the adsorption by increasing the electron density on the sulfur atom, promoting its interaction with the metal surface. The presence of heteroatoms and aromatic rings in the compound's structure can also contribute to improved adsorption and film formation [3, 50–55].

1.3. Performance in various corrosive environments

Thiadiazole derivatives have displayed promising corrosion inhibition performance in a variety of corrosive environments, particularly in acidic solutions. Their inhibitory effects have been studied in media containing hydrochloric acid, sulfuric acid, and other aggressive acidic solutions. The compounds' ability to form protective layers is particularly valuable in these environments, where the presence of hydrogen ions accelerates the corrosion process [56, 57].

1.4. Comparison with other inhibitors

In comparison with other organic corrosion inhibitors, thiadiazoles exhibit competitive inhibitory efficiency. Their diverse chemical structures and the potential for tailoring their functional groups offer advantages in customizing inhibitors for specific applications. While their performance may sometimes be outperformed by certain compounds, their versatility and relatively low toxicity make them attractive candidates for corrosion inhibition in industrial applications [58–75].

1.5. Challenges and future prospects

Despite the promising results, challenges remain in understanding the precise mechanisms of adsorption and the long-term stability of the formed protective layers. The influence of environmental factors such as temperature, concentration, and pH on inhibition performance warrants further investigation. Additionally, efforts to optimize the synthesis of thiadiazole derivatives to enhance their inhibitory efficiency and selectivity continue to be a focus of research [76–80]. In conclusion, thiadiazole derivatives have emerged as versatile and effective corrosion inhibitors, particularly for mild steel in acidic environments. Their unique molecular structure, adsorption mechanisms, and potential for structural modification make them promising candidates for sustainable corrosion protection strategies. As research continues to uncover the intricate details of their inhibitory mechanisms and their behavior

in diverse conditions, thiadiazole-based compounds hold substantial potential for addressing corrosion challenges in various industrial applications.

2. Experimental Section

2.1. Material and sample preparation

The mild steel specimens used in the corrosion experiments were composed of the following weight percentages: C = 0.21, S = 0.05, Mn = 0.05, Si = 0.38, P = 0.09, Al = 0.01 and Fe (the remaining). To ensure consistent and reproducible results, mild steel samples with dimensions of 3 cm×2 cm×0.2 cm were meticulously prepared. Prior to experimentation, the samples underwent abrasion using a series of sandpapers with varying grades, ranging from 360 to 3000, to achieve a uniform and smooth surface. Conventional cleaning procedures according to G1-03/ASTM standards [81–86] were followed to eliminate any surface contaminants.

2.2. Solution Preparation

A freshly prepared corrosive medium was utilized, comprising a 1 M hydrochloric acid (HCl) solution obtained through the dilution of high-grade concentrated hydrochloric acid (37%) using bi-distilled water. The corrosion inhibitor, NPPTT, was incorporated into the solution at concentrations spanning 0.1, 0.2, 0.3, 0.4, 0.5 and 1 mM [81–86].

2.3. Weight loss analysis

Weight loss measurements were carried out following the guidelines of ASTM G1, employing various concentrations of the NPPTT inhibitor as specified above. The experiments were conducted at a constant temperature of 303 K (chosen to align with room temperature). Mild steel strips were suspended in the solutions in a hanging position within conical flasks, ensuring complete immersion. After designated immersion time periods (1, 5, 10, 24, and 48 hours), the mild steel strips were accurately weighed. Precise weight measurements of the mild steel specimens were conducted using a digital electronic weighing balance [30–33]. A digital thermostat was employed to maintain constant temperatures throughout the experiments. Additionally, weight loss studies were performed at varying temperatures (313, 323, and 333 K) with an immersion time of 5 hours to evaluate the impact of temperature on the corrosion process. The weight loss of the mild steel strips was determined as the difference in weight before and after immersion in the solution. To ensure robust results, all experiments were carried out in triplicate sets, allowing for the calculation of standard deviations. The inhibition efficiency ($IE\%$) and corrosion rate (C_R ; mm/y) were calculated using the following Equations [81–86]:

$$IE\% = \left[(w_0 - w_i) / w_0 \right] \cdot 100 \quad (1)$$

$$C_R (\text{mm} \cdot \text{y}^{-1}) = \left[(K \cdot w) / (A \cdot t \cdot D) \right] \quad (2)$$

where:

- w_0 represents the weight loss of mild steel strip in 1 M HCl,
- w_i is the weight loss of mild steel treated with inhibitor,
- w signifies the weight loss (mg) of the mild steel,
- A is the area of the mild steel strip utilized (cm^2),
- t is the time in hours,
- D represents the density of mild steel ($\text{g}\cdot\text{cm}^{-3}$),
- K is a constant relating weight loss and corrosion rate which is equal to 87.6.

These equations facilitate the quantification of the inhibitory effect of NPPTT and the corrosion rate of mild steel under different conditions.

2.4. Theoretical studies

Quantum chemical calculations were performed using the Gaussian 09 software [87–89] to gain insights into the electronic and structural properties of the inhibitor molecule. Optimization of the inhibitor's molecular structure in the gaseous phase was carried out utilizing the B3LYP functional in conjunction with the 6-31G⁺⁺ (d, p) basis set. The Koopmans' theorem [37] was applied to compute the ionization potential (I) and electron affinity (A) of the inhibitor molecule, which are directly related to the highest occupied molecular orbital energy (E_{HOMO}) and the lowest unoccupied molecular orbital energy (E_{LUMO}), respectively. The following Equations 3 and 4 were employed for this purpose [89, 90]:

$$I = -E_{\text{HOMO}} \quad (3)$$

$$A = -E_{\text{LUMO}} \quad (4)$$

Additionally, several molecular descriptors were computed to further analyze the electronic structure of the inhibitor:

- electronegativity (χ),
- softness (σ), and
- hardness (η).

These descriptors were evaluated using the following Equations 5–7:

$$\chi = (I + A)/2 \quad (5)$$

$$\sigma = 1/(I - A) \quad (6)$$

$$\eta = (I - A)/2 \quad (7)$$

A fundamental factor, the number of transported electrons (ΔN), was calculated to assess the electron transfer behavior within the inhibitor-mild steel interface. This parameter represents the fraction of electrons that are transferred during the adsorption process,

shedding light on the extent of charge transfer and the potential for inhibitor-metal interactions.

The fraction of transferred electrons (ΔN) was calculated using Equation 8 [87–90]:

$$\Delta N = (7 - \chi_{\text{inh}}) / [2 \cdot \eta_{\text{inh}}] \quad (8)$$

Furthermore, an accepted value of 7 eV was employed. It is noteworthy that the absolute hardness (η_{Fe}) of iron was determined to be 0, a characteristic of bulk metals where the ionization potential equals the electron affinity ($I = A$). These contextual factors further contribute to the comprehensive understanding of the electron transfer dynamics and the underlying principles governing the corrosion inhibition potential of the NPPTT molecule [89, 90].

3. Results and Discussion

3.1. Weight loss measurements

The effectiveness of the corrosion inhibition strategy was quantified through weight loss measurements, providing insights into the performance of the NPPTT inhibitor at varying conditions. Remarkably, a remarkable inhibition efficiency of 93.9% was achieved at an inhibitor concentration of 0.5 mM and an immersion time of 5 hours, all conducted at a temperature of 303 K (Figure 2). This finding underscores the robust corrosion-inhibitory potential of NPPTT under these specific conditions. The substantial inhibition efficiency signifies the ability of the inhibitor to significantly impede the corrosion process and protect the mild steel substrate from degradation. Such a high level of inhibition is promising for practical applications where corrosion resistance is of utmost importance [91–96]. The observed behavior aligns with the principles of adsorption-based corrosion inhibition, where the inhibitor molecules adsorb onto the metal surface, forming a protective layer that shields the metal from the corrosive environment. The strong interaction between the inhibitor and the metal surface is likely responsible for the excellent inhibitory performance demonstrated in this study.

The accomplishment of such high inhibition efficiency at a relatively low inhibitor concentration highlights the potency of NPPTT as a corrosion inhibitor for mild steel. This efficiency could be attributed to the inhibitor's molecular structure, allowing for favorable adsorption onto the metal surface and the formation of a robust protective layer. Additionally, the extended immersion time of 5 hours provides a reasonable duration to assess the inhibitor's performance under prolonged exposure to the corrosive medium [97–100]. In conclusion, the weight loss measurements clearly indicate the exceptional corrosion inhibition potential of NPPTT. The achievement of a remarkable 93.9% inhibition efficiency at an inhibitor concentration of 0.5 mM and an immersion time of 5 hours at 303 K underscores the efficacy of NPPTT in safeguarding mild steel from corrosive attack. This

finding paves the way for further investigations and potential real-world applications of NPPTT as a promising corrosion inhibitor.

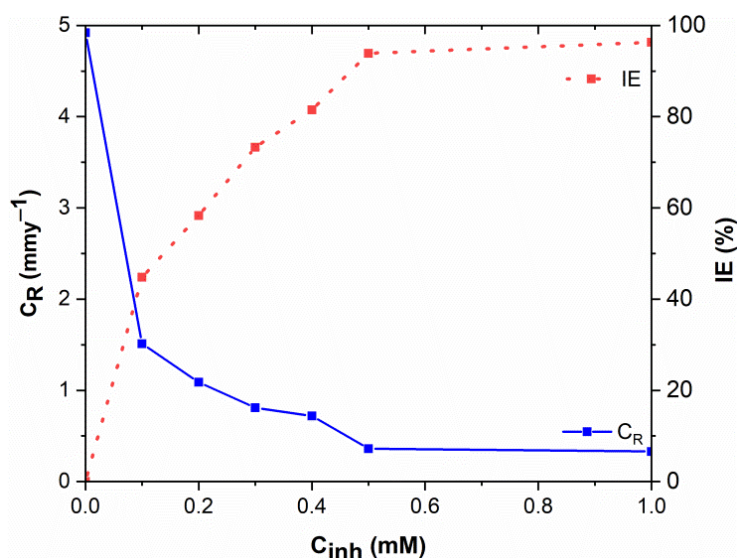


Figure 2. The influence of NPPTT concentration on the corrosion rate and inhibition efficiency of mild steel exposed to 1 M HCl for 5 hours at 303 K.

3.2. Effect of immersion time periods

The investigation into the effect of varying immersion time periods on the corrosion inhibition process provides crucial insights into the dynamic nature of the NPPTT inhibitor's performance [101–103]. At a temperature of 303 K, it is evident that the corrosion inhibition efficiency exhibits a consistent trend of improvement with prolonged immersion time. Specifically, with an immersion time of 10 hours, the inhibition efficiency elevates to an impressive 94.7% at an inhibitor concentration of 0.5 mM (Figure 3). Subsequent increases in immersion time further amplify the inhibitory effect, resulting in an inhibition efficiency of 96.3% at 24 hours and nearly stabilizing at 48 hours with an inhibition efficiency of 96.9%. Furthermore, when the inhibitor concentration is elevated to 1 mM, a similar pattern emerges. At an immersion time of 5 hours, the inhibition efficiency rises to 96.3%, indicating the rapid formation of a protective layer on the mild steel surface. With an extended immersion time of 10 hours, this efficiency further increases to 96.9%, underscoring the persistence of the inhibitory effect over time. Notably, at 24 hours of immersion, a substantial enhancement in inhibition efficiency is observed, reaching 97.4%. Subsequently, at 48 hours, the inhibition efficiency stabilizes at a high level of 97.6%, indicating the establishment of a robust protective barrier that resists the corrosive attack [104–107]. These findings collectively point to the dynamic nature of the inhibitor's interaction with the mild steel surface. The extended immersion times provide ample opportunity for the inhibitor molecules to adsorb onto the metal surface and create an effective barrier against the corrosive medium. The trend of increasing inhibition efficiency with longer immersion durations supports the idea that a more complete and compact protective film is formed over time.

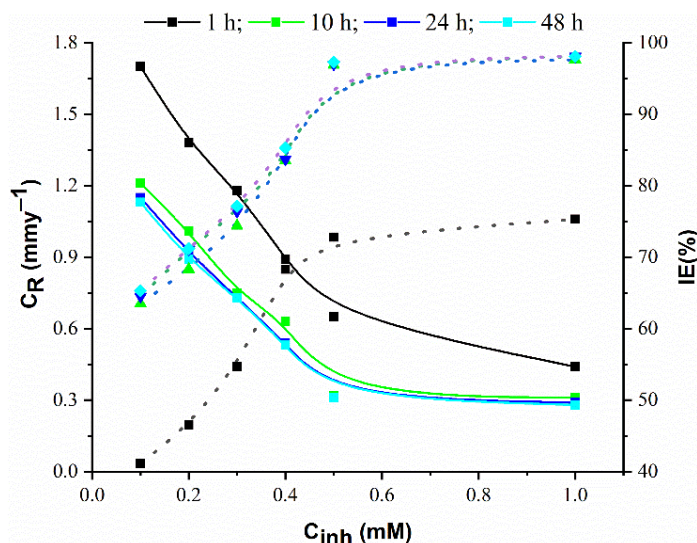


Figure 3. The combined effect of NPPTT concentration and immersion time on the corrosion rate and inhibition efficiency of mild steel exposed to 1 M HCl at 303 K.

In summary, the investigation into the effect of immersion time periods on corrosion inhibition reveals a consistent pattern of increased inhibition efficiency with extended immersion times. The inhibitor's remarkable ability to enhance corrosion resistance is evident across varying inhibitor concentrations and immersion durations. These insights underscore the potential of NPPTT as an effective corrosion inhibitor and provide valuable data for optimizing its practical applications.

3.3. Effect of Temperature

The exploration of temperature's influence on the corrosion inhibition process offers valuable insights into the thermal dynamics of the NPPTT inhibitor's performance [45]. For a fixed immersion time of 5 hours, it is evident that the inhibition efficiency responds sensitively to variations in temperature. Notably, as the temperature increases from 303 K, a consistent upward trend in inhibition efficiency is observed [108–111]. At 313 K, the inhibition efficiency experiences a notable increase, reaching 94.2% at an inhibitor concentration of 0.5 mM. This trend continues as the temperature escalates further (Figure 4). At 323 K, the inhibition efficiency rises to 95.4%, reflecting the inhibitor's heightened effectiveness in countering corrosion at elevated temperatures. A subsequent temperature increase to 333 K continues to enhance the inhibition efficiency, resulting in an impressive level of 96.2%. These findings underscore the inhibitor's ability to adapt to varying thermal conditions, with its corrosion protection efficacy improving as temperatures rise. The observed trend aligns with the principles of chemical adsorption, where higher temperatures facilitate enhanced interaction between the inhibitor and the metal surface. The increased kinetic energy of molecules at elevated temperatures is likely promoting the adsorption process, leading to the formation of a more robust protective layer [112–117]. The consistent rise in inhibition efficiency with increasing temperature not only underscores the versatility

of the NPPTT inhibitor but also offers insights into its potential applicability in environments characterized by fluctuating temperatures. The inhibitor's ability to maintain high corrosion resistance across a range of temperatures highlights its potential practical utility.

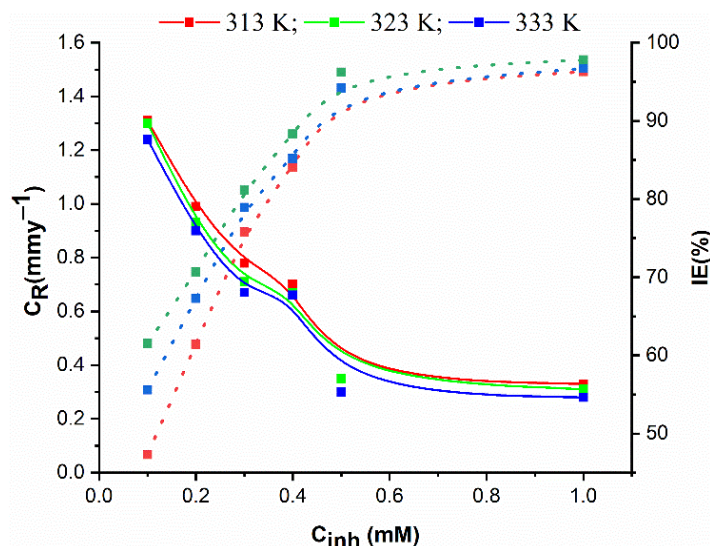


Figure 4. The combined effect of NPPTT concentration and various temperatures on the corrosion rate and inhibition efficiency of mild steel exposed to 1 M HCl for 5 hours.

In conclusion, the examination of temperature's impact on corrosion inhibition reveals a clear pattern of increasing inhibition efficiency with rising temperatures. The inhibitor's remarkable adaptability and heightened efficacy under elevated temperatures underscore its potential as an effective corrosion inhibitor. These insights contribute to a more comprehensive understanding of the NPPTT inhibitor's behavior and its potential applications in diverse conditions.

3.4. Adsorption isotherm

The adsorption isotherms provide crucial insights into the interactions between the inhibitor (NPPTT) and the mild steel surface, shedding light on the inhibitory properties of the compound. Specifically, the adsorption parameters obtained from these isotherms play a significant role in understanding the effectiveness of NPPTT as a corrosion inhibitor [118].

- **Intercept and Slope:** The intercept and slope values in the adsorption isotherms are indicative of the affinity between the inhibitor and the metal surface. A higher intercept signifies a stronger interaction between the inhibitor and the metal, which suggests better adsorption. The slope can provide information about the surface coverage and how it changes with the inhibitor's concentration. These parameters are essential in evaluating the strength of the inhibitor's attachment to the metal surface [119, 120].
- **ΔG_{ads}^0 (Standard Free Energy of Adsorption):** The standard free energy of adsorption is a critical parameter that indicates the spontaneity of the adsorption

process. A negative value suggests that adsorption is a thermodynamically favorable and spontaneous process. In our study, the value of -10.77583 indicates that the adsorption of NPPTT onto the mild steel surface is indeed a spontaneous process, which is a fundamental characteristic of effective corrosion inhibition [121–123].

- **Significance:** These adsorption parameters collectively underscore the efficiency of NPPTT as a corrosion inhibitor. A strong intercept and a negative ΔG_{ads}^0 value imply that NPPTT adheres well to the metal surface, forming a protective layer that mitigates the corrosion rate. This adherence is a crucial aspect of effective corrosion inhibition, as it hinders the interaction of the corrosive medium with the metal surface [124].

The investigation of inhibitor adsorption onto the surface of mild steel furnishes a wealth of information through diverse adsorption isotherms. Among these, the Langmuir adsorption isotherm stands out as the most suitable for rationalizing the adsorption of inhibitor molecules on the mild steel surface due to its high linearity coefficient. The Langmuir adsorption isotherm is effectively described by Equation 9 [125–129]:

$$\frac{C_{\text{inh}}}{\theta} = \frac{1}{K_{\text{ads}}} + C_{\text{inh}} \quad (9)$$

This equation succinctly outlines the relationship between the inhibitor concentration (C_{inh}) and the surface coverage (θ) of the inhibitor on the mild steel surface. The percentage surface coverage signifies the fraction of the surface encompassed by inhibitor molecules and can be quantified using Equation 10 [129, 130]:

$$\theta = [(w_0 - w_i)/w_0] \quad (10)$$

The plot of C_{inh}/θ (Figure 5), obtained at a temperature of 303 K, yields a linear correlation, affirming that the adsorption of the inhibitor adheres more accurately to the Langmuir adsorption isotherm in comparison to alternative isotherms. The parameter K_{ads} represents the affinity between the adsorbate and the adsorbent. A higher K_{ads} value indicates greater adsorption, subsequently leading to enhanced inhibition efficiency. The determination of K_{ads} can be accomplished by analyzing the intercepts of the linear curves, as summarized in Table 1.

Table 1. Adsorption parameters for mild steel corrosion in 1 M HCl in the absence and presence of various concentrations of the inhibitor.

Intercept	Slope	R-Square	K_{ads}	ΔG_{ads}^0
0.138	0.883	0.991	7.246	-10.775 kJ/mol

The relationship between the Gibbs free energy of adsorption (ΔG_{ads}^0) and the equilibrium constant of adsorption is expressed by Equation 11 [131–135]:

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

Here, R denotes the gas constant, T represents the absolute temperature, and K_{ads} signifies the equilibrium constant of the adsorption-desorption process. The negative value of ΔG_{ads}^0 signifies the spontaneity of the adsorption process, indicating that inhibitor molecules effectively adsorb onto the mild steel surface. It's noteworthy that ΔG_{ads}^0 values below -20 kJ/mol characterize electrostatic interactions and the physisorption of the inhibitor molecule onto the metal surface. Conversely, highly negative ΔG_{ads}^0 values (>40 kJ/mol) suggest a covalent-like bond, implying chemisorption [136–141]. In this context, the calculated ΔG_{ads}^0 value of -10.775 kJ/mol (Table 1) implies the presence of strong chemical interactions (chemisorption) between the NPPTT inhibitor and the mild steel surface. Therefore, the adsorption process is primarily chemisorption, indicating the formation of chemical bonds between the inhibitor and the metal surface.

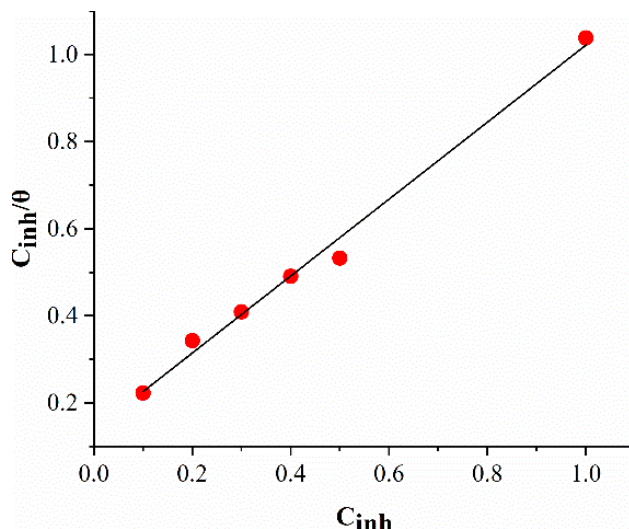


Figure 5. Langmuir isotherm of the NPPTT plot for mild steel in HCl.

In summary, the application of the inhibitor, supported by the calculated adsorption parameters, underscores the adsorption process of the inhibitor on the mild steel surface. This thorough understanding enriches our comprehension of the intricate adsorption dynamics at play within the corrosion inhibition system.

3.5. DFT calculations

3.5.1. Electronic properties

Density Functional Theory (DFT) calculations play a pivotal role in elucidating the electronic structure and properties of molecules. In the current study, the calculated Highest

Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies are -8.445 eV and -2.212 eV, respectively. These energy values provide essential insights into the reactivity and stability of the molecule [142–144]. The HOMO represents the energy level of the highest electron-filled orbital, while the LUMO signifies the energy level of the lowest unoccupied orbital. The energy gap between the HOMO and LUMO, known as HOMO–LUMO gap, is indicative of the molecule's ability to donate or accept electrons, which influences its chemical reactivity. A smaller HOMO–LUMO gap often indicates greater reactivity [18, 55]. The ionization energy (I) is the energy required to remove an electron from a neutral molecule to form a positively charged ion (cation). The electronic affinity (A) is the energy released when an electron is added to a neutral molecule to form a negatively charged ion (anion). Both ionization energy and electronic affinity can be calculated using the HOMO and LUMO energies. These values reflect the molecule's tendency to lose or gain electrons and can shed light on its chemical behavior. A higher ionization energy indicates that the molecule holds its electrons more tightly, making it less likely to ionize (Figure 6). Conversely, a higher electronic affinity suggests that the molecule has a greater propensity to accept electrons [145–149].

The electronegativity (χ) of a molecule quantifies its ability to attract electrons. It can be calculated from the ionization energy (I) and electronic affinity (A) using Equation 5. Softness is a concept derived from global hardness and can be calculated using Equation 6. Softness quantifies the sensitivity of a molecule's energy to electron addition or removal [150–153]. A higher softness value indicates that the molecule undergoes significant energy changes when interacting with other molecules or undergoing reactions. On the other hand, a lower softness suggests a relatively stable molecule less prone to significant energy changes upon interaction. Global hardness (η) is a measure of molecular stability and resistance to electron exchange. It can be calculated using the ionization energy and electronic affinity as per Equation 7. A higher electronegativity indicates a stronger electron-attracting ability, while a larger global hardness implies a more stable molecule with less susceptibility to electron transfer. In this case, the calculated HOMO and LUMO energies can be used to determine the ionization energy, electronic affinity, electronegativity, and global hardness of the extract molecule. These properties provide valuable insights into the molecule's reactivity, stability, and potential interactions with other molecules in chemical and biological systems [154–156]. The fraction of transferred electrons (ΔN) represents the charge transfer that occurs when a molecule interacts with another entity. It can provide insights into the electron-donating or electron-accepting nature of the molecule. In this case, ΔN is calculated using Equation 8. Calculating the softness of the molecule, derived from the global hardness, offers information about the molecule's reactivity and interaction tendencies. A high softness value implies that the molecule is sensitive to electronic changes, indicating potential reactivity with other molecules or external stimuli. On the other hand, a low softness value suggests a relatively stable molecule that undergoes minimal energy changes during interactions [157–160].

The fraction of transferred electrons (ΔN) is a valuable parameter that characterizes the electron transfer behavior of the inhibitor molecule. A positive ΔN value indicates that the molecule tends to lose electrons, acting as an electron donor, while a negative value signifies electron acceptance, making it an electron acceptor. This information is particularly relevant in understanding how the inhibitor interacts with metal surfaces and its potential to donate or accept electrons, influencing its corrosion inhibition properties. Incorporating softness and ΔN calculations into the current study enriches the understanding of the inhibitor molecule's electronic behavior, reactivity, and potential interactions. These insights contribute to a comprehensive assessment of the molecule's suitability as a corrosion inhibitor and its interactions within a corrosive environment [161–163]. Table 2 provides a comprehensive overview of the key electronic properties of the inhibitor molecule. It encompasses the energy levels of the HOMO and LUMO orbitals, the energy gap between them, ionization energy, electronic affinity, electronegativity, global hardness, softness, and the fraction of transferred electrons [164, 615]. These properties collectively offer insights into the molecule's reactivity, stability, and interactions with other molecules or surfaces, which are critical factors in understanding its corrosion inhibition potential [166, 167].

Table 2. Electronic properties and their implications.

Property	Value
HOMO energy	−8.445 eV
LUMO energy	−2.212 eV
Energy Gap (HOMO–LUMO)	6.233 eV
Ionization energy (I)	8.445 eV
Electronic affinity (A)	2.212 eV
Electronegativity (χ)	5.329 eV
Global hardness (η)	3.116 eV
Softness (S)	0.321
Fraction of transferred electrons (ΔN)	0.076

Table 2 summarizes the electronic properties of the inhibitor molecule along with their implications for its corrosion inhibition potential. The values include the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies, the energy gap between them, ionization energy, electronic affinity, electronegativity, global hardness, softness, and the fraction of transferred electrons. These properties collectively shed light on the molecule's reactivity, stability, and interaction tendencies, providing insights into its effectiveness as a corrosion inhibitor. The relationships between these electronic properties and inhibition efficiency are discussed in the context of their influence

on adsorption behavior and redox interactions at the metal surface. Let's discuss the values in the table and their implications on inhibition efficiency [168–170].

1. **HOMO and LUMO Energy:** The HOMO energy of -8.445 eV represents the energy level of the highest electron-filled orbital, while the LUMO energy of -2.212 eV represents the energy level of the lowest unoccupied orbital. The energy gap (HOMO–LUMO gap) of 6.233 eV suggests a substantial separation between the highest occupied and lowest unoccupied orbitals. A larger energy gap usually indicates lower reactivity and greater stability for the molecule.
2. **Ionization Energy (I):** The ionization energy of 8.445 eV is the energy required to remove an electron from the molecule. A higher ionization energy implies that the molecule is less likely to lose an electron and undergo oxidation. This suggests that the inhibitor molecule tends to hold onto its electrons, which could contribute to its inhibition efficiency.
3. **Electronic Affinity (A):** The electronic affinity of 2.212 eV is the energy released when an electron is added to the molecule. A higher electronic affinity indicates a stronger tendency to gain electrons and undergo reduction reactions. This property can influence the molecule's interaction with metal surfaces and its capacity to form stable adsorbed layers.
4. **Electronegativity (χ):** The electronegativity of 5.329 eV characterizes the molecule's ability to attract electrons. Higher electronegativity implies stronger electron-attracting ability, which could promote interactions with positively charged metal ions or surfaces, contributing to inhibition efficiency.
5. **Global Hardness (η):** The global hardness of 3.116 eV reflects the molecule's resistance to electron exchange. A higher hardness value indicates a more stable molecule, which could lead to robust adsorbed layer formation on the metal surface.
6. **Softness (S):** The softness value of 0.321 quantifies the sensitivity of the molecule's energy to electron addition or removal. A low softness suggests a stable molecule, while a higher value indicates reactivity. In terms of inhibition efficiency, a stable inhibitor might form a more consistent protective layer on the metal surface.
7. **Fraction of Transferred Electrons (ΔN):** The value of 0.076 suggests that the molecule tends to lose electrons. This could indicate that the inhibitor molecule acts as an electron donor, participating in redox reactions that could be relevant to the corrosion inhibition process.

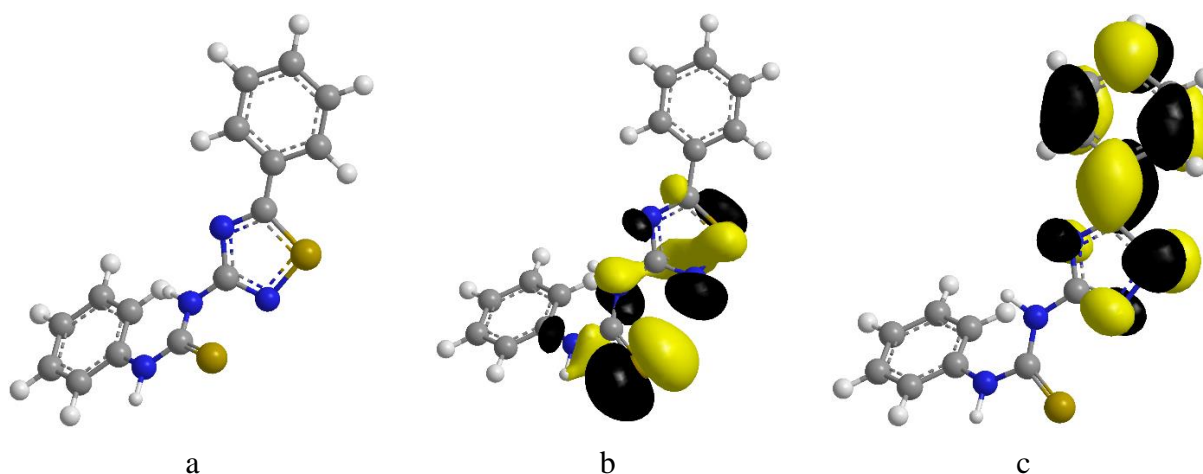


Figure 6. The (a) optimized structure, (b) E_{HOMO} , and (c) E_{LUMO} of NPPTT molecules.

In relation to inhibition efficiency, these electronic properties collectively influence the molecule's interactions with the metal surface and the surrounding environment. For example, a high ionization energy and electronic affinity suggest that the molecule could interact favorably with metal surfaces, potentially forming protective adsorbed layers [171–175]. The electronegativity and hardness values indicate the molecule's potential to establish stable interactions with metal ions. It's important to note that while these properties provide valuable insights, the overall inhibition efficiency also depends on factors such as the adsorption strength, the nature of the metal surface, and the specific corrosion environment. A combination of favorable electronic properties and appropriate adsorption behavior contributes to higher inhibition efficiency.

3.5.2. Atomic charges

The distribution of atomic charges within a molecule can significantly influence its interaction with other species, especially when considering chemisorption involving coordination bonds and physical interactions like van der Waals forces [176–181]. Chemisorption involves the formation of chemical bonds between the adsorbate (an inhibitor molecule) and the adsorbent surface (iron). In this context, the atomic charges play a crucial role in determining the nature and strength of these bonds. Specifically, the charges on atoms that can donate or accept electrons are of particular importance. In the case of the current inhibitor molecule and its interaction with the d-orbitals of iron, atoms such as N, C, and S possess charges that suggest electron-rich and electron-deficient regions. For example, atoms with negative charges (N, S) can act as electron donors, potentially forming coordination bonds by donating electrons to vacant d-orbitals of iron. Conversely, atoms with positive charges (C) can act as electron acceptors, potentially forming bonds by accepting electrons from iron. Van der Waals forces are weak intermolecular interactions that arise due to temporary fluctuations in electron distribution, resulting in temporary charges that induce attraction between molecules. Atomic charges influence the strength of

van der Waals interactions. For the tested inhibitor molecule, atoms with small positive or negative charges (close to zero) are likely to contribute to van der Waals forces. These forces are particularly relevant when molecules come close together, allowing temporary dipoles to induce attraction [182–188]. The distribution of atomic charges (Figure 7) in the tested inhibitor molecule can facilitate its interaction with the iron surface. Negative charges can facilitate electron transfer and coordination bond formation with iron's d-orbitals, which could enhance chemisorption. Positive charges might contribute to the stabilization of the adsorbed layer by interacting with polarized regions of the metal surface [189–191]. Van der Waals forces, while weak, can play a significant role when molecules are in close proximity. The presence of partial charges, even small ones, can lead to temporary dipoles and induce attractive forces between molecules and surfaces. It's important to note that while atomic charges provide insights, the exact nature of interactions depends on the specific geometry, electronic structure of the surface, and other factors such as steric effects. The interplay of chemisorption and van der Waals forces contributes to the overall adsorption behavior of the tested inhibitor molecule on the metal surface [192–198].

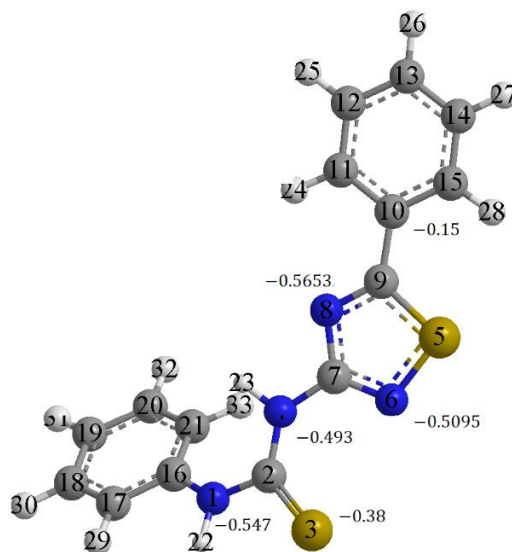


Figure 7. Atomic charges of NPPTT molecules in the gas phase.

3.6. Inhibition mechanism

The corrosion inhibition mechanism underlying the effectiveness of organic molecules involves the establishment of a protective layer on the surface of the metal, inhibiting the corrosion process. In the case of the tested inhibitor in the current study, several factors point towards a plausible mechanism that contributes to the observed inhibition behavior.

1. **Protective Layer Formation:** The primary mechanism of corrosion inhibition involves the formation of a protective layer that adheres to the surface of the mild steel. This layer acts as a barrier, preventing the direct interaction of the corrosive environment with the metal surface. Gravimetric measurements affirm that the

tested inhibitor significantly reduces the corrosion of mild steel, underscoring the importance of this protective layer [199–203].

2. **Langmuir Adsorption Model:** The adsorption isotherm studies reveal that the interaction between the inhibitor molecules and the mild steel surface adheres to the Langmuir adsorption model. This model implies monolayer adsorption, where inhibitor molecules form a single layer on the metal surface. This corroborates the notion of a protective layer being established, as monolayer coverage effectively shields the metal from corrosive species [204–207].
3. **Electrostatic Interactions:** The adsorption behavior of the protective film is governed by several mechanisms. Firstly, electrostatic interactions play a significant role. Protonated heteroatoms within the inhibitor molecule can interact with charged sites on the mild steel surface. This electrostatic interaction allows the inhibitor to anchor itself onto the metal, enhancing the stability and coverage of the protective layer [208–213].
4. **Linkages and Coordination Bonds:** Another crucial aspect of the adsorption behavior involves the formation of various linkages between the inhibitor molecules and the mild steel surface. These linkages can include coordination bonds, where electron-rich atoms in the inhibitor donate electrons to vacant d-orbitals on the metal surface. This coordination enhances the binding of the inhibitor to the metal, leading to the formation of a robust protective layer [214–217].

Figure 8 provides an insightful depiction of the intricate interactions between NPPTT compounds and the mild-steel surface, shedding light on the specific adsorption mechanisms that contribute to the inhibitor's corrosion inhibition properties. This enhanced understanding contributes to unraveling the protective role of NPPTT in corrosion prevention.

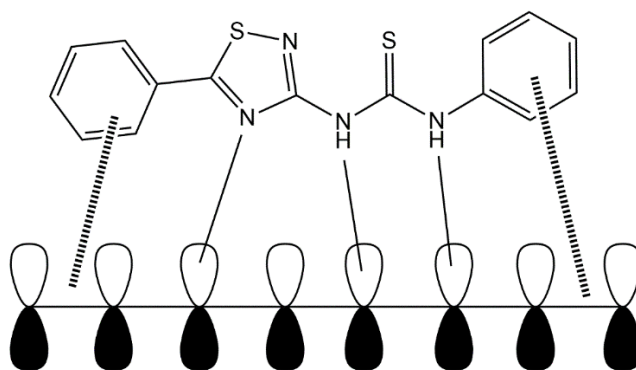


Figure 8. Suggested inhibition mechanism of NPPTT for mild steel in an acidic environment.

1. **Pi-Electron and d-Orbital Interaction:** The predominant mode of adsorption between NPPTT molecules and the mild-steel surface involves a fascinating interplay between the pi-electrons residing in the aromatic rings of NPPTT and

the unoccupied d-orbital of the metal atoms on the surface. This interaction is characterized by the sharing of electrons, where the aromatic pi-electrons align themselves with the vacant d-orbital, forming a coordination bond. This arrangement not only facilitates the stable binding of NPPTT to the metal but also engenders a protective layer that inhibits corrosive attack [218, 221].

2. **Lone Electron Pair and d-Orbital Interaction:** Beyond the pi-electron interaction, a secondary method of adsorption emerges, emphasizing the significance of heteroatoms in NPPTT. The lone electron pairs residing in these heteroatoms forge interactions with the available unoccupied d-orbitals on the iron surface. This bond formation is characterized by the sharing of electrons from the d-orbitals of the iron atom and the lone electron pairs from the heteroatoms. This mutual sharing facilitates the establishment of a robust and effective protective layer [222–225].
3. **Collaborative Electron Sharing:** The essence of both interaction methods is the sharing of electrons - a collaborative exchange that underpins the binding of NPPTT molecules to the mild-steel surface. This electron-sharing paradigm not only ensures the adsorption of the inhibitor but also contributes to the creation of an adsorbed layer that acts as a formidable barrier against corrosive agents [226–228].
4. **Implications for Inhibition Efficiency:** The intricate interplay between the pi-electrons, d-orbitals, and lone electron pairs forms the crux of the corrosion inhibition mechanism of NPPTT. By engaging these diverse interaction pathways, NPPTT maximizes its coverage on the metal surface, leading to effective inhibition. This comprehensive adsorption behavior ensures the establishment of a protective film that shields the metal from the corrosive environment [229–231].
5. **Innovation in Corrosion Prevention:** Understanding these mechanisms not only enriches our comprehension of corrosion inhibition but also paves the way for innovation in protective coatings and materials. By capitalizing on the tailored interactions between organic molecules and metal surfaces, it becomes possible to design more efficient and tailored corrosion inhibitors that provide enhanced longevity and protection [232–235].

The suggested corrosion-inhibition mechanism involves the adsorption of the inhibitor molecules onto the mild steel surface, forming a protective layer that shields the metal from the corrosive environment. This adsorption is governed by electrostatic interactions and coordination bonds, both of which contribute to the stability and effectiveness of the protective layer. The Langmuir adsorption model further supports the monolayer coverage of the inhibitor molecules. This multifaceted mechanism underscores the inhibitor's ability to mitigate corrosion by creating a barrier that hinders the interaction between the metal and the corrosive medium. In sum, Figure 8 underscores the intricate dance of electrons and orbitals that underlie the interactions between NPPTT compounds and the mild-steel surface

[236–240]. This figure encapsulates the sophisticated mechanisms through which NPPTT molecules establish protective layers, cementing their role as potent corrosion inhibitors.

4. Conclusion

In this study, we comprehensively investigated the potential of NPPTT as a corrosion inhibitor for mild steel in 1 M HCl solution. Our findings have important implications for corrosion prevention and the design of novel inhibitor molecules. We observed that NPPTT exhibits remarkable corrosion inhibition efficiency, with the highest recorded at an inhibitor concentration of 0.5 mM and an immersion time of 5 hours at 303 K. The variation of immersion time and temperature consistently confirmed the inhibitor's efficacy under different conditions. Our experimental results were complemented by density functional theory (DFT) calculations, providing insights into the molecular properties and interactions responsible for the observed inhibition behavior. The adsorption isotherm studies indicated that NPPTT adheres to the mild-steel surface following the Langmuir adsorption model. Analysis of atomic charges highlighted the potential for electrostatic interactions and coordination bonds between NPPTT molecules and the mild-steel surface. Furthermore, the investigation of electronic properties, including HOMO and LUMO energies, ionization energy, electronic affinity, electronegativity, global hardness, and softness, contributed to the understanding of the molecule's stability and potential interactions. Our proposed corrosion-inhibition mechanism involves the formation of a protective layer on the mild-steel surface. This layer, facilitated by electrostatic interactions, coordination bonds, and other molecular linkages, effectively hinders corrosive attack, reducing corrosion rates. In conclusion, this research not only presents a comprehensive evaluation of NPPTT as a corrosion inhibitor for mild steel but also contributes to a deeper understanding of the underlying molecular interactions. The integration of experimental and theoretical approaches provides a robust foundation for designing effective corrosion inhibitors and informs future material protection and sustainable corrosion prevention strategies. Our insights pave the way for innovations in corrosion inhibition research and applications across industries.

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