

Evaluating the corrosion inhibition efficiency of 5-(4-pyridyl)-3-mercapto-1,2,4-triazole for mild steel in HCl: insights from weight loss measurements and DFT calculations

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Abstract

Metals are frequently exposed to corrosion by a wide variety of sources in various manufacturing environments. Effective inhibitors are urgently necessary to put an end to this situation. The investigation that follows requests to evaluate the potential of 5-(4-pyridyl)-3-mercapto-1,2,4-triazole (PMT) to prevent mild steel from corroding in an acid environment. PMTs inhibitory mechanisms were identified by weight loss experiments, Density Functional Theory (DFT) calculations and Langmuir adsorption isotherm analysis. The study found that when mild steel was dipped into 1 M HCl under optimal inhibitor conditions and at a concentration of 0.5 mM, the inhibition efficiency reached 97.1% at 303 K. Experiments of weight loss and density functional theory (DFT) are utilized to explore inhibitory mechanisms, and are also offered indicates about PMT's adsorption behavior on metal surfaces. The Langmuir adsorption isotherm suggestions a first indication about the compound's effectiveness, but it may also assist as a starting point for future developments in research on corrosion inhibition. These results provide some important knowledge to us about the fundamental mechanism of corrosion protection, and have important applications to industries trying to protect metals from corroding threatened in aggressive environments.

Keywords: corrosion inhibition, PMT, weight loss experiments, DFT quantum chemical calculations, Langmuir adsorption isotherm.

1. Introduction

Corrosion presents a widespread risk to the structural stability of metallic components within various industrial sectors, including critical infrastructure, transportation, and the oil and gas industry [1–8]. This natural process results in compromised safety, reduced operational efficiency, and substantial economic losses. Substantial efforts have been devoted to identifying effective strategies to mitigate corrosion, with corrosion inhibitors emerging as a prominent solution. These chemical compounds are intricately formulated to create protective layers on metal surfaces, thereby inhibiting the electrochemical reactions that lead to corrosion [9–16]. These chemical compounds have been meticulously formulated to create protective layers on metal surfaces, thereby inhibiting the electrochemical reactions that lead to corrosion [17–22]. Their widespread use can be attributed to their cost effectiveness, ease of application and ability to extend the lifespan of materials [23–27]. Organic corrosion inhibitors, whether derived from natural or synthetic sources have shown effectiveness and sustainability [28–33]. When these organic inhibitors are applied to metal surfaces they create films that assistance defend against corrosive attacks. The growing popularity of inhibitors, in corrosion prevention efforts is due, to their friendly nature ability to biodegrade and diverse range of inhibitive properties [34–66]. The basic process of inhibiting corrosion involves the adsorption of molecules, onto metal surfaces. In environments these molecules selectively attach to metal surfaces through chemisorption and physisorption [37–42]. Chemisorption involves the formation of chemical bonds creating a layer that limits the entry of corrosive agents. On the hand physisorption is a less stable and reversible process that lacks strong chemical bonding [43–46]. The ability of corrosion inhibitors to effectively adhere to metal surfaces and form shields depends on various factors, including the concentration of the inhibitor, temperature and duration of immersion. These factors have an impact, on how the inhibitors adsorb and ultimately affect their inhibitory efficiency [47–52]. The Langmuir adsorption isotherm plays a role, in studying the impact of adsorption inhibitors on metal surfaces. It offers insights into surface coverage and the equilibrium constant (K_{ads}), for adsorption [53–55]. Understanding the adsorption isotherm plays a role, in enhancing our knowledge of how organic inhibitors and metal surfaces interact. This in turn aids in the advancement of corrosion inhibitors that're more efficient [57–59]. The recent study focused on examining the properties of 1,2,4-triazole derivatives as potential organic substances that can prevent mild steel corrosion in acidic environments containing hydrochloric acid (HCl). Both weight loss measurements and advanced calculations based on Density Functional Theory (DFT) have been used to understand mechanisms that inhibit corrosion [60–66]. The analyses have produced significant findings, paving the way for the primary aim of this research: to investigate the corrosion inhibition capacity of PMT (Figure 1) and reveal its outstanding effectiveness in

protecting mild steel from corrosive deterioration. The study utilizes a research approach that involves conducting weight loss experiments, analyzing Langmuir adsorption isotherm and performing calculations using DFT quantum chemistry methods.

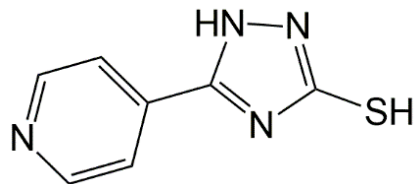


Figure 1. Shows the chemical structure of PMT.

Organic corrosion inhibitors have become a selection for protecting metals against corrosion [67–70]. Industries are drawn to their advantages such as being friendly versatile, cost effective compatible, with existing systems and sustainable. However, there are still challenges that must be overcome to fully harness the potential of these inhibitors in promoting corrosion protection strategies. These challenges are important to address in order to achieve long term stability, compatibility, with coatings and a better understanding of environments [71–74]. It is crucial to tackle these challenges if we want to harness the potential of organic inhibitors in promoting sustainable corrosion protection strategies [75–80]. In industries inhibitors are highly interesting due to their eco-friendliness, flexibility, cost effectiveness, compatibility, with existing systems and sustainability. However further research and development are necessary to address challenges such as long term stability, compatibility, with coatings and the understanding of environments [71–74]. It is crucial to overcome these challenges in order to fully unleash the potential of inhibitors in promoting corrosion protection strategies [75–80]. The research findings demonstrate that PMT exhibits inhibition efficiency of 97.1% at 303 K in a demanding 1 M HCl solution when used at an inhibitor concentration of 0.5 mM. PMT demonstrates an ability to inhibit corrosion, in environments production it an effective corrosion inhibitor for mild steel. The study reveals information, about how PMT molecules interact with the metal surface, their adsorption behavior. According to the Langmuir adsorption isotherm, PMT molecules adhere strongly and favorably to the surfaces of steel resulting in high surface coverage and a significant equilibrium constant of adsorption (K_{ads}). This comprehensive understanding establishes a robust foundation for further advancements in corrosion inhibition research, holding promising implications for industries seeking robust solutions to protect metals in challenging environments. The research objectives were to quantitatively evaluate the corrosion inhibition efficiency of PMT under specific conditions, in particular in 1 M HCl solid solution at an inhibitor concentration of 0.5 mM and a temperature of 303 K. The second aim is to use Langmuir adsorption isotherms for exploration adsorption behavior of the inhibitor on the metal surface. Finally, advanced quantum chemical DFT calculations were employed to explore the interactions between the PMT inhibitor and the mild steel surface. This research aims to develop a comprehension of PMTs mechanism for inhibiting

corrosion aiding in the enhancement of efficient and environmentally friendly strategies for corrosion protection. The consequences clarify important promise for industries demanding strong solutions to protection metallic materials, contributing to the improvement of corrosion science and engineering. Through highlighting on the inhibitory properties and mechanisms of this triazole derivative, this research aims to assist the adoption of novel and potent corrosion inhibitors, furthering the field of corrosion science and engineering.

2. Experimental Methodology

2.1. Materials and reagents

We obtained all the materials and reagents for this study from Sigma Aldrich Malaysia. To create a solution for our experiments, we prepared an acid (HCl) solution with a concentration of 1 M by diluting a high quality 37% HCl solution with double distilled water. In order to achieve inhibitor concentrations ranging from 0.1, to 1.0 mM we diluted the inhibitor in the 1 M HCl solution [81].

2.2. Sample preparation

The mild steel tests applied in this study underwent analysis for their chemical composition using X-ray fluorescence spectrometry. 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). The samples were prepared following the ASTM G1-03 protocol and polished using silicon carbide series plates (120, 600, and 1200). Before immersion, the mild steel coupons were thoroughly cleaned with double-distilled water and acetone and then dried in an oven [80, 81].

2.3. Weight loss measurements

The weight loss measurements were performed by immersing the mild steel samples in 500 ml glass beakers containing 400 ml of the prepared 1 M HCl solution with varying concentrations of the inhibitor. The experiments were carried out at a temperature of 303 K using a water bath, following the NACE TM0169/G31 protocol. The samples were exposed for different time periods (1, 5, 10, 24, and 48 hours), and the products of corrosion were carefully wiped off the surface before the coupons were dried and weighed. The difference in weight was recorded, and the mass variation at the estimated time, along with the original mass of the metallic sample, represented the weight loss attained. The mild steel coupons were immersed in corrosive media (1 M HCl) containing different inhibitor concentrations (0.1, 0.2, 0.3, 0.4, 0.5, and 1 mM) at temperatures of 303, 313, 323, and 333 K using a water bath to examine the effect of temperature [80, 83]. The average rate of corrosion was calculated after being exposed in triplicate, and the rate of corrosion and inhibition efficiency were determined using the following Equations (1, 2) [80–88]:

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

$$IE\% = \left[1 - \frac{C_{R(i)}}{C_{R_0}} \right] \times 100 \quad (2)$$

where W is the weight loss (mg) of the sample, a is the surface area of mild steel (cm^2), d is the density of the mild steel coupon (g/cm^3), and t is the exposure time (h). The corrosion rates in the absence and presence of the inhibitor were denoted as C_{R_0} and $C_{R(i)}$, respectively.

The coverage area (θ) for both uninhibited and inhibited solutions was determined using the following equation [80–88]:

$$\theta = 1 - \frac{C_{R(i)}}{C_{R_0}} \quad (3)$$

2.4. DFT calculations

ChemOffice software was utilized for conducting quantum chemical calculations. To investigate the interactions between the inhibitor and the metal surface, Density Functional Theory (DFT) calculations were performed using Gaussian 09 Revision C.01 software. The optimization of the inhibitors structure, in its form was achieved through the B3LYP method. The basis set “6 31G⁺⁺(d, p)”. By applying the Koopmans theory, we determined the ionization potential (I) and electron affinity (A) based on the occupied orbital (E_{HOMO}) and lowest unoccupied molecular orbital (E_{LUMO}) respectively. Equations (4, 5) were used to calculate I and A [89, 90].

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

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

The values for electronegativity (χ), hardness (η), and softness (σ) were determined using Equations (6–8).

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

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

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

Additionally, we determined the number of electrons transferred (ΔN) by applying Equation (9) mentioned in references [90–93]. The electronegativity value of iron was set at

7 eV while the hardness value was considered to be zero eV. Taking these findings into account, we formulated Equation (10).

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

$$\Delta N = \frac{7 - \chi_{\text{inh}}}{2(\eta_{\text{inh}})} \quad (10)$$

2.5. Adsorption isotherm studies

To gain comprehensive insights into the properties of the studied molecules, various types of adsorption isotherms, including Frumkin, Temkin, and Langmuir, were employed. These isotherms aid in determining the extent of inhibitor coverage on the metal surface. Weight-loss measurements were conducted to assess the surface coverage of the inhibitor at various concentrations in corrosive media [94–96].

3. Results and Discussion

3.1. Weight loss measurements

Weight loss measurements were performed to evaluate the corrosion behavior of mild steel samples in a corrosive environment. The experiments were conducted at 303 K, and the samples were immersed for 5 hours in a 1 M HCl solution with varying concentrations of the inhibitor, namely “PMT”. The obtained results, represented in Figure 2, illustrate the corrosion rate and inhibition effectiveness [97–100]. As shown in Figure 2, the addition of PMT to the corrosive solution leads to a significant reduction in the corrosion rate of the mild steel samples. The inhibitory effect exhibits an increasing trend with rising PMT concentrations, reaching its highest efficiency at 0.5 mM. This behavior can be attributed to the higher concentration of PMT molecules available for adsorption onto the mild steel surface. The adsorption of PMT molecules forms a protective layer that acts as a barrier, hindering the corrosive attack and thereby enhancing the inhibition effectiveness [101–105]. Formation of this barrier film on the metallic surface protects the metal against an aggressive environment and thereby reduces the corrosion rate. Nevertheless, it should be noted that with higher PMT concentrations than 0.5 mM the inhibition efficiency decreases. High concentrations of dissolved oxygen lead to desorption of excessive PMT molecules from mild steel surface. The desorption process weakens the protective layer, reducing its ability to prevent corrosion effectively [106–109]. Overall, the weight loss measurements clearly demonstrate the corrosion inhibition potential of PMT for mild steel in a 1 M HCl solution. The results highlight the importance of alteration the concentration of PMT to achieve its inhibitory impact [110–112]. Moreover, these findings offer insights into how PMT molecules adhere to the surface of steel revealing the mechanisms that prevent corrosion.

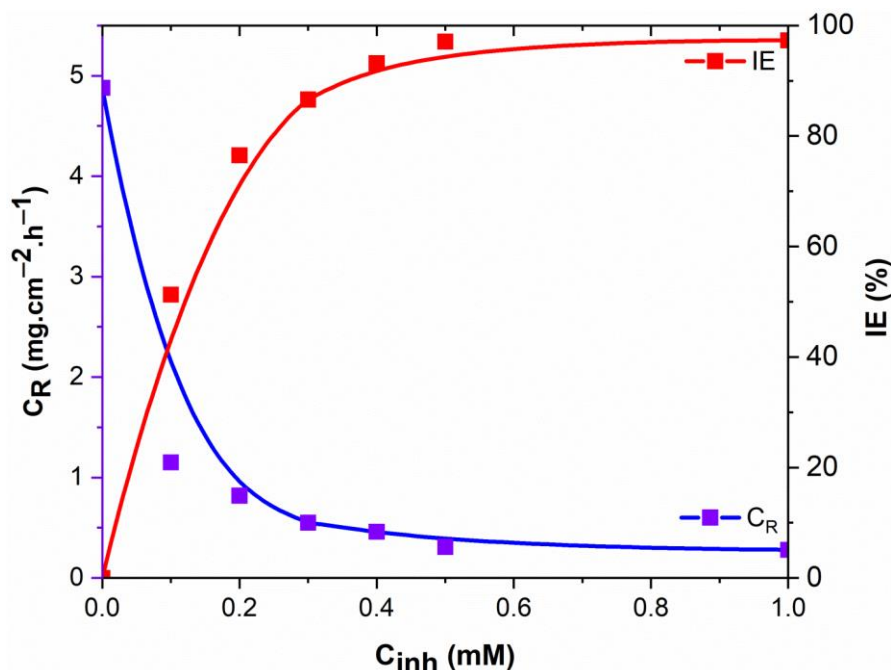


Figure 2. The corrosion rates and inhibition effectiveness on mild steel in hydrochloric acid solutions with and without the inhibitor after immersing the samples for a period of 5-hour at 303 K.

In this research we conducted a study to examine how the length of time something is immersed affects the effectiveness of preventing corrosion, on steel in a solution [113–118]. We submerged samples of steel in a solution containing hydrochloric acid and different amounts of an inhibitor for periods (1, 5, 10, 24 and 48 hours) at a temperature of 303 K. The results we obtained are shown in Figure 3. Demonstrate how the efficiency of corrosion prevention changes based on the duration of immersion [119–122]. Figure 3 clearly indicates that as the immersion time increases up to 5 hours there is an improvement in corrosion prevention. The efficiency continues to improve up to 24 hours before experiencing a decline in protective performance [123–125]. Finally, after 48 hours the efficiency stabilizes. We believe that this increase, in efficiency can be attributed to inhibitor molecules attaching themselves to the surface of steel thereby forming a protective layer. This interaction allows the van der Waals forces to come into play, facilitating the adsorption of the inhibitor molecules onto the metal surface [126–131]. Although some inhibitor molecules may detach from the surface during longer exposure durations, reducing the coverage area and overall effectiveness, the sustained high inhibition efficiency observed during extended exposure demonstrates the stability of the adsorbed inhibitor layer in the corrosive solution. The protective layer formed by the inhibitor molecules acts as a barrier, preventing direct corrosive attacks on the metal surface and, consequently, reducing the corrosion rate [132–135]. These findings highlight the significance of how an object's immersed in the corrosion inhibition process. When objects are exposed for a period it allows for an absorption of inhibitor molecules and the creation of a strong protective layer. This

knowledge can be valuable, in determining the time and concentration required for use thus maximizing corrosion protection, for metals in corrosive environments [136–139].

As the inhibitor concentration increases, there is a consistent reduction in corrosion rates at all immersion times. After 1-hour immersion, notable reductions in corrosion rates are observed, indicating a rapid inhibitive effect even at low concentrations [140–143]. After 5 to 24-hour immersion, the inhibitory effect persists and becomes more pronounced with time, emphasizing the concentration-dependent corrosion inhibition capacity. At low concentrations, the corrosion rates generally decrease with longer immersion times, suggesting a gradual development of the inhibitive effect [144–147]. At moderate concentrations (0.4–0.5 mM), the initial reduction in corrosion rates is significant within the first hour, and further immersion (5–24 hours) continues to enhance the inhibitive effect, albeit at a diminishing rate. At high concentrations, the corrosion rates are already low at the 1-hour mark, and further immersion yields marginal additional reduction, indicating a saturation effect. 0.5 mM concentration stands out, consistently offering low corrosion rates across all immersion times. It demonstrates an optimal balance between concentration and inhibitory effectiveness [148–152]. Within 1 to 5 hours, significant reductions in corrosion rates occur within the first 5 hours, indicating rapid adsorption and the initiation of the inhibitive process. Within 5 to 24 hours, the continued decline in corrosion rates suggests the formation of a more stable and robust inhibitor layer over prolonged exposure. For scenarios requiring short-term protection, concentrations as low as 0.1 mM already exhibit substantial inhibitory effects within the first hour [153–155]. Concentrations of 0.5 mM show promising prolonged inhibition, making them suitable for applications where extended protection is crucial. In conclusion, the data underscores the concentration-dependent and time-sensitive nature of the inhibitory effects of the studied compound. Higher concentrations and longer immersion times consistently lead to lower corrosion rates, emphasizing the need for a nuanced approach to inhibitor selection based on specific application requirements [156–159]. Further analysis, including statistical methods and modeling, could provide deeper insights into the correlation between inhibitor concentration, immersion time, and corrosion rates, aiding in the optimization of corrosion protection strategies.

The results obtained in this study reveal a significant reduction in the inhibition efficiency of the tested inhibitor derivative “PMT” as the temperature increases from 303 K to 333 K (Figure 4). At 303 K, a concentration of 0.5 mM of the inhibitor demonstrated an impressive inhibition efficiency of 97.1%, indicating its effectiveness in protecting the metallic substrate from corrosion. However, at 333 K, the inhibition efficiency decreased to 91.6%, indicating a decrease in the inhibitory performance of “PMT” at higher temperatures. Several factors may contribute to this observed reduction in inhibition efficiency with increasing temperature. Firstly, elevated temperatures intensify the thermal agitation of the “PMT” molecules and the corrosive solution [160–166]. This increased thermal agitation can disrupt the adsorption process of the inhibitor onto the metal surface, leading to a

reduction in the formation of a protective layer. Additionally, higher temperatures can enhance the reactivity of the corrosive environment, resulting in increased corrosion rates even in the presence of the inhibitor [167–169].

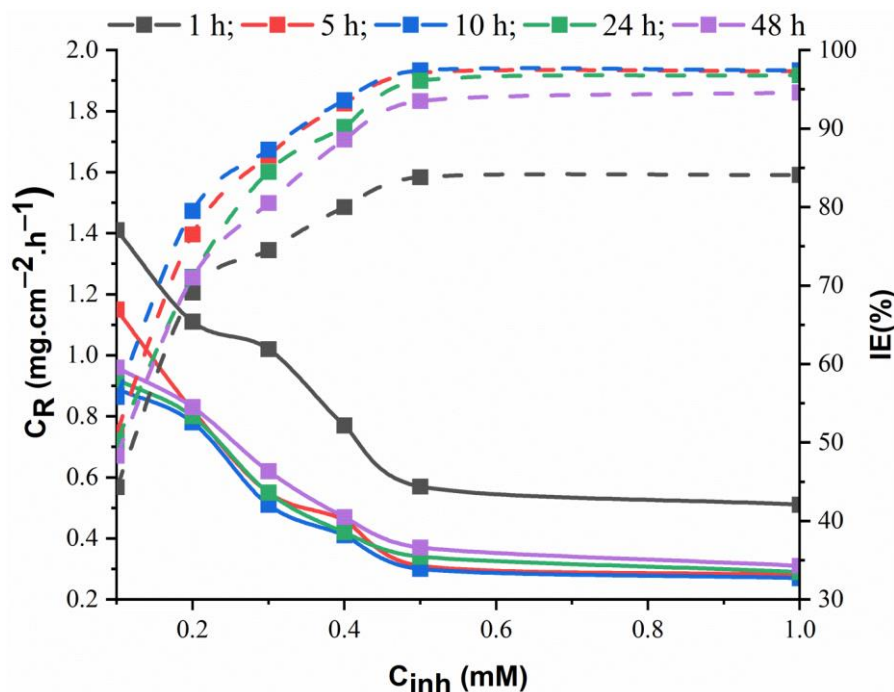


Figure 3. A comparison of corrosion rates and inhibition effectiveness in hydrochloric acid solutions with and without the inhibitor for 1, 5, 10, 24, and 48 h immersion time at different temperatures.

In addition, elevated temperatures can cause the displacement of inhibitors from metal surfaces. This high thermal energy weakens the bonding between the PMT molecules and the metal surface resulting in some molecules detaching thus decreasing the effective coating region. The desorption process that occurs during this stage can render the inhibitor ineffective [170–174]. Significant corrosion protection is provided by “PMT” especially at higher temperature conditions although its inhibition efficiency is reduced under these conditions. Nevertheless, one should bear in mind that the effectiveness of the inhibitor depends on temperature variation. In order to better optimize PTM as a corrosion inhibitor, further researches and studies are required to reveal the exact reasons why inhibiting efficiency reduces with increasing temperatures. Such knowledge could be used in designing measures that would increase the efficacy and stability of “PMT” inhibition especially in high temperatures [175–179]. Exploring other parameters including dosage, time exposure, and potential interactions between PMT and other additives would provide deeper insights into its corrosion inhibition mechanism. However, in conclusion, the decrease in inhibitor efficiency from 97.1% at 303 K to 91.6% at 333 K when “PMT” concentration was increased to 0.5 mM suggests that the inhibitor response may be temperature-dependent. Such findings underscore the importance of considering temperature variations when developing corrosion

inhibition strategies, highlighting the need for future studies to enhance “PMT” protection efficiency across different temperature ranges.

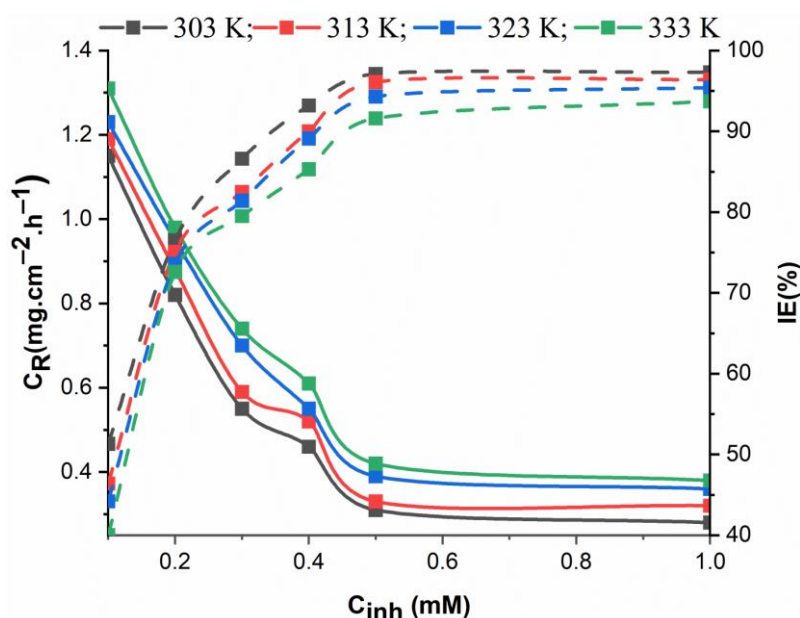


Figure 4. Comparison of corrosion rate and inhibition efficiency in hydrochloric acid solution with and without the inhibitor during a 5-hour immersion at various temperature.

The obtained results show that the inhibition efficiency of PMT decreases significantly with increase in temperature from 303 K to 333 K. For instance, at 303 K, 0.5 mM of the inhibitor exhibited a notable inhibition efficiency from corrosion. Nevertheless, PMT efficiency lowered down to 91.6% with temperature increasing up to 333 K, thus showing reduced inhibition effect at elevated temperatures. This apparent decrease in inhibition efficiency at increased temperatures could be due to several factors. Firstly, the presence of thermal stress in PMT particles and corrosive solutions become more severe due to increase in the temperature. Increased thermal excitation may prevent the deposition of an inhibitor film resulting in a reduced barrier thickness. Moreover, high temperature would heighten reactivity of the destructive environment and would boost up corrosion rate despite presence of the inhibitor. Higher temperature could even lead to desorption of the inhibitor molecules from the surface of metal. The high thermal energy might lower the degree of interaction between PMT molecules and the coated metal surface leading to a few of these molecules falling away and lowering the area covered by the protective coat. The inhibition mechanism is affected by this adsorption process and contributes to the reduction in inhibition effectiveness [186–189]. Nevertheless, it should be stated that at elevated temperatures inhibition efficacy tends to decline, and this does not cancel out protection by PMT. Although reduced, it still offers adequate resistance to a high temperature corrosion. Nevertheless, it is very important to take into account the weak sides of the inhibitor’s operation in various temperatures. Therefore, more investigations would be necessary to find

out the reasons for decreasing inhibition efficiency with increasing temperatures of the PMT. Such knowledge could be useful in formulating new PMT measures aimed at boosting its performance against severe corrosion conditions at elevated temperatures. Moreover, other factors like inhibitor amount, soaking period and compatibility effect among other additives could be explored to improve on the efficiency of the PMT at high temperatures [190–192]. Overall, it can be seen that with regard to the PMT at the same concentration, the efficiency decreased from 97.1% to 91.6% between 303 K and 333 K indicating the temperature sensitivity. The finding points out that in order for appropriate corrosion inhibition strategy, one must take into account temperature effect and calls for more studies in this field.

3.2. Adsorption isotherm analysis

For evaluation of PMT adsorption process in the corrosion inhibition of mild steel in HCl solutions, we utilized Frumkin, Temkin and Langmuir isotherms as presented in Table 1. These isotherms provide valuable insights into the adsorption behavior and the effectiveness of the inhibitors. Among these, the Langmuir isotherm stood out as the most suitable for describing the adsorption process of PMT on the mild steel surface. This isotherm, commonly used for studying inhibitor adsorption on metal surfaces, assumes monolayer adsorption on a homogeneous surface [193–198]. Table 1 and Figure 5 demonstrate a good fit of the PMT inhibitor's adsorption isotherm to the Langmuir model. The Langmuir adsorption isotherm, represented by Equation (11), establishes the relationship between surface coverage and inhibitor concentration. The equilibrium constant of adsorption (K_{ads}) derived from the Langmuir isotherm indicates the extent of adsorption inhibitor on the mild steel surface. The results reveal significant adsorption of PMT on the mild steel surface, as evidenced by its relatively high K_{ads} value. Additionally, the negative value of the standard free energy of adsorption (ΔG_{ads}^0), calculated using Equation (12), suggests a spontaneous and favorable adsorption process, indicating the formation of a stable inhibitor layer on the mild steel surface.

Table 1. The adsorption isotherms for PMT on mild steel surface.

Parameter	The adsorption isotherms					
	Langmuir				Frumkin	Temkin
	Temperature				Temperature	
	303 K	313 K	323 K	333 K	303 K	303 K
R-Square	0.995	0.093	0.087	0.071	0.486	0.857
Slope	0.937	0.933	0.929	0.937	0.902	0.378
Intercept	0.071	0.992	0.993	0.995	0.018	0.204

We also compared the adsorption behaviour of PMT using the Frumkin and Temkin isotherms in addition to the Langmuir isotherm. Nevertheless, the Langmuir isotherm showed more adequacy with a larger R^2 value, and fitted closer to the experiment values. Such things as electrostatic forces, unshared electron pair interactions, and p-electron interactions play a part in this understanding. Nitrogen atoms, heterocycle rings and pyridinic rings are present in PMT. These act as donor ligands for PMT, and thus improve the bioavailability of the drug as well [199–201]. Summing up, the Langmuir adsorption isotherm adequately characterizes PMT's adsorption behavior as a corrosion inhibitor for mild steel in HCl solutions. This model gives useful information, the intensity (K_{ads}), and strength (ΔG_{ads}^0). Adsorption mechanism comprises of the addition of unshared electron pairs, electrostatics interaction and the π interaction with the mild steel surface, leading to its corrosion inhibition function by PMT.

$$\frac{C}{\theta} = (K_{\text{ads}})^{-1} + C \quad (11)$$

$$\Delta G_{\text{ads}}^0 = -RT \ln(55.5K_{\text{ads}}) \quad (12)$$

where K_{ads} is an adsorption constant whereas θ is the surface coverage.

The intercept, R-square, and slope values from linear regression analysis of Langmuir adsorption isotherm data provide important information about the fit of the experimental data to the Langmuir model. An R-square value close to 1 (in this case, 0.995) indicates a good fit of the data with the model, indicating that the Langmuir isotherm accurately describes the adsorption behavior of PMT on the mild steel surface. The slope value (0.937 ± 0.033) reflects the relationship between surface coverage (θ) and the concentration of the inhibitor (C), while the intercept value (0.071 ± 0.016) has a less significant meaning in the context of adsorption analysis [202–204].

The thermodynamic parameters obtained from weight loss measurements at various concentrations are determined. The negative value of ΔG_{ads}^0 suggests a spontaneous adsorption process, leading to the formation of a stable layer of inhibitor molecules on the mild steel surface. The strength of the adsorption process is typically evaluated based on the ΔG_{ads}^0 value, with values less than $-20 \text{ kJ} \cdot \text{mol}^{-1}$ indicating Van der Waals forces and more negative values exceeding $-20 \text{ kJ} \cdot \text{mol}^{-1}$ suggests chemisorption. Unpaired electrons from the heteroatoms of the inhibitor molecule transfer to the d-orbitals of iron atoms on the metal surface, forming coordination bonds. Our findings indicate the occurrence of both physisorption and chemisorption mechanisms, as demonstrated by the ΔG_{ads}^0 values ranging from -39.11 kJ . Chemisorbed molecules are expected to provide enhanced protection by reducing reactivity at the bonded sites on the metal surface. It is important to note that distinguishing between chemisorption and physisorption based solely on ΔG_{ads}^0 values is

challenging, as there is some overlap between the two mechanisms, and physical adsorption is believed to precede chemical adsorption [205–207].

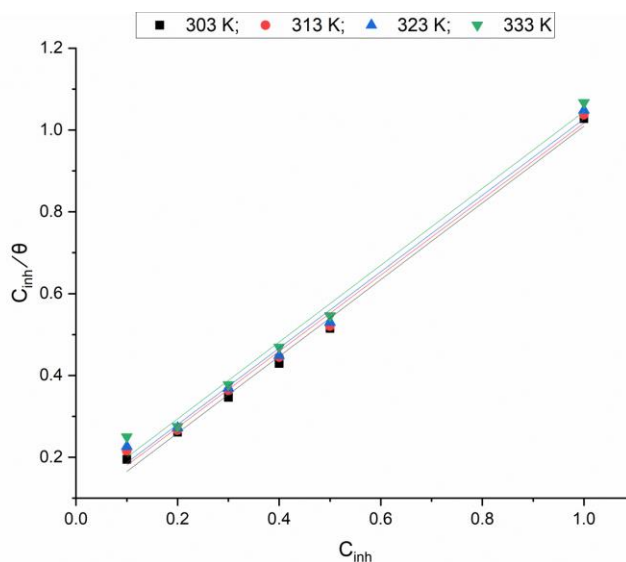


Figure 5. Langmuir adsorption isotherm for the tested inhibitor.

3.3. DFT calculations and molecular interactions

Quantum chemical calculations offer valuable insights into the structural properties of the PMT molecule and various thermodynamic parameters. The Gaussian [80–81] records at the B3LYP/6-311G(d,p) level are utilized for determining these parameters based on the structural characteristics of PMT. An example of the information obtained from this analysis is shown in Figure 6.

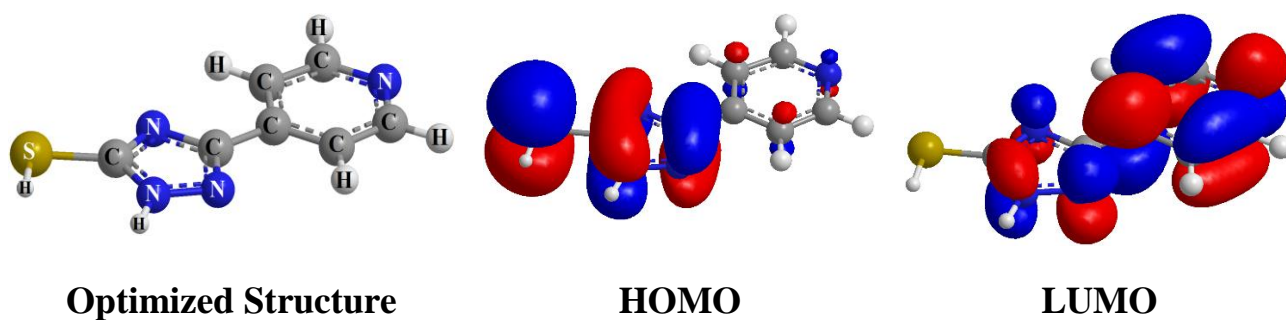


Figure 6. Optimized structure, HOMO, and LUMO of PMT.

The quantum chemical analysis carried out in this investigation provides significant insights into the structural characteristics and thermodynamic parameters of PMT molecules, elucidating their potential as corrosion inhibitors. Figure 6, shows the findings that offer an insight into the characteristics of PMT and how it interacts with the metal surface [208–211]. In order to identify the sites for adsorption, we utilize Mulliken charges, which indicate that nitrogen atoms possess negative charges, constructing them suitable sites for adsorption.

This behavior occurs because of the interactions between these atoms and the metal surface as represented in Figure 6. The functional groups located in the PMT molecules assist form a connection with the metal surface, which improves the process of adsorption. Additionally examining the occupied orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) provides insights, into the PMT molecules ability to donate or accept electrons. The HOMO signifies positions in the molecule that easily give away electrons whereas the LUMO indicates its capacity to accept electrons. In the instance of PMT the HOMO emphasizes that sulfur and nitrogen atoms are more inclined to transfer electrons to the substrate indicating their potential for creating a coating on the metal surface. On the hand when we look at the LUMO analysis it suggests that the nitrogen and carbon atoms in PMT tend to be more reactive and have a probability of accepting electrons. This in turn plays a role in the process of inhibition [16, 24]. The quantum chemical parameters listed in Table 2 including E_{HOMO} , E_{LUMO} , ΔE , electronegativity (χ) softness (σ) hardness (η) and the number of transferred electrons (ΔN) offer understanding of how PMT inhibits behaviors. E_{HOMO} values indicate a capacity, for electron donation, which is a desirable characteristic, for an effective corrosion inhibitor. On the hand lower E_{LUMO} values imply ability to accept electrons. The low ΔE values and high σ values indicate that PMT has corrosion inhibition properties effectively protecting steel from corrosion. The ΔN values, which represent the number of electrons transferred further confirm PMT's ability to assist electron exchange thereby contributing to its action [81, 213–215]. In general this analysis of quantum chemistry offers understanding of the characteristics and thermodynamic factors related to PMT molecules. It assists explain why they act as inhibitors for corrosion and aligns, with what we observe in experiments. By examining how the molecule interacts with the metal surface and its ability to transfer electrons, this study confirms that PMT has potential in reducing corrosion processes [206–220].

Table 2. DFT variables for PMT molecules in the gas phase.

E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	χ (eV)	η (eV)	σ (eV ⁻¹)	ΔN (eV)
-9.204	-1.756	-7.448	5.480	3.722	0.2686	0.204

Mulliken charges are commonly used to identify favorable adsorption sites for inhibitors. For PMT, nitrogen atoms exhibit negative charges and are preferred adsorption locations due to their donor-acceptor interactions with metal surfaces, as depicted in Figure 7. The functional groups within the PMT molecules facilitate complexation between the adsorbate and surface coordination bonds. Additionally, the examination of the highest occupied molecular orbital (HOMO) of the PMT component reveals the sites for electron donation within the molecules. The HOMO suggests that the nitrogen atoms can transfer electrons to the metallic substrate, while the lowest unoccupied molecular orbital (LUMO) represents the molecule's capacity to accept electrons [221–226]. Figure 7 illustrates that the most reactive LUMO locations in PMT are the nitrogen, sulfur, and carbon atoms.

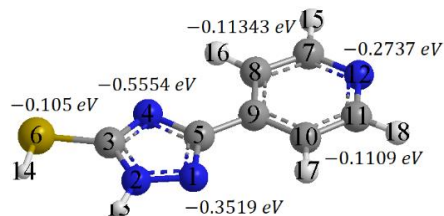


Figure 7. The atomic charges of PMT.

3.4. The inhibition mechanism of PMT as a corrosion inhibitor

Chemical adsorption, also known as chemisorption, involves strong interactions between the inhibitor molecules and the metal surface. The high inhibitory efficiency of PMT is attributed to the presence of pyridine rings, nitrogen atoms, and heterocyclic ring. Because these atoms have unpaired electron pairs, they can serve as coordinating sites to help metal ions form coordination bonds [227–231]. The unpaired electrons from the inhibitor's nitrogen atoms and the d-orbitals of the iron atoms on the mild steel surface might interact during the adsorption process. Conversely, lower Van der Waals forces or electrostatic contacts between the inhibitor molecules and the metal surface cause physical adsorption, also referred to as physisorption. These weaker connections with the mild steel surface are made possible by the functional groups present in the PMT molecules. These interactions help PMT to absorb onto the metal surface and increase corrosion prevention efficiency. One of the elements involved in the damping process is the formation of coordination bonds, between the molecules in PMT and the iron orbitals, on the surface of steel. The empty energy levels of the iron ions, on the metal surface can interact with the electron pairs from the nitrogen atoms, in the inhibitor molecule. By improving the attachment of the inhibitor to the surface of the metal the coordination bond protections steel against corrosion in environments by forming a protective layer. In general both chemical and physical processes contribute to the adsorption of PMT on the surface of steel (Figure 8). Chemisorption plays a role by establishing coordination bonds between the inhibitor molecules and iron atoms while physisorption involves interactions that assistance, in the adsorption process. The effective ability of PMT to prevent corrosion in HCl solutions for steel occurs due to the actions of these processes [232–240].

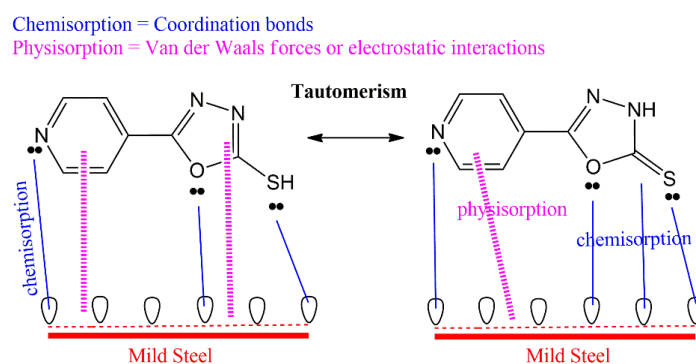


Figure 8. Assumed inhibitive mechanism.

4. Conclusion

The primary objective of the study was to examine how PMT behaves as a corrosion inhibitor, in HCl solutions for steel and understand its inhibition mechanism. To summarize the main focus was on investigating PMTs adsorption behavior and its role, in preventing corrosion. Quantum chemical analysis provided insights, into the structure and thermodynamic properties of the inhibitor molecule shedding light on its potential, as a corrosion inhibitor. According to the adsorption isotherm study it was determined that the Langmuir isotherm provides the model, for explaining the adsorption process of PMT on the surface of mild steel. The Langmuir isotherm provides crucial characteristics, such as the equilibrium constant of adsorption (K_{ads}), to define the adsorption process. The Langmuir isotherm is a tool for understanding the adsorption process as it provides information, such, as the equilibrium constant of adsorption (K_{ads}). It does this by assuming monolayer adsorption and a homogenous surface. It achieves this by assuming that adsorption occurs at the monolayer adsorption and a homogenous surface. The corrosion inhibitors ability to prevent corrosion was improved because it had a high K_{ads} value indicating that it strongly attached to the surface of the mild steel. Furthermore the metal surface showed the formation of an inhibitor layer due to a spontaneous and beneficial adsorption process as suggested by the values of the standard free energy of adsorption (ΔG_{ads}^0). Both chemical and physical processes were involved in the mechanism of PMT adsorption. The interaction between the d-orbitals of iron ions on the surface of steel is coordinated with the inhibitor molecule. This coordination promotes chemisorption through the presence of nitrogen atoms, heterocyclic rings and pyridine rings. The strong bond between the inhibitor and the metal surface enhanced its ability to prevent corrosion. Furthermore, the reduction in electrostatic contacts and the contribution of Van der Waals forces played a role in assisting physisorption. As a result, it enhanced the adsorption process to an extent. The effectiveness of PMT in preventing corrosion processes was determined by the combined effects of bonding and physical adsorption mechanisms. The inhibitor effectively reduces reactivity at the bonded sites and prevents corrosive attacks, resulting in the formation of a stable and protective layer on the surface of the metal. Through the analysis of quantum chemistry and adsorption isotherm studies we were able to gain an understanding of how PMT acts as an inhibitor for steel corrosion in acidic conditions. This suggests that PMT could potentially be used as a corrosion inhibitor in environments. The findings of the study provide insights into the development and improvement of inhibitors to prevent metal corrosion. Additionally, they contribute to the advancement of techniques for corrosion inhibition. The exploration of PMT, as a substance that prevents corrosion opens up possibilities for research in the field of corrosion science and materials protection.

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