

Effect of TMN on the Corrosion Inhibition of Carbon Steel in 1 M HCl Solution: Experimental and DFT Studies

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This work aimed to elucidate effect of 1-((thiazol-2-ylimino)methyl)-2-naphthol (TMN) on corrosion inhibition of carbon steel in 1 M HCl medium. Corrosion inhibition efficiencies were assessed based pm weight loss measurements and computational Density Functional Theory (DFT) studies. TMN, a very strong adsorbate on surface steel, is expected to show high values of inhibition efficiency since it has excellent electronic properties based on DFT analysis. Inhibition efficiency of TMN increased with increasing concentration. The maximum value was 91.2 at 0.5 mM concentration after 5 hours of immersion at 303 K. Study of immersion time at 303 K for different concentrations of the inhibitor indicated an increase in inhibition efficiency with time until 10 hours, followed by a slight decrease until 48 hours. After immersion of 5 hours, corrosion inhibition efficiency increased with increasing temperature from 303 K to 333 K. Adsorption behavior of TMN followed Langmuir adsorption isotherm. For this study, DFT calculations supported the data observed experimentally, confirming that TMN could be utilized as an efficient corrosion inhibitor with a strong efficacy.

Keywords: Schiff base, Corrosion inhibitor, Carbon steel, Weight loss measurements, DFT analysis

1. Introduction

Corrosion is a natural degradation process to which materials are subjected, mainly metals, and it is induced by an environmental medium. This concern, although of paramount importance in different industries, prohibits the failure of materials, resulting in economic losses and thus further safety concerns [1,2]. These impacts must run into billions of dollars on an annual basis in maintenance, repair, and replacement of destroyed equipment and infrastructure. Industries suffering the effects of corrosion damage: chemical processing, oil refining, and power generation, often have to cope with the use of aggressive environments such as HCl [3]. The production of highly concentrated hydrochloric-industry applications for acid cleaning, oil well acidifying, descaling, and many more processes becomes significant in steel corrosion because

it poses severe threats to structures made of metals, especially carbon steel, which is very widely employed for its cost efficiency and mechanical properties. The area of research development and application of corrosion inhibitors is therefore of critical importance to solving these problems [4]. Corrosion inhibitors are substances which - when applied in small concentration on metals - can greatly reduce the rate of corrosion. Organic inhibitors, especially containing heteroatoms like nitrogen, sulfur, and oxygen, have gained interest owing to their efficiency and very negligible impacts on the environment [5]. Schiff bases have gained significant attention as effective corrosion inhibitors due to their structural versatility, ease of synthesis, and strong adsorption properties. Recent studies have demonstrated that Schiff base compounds containing heteroatoms (N, S, O) and conjugated π -electrons can efficiently protect metal surfaces by forming stable adsorption layers. The presence of the azomethine (-C=N-) functional group enhances their electron-donating

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ability, facilitating strong interactions with metal surfaces through chemisorption or physisorption mechanisms. Verma et al. (2021) reported that Schiff bases derived from salicylaldehyde and aromatic amines exhibit high inhibition efficiency (>90%) due to their strong adsorption on mild steel surfaces in acidic media [5]. Modified Schiff bases incorporating additional donor atoms, such as sulfur and oxygen, have been found to enhance corrosion protection through synergistic effects. Several investigations, including those by Verma *et al.* (2021), have demonstrated that Schiff bases maintain or even improve inhibition efficiency at elevated temperatures due to chemisorption dominance [7].

Organic inhibitors have also been exploited in coatings to inhibit corrosion in HCl. Sorts of majorly researched organic inhibitors are as follows: aliphatic, aromatic amines to name a few, which gives good improvement in corrosion inhibition properties by having the ability to form stable adsorption films on the metal surface. However, they are limited in applications due to their environmental impact and reasonable efficiencies at elevated temperatures [8,9]. Imidazole and benzimidazole derivatives have been reported to show prolific results of corrosion inhibition in HCl media because of the high electron density and planar structure that promotes robust adsorption onto the metal surface. However, the cheap and synthetic complexities can prove unhelpful especially when their usages are planned at the large scale [10,11]. Recent studies have shown that Schiff bases have better inhibition performance than N,N'-bis(salicylidene)ethylenediamine and 2-((E)-((1H-indol-3-yl)methylene)amino)ethanol because of their electron-donation capabilities towards the metal surfaces while providing stable complexes [12,13]. Moreover, Schiff bases offer temperature stability and long-term adsorption, thus making them applicable in the industry [14,15]. The research with such inhibitors opened doors under applications extending to a certain level; however, the efficiency protractedness of immersion and heat has remained unsolved. A close comparative analysis indicates that Schiff bases always stand above other classes of inhibitors in terms of efficiency, thermal stability, and indeed environmental safety [16,17]. While Schiff bases have emerged as promising candidates for corrosion inhibition, there remain gaps in understanding their

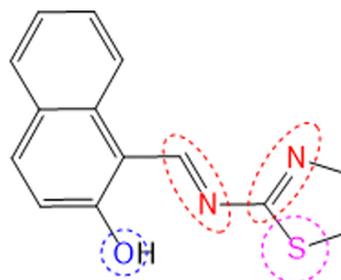


Fig. 1. The chemical structure of TMN

behavior under different conditions similar to those encountered in the industry; some of these include:

1. Few long-term data exist about the performance of Schiff bases under prolonged immersion.
2. Changes in temperature and concentration can cause fluctuations in inhibition efficiency.
3. Limited studies exist on correlating experimental results with theoretical calculations for mechanistic insights, e.g., Density Functional Theory (DFT).

Addressing these gaps will enhance the applicability and reliability of Schiff bases in industrial settings. This study introduces a novel Schiff base, 1-((thiazol-2-ylimino)methyl)-2-naphthol (Fig. 1), synthesized specifically for corrosion inhibition of carbon steel in 1 M HCl solution. Unlike conventional inhibitors, TMN combines the heteroatoms from the thiazole ring and the electron-rich azomethine group, enabling enhanced adsorption on the metal surface. The study integrates experimental techniques and DFT calculations to provide a comprehensive understanding of its performance and mechanism. The main objectives of this work can be summarized as follows:

1. To evaluate the corrosion inhibition efficiency of TMN using weight loss measurements under varying conditions of concentration, immersion time, and temperature.
2. To analyze the adsorption mechanism of TMN through experimental adsorption isotherms.
3. To correlate experimental findings with DFT studies, providing theoretical insights into the electronic and adsorption properties of TMN.
4. To compare the performance of TMN with other organic inhibitors, highlighting its advantages in terms of efficiency and environmental compatibility.

2. Experimental Details

2.1 Materials

Carbon steel was used in this study, with a chemical composition of 0.21 wt% carbon (C), 0.005 wt% manganese (Mn), 0.38 wt% silicon (Si), 0.05 wt% sulfur (S), 0.01 wt% aluminum (Al), and 0.09 wt% phosphorus (P), with the remainder being iron (Metal supplies company-Malaysia). The corrosion inhibition effectiveness of 1-((thiazol-2-ylimino)methyl)-2-naphthol (TMN) was evaluated in a 1 M hydrochloric acid (HCl) solution. Steel samples with dimensions of 4.0 cm × 2.5 cm × 0.1 cm were prepared. The surfaces of the samples were polished using abrasive papers of varying grit sizes (400, 600, and 1200) to achieve a smooth finish. Polished samples were washed with double-distilled water, rinsed with ethanol to remove residual contaminants, dried at room temperature, and weighed to record their initial dry weight for subsequent comparisons [18,19].

2.2 Preparation of Hydrochloric Acid Solutions

A 1 M HCl solution was prepared by diluting analytical-grade hydrochloric acid (37% purity) obtained from Merck, Malaysia, with double-distilled water. Different concentrations of TMN were dissolved in this solution to ensure homogeneous mixing and distribution. Carbon steel samples were immersed in the prepared solutions for specific time intervals. Visual observations were made to detect signs of corrosion, such as discoloration or surface roughening, while weight loss measurements provided quantitative data for corrosion analysis [20,21].

2.3 Weight Loss Measurements

The weight loss method was utilized to determine the corrosion rate and evaluate the inhibition efficiency of TMN on carbon steel in a 1 M HCl medium. Each experiment involved immersing polished steel samples, with a 1 cm² exposed surface area, in 500 mL of the acid solution within a glass beaker. TMN concentrations ranged from 0.1 mM to 1 mM, with experiments conducted at temperatures between 303 K and 333 K, maintained using a thermostat water bath. Samples were immersed for time intervals of 5 hours, 10 hours, 24, and 48 hours in a selected immersion medium. Thereafter, the samples were washed by ultrasonic cleaner with ultrapure

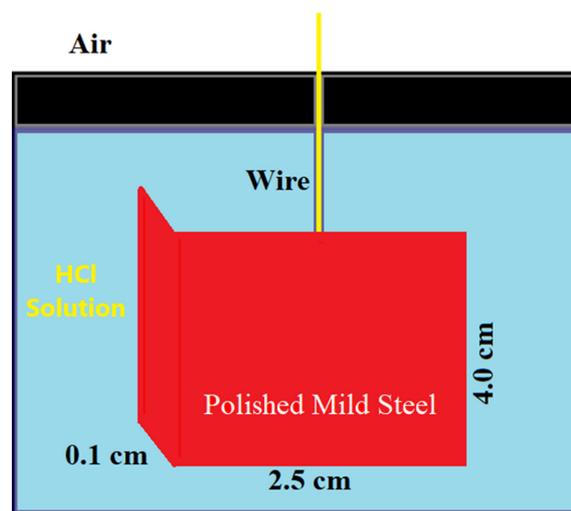


Fig. 2. Experimental Setup for Weight Loss Corrosion Test

water and ethanol before drying the samples for weighing for weight loss calculation. The collected data were utilized to calculate corrosion rate, inhibition efficiency, and surface coverage [21,22]. The experimental setup shown in Fig. 2 comprised the steel sample suspended in an HCl solution in a glass beaker by means of a wire. The wire used to suspend the polished carbon steel specimen in the corrosive medium was a non-metallic coated wire to prevent unwanted electrochemical reactions that could influence the corrosion rate measurements. The wire was made of non-reactive polymer-coated material (nylon-coated wire) to ensure that it did not introduce additional metal ions into the solution or interfere with the inhibitor's adsorption mechanism. This setup followed NACE standards for corrosion studies for reliable and reproducible results [21,22]. Samples were immersed for time intervals of 5 hours, 10 hours, 24, and 48 hours in a selected immersion medium. Thereafter, the samples were washed by ultrasonic cleaner with ultrapure water and ethanol before drying the samples for weighing for weight loss calculation. The collected data were utilized to calculate corrosion rate, inhibition efficiency, and surface coverage [21,22]. The experimental setup shown in Fig. 2 comprised the steel sample suspended in an HCl solution in a glass beaker by means of a wire. This setup followed NACE standards for corrosion studies for reliable and reproducible results [21,22].

The relations (1-3) were used for calculations:

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

W is the weight loss in grams, a is the exposed surface area of the steel sample (cm^2), and t is the immersion time (hours).

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

Where: $C_{R(o)}$ is the corrosion rate without inhibitor (control) and $C_{R(i)}$ is the corrosion rate with inhibitor.

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

2.4 Theoretical Study

Theoretical Study Quantum chemical calculations were carried out with GAMESS software for the study of electronic properties of TMN inhibitor. The molecular structure of TMN has been optimized level with the use of DFT-B3LYP/6-31G(d) theory (ChemOffice). Important quantum chemical parameters such as the highest occupied molecular orbital (HOMO) energy, lowest unoccupied molecular orbital (LUMO) energy, and some additional indices related to molecular reactivity were calculated according to equations (4-8):

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

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

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

$$\text{Chemical hardness } (\eta): \eta = \frac{I-A}{2} \quad (7)$$

$$\text{Chemical softness } (\sigma): \sigma = \eta^{-1} \quad (8)$$

The electron transfer fraction (ΔN) between the inhibitor and the carbon steel surface was also computed based on equation (9):

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

Where χ_{inh} and η_{inh} refer to the electronegativity and hardness of the inhibitor, respectively. For this, the

reference values for iron (Fe) were adopted: $\chi_{Fe} = 7 \text{ eV}$ and $\eta_{Fe} = 0 \text{ eV}$.

Such calculations yield the electronic interactions involved in TMN onto steel surface and decipher molecular mechanisms involved in performance regarding the corrosion inhibition capacity of the molecule.

3. Results and Discussion

3.1 Weight loss measurements

3.1.1 effect of inhibitor concentration

The investigations into the performance of TMN as a corrosion inhibitor for carbon steel in the concentration of 1 M HCl involved the determination of the corrosion rate (CR) and inhibition efficiency (IE%) at various concentrations of inhibitors at 303 K. As illustrated in Fig. 3, the data clearly show the dependency of C_R and IE% on TMN concentration. The recorded measure for carbon steel without an inhibitor in 1 M HCl solution was $4.89 \text{ mg}\cdot\text{cm}^{-2}\cdot\text{h}^{-1}$, suggesting intense corrosion in the absence of such an inhibitor. On increasing the concentration of TMN from 0.1 mM to 0.5 mM, sharp decreases in CR were observed. The CR recorded at 0.5 mM TMN was only $0.32 \text{ mg}\cdot\text{cm}^{-2}\cdot\text{h}^{-1}$, confirming the efficiency of TMN in corrosion control. The increasing IE% is proportional to increased concentration of TMN. At 0.1 mM, the IE% was 41.7%, reflecting moderate inhibition performance. With increasing TMN concentration,

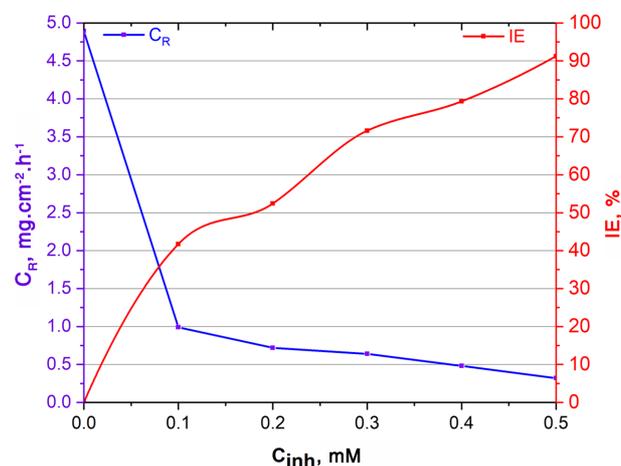


Fig. 3. Variation of Corrosion Rate and Inhibition efficiency of TMN with Inhibitor Concentration for carbon Steel in 1 M HCl at 303 K

the IE% rose significantly, reaching a maximum of 91.2% at 0.5 mM, demonstrating the superior performance of TMN as an effective inhibitor at this concentration.

The sharp decline in C_R and the corresponding rise in IE% with increasing TMN concentration suggest strong adsorption of TMN molecules on the carbon steel surface. TMN likely forms a protective barrier on the steel surface, reducing the direct interaction between the metal and the corrosive environment. TMN, as a Schiff base, contains nitrogen, sulfur, and oxygen heteroatoms, along with π -electrons in its molecular structure. These features enhance its ability to donate electrons to vacant d-orbitals of iron atoms, leading to strong chemisorption. The adsorption of TMN molecules likely follows the Langmuir adsorption isotherm, as indicated by the linear relationship between IE% and concentration [23]. The high IE% at relatively low concentrations demonstrates the economic feasibility of using TMN as a corrosion inhibitor in industrial applications. That increasing TMN concentration improves inhibition efficiency is confirmed by the data, leading toward possibly effective solutions for corrosion inhibition in HCl medium [24]. The findings of weight loss tests suggest TMN is quite effective in lowering corrosion rates on carbon steel in 1 M HCl. The highest improvement in IE% with TMN increment holds promise for a green alternative in the manufacture of such inhibitors. The maximum inhibition efficiency at 91.2% at 0.5 mM concentration indicates TMN as one of the most suitable candidates for corrosion protection in a highly acidic environment.

3.1.2 effect of immersion time

The time of immersion was found to act on the corrosion inhibition efficiency (IE%) and corrosion rate (C_R) of TMN for carbon steel in 1 M HCl solution, and at different concentrations of the inhibitor, time was varied. As demonstrated in Figs. 4, it was found that for each of the TMN concentrations, the C_R was markedly reduced after the immersion time was increased to 10 hours. This can depict the progressive formation of a protective inhibitor layer on the carbon steel surface between the aggressive acidic environment and the steel. After 10 hours of immersion, the C_R was increased at most concentrations, probably due to partial desorption or degradation of the adsorbed inhibitor layer over a long immersion period.

For instance, with the case for 0.1 mM, the C_R at 10 hours was $0.72 \text{ mg}\cdot\text{cm}^{-2}\cdot\text{h}^{-1}$, and at 48 hours it increased to $1.04 \text{ mg}\cdot\text{cm}^{-2}\cdot\text{h}^{-1}$.

Further, IE% showed a steady and consistent increases with immersion time up to 10 hours for all TMN concentrations. This improvement also emphasizes the time-dependent adsorption and stabilization of TMN molecules in the carbon steel surface. At 48 hours, a minor decline in IE% was noted to suggest partial degradation or weakening of the inhibitor layer in course of time. At 0.5mM of concentration, for instance, the IE% dropped from 92.3% at 10 hours to 89.4% at 48 hours. Then, the highest IE% values were recorded at 0.5mM TMN for all immersion times; that demonstrates the higher concentrations of the inhibitor fortified the corrosion protection. For instance, 0.5mM reflected an IE% of 62.9% at 1 hour as opposed to 29.4% at 0.1mM. Therefore, at weak TMN concentrations, for instance 0.1mM, the IE% was also much lower, implying that not enough inhibitor molecules were available to complete the protective layer on the steel surface.

The weight loss measurements showed that inhibition efficiency (IE%) increased up to 10 hours of immersion but gradually declined afterward. The weight loss measurements showed that inhibition efficiency (IE%) increased up to 10 hours of immersion but gradually declined afterward. This trend suggests that while the TMN inhibitor initially forms a strong protective adsorption layer, prolonged exposure leads to a slight decrease in surface coverage or reorganization of adsorbed molecules. At 10 hours, IE% was at its peak, but at 24 and 48 hours, IE% slightly decreased, indicating some desorption or weakening of the adsorbed inhibitor film. In acidic environments (1 M HCl), H^+ and Cl^- ions compete with the inhibitor molecules for adsorption sites on the carbon steel surface. Over extended immersion, these aggressive ions may gradually disrupt the inhibitor layer, leading to partial desorption or rearrangement of TMN molecules. Prolonged exposure to HCl may lead to localized dissolution of the steel surface, altering the adsorption dynamics. Corrosion products (e.g., FeCl_2 , FeCl_3) may accumulate over time, hindering the inhibitor's effectiveness by reducing the available adsorption sites. Physical adsorption components of the inhibitor layer (weak Van der Waals interactions) may

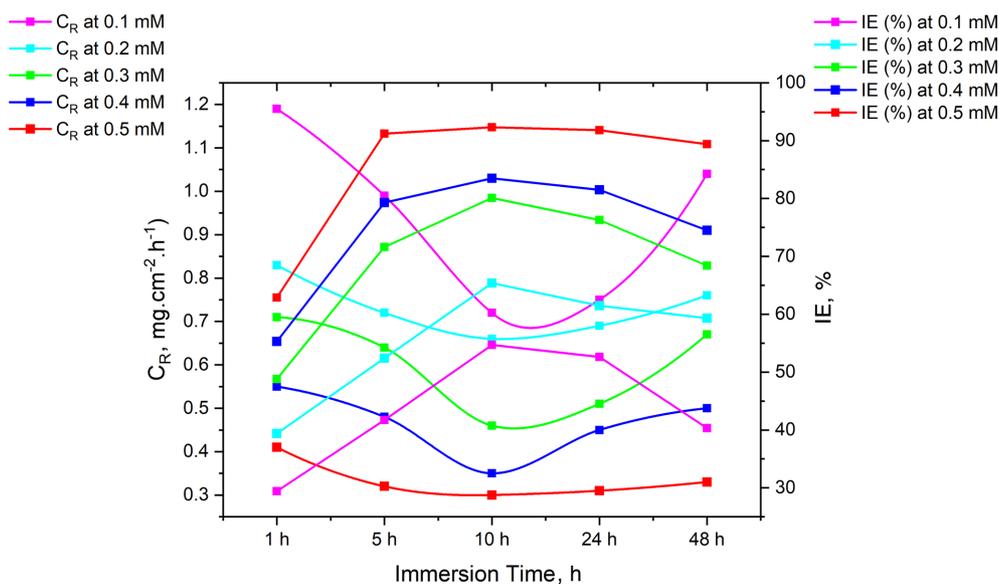


Fig. 4. Effect of Immersion Time on Corrosion Rate and Inhibition Efficiency of TMN for Carbon Steel in 1 M HCl at Various Concentrations

become destabilized over time, leading to gradual desorption. The Langmuir adsorption isotherm suggests dynamic equilibrium between adsorbed and desorbed species, which may shift with prolonged immersion due to weakening interactions [24,25].

It is the continued and deeper adsorption of the TMN molecules over the virgin surface steel which gives the increased IE% with time till about 10 h, thus producing a dense and stable protective layer. The reduced value of IE% after 10 h exposure suggests that prolonged acidic environment exposure weakened the attraction responsible for adsorption or perhaps H^+ competitive adsorption, which reduced the effectiveness of the protective film. The data, however, shows that TMN is effective for short and medium duration protection of carbon steel in 1 M HCl, even more so at higher dosage levels. For very long times of immersion, possibly another means of stabilization-(co-additives or multilayer inhibitors)-may be needed to maintain high inhibition efficiency [26]. Immersion time plays a decisive role in the efficiency of corrosion inhibition provided by TMN. Under shorter immersion times, the protective layer formed by TMN builds progressively leading to the increment of inhibition efficiency. On the other hand, for extended times of immersion, their efficiency is reduced a little since the film has already suffered partial degradation or desorption. This reinforces the need to optimize both inhibitor

concentration and exposure time for sustainable corrosion protection of carbon steel in an acidic medium.

3.1.3 Effect of Temperature

The effect of temperature on the IE% and C_R of TMN for carbon steel in 1M HCl was evaluated at varying concentrations of the inhibitor. All these are as shown in Fig. 5, which are the summary to the following observations: the C_R , which reduces considerably with an increase in TMN concentration at any temperature (303 K, 313 K, 323 K, and 333 K). For instance, at 303 K, the C_R decreased from $0.99 \text{ mg}\cdot\text{cm}^{-2}\cdot\text{h}^{-1}$ (0.1 mM TMN) to $0.32 \text{ mg}\cdot\text{cm}^{-2}\cdot\text{h}^{-1}$ (0.5 mM TMN). As the temperature increases, the C_R slightly decreases for all inhibitor concentrations. For example, at 0.5 mM TMN, the C_R decreased from $0.32 \text{ mg}\cdot\text{cm}^{-2}\cdot\text{h}^{-1}$ at 303 K to $0.28 \text{ mg}\cdot\text{cm}^{-2}\cdot\text{h}^{-1}$ at 333 K, suggesting that the inhibition efficiency improves with increasing temperature. This behavior indicates that the adsorption mechanism of TMN on the carbon steel surface is predominantly chemisorption, as higher temperatures typically enhance chemical interactions between the inhibitor molecules and the metal surface. The increasing inhibition efficiency with temperature suggests stronger bonding interactions between TMN and the steel surface, which is characteristic of chemisorption-driven adsorption mechanisms. However, the increase in CR with temperature is less pronounced for higher TMN concentrations. The IE% improves

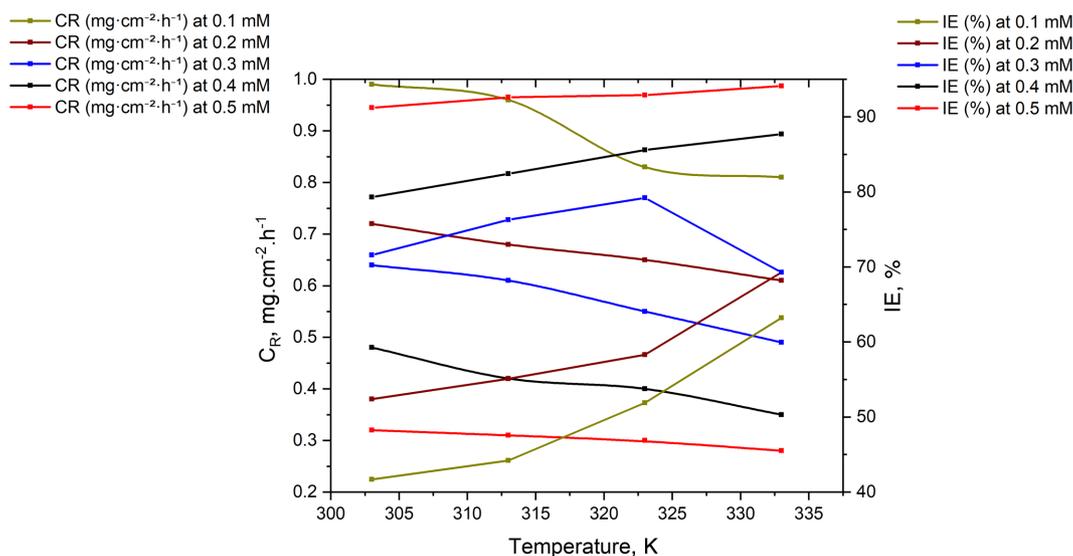


Fig. 5. Effect of Temperature on Corrosion Rate and Inhibition Efficiency of TMN for Carbon Steel in 1 M HCl at Various Concentrations

consistently with increasing TMN concentration at all temperatures, indicating better surface coverage and enhanced inhibition with higher inhibitor concentrations [27]. As the temperature rises, the IE% also increases slightly for each concentration. For instance, at 0.5 mM TMN, the IE% improved from 91.2% at 303 K to 94.1% at 333 K. This behavior suggests a chemisorption mechanism for TMN adsorption, where chemical bonding between TMN molecules and the steel surface strengthens with temperature.

The increase in IE% with temperature suggests that the adsorption of TMN on the steel surface is not solely physisorption, which typically weakens at higher temperatures. Instead, chemisorption likely dominates, where TMN forms covalent bonds with the steel surface, improving the stability of the protective layer. The results imply that TMN adsorption aligns with the Langmuir adsorption isotherm, with higher temperatures enhancing the adsorption process. At 0.1 mM TMN, the IE% increased from 41.7% at 303 K to 63.2% at 333 K, demonstrating moderate inhibition at low concentrations. At a TMN concentration of 0.5 mM, the IE% value surpassed the 90% figure for all the temperatures, attaining a maximum of 94.1% at 333 K. It thus underscores the superlative action of TMN at higher concentration levels even under high temperatures. Exceptionally high inhibition efficiency levels are also

retained by TMN in a temperature range, making it possible for application in industries whose systems face elevated temperature conditions. Slight increase in IE% with rise in temperature backs up TMN as a firm and effective corrosion inhibitor for carbon steel under acidic environments. The study on temperature proves the possibility of very deep corrosion inhibition due to the fact of TMN within which the steel is in 1 M HCl over a vast temperature range. The better IE% at elevated temperatures corroborated the chemisorption-based adsorption mechanism, in which TMN creates a potent and firm protective barrier on the surface of the steel. The high efficiency of TMN, even at elevated temperatures, underscores its potential for use in various industrial applications requiring corrosion protection under harsh conditions.

3.2 Adsorption Isotherm

The adsorption behavior of TMN on the carbon steel surface in 1 M HCl was analyzed using the Langmuir adsorption isotherm, as shown in Fig. 6. The linear fit of C_{inh}/θ versus C_{inh} confirms that the adsorption of TMN follows the Langmuir model. This indicates a monolayer adsorption of TMN molecules on the carbon steel surface, where the adsorbed molecules do not interact with each other. The slope of the line is 0.739, and the intercept is 0.196. The high R² value (0.975) indicates excellent

adherence of the experimental data to the Langmuir adsorption model, validating the monolayer adsorption assumption [28]. The adsorption equilibrium constant was calculated as:

$$K_{ads} = \frac{1}{\text{Intercept}} = \frac{1}{0.196} = 5.10 \text{ L/mol}$$

A higher K_{ads} value indicates strong adsorption of TMN molecules on the carbon steel surface, suggesting a stable inhibitor layer.

The Gibbs free energy of adsorption was calculated using the formula:

$$\begin{aligned} \Delta G_{ads} &= -RT \ln(K_{ads}) \\ \Delta G_{ads} &= -8.314 \times 303 \ln(5.10) = -4.105 \text{ kJ/mol} \end{aligned}$$

The Gibbs Free Energy of Adsorption ΔG_{ads} calculated from the Langmuir adsorption isotherm suggests that the adsorption of TMN onto the carbon steel surface is primarily physisorption. This conclusion is based on the typical threshold for physisorption, where ΔG_{ads} values are generally less negative than -20 kJ/mol . Physisorption involves weak van der Waals forces between the inhibitor molecules and the metal surface, indicating spontaneous but low-energy adsorption. However, the experimental results also show that the inhibition efficiency (IE%) increases with increasing temperature, as observed in the temperature-dependent weight loss measurements. This

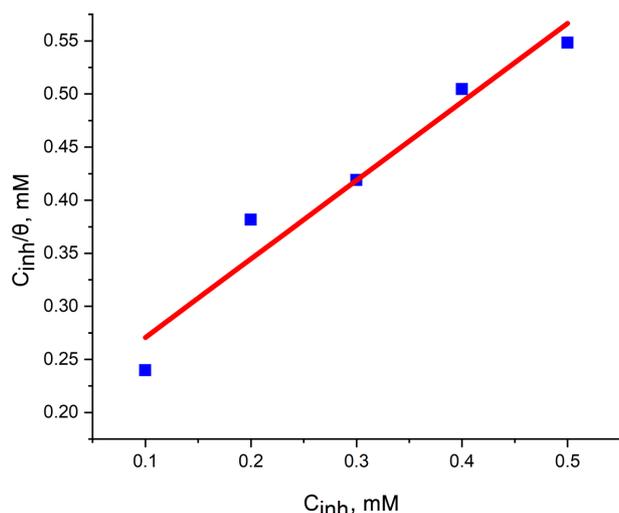


Fig. 6. Langmuir Adsorption Isotherm Plot for TMN Adsorption on Carbon Steel in 1 M HCl Solution

behavior contradicts the typical trend for pure physisorption, where adsorption weakens at elevated temperatures due to the desorption of physically adsorbed molecules [29]. The increase in IE% with temperature suggests a chemisorption mechanism, where chemical bonds form between TMN molecules and the steel surface, resulting in stronger and more stable adsorption at higher temperatures.

The low value ΔG_{ads} indicates that TMN adsorption initially involves physical interactions, such as van der Waals forces and electrostatic attractions, between the inhibitor molecules and the steel surface. These interactions facilitate the formation of a protective monolayer, reducing the direct interaction between the metal and the corrosive medium. The increase in IE% with temperature reflects the transition from weaker physical interactions to stronger chemical adsorption. Chemisorption involves the formation of covalent or coordinate bonds between the TMN molecules and the steel surface, which enhances the stability of the adsorbed layer. The presence of nitrogen, sulfur, and oxygen heteroatoms in TMN enables electron donation to the vacant d-orbitals of iron atoms, further supporting a chemisorption mechanism [30]. The negative value of ΔG_{ads} confirms the spontaneous nature of TMN adsorption on the carbon steel surface. The physisorptive nature of adsorption corroborated with little contribution from chemisorption is indicated by the magnitude ($-4.11 \text{ kJ mol}^{-1}$) as it is lower than the -20 kJ mol^{-1} threshold value generally associated with stronger chemisorption. The analysis of the Langmuir adsorption isotherm shows that TMN forms a strong and stable monolayer on the surface of carbon steel in 1 M HCl. The developed values of K_{ads} and ΔG_{ads} show that adsorption is favorable and spontaneous, further supporting the utility of the inhibitor for corrosion rate reduction [31]. Based on experimental trends, it is suggested that chemisorption dominates above 323 K.

3.3 DFT and Its Relation to Corrosion Inhibitors

Density Functional Theory (DFT) is a powerful tool for computational modelling so much that it can help disentangle the electronic properties of molecules as used as inhibitors for corrosion. It provides a view of the interaction between inhibitor molecules and metal

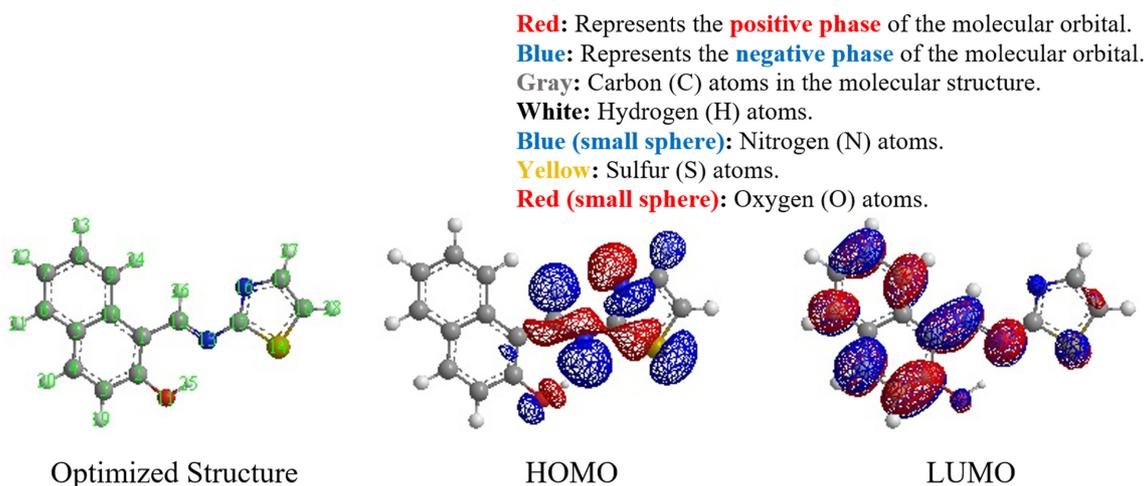


Fig. 7. Optimized Structure, HOMO, and LUMO of TMN Molecule Showing Electron Distribution and Reactivity Centers

surfaces at the quantum mechanical level. Energy values like HOMO, LUMO, ΔE , and others are parameters associated with the reactivity, adsorption capability, and inhibition efficiency of the molecule. HOMO specifies the electron donating ability of a molecule. Higher-energy HOMOs indicate better electron-donating capability, thus higher attachment to the surface of the metal. LUMO indicates the electron accepting ability of the molecule, with lower energies indicating better acceptance of back-donated electrons from the metal. HOMO and LUMO energy provide energy gap which is calculated by EMO-ELUMO. Lower energy difference indicates higher chemical reactivity and the strength of the adsorption on metal surface [32]. Furthermore, these quantum chemical parameters enhance the understanding of how inhibitors interact with metal surfaces and set the groundwork for establishing very strong inhibitors. Optimized structures and molecular orbitals (HOMO and LUMO) of TMN in Fig. 7 give critical insight into the behavior of TMN as a corrosion inhibitor. The molecular structure of TMN reveals a heteroatom (N, O, S) and π -electrons contained within a conjugated system. These groups and these electronic properties are vital for adsorption on the steel surface. The HOMO was primarily localized around the azomethine (C=N) group and the heteroatoms, especially the sulfur. This suggests that such areas are the active electron-donating centers. The capacity of TMN to donate electrons from these sites facilitates coordinate covalent bond formation with the vacant d-orbitals of iron atoms

which supports chemisorption [33]. The LUMO is distributed over the aromatic rings and heteroatoms, suggesting that TMN can accept electrons back-donated from the metal surface. This mutual electron exchange strengthens adsorption and enhances the inhibitor's stability on the metal surface. The complementary nature of HOMO and LUMO ensures strong and stable adsorption of TMN on the steel surface, forming a protective barrier that reduces metal dissolution in the acidic environment. The concentration of electron density in specific regions aligns with experimental observations of high inhibition efficiency [34].

The quantum chemical parameters of TMN are summarized in Table 1. A higher ionization potential indicates that TMN has strong electronic stability and is less prone to losing electrons. However, it can still act as a good electron donor through the azomethine group and heteroatoms. A moderate electron affinity suggests that TMN can accept back-donated electrons from the metallic surface, stabilizing the adsorbed layer. The small energy gap indicates high chemical reactivity, which enhances TMN's ability to interact with the steel surface [35]. The low ΔE reflects the dual role of TMN as both an electron donor and acceptor. The electronegativity of TMN is close to that of iron ($\chi_{\text{Fe}} = 7 \text{ eV}$), indicating compatibility for forming stable adsorption interactions with the steel surface. Moderate hardness suggests that TMN is stable but reactive enough to facilitate strong adsorption on the metal surface. The balance between efficiency and

Table 1. Quantum Chemical Parameters of TMN and Their Implications for Corrosion Inhibition

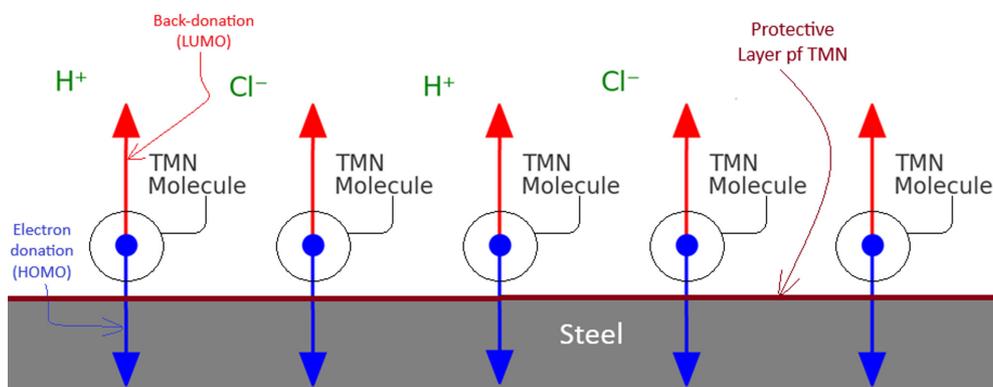
Parameter	Value
Ionization Potential (I) (eV)	9.215
Electron Affinity (A) (eV)	4.393
HOMO Energy (eV)	-9.215
LUMO Energy (eV)	-4.393
Energy Gap (eV)	6.804
Electronegativity (χ) (eV)	-4.822
Chemical Hardness (η) (eV)	2.411
Chemical Softness (σ) (eV ⁻¹)	0.415
Electron Transfer Fraction (ΔN)	0.041

inhibition of corrosion is critically important. A moderate softness value indicates that TMN can easily adapt its electronic structure during interactions with the metal, improving adsorption and inhibition efficiency [36]. This small positive value thus confirms that TMN donates electrons to the steel surface, leading to stable bonds. This electron donation is in agreement with chemisorption mechanism empirically found. The quantum chemical parameters of TMN, consisting of HOMO and LUMO analysis emphasized in confirmatory evidence of the dual role as electron donor and acceptor, is expected to result in powerful chemisorption on the surface of steel. The tiny energy gap, as well as the favorable values of hardness, softness, and electron transfer fraction, will further emphasize TMN's efficiency as a corrosion inhibitor. These findings from computational forecast find endorsing evidence from the experimental work stating TMN's potential applicability in acidic environments [37].

3.4 Suggested Inhibition Mechanism

The combined action of physical and chemical adsorption of TMN on carbon steel in 1 M HCl, as established experimentally and through quantum chemical studies, suggests the corrosion inhibition mechanism. The physical is the type of adsorption identified as the chemical goes well. It means that physisorption precedes chemisorption. The TMN molecules create weak van der Waals bonds and electrostatic forces with the steel surface [38,39]. Heteroatoms (N, S, O) and the π -electrons in the structure of TMN provide active centers for such interactions, which lead to an initial protective layer formation. TMN molecules donate electrons from their HOMO mainly from the azomethine (C=N) group and from heteroatoms: N, S, and O, into vacant d-orbitals of iron atoms on the steel surface [38]. This ensures strong coordinate covalent bonds that fix TMN molecules onto the steel surface [40]. At the same time, the LUMO of TMN takes the back-donated electrons from the metal surface thus further stabilizing the adsorbed layer [41].

The dense and uniform adsorption of TMN molecules hereby leads to the formation of a monolayer, becoming barrier which prevent direct access of as much as possible of the metal surface to the corrosive acid environment [42,43]. This barrier restricts the diffusion of corrosive species (H^+ and Cl^- ions) toward the surface of the steel, thus retarding corrosion. At elevated temperatures, chemisorption becomes more pronounced, as higher energy promotes stronger bonds between TMN molecules and the steel surface. This results in an increase in inhibition efficiency [44,45]. Fig. 8, illustrating the

**Fig. 8. Proposed Inhibition Mechanism of TMN on Carbon Steel Surface in 1 M HCl Solution**

proposed inhibition mechanism of TMN on the carbon steel surface in 1 M HCl solution.

4. Conclusion

This study comprehensively examined the corrosion inhibition efficacy of 1-((thiazol-2-ylimino)methyl)-2-naphthol (TMN) for carbon steel in 1 M HCl solution, employing both experimental weight loss measurements and quantum chemical calculations. The findings confirm that TMN is a highly effective corrosion inhibitor, exhibiting a maximum inhibition efficiency of 91.2% at 0.5 mM and 303 K.

The inhibition performance of TMN was found to be strongly dependent on concentration, immersion time, and temperature:

- Effect of Concentration: Inhibition efficiency increased with higher TMN concentrations, indicating effective surface coverage and adsorption on the steel surface.
- Effect of Immersion Time: The inhibition efficiency increased progressively up to 10 hours, after which a slight decrease was observed, suggesting possible desorption or reorganization of adsorbed molecules over extended exposure periods.
- Effect of Temperature: Higher temperatures resulted in an increase in inhibition efficiency, confirming that chemisorption dominates the adsorption mechanism at elevated temperatures.

The adsorption of TMN followed the Langmuir isotherm model, indicating the formation of a stable monolayer on the steel surface. The calculated Gibbs free energy of adsorption ($\Delta G_{\text{ads}} = -4.11$ kJ/mol) suggests a mixed adsorption mechanism involving both physisorption and chemisorption, with a stronger contribution from chemisorption at higher temperatures.

Quantum chemical calculations (DFT) provided further insights into the electronic properties of TMN, supporting its inhibitory performance:

- HOMO Distribution: TMN's HOMO is localized on active sites such as the azomethine (-C=N) group and heteroatoms (N, S, and O), enhancing its ability to donate electrons to the steel surface for strong adsorption.
- Energy Parameters: A small HOMO-LUMO gap ($\Delta E = -4.822$ eV), high electronegativity ($\chi = 6.804$ eV), and favorable softness ($\sigma = 0.415$ eV⁻¹) reinforce

TMN's strong adsorption tendency and high reactivity.

- Adsorption Mechanism: TMN acts as a dual-function inhibitor, donating electrons through its HOMO and accepting back-donated electrons through its LUMO, facilitating strong chemisorption on the steel surface.

The heteroatoms (N, S, and O) and π -electronic systems in TMN play a crucial role in corrosion protection, as they facilitate strong interactions with the steel surface, blocking aggressive H⁺ and Cl⁻ ions from reaching the metal. The results establish TMN as a promising, eco-friendly corrosion inhibitor for protecting carbon steel in acidic environments, particularly at elevated temperatures.

This study provides a comprehensive experimental-theoretical approach to understanding the corrosion inhibition mechanism of TMN, confirming its high inhibition efficiency due to a biphasic physical-chemical adsorption mechanism. Given its phenomenal performance, TMN presents an attractive alternative for acid-resistant corrosion inhibition applications. Future research should focus on scaling up its practical application and assessing its environmental impact to optimize its industrial utilization.

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