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Schiff's Base Performance in Preventing Corrosion on Mild Steel in Acidic Conditions

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ABSTRACT

Many industries, particularly the oil and gas industry, extensively use metallic materials. However, steel is negatively impacted by corrosion, which decreases the functioning of its surfaces. Therefore, finding a solution to the corrosion challenge is imperative. To prevent mild steel from corroding in a 1 M hydrochloric acid medium, a Schiff base named methyl 5-(((((2-hydroxynaphthalen-1-yl)methylene)amino))-1-methyl-1H-pyrazole-4-carboxylate (MMPC) was utilized. Weight loss measurements and theoretical calculations were conducted to explore the effectiveness and mechanism of corrosion protection. MMPC adsorbs onto mild steel, blocking active sites, and the adsorption follows the Langmuir adsorption isotherm model. Based on a free energy (ΔG^o_{ads}) value of -37.25 KJmol^{-1}, physical adsorption and chemical adsorption are two separate adsorption modes. At a concentration of 0.5 mM and 303 K, the findings demonstrate that MMPC showed an excellent inhibitor effectiveness of 97.13 %. The acid reaction site is blocked by the inhibitor adsorbed onto the mild steel surface. Density Functional Theory (DFT) at the B3LYP/6-311 G^{++} basis set was also used to determine the effectiveness of the inhibitor, and the results demonstrated that MMPC is an effective inhibitor. Prog. Color Colorants Coat. 16 (2023), 319-329© Institute for Color Science and Technology.

1. Introduction

Due to its superior mechanical and thermal properties, mild steel is one of the most significant steel alloys used in various sectors to build factories, appliances, storage facilities, and more [1]. However, because of how quickly mild steel corrodes when exposed to acids, corrosion prevention is of great industrial and scientific interest [2]. Corrosive environments are utilized in various manufacturing processes, such as scaling, cleaning (oil well cleaning), and pickling [3]. Anticorrosion technology is a realistic, reliable, and economical corrosion reduction technology [4]. Effective corrosion inhibitors should greatly reduce the rate of metal corrosion during acidifying treatments. Corrosion inhibitors are adsorbed onto the metallic substrate to inhibit corrosion through their active

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functions. Several natural substances are used as corrosion inhibitors due to the well-documented risks associated with most synthetic corrosion inhibitors [5]. Corrosion inhibitor engineering is developing from the perspective of environmental sustainability. Green inhibitors, which are more ecologically responsible, are currently the subject of recent rules everywhere [6].

Hazardous compounds used as corrosion inhibitors, such as triazoles, heterocyclic rings, chromate ions, and molybdate ions, are believed to significantly slow corrosion rates. However, they contain carcinogenic compounds that kill plants and animals, heavy metals that wash into streams and ruin ecosystems, and are often very expensive to dispose of after being used in metal pipes. As a result, the usage of novel inhibitors with fewer side effects has increased due to concerns about toxicity, degradability, bioaccumulation, and affordability [7]. The much more significant and effective strategy for preventing iron corrosion is the application of organic inhibitors [8]. Widely utilized organic inhibitors include aromatic rings, double and triple bonds, nitrogen, sulfur, and oxygen as heteroatoms [9]. The effectiveness of such chemical compounds in preventing corrosion depends on their ability to remove adsorbed water molecules at the interface and create a tight protective film that shields the metal surface from the corrosive fluid [10]. The amount of adsorption is influenced by these organic molecules' molecular weight, projected surface area, and heteroatom content [11, 12].

Most of these substances have a poisonous character and stick poorly to metal surfaces. Therefore, in this study, a Schiff base (Figure 1) was assessed as a mild steel corrosion inhibitor in a 1 M HCl solution. The effects of concentration (0.1, 0.2, 0.3, 0.4, 0.5, and 1 mM), immersion duration (1, 5, 10, 24, and 48 h), and temperature (303, 313, 323, and 333 K) on the corrosion inhibition ability of the Schiff base were investigated using weight loss techniques. The evaluated Schiff base was subjected to computational investigations using density functional theory (DFT) to validate and support the experimental findings. The article presents a study on the use of a Schiff base named MMPC as a corrosion inhibitor for mild steel in a 1 M hydrochloric acid medium. The study combines experimental techniques such as weight loss measurements with theoretical calculations using Density Functional Theory (DFT) to explore the effectiveness and mechanism of corrosion protection. The objective of the article is to present the findings of the study on the effectiveness of MMPC as a mild steel corrosion inhibitor in a 1 M HCl solution. The investigation includes analyzing the effects of concentration, immersion duration, and temperature on the corrosion inhibition ability of the Schiff base, using weight loss techniques. The study also validates and supports the experimental findings with computational investigations using DFT.

2. Experimental

2.1. Materials and methods

The sample company provided the mild steel used in this research, and Table 1 specifies the element content by composition (by wt. %). The steel was cut into measurements of 35×20×4 mm and cleaned with silicon carbide paper. After treatment with acetone as a cleaning agent, the steel was rinsed with double distilled water and oven-dried before being weighed.

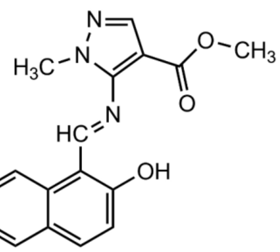

Figure 1: The structure of MMPC.

Table 1: Shows the weight percentage chemical composition of the metallic substrate.

Iron	Phosphorous	Sulphur	Aluminium	Silicon	Manganese	Carbon
Balance	0.09 %	0.05 %	0.01 %	0.38 %	0.05 %	0.21 %

2.2. Weight loss techniques

The metallic substrate was subjected to untreated and treated solutions of 1 M HCl. The treated solution had the tested inhibitor with concentrations of 0.1, 0.2, 0.3, 0.4, 0.5, and 1.0 mM. Exposure durations were 1, 5, 10, 24, and 48 hours at 303 K. To study the effect of temperature, the inhibited and uninhibited solutions were investigated for 5 hours at solution temperatures of 313, 323, or 333 K in accordance with NACE TM0169/G31 [13]. The tested coupons were then removed and treated in line with ASTM standard G1-03. Continuing the computations, the mean mass loss was used to calculate the rate of corrosion [14]. The rate of corrosion (C_R), the inhibitory performance (IE %), and the surface coverage (θ) were determined using Equations 1-3 [13,14]:

$$C_R\ (mg.cm^{-2}.h^{-1})=\frac{W}{a} \quad (1)$$

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

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

where W is the mass loss of metallic substrate (mg), a is the area of investigated coupon (cm^2), t is the immersion durations (h) [13, 14].

2.3. Theoretical calculations

The molecular modeling computations were carried out using Gaussian 09 [15]. The inhibitor structure in the gas phase was optimized using the B3LYP method and the principle group "6-31G^{++} (d,p)". According to Koopman's hypothesis [16], the ionization potential (I) and electron affinity (A) correspond to E_{HOMO} and E_{LOMO}, respectively. The ionization potential and electron affinity were calculated using equations 4 and 5, respectively:

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

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

To determine the hardness (η), softness (σ), and electronegativity (χ), utilize equations 6-8:

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

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

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

To calculate the proportional number of transported electrons (ΔN), [16] can utilize equation 9:

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

Thus, χ_{Fe} and χ_{inh} referred to iron and inhibitor electronegativities, whereas η_{Fe} and η_{inh} signify to iron and inhibitor hardness respectively.

For the metallic substrate the value of ΔN was determined based Equation 10, and the χ_{Fe} = 7 eV, η_{Fe} = 0 eV [16]:

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

3. Result and Discussion

3.1. Weight loss investigations

Figure 2 presents an overview of the weight loss assay results for metallic samples in HCl without and with the addition of MMPC. The findings show that MMPC protects the coupon surface from corrosion, and its ability to do so increases with its concentration. For a 5-hour exposure, the corrosion rate was slowed down by increasing the MMPC concentration. The maximum inhibitory potency concentration (97.13 %) was observed at 0.5 mM MMPC. It is believed that the large molecular structure of MMPC and the abundance of heteroatoms (three nitrogen atoms plus three oxygen atoms) contribute to the strong inhibitory ability of the material [15].

The corrosion inhibition performance of MMPC was enhanced by increasing its dosage up to 0.5 mM as the MMPC molecules were adsorbed onto the metal sample surface to form a protective barrier. However, when inhibitor concentrations climbed above 0.5 mM and approached 1.0 mM, the inhibitor molecules were attracted to the surface of the steel substrate, virtually retaining the inhibitory efficiency constant.

3.2. The effect of exposure time

The metal substrate was exposed to an HCl solution with inhibitory concentrations ranging from 0.1 to 1.0 mM for 1 to 48 hours at 303 K to examine the effect of exposure duration on the corrosion inhibition efficacy of MMPC (Figure 3). Up to 10 hours of immersion time, rapidly increasing damping efficiency was observed. After that, it decreased steadily to 24 hours, and then more rapidly to 48 hours. By increasing the amount of MMPC adsorbed on the mild steel surface as a result of increasing the concentration and exposure time, the inhibitory efficiency was increased. Additionally, as even more inhibitor molecules were adsorbed on the metallic substrate, the inhibitor's adsorption density notably rose, enabling both Van Der Waals forces (physisorption) and the formation of coordination complexes (chemisorption). If some inhibitor molecules leave the surface, the effective area that the inhibitor covers and the inhibitory activity may both be lowered. Evidence that the inhibitor layer adsorbed in the inhibited media comes from the comparatively high inhibitive efficacy observed over the prolonged immersion period.

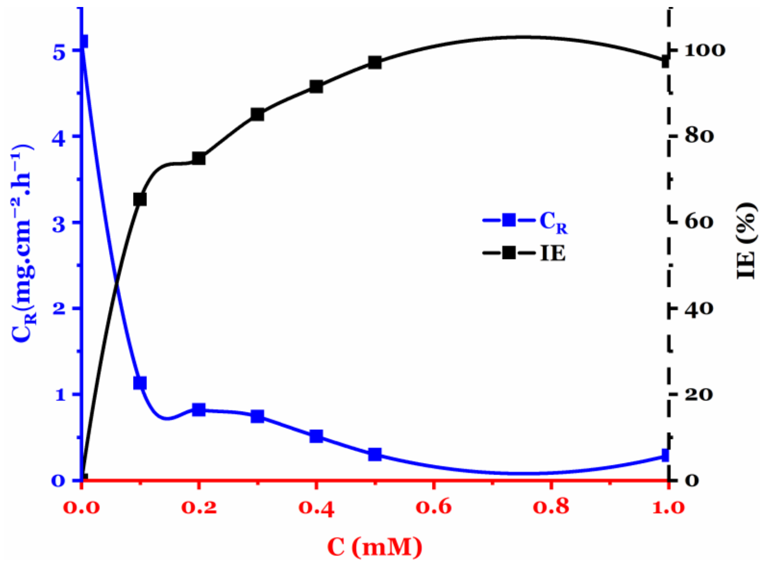

Figure 2: C_R vs IE % for various MMPC concentrations of metallic substrate subjected to corrosive media for 5 hours at 303 K.

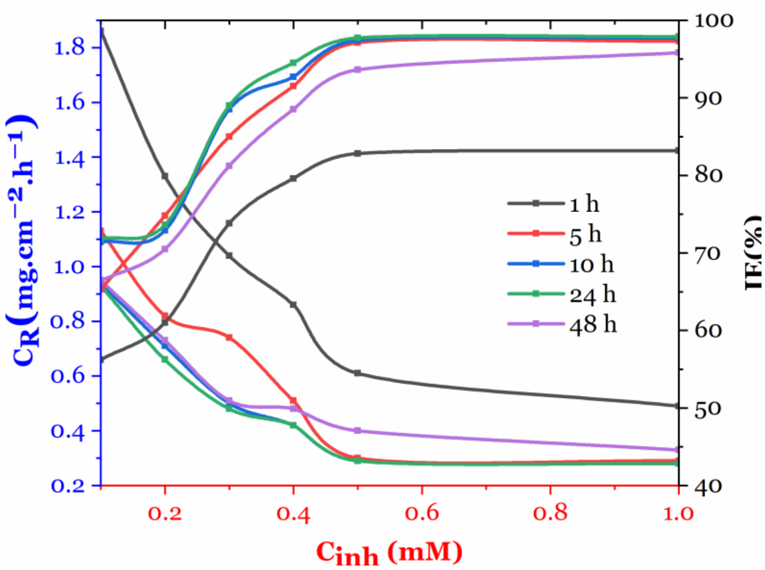

Figure 3: Various dosages effect of MMPC on the C_R and IE % of metallic substrate immersed in 1 M HCl solution for 1 to 48 h at 303 K.

3.3. The effect of temperature

The weight loss method was utilized to investigate the corrosion inhibitory effectiveness of MMPC on mild steel under acidic conditions with various concentrations (0.1-1.0 mM) at different temperatures (303-333 K) after 5 hours of exposure. As shown in Figure 4, at a constant inhibitor concentration, the corrosion rate increased with increasing temperature, while the effectiveness of corrosion protection decreased as the temperature rose from 303 to 333 K. At normal temperatures, MMPC performed optimally. Physisorption was observed, with a decrease in inhibitory activity as the temperature increased at all concentrations. Additionally, at high temperatures, desorption occurs, resulting in the loss of MMPC molecules from the surface of the sample.

3.4. Adsorption isotherm

The comprehension of the interaction between the inhibitor molecules and the metallic substrate is made easier by the adsorption temperature. The surface coverage (θ) value, obtained by graphemetrical measurments, was used to decide which isotherm best fits the data. To ascertain if MMPC molecules attested inhibitor to the surface of the metallic substrate physically or chemically, a number of adsorption isotherms, including the Temkin, Freundlich, and Langmuir isotherms, were utilized to analyze the adsorption mechanism. The regression coefficient (R^2) for the MMPC of 0.9989 and the computed slope and intercept values for the Langmuir isotherms of 9.591E-4 ± 2.21372E-5 and 0.05926 ± 0.01125, respectively at 303 K, show that the Langmuir absorption isotherms appear to suit the data well. Equation 12 and the isothermal plot of Langmuir absorption between C/θ and C are shown in Figure 5

$$\frac{C}{\theta}=\frac{1}{K_{ads}}+C \tag{12}$$

where C is the concentration of MMPCs and K_{ads}, which stands for surface area, is the equilibrium constant.

To use the K_{ads} value and a linear straight fitted plot between C/θ and C, the free energy of adsorption, ΔG^{o}_{ads}, was computed. K_{ads} and ΔG^{o}_{ads} are connected by equation 13 in this way.

$$\Delta G^{o}_{ads} = -RT\ ln(55.5K_{ads}) \tag{13}$$

where T is the temperature, R is the gas constant, and 55.5 is the water content measurement. The "K_{ads}" constant was added to the calculation above to produce the "ΔG^{o}_{ads}" value.

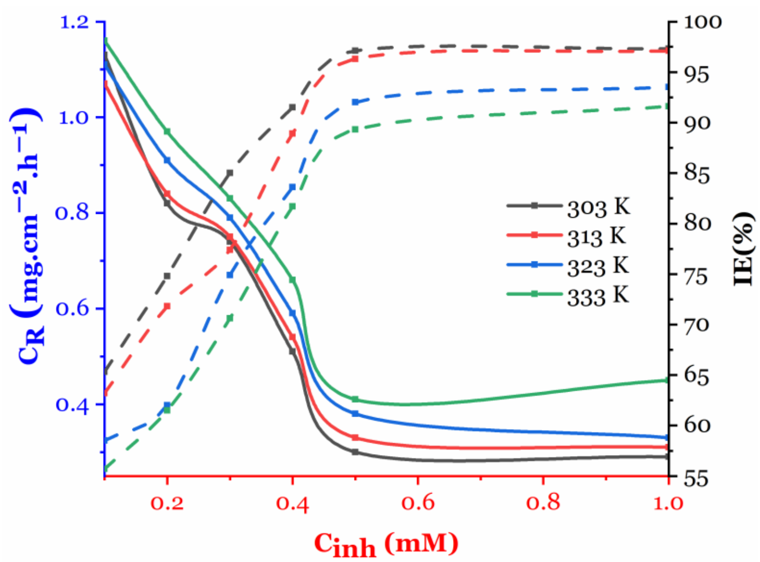

Figure 4: Various dosages effect of MMPC on the C_R and IE % of metallic substrate immersed in 1 M HCl solution for 5 h at 303-333 K.

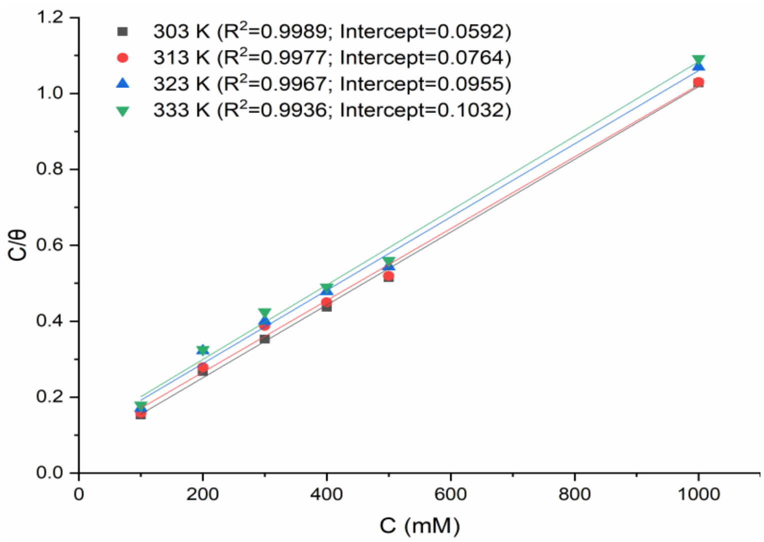

Figure 5: Langmuir adsorption isotherm for metallic substrate in acidic solution at different temperatures.

A value of ΔG^o_{ads} approximately or even less negative than -20 kJmol^{-1} suggests physisorption, but a value of ΔG^o_{ads} ranging from -40 kJmol^{-1} and larger negative value suggests chemisorption [22, 23]. Physical adsorption and chemical adsorption are two separate adsorption modes, according to the MMPC ΔG^o_{ads} value of -37.25 kJmol^{-1}.

3.5. DFT calculations

Numerous applications use density functional theory (DFT) to assess the effectiveness of inhibitors and the behavior of the coupon surface. In this study, geometrical optimization of the tested inhibitor molecule was performed using the DFT/B3LYP approach with the basis set 6-311G^{++}(d,p) and Gaussian 09. Quantum chemical descriptors were calculated using the optimized geometry to determine the ionization potential (IP) and electron affinity (EA). Figure 6 displays the structure of the optimized tested inhibitor molecule. Quantum chemical calculations are frequently employed to explore the reaction mechanism process, which has been verified as an effective way to prevent corrosion activities of chemicals in connection to their electronic structure [17-19]. As a result, the effectiveness of the tested inhibitor to resist corrosion has been studied. Table 2 shows the values of the quantum chemical characteristics, which include E_{HOMO}, E_{LUMO}, ΔE, χ (Electronegativity), Softness (σ), and Hardness (η). The frontier orbitals play an important role in understanding the reactivity of chemical compounds when determining the corrosion behavior of any organic substance [20]. The values for E_{HOMO}, E_{LUMO}, and ΔE are -9.067, -4.203, and 4.864 eV, respectively. A lower E_{LUMO} is accountable for mild steel's ability to receive electrons into the vacant d-orbital of the inhibitor, and a lower E boosts corrosion efficiency. E_{HOMO} is responsible for the compound's ability to donate electrons; the higher the E_{LUMO}, the better the compound's donating potential. This determines the covalent bond's polarity and the distribution of charges that enable molecules to adsorb on metallic surfaces, making the tested inhibitor an effective corrosion inhibitor. The electronegativity (χ) value of 6.635 eV, which explains how the molecule attracts electrons toward itself, and a higher electronegativity leads to better inhibition efficiency, are other quantum chemical property values that help to explain the potential of the tested inhibitor as a corrosion inhibitor. The computed values for the ionization energy (I), hardness (η), softness (σ), and electron affinity energy are shown in Table 2 as 9.067, 2.432, 0.41118, and 4.203 eV, respectively. A greater E_{HOMO} offers low ionization energy and electron affinity, which leads to improved inhibition efficiency. As a result, the tested inhibitor is a better inhibitor to corrosion on mild steel. Ionization and electron affinity describe the properties of compounds based on electron density. Additionally, the hardness and softness listed in Table 2 were verified. This information illustrates the compound's molecular stability and reactivity and is favorable for preventing corrosion on mild steel.

Table 2: Quantum chemical parameters of tested inhibitor molecule.

Inhibitor	E_{HOMO}	E_{LUMO}	ΔE	χ	σ	η	*I*	A	Δ*N*
MMPC	-9.067 eV	-4.203 eV	4.864 eV	6.635	0.41118	2.432	9.067 eV	4.203 eV	0.075

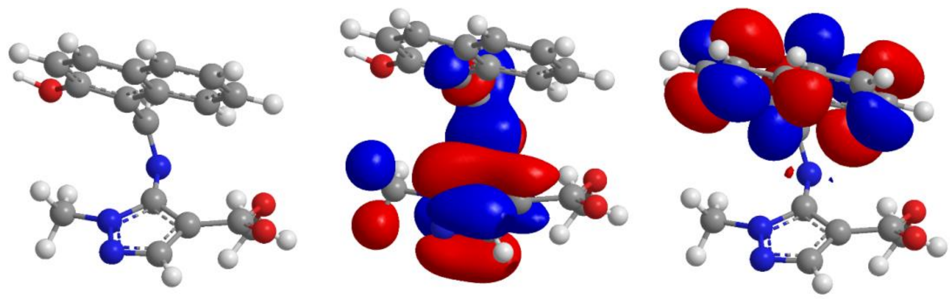

Figure 6: Optimized structure, HOMO, and LUMO for the AAQQQ4 tested inhibitor molecule.

3.6. Mechanism of inhibition

Corrosion is the process by which materials deteriorate due to chemical reactions with their environment, typically involving oxidation or reduction reactions. Corrosion inhibitors are substances that can be added to a system to prevent or slow down the corrosion process [21-23].

Organic synthesized inhibitors are a common type of corrosion inhibitor that work by forming a protective film on the metal surface, which helps to prevent or slow down the corrosion process. The mechanism of corrosion inhibition by organic synthesized inhibitors can be explained in the following steps:

1. Adsorption: The inhibitor molecules adsorb onto the metal surface by weak chemical forces, such as Van der Waals forces, electrostatic forces, and hydrogen bonding. The adsorption process is influenced by factors such as the chemical structure and size of the inhibitor molecules, the nature of the metal surface, and the pH and temperature of the solution.
2. Formation of a protective film: The adsorbed inhibitor molecules react with the metal ions and other species in the corrosive environment to form a protective film on the metal surface. This film acts as a barrier between the metal and the corrosive environment, preventing or slowing down the corrosion process.
3. Inhibition of cathodic and anodic reactions: The inhibitor molecules can also inhibit the cathodic and anodic reactions that occur during the corrosion process. For example, the inhibitor can block the reaction sites on the metal surface where oxygen reduction occurs during the cathodic reaction. This inhibition reduces the rate of the corrosion process.

The effectiveness of an organic synthesized inhibitor depends on a number of factors, including the chemical structure of the inhibitor, the concentration of the inhibitor in the solution, and the nature of the corrosive environment. These factors need to be optimized to achieve the best corrosion inhibition performance.

Using weight loss measurements, it was observed that the chemical azomethine forms protective films against mild steel corrosion in hydrochloric acid medium. The inhibition efficiency increases with higher inhibitor concentrations. When 0.5 mM of the inhibitor was present at 303 K for 5 hours of immersion, the material showed a protective capacity between 65 and 97 %. The investigated inhibitor utilizes the Langmuir model, which takes into account both decomposition and chemisorption adsorption at the metal interface. Figure 7 illustrates the adsorption of an imine molecule on the metal surface, showing the chemical attraction of the unshared electron pairs of the azomethine molecule to the unoccupied iron d-orbitals of the metallic substrate surface, as well as the electrostatic attractions of the negatively charged steel surface.

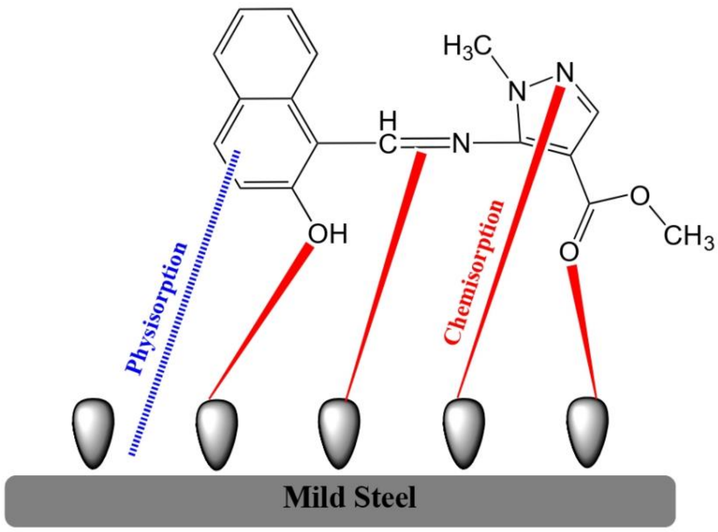

Figure 7: The suggested mechanism of tested inhibitor molecule on mild steel surface in in corrosive solution.

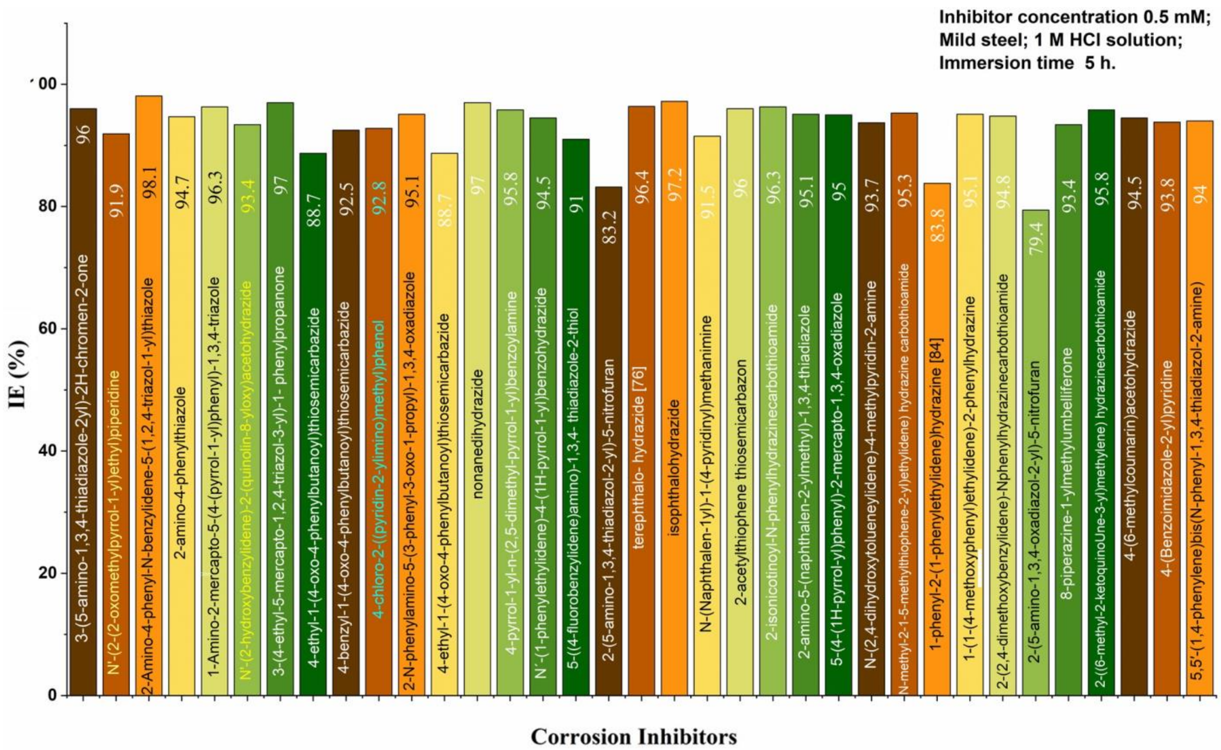

Figure 8: Comparison between several synthesized organic corrosion inhibitors.

3.7. Comparison studies

In this research, we conducted a comparative analysis of the inhibitory effectiveness of various organic corrosion inhibitors that have been previously synthesized and published [24, 56]. We evaluated the inhibitory efficiency of each inhibitor and presented our findings in Figure 8.

Figure 8 provides an overview of the inhibition efficiencies of several synthesized organic corrosion inhibitors. The chart displays the inhibitors' inhibition efficiency as a percentage, with a higher percentage indicating a more effective inhibition. The inhibitors are identified on the x-axis, and the y-axis represents the percentage of inhibition efficiency.

The comparison enables us to determine which synthesized organic corrosion inhibitor is the most effective at inhibiting corrosion. This information can help in selecting the most suitable inhibitor for specific applications, such as in the chemical, petroleum, or manufacturing sectors. Furthermore, the study's results may offer insights into the mechanisms of corrosion inhibition and guide future research and development of corrosion inhibitors.

4. Conclusions

In conclusion, the research findings show that MMPC is an effective inhibitor for preventing the corrosion of mild steel in a 1 M hydrochloric acid medium. The use of weight loss measurements and theoretical calculations, including the Langmuir adsorption isotherm model and Density Functional Theory, provided insight into the mechanism and effectiveness of the corrosion protection. The results indicate that MMPC adsorbs onto mild steel, blocking active sites and exhibiting excellent inhibitor effectiveness of 97.13 % at a concentration of 0.5 mM and 303 K. Overall, this study offers valuable insights into the development of effective inhibitors for protecting metallic materials, particularly in the oil and gas industry, where corrosion is a significant challenge.

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