

# Comprehensive Analysis of the Corrosion Inhibition Performance of 4-Piperonylideneaminoantipyrine for Mild Steel in HCl Solution: Concentration, Time, Temperature Effects, and Mechanistic Insights

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Metal corrosion in acidic environments is a major issue in various industrial applications. This study evaluates the 4-piperonylideneaminoantipyrine (PPDAA) corrosion inhibition efficiency for mild steel in a hydrochloric acid (HCl) solution. The weight loss method was used to determine the corrosion inhibition efficiency at different concentrations and immersion time periods. Results revealed that the highest inhibition efficiency (94.3%) was achieved at 5 mM concentration after 5 hours of immersion time. To inspect the surface morphology of the inhibitor film on the mild steel surface, scanning electron microscopy (SEM) was used before and after immersion in 1.0 M HCl. Density functional theory (DFT) calculations were performed to investigate the molecular structure and electronic properties of the inhibitor molecule to understand the corrosion inhibition mechanism. Theoretical results showed that the inhibitor molecule can adsorb onto the mild steel surface through its nitrogen and oxygen atoms, forming a protective layer that prevents HCl corrosive attack. These findings highlight the potential of PPDAA as an effective corrosion inhibitor for mild steel in HCl solution. Moreover, combining experimental and theoretical approaches provides insights into the mechanism of corrosion inhibition, which is essential for developing effective strategies to prevent metal corrosion in acidic environments.

**Keywords:** Corrosion inhibition, 4-(Piperonylideneamino)antipyrine (PPDAA), Mild steel, Hydrochloric acid (HCl), Density functional theory (DFT)

## 1. Introduction

Mild steel stands as a widely employed material in various industries, appreciated for its commendable mechanical attributes and cost-efficiency. However, its susceptibility to corrosion, particularly in acidic environments, poses a significant challenge leading to economic losses and safety concerns [1-3]. Notably, hydrochloric acid (HCl), a prevalent industrial chemical, can trigger severe corrosion in mild steel, making the utilization of corrosion

inhibitors pivotal to mitigate HCl-induced corrosion [4,5]. Organic inhibitors have garnered substantial attention due to their efficacy in shielding mild steel against corrosion in acidic surroundings. Their ability to adsorb onto the metal surface, forming a protective film that thwarts acid attacks, underscores their importance [6,7]. Recent investigations have delved into numerous organic inhibitors, assessing their effectiveness in combatting HCl-induced corrosion in mild steel [8-11]. Moreover, researchers have directed their efforts toward developing novel organic inhibitors, aiming for both enhanced corrosion inhibition efficacy and environmental

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friendliness [12-14]. For instance, Al-Amiery *et al.* explored a novel Schiff base derivative, reporting corrosion inhibition efficiency of up to 96.7% at 0.5 mM concentration [15]. Similarly, in 2022, a Nicotinehydrazide-based inhibitor displayed remarkable efficiency in curbing mild steel corrosion in HCl solution, achieving up to 97% inhibition at 5 mM concentration [16]. In tandem with experimental studies, theoretical calculations have emerged as valuable tools to elucidate the molecular underpinnings of corrosion inhibition [17-20]. The application of Density Functional Theory (DFT) calculations has become a prevalent approach for predicting the adsorption behavior and electronic characteristics of organic inhibitors on metal surfaces [21-23]. A pertinent example is Mustafa *et al.*'s employment of DFT calculations to decipher the inhibition mechanism of a novel -2-mercapto-1,3,4-oxadiazole compound on mild steel in HCl solution. Their findings suggested that the inhibitor could adsorb onto the mild steel surface, engendering a protective layer that counteracted the corrosive impact of HCl [24].

The choice of corrosion inhibitor is a pivotal decision, dictated by the intricate interplay of multiple factors. Within this tapestry of considerations, the rationale behind the selection of 4-piperonylideneaminoantipyrene (PPDAA) emerges as a critical facet, one that merits comprehensive exploration. The omnipresent challenge of corrosion has spurred intensive research into effective mitigation strategies. Mild steel, revered for its mechanical properties and cost-effectiveness, remains particularly vulnerable in acidic environments. Among these, hydrochloric acid (HCl) stands as a potent adversary, capable of inducing swift and damaging corrosion. In this milieu of challenges, the quest for corrosion inhibitors becomes paramount. Amid the landscape of potential corrosion inhibitors, 4-piperonylideneaminoantipyrene (PPDAA) emerges as a subject of interest, igniting curiosity for its unique attributes. This choice is fueled by a combination of factors that sets it apart from the rest. PPDAA's molecular architecture, brimming with nitrogen and oxygen atoms, heterocyclic, and benzene rings, beckons as a canvas for potential corrosion inhibition. The presence of unpaired electron pairs within these elements tantalizingly hints at its suitability for interaction with metallic surfaces. The allure of PPDAA extends beyond its molecular structure.

Preliminary indications suggest that it might yield a protective layer when interacting with mild steel surfaces, mitigating the corrosive onslaught. This dualistic mechanism, rooted in both its physical composition and anticipated interactions, positions PPDAA as a multifaceted contender. Modern times demand not only efficiency but also environmental compatibility. PPDAA's exploration aligns with this ethos, as research steers towards inhibitors that demonstrate both potency and eco-friendliness. As our investigation delves into the efficacy of 4-piperonylideneaminoantipyrene (PPDAA) as a corrosion inhibitor, the rationale behind its selection becomes increasingly profound. The undercurrents of molecular potential, holistic inhibition mechanisms, and environmental alignment serve as the driving forces propelling this study forward. With each step, we inch closer to unraveling the depth and promise that PPDAA holds within the realm of corrosion inhibition.

This research is geared towards a comprehensive assessment of the corrosion inhibition potential of 4-(Piperonylideneamino)antipyrene (Fig. 1) for mild steel in HCl solution, employing a dual-pronged strategy involving experimental and theoretical approaches. The principal objectives encompass:

#### 1. Measurement of Corrosion Inhibition Efficiency:

Through the weight loss method, the corrosion inhibition efficiency of the inhibitor shall be gauged at varying concentrations and immersion durations. This endeavor aims to elucidate the impact of concentration and time on the inhibitor's effectiveness.

#### 2. Exploration of Adsorption Behavior and Electronic Properties:

Leveraging density functional theory calculations, the adsorption behavior and electronic traits of the inhibitor molecule on the mild steel surface shall be probed. Insights into the fundamental interactions between the inhibitor and the metal surface are anticipated.

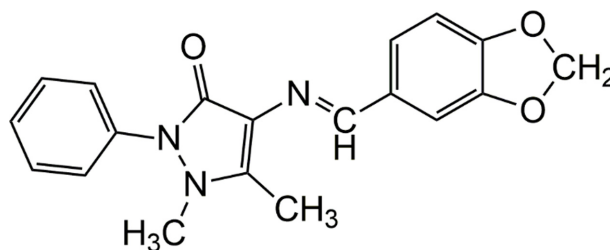


Fig. 1. PPDAA chemical structure

**3. Unveiling Corrosion Inhibition Mechanism:** A meticulous analysis of the corrosion inhibition mechanism of the 4-(Piperonylideneamino)antipyrine inhibitor will be pursued. This includes an investigation into the factors governing its protective effects and its potential as a robust corrosion inhibitor for mild steel in the realm of HCl-induced corrosion.

In amalgamation, this research endeavors to contribute to the understanding of corrosion inhibition strategies by assessing a novel organic inhibitor's efficacy through empirical and theoretical avenues. The insights garnered are poised to have implications for the development of more potent corrosion prevention methodologies for mild steel in the context of HCl environments.

## 2. Experimental Techniques

### 2.1 Weight loss Analysis

In this study, the mild steel samples were analyzed for their chemical composition using X-ray fluorescence spectrometry. The samples were prepared according to the ASTM G1-03 [25] protocol and polished with silicon carbide series plates. Prior to immersion, the mild steel coupons were cleaned with double-distilled water and acetone, and then dried in an oven. To create a corrosive media for the experiments, a 1 M HCl solution was prepared by diluting analytical grade 37% HCl solution with double-distilled water. Inhibitor concentrations ranging from 0.1 to 1.0 mM were achieved by diluting the inhibitor in 1 M HCl solution. The mild steel samples were immersed in 500 mL glass beakers containing 400 mL of 1 M HCl solution with varying concentrations of the inhibitor. The experiments were conducted at 25 °C using a water bath, following the NACE TM0169/G31 [26] protocol. The samples were exposed for different periods (1, 5, 10, 24, and 48 hours), and the products of corrosion were wiped off the surface before the coupons were dried and weighed. The weight difference was recorded, and the mass variation at the estimated time and original mass of the metallic sample represented the weight loss attained [27]. 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 25, 35, 45, and 55 °C using a water bath to determine the effect of temperature. The average rate

of corrosion was calculated after being exposed in triplicate, and the rate of corrosion was calculated using relation (1) [28].

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

To calculate the inhibition efficiency, equation (2) was used, where  $W$  is the weight loss (mg) of the sample,  $a$  is the surface area of mild steel (cm<sup>2</sup>),  $d$  is the density of the mild steel coupon (g/cm<sup>3</sup>), and  $t$  is the exposure time (h) [29].

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

The corrosion rates in the absence and presence of inhibitor were denoted as  $C_{R_o}$  and  $C_{R(i)}$ , respectively. Equation (3) was used to determine the coverage area ( $\theta$ ) for both uninhibited and inhibited solutions [30].

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

### 2.2 Adsorption Mechanism

To obtain a better understanding of the properties of the studied molecules, it is important to use various types of adsorption isotherms, such as Frumkin, Temkin, and Langmuir. These isotherms can help determine the amount of inhibitor coverage on the surface. Therefore, weight loss measurements were carried out in this study to determine the extent of surface coverage of the inhibitor at various concentrations in corrosive media [31].

### 2.3 Theoretical calculations

The Gaussian 09 software (ChemOffice molecular modeling package) was utilized in this study to conduct quantum chemical calculations [32]. The optimization of the inhibitor structure in the gaseous state was achieved through the B3LYP method and the basis set "6-31G<sup>++</sup>(d,p)". To determine the ionization potential (I) and electron affinity (A) based on Koopmans theory [33],  $E_{HOMO}$  and  $E_{LOMO}$  were used, respectively. Equations (4 and 5) were employed in determining I and A.

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

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

Equations (6-8) were used to determine the electronegativity ( $\chi$ ), hardness ( $\eta$ ), and softness ( $\sigma$ ) values.

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

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

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

Equation (9) from [33] was utilized to calculate the number of electrons transferred ( $\Delta N$ ).

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

The electronegativity value of iron was determined as 7 eV, and its hardness value was found to be zero eV. Based on these results, equation (10) was developed.

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

### 3. Result and Discussion

#### 3.1 Effect of concentration

Weight loss measurements were used to evaluate the corrosion performance of mild steel samples in a 1 M corrosive environment, both with and without the addition of various doses of PPDA, after 5 hours of immersion at 25 °C. The rate of corrosion and inhibition effectiveness

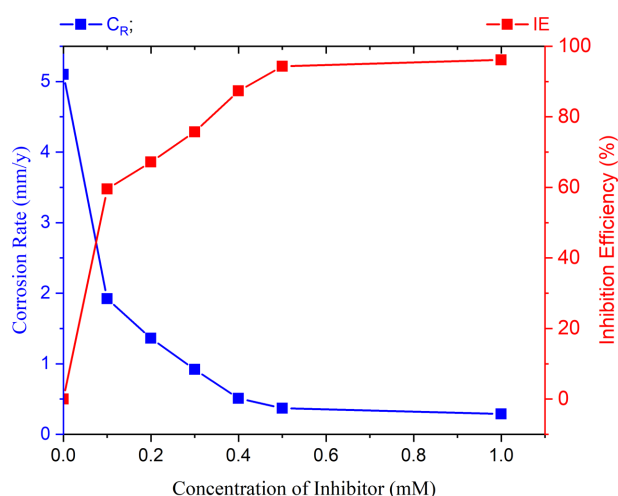


Fig. 2. Impact of Inhibitor Concentration on Corrosion Rates and Inhibition Efficiency in Hydrochloric Acid Solutions after 5 Hours at 25 °C

are presented in Fig. 2. The results show that the inhibitor's ability to prevent corrosion increases with concentration up to 0.5 mM. This can be attributed to a higher concentration of PPDA molecules binding to the mild steel surface, creating a protective layer that increases inhibition effectiveness [34]. However, at concentrations exceeding 0.5 mM, the PPDA molecules start to desorb from the mild steel surface, reducing the effectiveness of the protection.

#### 3.2 Exposure periods effect

The impact of exposure duration on the corrosion inhibition efficiency of a metallic substrate in a corrosive solution was investigated in this study. The corrosion experiments were carried out by immersing mild steel samples in a hydrochloric acid solution containing different concentrations of the inhibitor for various immersion periods (1, 5, 10, 24, and 48 hours) at a temperature of 25 °C. The obtained results depicted in Fig. 3 demonstrate that the inhibition efficiency rises substantially as the immersion duration increases up to 5 hours, and gradually increases up to 24 hours, followed by a reduction in protective performance. After 48 hours, the inhibition efficiency stabilizes. The increase in inhibition efficiency is attributed to the larger number of inhibitor molecules attaching to the mild steel surface, resulting in the formation of a protective layer. This interaction allows the van der Waals force to interact with

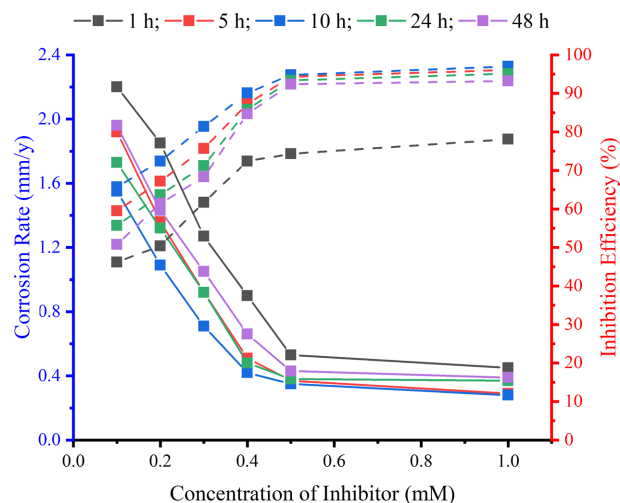
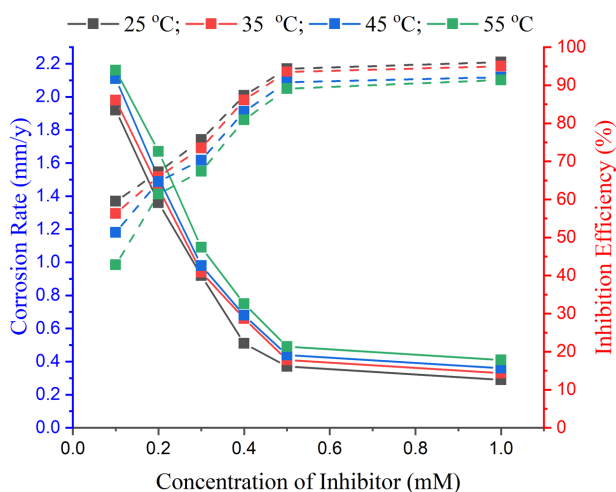


Fig. 3. Influence of Immersion Time on Corrosion Rates and Inhibition Efficiency in Hydrochloric Acid Solutions with and without Inhibitor at 25 °C

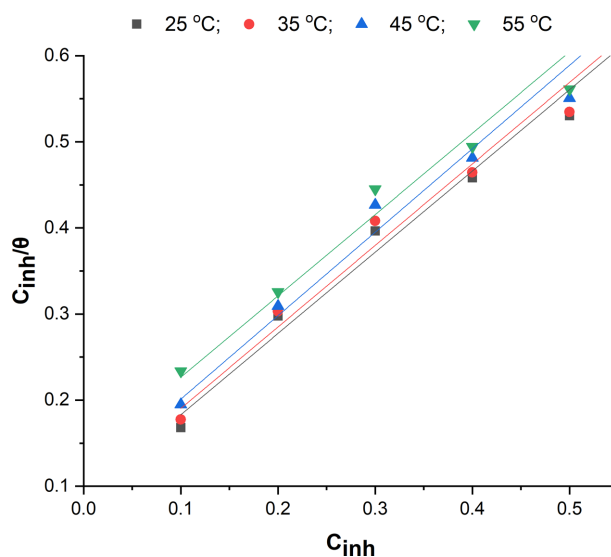


**Fig. 4. Comparative Analysis of Corrosion Rates and Inhibition Efficiency in Hydrochloric Acid Solutions with and without Inhibitor for a 5-hour Immersion Period at Various Temperatures**

the inhibitor molecules. Although some inhibitor molecules may leave the surface, reducing the active area that the inhibitor covers and its effectiveness, the high inhibition efficiency observed during a longer exposure duration demonstrates the stability of the adsorbed inhibitor layer in the corrosive solution [35,36].

### 3.3 Temperature effects

The effectiveness of PPDA in reducing weight loss and activation variables were calculated through weight loss experiments performed at different temperatures (25, 35, 45, and 55 °C) [37]. Fig. 4 illustrates that increasing temperature leads to a slightly higher corrosion rate of the metallic substrate in inhibited and uninhibited solutions, likely due to increased thermal agitation of PPDA particles in the corrosive environment at higher temperatures, resulting in higher conductivity and acidic activity of the solution. As a result, inhibition efficiency decreases with increasing temperature, leading to an increase in the corrosion rate [38]. At 25 °C in a 1 M HCl medium, an inhibitor concentration of 0.5 mM exhibited an inhibition efficiency of 94.3%, indicating a new inhibitor suitable for hydrochloric acid solution that has not been previously reported. This inhibitor performed better than previously reported inhibitors, highlighting the importance of maintaining protection performance at high temperatures, as downhole temperatures are typically high in the petroleum sector [39].



**Fig. 5. Langmuir model plot**

### 3.4 Adsorption isotherm

Chemical inhibitors function by adsorbing inhibitor molecules onto the metal surface. To understand this adsorption process, three adsorption isotherms (Frumkin, Temkin, and Langmuir) were studied to calculate the percentage of surface coverage. Among these isotherms, the Langmuir isotherm was deemed the most suitable, given its high regression coefficient ( $R^2$ ) value close to unity and straight line, as demonstrated in Fig. 5. Equation (11) is commonly used to represent the Langmuir adsorption isotherm [40]:

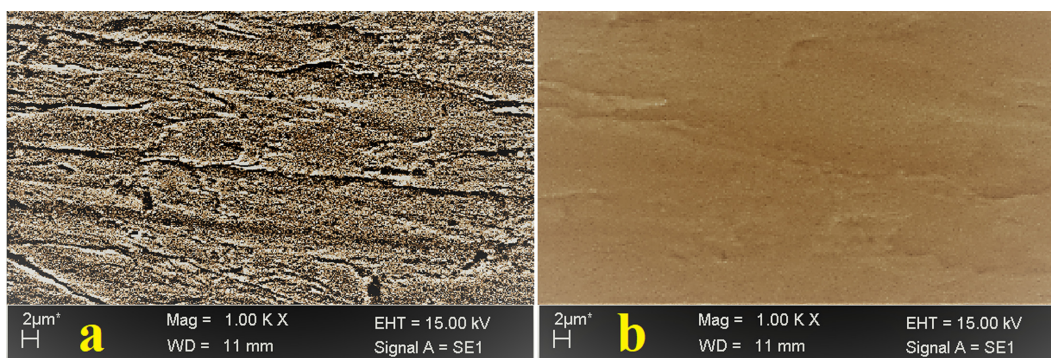
$$C_{inh}/\theta = (K_{ads})^{-1} + C \quad (11)$$

where  $K_{ads}$  is the constant of adsorption and  $\theta$  is the surface coverage.

Fig. 5 displays the adsorption isotherm of the tested inhibitor, and the Langmuir model was found to be the most appropriate option among the analyzed isotherms. The equation commonly used to represent the Langmuir adsorption isotherm is equation (11) [41]. The  $K_{ads}$  value of the tested inhibitor, which signifies the extent of inhibitor adsorption on the mild steel surface, is summarized in Table 1. A higher  $K_{ads}$  value represents stronger adsorption and better corrosion inhibition performance. The tested inhibitor has the highest  $K_{ads}$  value, indicating the highest adsorption on the mild steel surface. Equation (12) can be employed to calculate the

**Table 1. The thermodynamic parameters computed based on weight loss measurements at different temperatures**

Parameters	25 °C	35 °C	45 °C	55 °C
Intercept	0.088 ± 0.017	0.095 ± 0.018	0.104 ± 0.019	0.132 ± 0.020
Slope	0.943 ± 0.033	0.94689 ± 0.036	0.969 ± 0.037	0.944 ± 0.040
R-Square	0.9949	0.9941	0.9939	0.9926



**Fig. 6. Scanning Electron Microscopy (SEM) Exploration, (a) Mild steel surface in absence of PPDAA, and (b) Mild steel surface in presence of PPDAA**

standard free energy of adsorption ( $\Delta G_{ads}^{\circ}$ ) utilizing  $K_{ads}$  values [42].

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

Table 1 presents the calculated thermodynamic parameters based on weight loss measurements at different temperatures. The negative values of  $\Delta G_{ads}^{\circ}$  indicate a spontaneous adsorption process resulting in a stable layer of inhibitor molecules on the mild steel surface.

The strength of the adsorption process is often described by the value of  $\Delta G_{ads}^{\circ}$ , where values less than  $-20 \text{ kJ}\cdot\text{mole}^{-1}$  typically signify Van der Waals forces, while more negative values than  $-40 \text{ kJ}\cdot\text{mole}^{-1}$  suggest chemisorption. In chemisorption, unpaired electrons from the inhibitor molecule's heteroatoms transfer to the metallic surface's iron atom d-orbitals, resulting in coordination bonds. Our results showed that both physisorption and chemisorption mechanisms occurred in this study, with  $\Delta G_{ads}^{\circ}$  values ranging from  $-33.5$  to  $-36.3 \text{ kJ}\cdot\text{mole}^{-1}$ . Chemisorbed molecules are expected to provide better protection by reducing reactivity at the linked spots on the metal surface. It is challenging to differentiate between chemisorption and physisorption solely based on  $\Delta G_{ads}^{\circ}$  values, as there is some overlap between the two mechanisms, and physical

adsorption is believed to occur before chemical adsorption [43].

### 3.5 SEM

A probing inquiry into the intricate interaction between mild steel and its corrosive environment necessitates the lens of Scanning Electron Microscopy (SEM) analysis. In this endeavor, the surface morphology of mild steel, following a 3-hour immersion in 1.0 M HCl, unfolds as a pivotal narrative, artfully documented in Fig. 6. This journey of observation gains even more significance as it unfolds in the dual presence and absence of 0.5 mM PPDAA. In the absence of the protective embrace offered by 0.5 mM PPDAA, the surface of mild steel reveals the consequences of vulnerability. Here, the ravages of a high dissolution rate of iron, characteristic of this pH, manifest in the form of a damaged terrain. The magnified view casts light upon the pronounced deterioration of the surface – a visual testimony to the relentless attack of the corrosive environment (Fig. 6a). However, the narrative shifts when 0.5 mM PPDAA enters the equation. A transformation transpires, akin to the unfolding of a protective tapestry. The eyes discern a thin and uniform layer draping the metallic landscape. This visual spectacle bears the imprints of PPDAA's presence, serving as a testament to its role in orchestrating the symphony of



corrosion inhibition (Fig. 6b). The discerning eye might catch the presence of delicate cracks woven within the protective film. These fault lines emerge as a consequence of surface dehydration – a requisite step prior to SEM imaging. These cracks, while artifacts of the imaging process, underline the dynamic interplay between the experimental setup and the visualization tool. Each artifact underscores the intricate choreography that guides scientific observation. In the symphony of observations, a resounding note echoes – a note that serves as evidence of PPDAA's role in the narrative (Fig. 6b). The thin and uniform layer, meticulously imprinted upon the metallic surface, emerges as a testament to PPDAA's capacity to orchestrate a protective embrace. It is a shield that insulates the surface from the acidic medium's tenacious advances. The visual panorama encapsulates

the very essence of PPDAA's role – an agent of defense, a custodian of the surface, and a bulwark against the corrosive tempest.

In sum, the Scanning Electron Microscopy (SEM) analysis unfolds as more than an observation; it is a visual testament to the story of corrosion, inhibition, and resilience. Each detail inscribed upon the imagery serves as a fragment in the larger narrative of understanding – a narrative that transcends the visual and delves into the heart of scientific exploration.

### 3.6 DFT

The use of quantum chemical techniques can provide important insights into the structural properties of PPDAA molecules and various thermodynamic parameters. By examining Gaussian records at B3LYP/6-311G (d,p), such parameters can be determined based on the structural

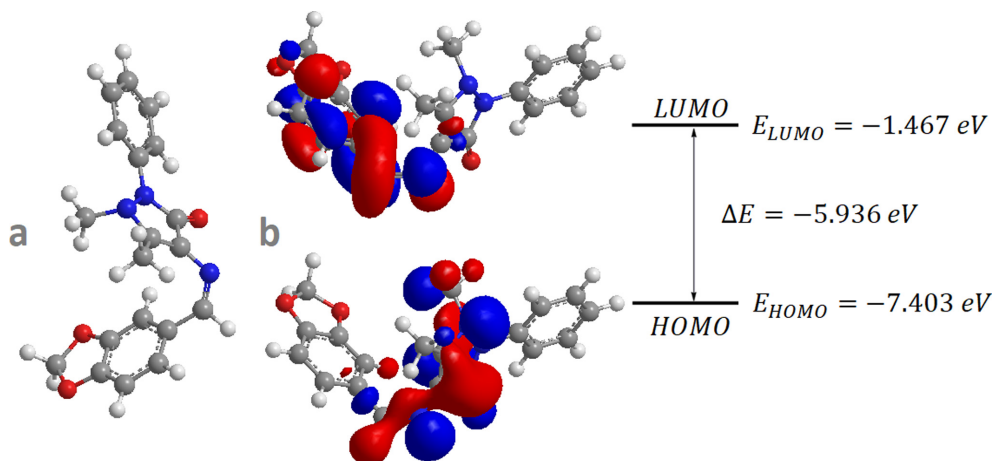


Fig. 7. (a) Optimized structure and (b) Energy gap plot of PPDAA

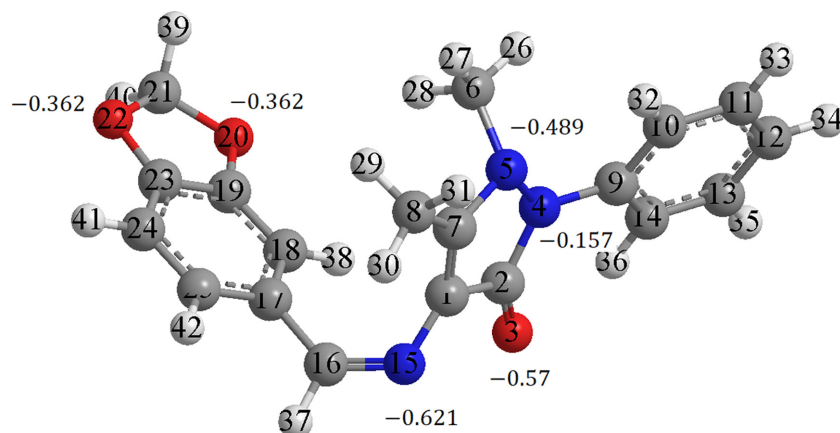


Fig. 8. Mulliken charges of PPDAA

**Table 2. DFT variables for PPDAA molecules in gas phase**

I (eV)	A (eV)	$E_{HOMO}$ (eV)	$E_{LUMO}$ (eV)	$\Delta E$ (eV)	$\chi$ (eV)	$\eta$ (eV)	$\sigma$ (eV <sup>-1</sup> )	$\Delta N$ (eV)
7.403	1.476	-7.403	-1.476	-5.936	4.435	2.968	0.3369	0.432

parameters of PPDAA [44]. Fig. 7 shows an example of the type of information that can be obtained.

Mulliken charges are often used to identify inhibitor adsorption sites. In PPDAA, the oxygen and nitrogen atoms with negative charges are favored adsorption locations due to their donor-acceptor interactions with metal surfaces, as shown in Fig. 8. The benzene ring in PPDAA molecules also facilitates the formation of complexations between the adsorbate and surface coordination bonds [45-47]. The highest occupied molecular orbital (HOMO) indicates the site for electron donation in the molecule, and for PPDAA, the HOMO reveals that the O and N atoms can transfer electrons to the metallic substrate. In contrast, the lowest unoccupied molecular orbital (LUMO) indicates the molecule's ability to accept electrons, and Fig. 8 shows that the N, O, and C atoms in PPDAA are the most reactive LUMO locations [48,49].

The quantum chemical technique can provide valuable information on the structural characteristics of PPDAA molecules, including various thermodynamic parameters. Gaussian records at B3LYP/6-311G (d,p) can be used to determine such parameters based on the structural parameters of PPDAA, as illustrated in Fig. 7. Table 2 summarizes the computed quantum chemical parameters, such as  $E_{HOMO}$ ,  $E_{LUMO}$ ,  $\Delta E$ , electronegativity ( $\chi$ ), softness ( $\sigma$ ), hardness ( $\eta$ ), and the number of electrons transported ( $\Delta N$ ). A molecule with a higher  $E_{HOMO}$  value can donate electrons more easily, while a smaller  $E_{LUMO}$  value indicates a molecule's ability to accept electrons. A good corrosion inhibitor should have low values of  $\Delta E$  but high values of  $\sigma$ . PPDAA has a low  $E_{HOMO}$  value, indicating its ability to donate electrons, and a high  $\Delta N$  value, indicating better electron exchange ability [50]. The calculated values in Table 2 suggest that PPDAA is an effective corrosion inhibitor, and there is good agreement between the test results and the quantum chemical parameters. When a metal shares electrons with the inhibitor (back donation), it establishes contact between the metal surfaces and the inhibitor.

### 3.7 Suggested mechanism

The adsorption mechanism of organic inhibitors onto metallic substrates is governed by a multitude of factors, including the inhibitor's chemical composition, metal type, surface charge, and distribution of charges within the inhibitor molecule. Various interaction modes, such as electrostatic interactions, unshared electron pairs interaction, and p-electron interactions, or their combinations, can play crucial roles in this process. The intricate mechanism through which inhibitors like 4-(Piperonylideneamino)antipyrine (PPDAA) interact with metallic surfaces encompasses several key aspects. PPDAA's structure is replete with contributing elements such as nitrogen and oxygen atoms, heterocyclic rings, and benzene rings, all of which collectively contribute to its remarkable inhibitory effectiveness. Specifically, the unpaired electron pairs associated with nitrogen and oxygen atoms serve as potential coordinating centers [51]. In the context of acidic environments, PPDAA primarily exists as protonated molecules when interacting with uncharged particles. The adsorption of inhibitor particles onto metallic surfaces is a complex process that involves multiple facets. These include interactions between donor and acceptor  $\pi$ -bonds and unoccupied iron d-orbitals, electrostatic interactions, and the interplay between unoccupied iron d-orbitals and the unpaired electrons of nitrogen and oxygen atoms. In scenarios where positively charged ion particles face challenges in reaching positively charged mild steel surfaces due to repulsion, protonated inhibitor molecules can still be effectively adsorbed through electrostatic interactions. Notably, inhibitor ions, exemplified by protonated inhibitor molecules, can interact with negatively charged chloride ions present on steel surfaces. This interaction results in chloride hydration and a favorable shift in charge, accentuating the positive charge of inhibitor ions. However, it is important to acknowledge the complexity of the adsorption process. No singular mechanism suffices to entirely explain the intricate interplay between inhibitor molecules and metallic substrates within corrosive



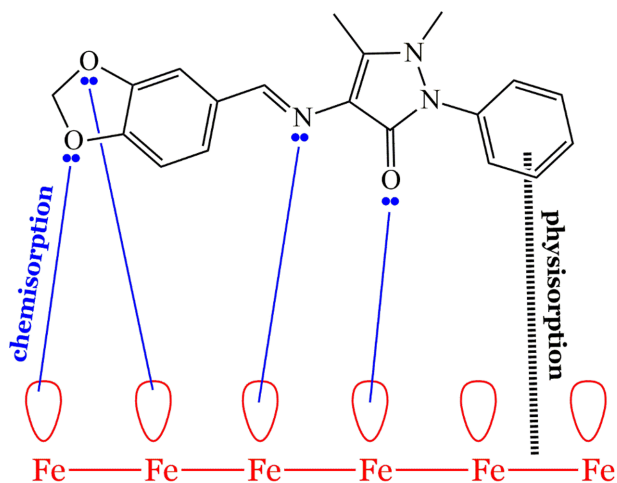


Fig. 9. Schematic Depiction of Potential Adsorption Mechanisms

environments. Rather, as illustrated in Fig. 9, a range of mechanisms may synergistically contribute to elucidating the nuanced process of inhibitor molecule adsorption onto metallic substrates. The interplay of these mechanisms unveils the intricate dance between inhibitors and metal surfaces in environments fraught with corrosive challenges.

#### 4. Conclusion: Embracing the Promise and Complexity of Corrosion Inhibition

The journey undertaken in this study has ushered us into the intricate realm of corrosion inhibition, with a keen focus on 4-piperonylideneaminoantipyrine's potential as a defender of mild steel within hydrochloric acid (HCl) solution. Our exploration unveils a landscape of discoveries that underscore both affirmative outcomes and prudent considerations. The heart of our study lies in unraveling the potency of 4-piperonylideneaminoantipyrine as a corrosion inhibitor. A resounding testament to its prowess is the resplendent corrosion inhibition efficiency of 94.3% achieved at a 0.5 mM concentration over a 5-hour immersion span. This accomplishment magnifies its potential as a robust sentinel, steadfastly guarding mild steel against the relentless march of corrosion.

Our exploration extends beyond empirical findings, delving into the very fabric of the inhibitor's behavior. Molecular structures and electronic properties are illuminated through the meticulous lens of Density

Functional Theory (DFT) calculations. These calculations paint a vivid portrait, revealing that the inhibitor's nitrogen and oxygen atoms orchestrate an adhesion symphony on the mild steel's surface. This virtuoso performance culminates in the creation of a protective shield, thwarting the corrosive ambitions of HCl. This intimate interplay between theory and experiment augments our understanding of corrosion inhibition mechanisms, breathing life into the intricate dance between inhibitor and metal. Our findings echo with the resonance of promise – a promise that 4-piperonylideneaminoantipyrine holds as a prospective corrosion inhibitor. Its robust corrosion inhibition efficiency and the elucidation of its molecular interactions on metallic surfaces underscore its potential significance within corrosion prevention strategies. Yet, the path from scientific discovery to practical implementation is threaded with due diligence.

While we bask in the glow of accomplishment, it is essential to embrace the comprehensive perspective that science mandates. Our study stands not only as a banner of success but also as a canvas of potential limitations. We must temper our enthusiasm with a recognition of the variables that remain unexplored – pH nuances, and intricate real-world interactions. This acknowledgement fosters an environment of balanced progress, where each step forward is accompanied by a cautious glance around. As we look ahead, the envisioned path carves a trajectory marked by rigorous validation and comprehensive simulations. The transition from the controlled laboratory environment to the dynamic real-world stage demands meticulous testing under diverse conditions. Only through these diligent endeavors can we confidently advance towards harnessing 4-piperonylideneaminoantipyrine's potential as a corrosion inhibitor.

In summation, the voyage embarked upon in this study intertwines the beauty of discovery with the humility of exploration. The high corrosion inhibition efficiency of 4-piperonylideneaminoantipyrine beckons as a beacon of hope for corrosion mitigation. Yet, this hope is accompanied by a clarion call for continued research, validation, and circumspect implementation. With every conclusion drawn, we set a compass for future investigations – a compass that aligns both aspirations and limitations, paving the way for corrosion prevention strategies that are as robust as they are informed.

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