

## Corrosion Inhibition of Mild Steel in HCl Solution by 2-acetylpyrazine: Weight Loss and DFT Studies on Immersion Time and Temperature Effects

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### ARTICLE INFO

Article history:

Received: 25 Nov 2023

Final Revised: 15 Jan 2024

Accepted: 15 Jan 2024

Available online: 11 Mar 2024

Keywords:

Corrosion inhibition

Mild steel

Hydrochloric acid

2-acetylpyrazine

DFT

### ABSTRACT

*This study systematically explores the corrosion inhibition potential of 2-acetylpyrazine for mild steel in a hydrochloric acid (HCl) solution, employing a comprehensive approach that integrates experimental weight loss measurements and Density Functional Theory (DFT) calculations. Investigating inhibitory performance across varying immersion times, inhibitor concentrations, and temperatures, our research aims to elucidate the corrosion inhibition mechanism. Numerical findings highlight a substantial inhibitory efficiency of 92.7 % at an inhibitor concentration of 0.5 mM, an immersion time of 5 hours, and a temperature of 303 K. Remarkably, the efficiency increases to 98.1 % after extending the immersion time to 48 hours at 303 K with the same inhibitor concentration. Furthermore, we demonstrate the temperature's impact on inhibition efficiency, reaching 97.3 % at 333 K with an immersion time of 5 hours and an inhibitor concentration of 0.5 mM. The Langmuir model, applied to adsorption isotherms, provides valuable insights into the adsorption behavior of 2-acetylpyrazine on mild steel surfaces. Additionally, scanning electron microscope (SEM) results indicate the formation of a protective film on the steel surface in the presence of the studied inhibitors. This combined experimental and computational approach not only enhances our comprehension of the corrosion inhibition mechanism but also emphasizes the practical viability of 2-acetylpyrazine as an effective and temperature-sensitive inhibitor in HCl environments. These findings contribute significantly to advancing corrosion mitigation strategies with potential implications for industrial applications. Prog. Color Colorants Coat. 17 (2024), 333-350 © Institute for Color Science and Technology.*

### 1. Introduction

Corrosion stands as a pervasive challenge across diverse industrial sectors, jeopardizing the structural integrity

and lifespan of metallic components and structures [1-4]. Among the materials susceptible to corrosion, mild steel faces particular vulnerability due to its extensive use in

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<https://doi.org/10.30509/pccc.2024.167231.1261>

various industrial applications [5-9]. The prevalent use of hydrochloric acid (HCl) in many industrial environments compounds the degradation of mild steel surfaces, intensifying the corrosive impact [10-13]. In the pursuit of robust corrosion mitigation strategies, organic inhibitors have emerged as promising solutions, especially those featuring heteroatoms within their molecular structures [14-17]. Hydrochloric acid finds extensive application in industries such as chemical processing, metal cleaning, and acid pickling, playing a pivotal role in various processes [18, 19]. However, the aggressive nature of HCl towards metals, notably mild steel, underscores the imperative for the development of effective corrosion inhibition techniques [20]. Inorganic inhibitors, while possessing certain merits, exhibit notable disadvantages [21-23]. These inhibitors, often metal-based, can be prone to precipitation and can introduce undesirable ions into the system, potentially causing secondary issues. Additionally, their effectiveness may be compromised under fluctuating environmental conditions [24]. This prompts the exploration of organic inhibitors, a class gaining prominence due to its distinct advantages. Organic inhibitors, particularly those incorporating heteroatoms in their molecular structures, have demonstrated remarkable corrosion inhibiting properties [25, 26]. The inclusion of heteroatoms, such as nitrogen and oxygen, enhances the inhibitor's electron density and facilitates stronger interactions with metal surfaces. Organic inhibitors, in contrast to their inorganic counterparts, are often more stable and effective under diverse environmental conditions [27, 28]. The presence of heteroatoms in organic inhibitors contributes significantly to their inhibitory performance. These heteroatoms influence the electronic structure of the inhibitor, affecting its electron-donating or accepting capabilities [29, 30]. Furthermore, molecules with double bonds and resonance structures enhance the stability of the inhibitor on the metal surface. The conjugation and delocalization of electrons in such systems contribute to a more robust protective layer, thus improving inhibition efficiency [31-36].

In recent years, the adoption of Density Functional Theory (DFT) has gained prominence in corrosion inhibition research [37-39]. Offering a robust theoretical framework, DFT facilitates an in-depth exploration of the electronic structure and properties of molecules, enabling a comprehensive investigation into the interactions between inhibitors and metal surfaces. This

computational approach has proven invaluable in predicting and elucidating the inhibitory performance of organic compounds, guiding experimental studies toward more effective corrosion inhibitors. This research endeavors to explore the corrosion inhibiting capabilities of 2-acetylpyrazine, an organic compound with heteroatoms, for mild steel in HCl solution. By combining experimental weight loss measurements and DFT studies, our goal is to unravel the intricate interplay between the inhibitor and the metal surface [40, 41]. The study encompasses a systematic investigation of immersion time, inhibitor concentration, and temperature effects to comprehensively evaluate the performance of 2-acetylpyrazine (Figure 1) as a corrosion inhibitor. The utilization of adsorption isotherms, with a specific focus on the Langmuir model, enhances our understanding of the adsorption behavior and efficiency of the inhibitor. The novelty of this work lies in its holistic approach, bridging experimental and computational methodologies to gain deeper insights into the corrosion inhibition mechanism of 2-acetylpyrazine under industrially relevant conditions. This research not only contributes to the fundamental understanding of corrosion processes but also holds practical implications for the development of effective and sustainable corrosion inhibition strategies in industrial applications.

## 2. Experimental

### 2.1. Materials and reagents

All materials and reagents utilized in this investigation were procured from Sigma-Aldrich/Malaysia. A 1 M HCl solution served as the corrosive medium for the experiments. The inhibitor, 2-acetylpyrazine, was employed at concentrations ranging from 0.1 to 1.0 mM. Mild steel samples, characterized by their chemical composition through X-ray fluorescence spectrometry, were employed for corrosion studies. Silicon carbide served as the abrasive material for sample preparation.

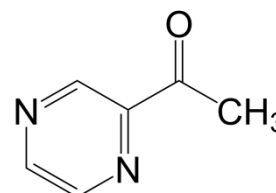


Figure 1: Chemical structure of 2-acetylpyrazine.

## 2.2. Sample preparation

Mild steel samples were prepared following the ASTM G1-03 protocol [42, 43]. Prior to immersion in the corrosive environment, samples underwent mechanical polishing to achieve a smooth finish using silicon carbide abrasive paper. Subsequently, samples were cleansed with double-distilled water and acetone to eliminate surface contaminants before thorough drying.

## 2.3. Weight loss measurements

Weight loss measurements were conducted to assess the corrosion rate of mild steel in the presence of 2-acetylpyrazine. Prepared mild steel samples were immersed in a 1 M HCl solution containing varying inhibitor concentrations (0.1, 0.2, 0.3, 0.4, 0.5, and 1 mM). Experiments were executed at different time intervals (1, 5, 10, 24, and 48 hours) and temperatures (303, 313, 323, and 333 K), adhering to the NACE TM0169/G31 protocol. The corrosion rate ( $C_R$ ) was calculated using equation 1 [43, 44]:

$$C_R = W/adt \quad (1)$$

where  $W$  represents the weight loss of the mild steel sample,  $a$  is the sample area,  $d$  is the density of mild steel, and  $t$  is the immersion time.

The inhibition efficiency (IE %) was determined using equation 2:

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

where  $C_{R(i)}$  is the corrosion rate in the presence of the inhibitor, and  $C_{R_0}$  is the corrosion rate in the absence of the inhibitor. The degree of surface coverage ( $\theta$ ) due to inhibitor adsorption was calculated using equation 3 [42-45]:

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

## 2.4. Density functional theory (DFT)

Density Functional Theory (DFT) calculations were conducted using Gaussian 09 software [46]. The B3LYP method with the "6-31G++(d,p)" basis set was employed to explore the molecular interactions between 2-acetylpyrazine and the mild steel surface. Koopmans theory [47] was utilized to estimate the energy of the Highest Occupied Molecular Orbital ( $E_{HOMO}$ ) and the Lowest Unoccupied Molecular Orbital ( $E_{LUMO}$ ). Electronegativity ( $\chi$ ) and chemical hardness

( $\eta$ ) were calculated using equations 4 and 5:

$$\chi = \frac{I+A}{2} \quad (4)$$

$$\eta = \frac{I-A}{2} \quad (5)$$

The softness ( $\sigma$ ) was obtained by taking the reciprocal of the chemical hardness as shown in equation 6:

$$(\sigma = \frac{1}{\eta}) \quad (6)$$

Additionally, the charge transfer ( $\Delta N$ ) between the mild steel surface and the inhibitor was determined using equation 7 [47]:

$$\Delta N = (\chi_{Fe} - \chi_{inh}) / 2(\eta_{Fe} + \eta_{inh}) \quad (7)$$

For the special case of metals where  $\eta_{Fe}$  is significantly larger than  $\eta_{inh}$ , equation 8 was applied:

$$\Delta N = \frac{7 - \chi_{inh}}{2(\eta_{inh})} \quad (8)$$

## 2.5. Adsorption isotherm studies

Adsorption isotherm studies were conducted to elucidate the adsorption behavior of 2-acetylpyrazine on the mild steel surface. These isotherms were constructed by plotting the degree of surface coverage ( $\theta$ ) against the inhibitor concentration [48, 49].

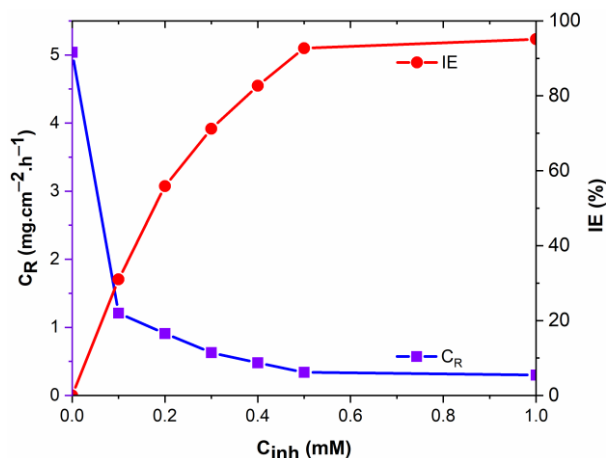
## 3. Results and Discussion

### 3.1. Weight loss measurements

The investigation into the corrosion inhibition properties of 2-acetylpyrazine for mild steel in HCl solution commenced with a thorough examination of weight loss measurements. These measurements provided crucial insights into the corrosion rate and inhibition efficiency under varying concentrations, immersion times, and temperatures.

#### 3.1.1. Effect of inhibitor concentration

The corrosion rate and inhibition efficiency of mild steel in the presence of 2-acetylpyrazine were assessed through weight loss measurements, offering crucial insights into the inhibitor's performance at various concentrations. Figure 2 portrays the corrosion rate and inhibition effectiveness during a 5-hour immersion period. The results showcase a noteworthy escalation in inhibition efficiency with increasing inhibitor concentration. At the optimum concentration of 0.5 mM,



**Figure 2:**  $C_R$  and IE % of mild steel in HCl with and without the inhibitor after a 5-hour immersion period at 303 K.

2-acetylpyrazine demonstrated the highest inhibition efficiency of 92.7 %, indicating its robust corrosion inhibitory properties. This phenomenon is attributed to the formation of a protective layer on the metal surface, which becomes more substantial and effective with higher inhibitor concentrations [50-53]. The protective layer acts as a barrier, impeding direct contact between the metal surface and the corrosive environment, resulting in a deceleration of the corrosion process. Notably, the concentration of 0.5 mM was identified as optimal for establishing a resilient protective layer on the mild steel surface [54]. However, it is crucial to consider that excessively high inhibitor concentrations may lead to saturation of adsorption sites on the metal surface, potentially limiting further adsorption and yielding diminishing returns in inhibition efficiency beyond a certain point [55]. Moreover, the protective layer formed is not permanent, undergoing desorption over time and reducing inhibition efficiency.

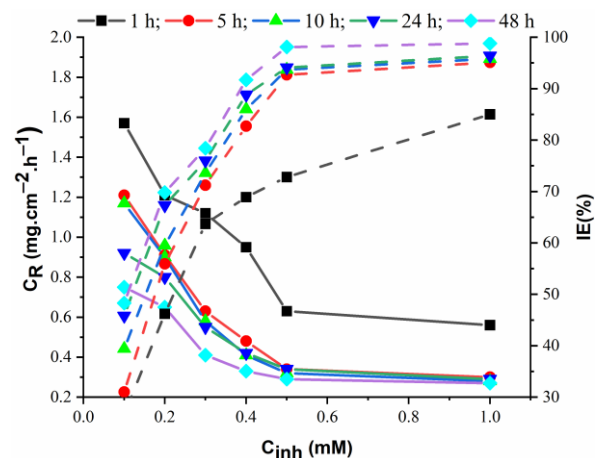
### 3.1.2. Effect of immersion periods

To explore the impact of immersion duration on corrosion inhibition, weight loss measurements were conducted at varying time intervals (1, 5, 10, 24, and 48 hours) at a constant temperature of 303 K. Figure 3 illustrates a substantial increase in inhibition efficiency within the initial 5 hours of immersion, reaching a peak of 98.1 % at 48 hours. This escalation suggests that 2-acetylpyrazine efficiently forms a protective layer during the initial immersion, hindering corrosive agents and retarding the corrosion process [56, 57]. Extended immersion durations allow for additional adsorption and

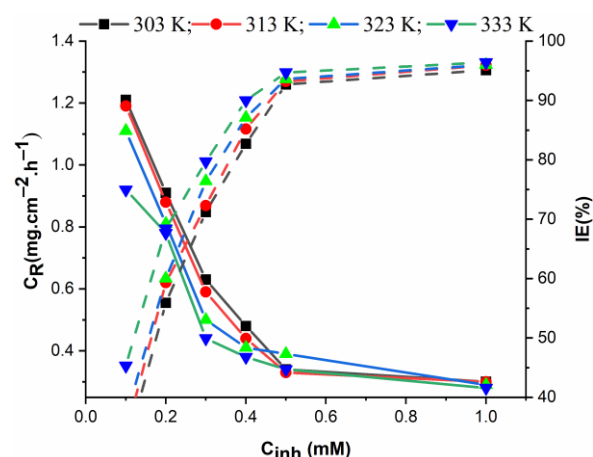
organization of inhibitor molecules on the mild steel surface, enhancing the protective layer's integrity. The observed time-dependent effectiveness underscores the significance of adequate immersion periods in establishing a robust protective layer, critical for prolonged corrosion protection in acidic environments [58-62].

### 3.1.3. Effect of temperatures

To examine the influence of temperature on corrosion inhibition, weight loss measurements were conducted at temperatures ranging from 303 to 333 K, maintaining an inhibitor concentration of 0.5 mM. Figure 4 reveals an increase in inhibition efficiency with rising temperature, reaching 97.3 % at 333 K. At lower temperatures (303 K), the inhibitor demonstrated significant efficiency, which further improved with elevated temperatures.



**Figure 3:** A comparison of  $C_R$  and IE % in hydrochloric acid solutions with and without the inhibitor for 1, 5, 10, 24, and 48 h immersion time at different temperatures.



**Figure 4:** Comparison of  $C_R$  and IE% in hydrochloric acid solution with and without the inhibitor during a 5-hour immersion at various temperature.

The temperature-dependent behavior can be attributed to the phenomenon of enhanced molecular activity and increased collision frequency at higher temperatures [63-65]. As the temperature rises, the kinetic energy of the molecules in the solution increases, leading to more vigorous interactions between the inhibitor molecules and the mild steel surface. This heightened activity facilitates greater adsorption of inhibitor molecules onto the metal surface, forming a more robust protective layer [66-69]. Additionally, the accelerated molecular movement disrupts the diffusion of corrosive species towards the metal surface, further contributing to the increased inhibition efficiency at elevated temperatures. Moreover, at higher temperatures, the thermodynamic aspects of the adsorption process become more favorable. The increased temperature provides additional thermal energy, enabling the inhibitor molecules to overcome activation barriers and adsorb onto the metal surface more effectively. This results in a more stable and organized protective layer, leading to a higher inhibition efficiency [70-74].

In summary, the weight loss measurements provide valuable insights into the temperature-dependent behavior of 2-acetylpyrazine as a corrosion inhibitor for mild steel in HCl solution, emphasizing the increased effectiveness at elevated temperatures [75-77]. The observed temperature dependence underscores the importance of considering the operational temperature conditions in real-world applications, where fluctuations may impact the inhibitor's performance. This temperature sensitivity enhances the practical utility of 2-acetylpyrazine as a corrosion inhibitor, showcasing its potential for effective corrosion protection in environments characterized by varying temperature conditions. Further studies could delve into the molecular mechanisms underlying the temperature-dependent behavior, providing a more comprehensive understanding of the corrosion inhibition process [78-82].

### 3.2. Adsorption isotherm analysis

Adsorption isotherm analysis was conducted to unravel the adsorption behavior of 2-acetylpyrazine on the mild steel surface. Among the diverse adsorption isotherms considered, the Langmuir isotherm emerged as the most fitting model for elucidating the inhibitor's adsorption process. The Langmuir isotherm assumes homogeneous surface adsorption with uniform adsorption sites, and its equation (equation 9) is given

by [83, 84]:

$$C_{inh}/\theta = (K_{ads})^{-1} + C \quad (9)$$

Where  $C_{inh}$  is the concentration of the inhibitor,  $\theta$  is the degree of surface coverage,  $K_{ads}$  is the adsorption equilibrium constant, and  $C$  is a constant linked to inhibitor-adsorbent interactions.

The experimental data were fitted to the Langmuir equation (Figure 5), and the obtained correlation coefficient (R2) value approached 1. This high R2 value underscores the excellent fit between the experimental data and the Langmuir model, affirming the accuracy of the Langmuir isotherm in describing inhibitor adsorption on the mild steel surface [85]. To comprehensively assess the model fits, we have included the R2 values for other adsorption isotherms in Figure 5, highlighting the superiority of the Langmuir model.

Based on the R2 values, it is evident that the Langmuir adsorption isotherm provides the best fit for our data, indicating its supremacy in describing the adsorption behavior of 2-acetylpyrazine on the mild steel surface. The slope value of the Langmuir plot and the intercept value elucidate the adsorption characteristics. The slope represents the adsorption equilibrium constant ( $K_{ads}$ ), signifying the affinity of the inhibitor for the metal surface. A higher  $K_{ads}$  value suggests stronger adsorption and a more stable inhibitor-metal surface interaction. The intercept value corresponds to the constant  $C$ , related to inhibitor-adsorbent interactions.

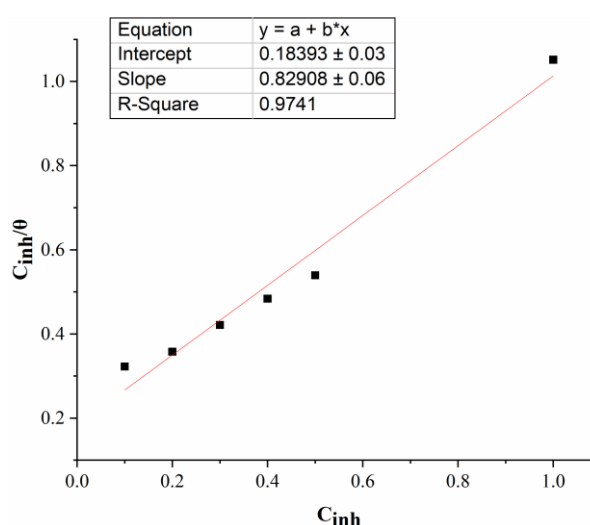


Figure 5: Langmuir adsorption isotherm model.



A non-zero intercept implies limited adsorption at very low inhibitor concentrations, likely due to the availability of only a restricted number of adsorption sites [86-88]. The Langmuir isotherm analysis provides insights into the thermodynamics of inhibitor adsorption. The calculated standard free energy of adsorption ( $\Delta G_{ads}^o$ ) (equation 10) ranged from  $-38.15 \text{ kJ}\cdot\text{mol}^{-1}$ , indicating a spontaneous and favorable adsorption process.

$$\Delta G_{ads}^o = -RT \ln(55.5K_{ads}) \quad (10)$$

Where R is the universal gas constant, T is the absolute temperature, and  $\ln$  is the natural logarithm [89].

The calculated  $\Delta G_{ads}^o$  values align with literature reports [90-93] for the adsorption process of the inhibitor "2-acetylpyrazine" on the mild steel surface, suggesting a thermodynamically favorable and spontaneous adsorption. The negative  $\Delta G_{ads}^o$  indicates an exothermic process, releasing energy upon adsorption, driven by attractive interactions between the inhibitor molecules and the metal surface. The calculated  $\Delta G_{ads}^o$  value of  $-38.15 \text{ KJ}\cdot\text{mol}^{-1}$  falls within the range reported for chemisorption processes, indicating robust and stable interactions between the inhibitor and the metal surface. However, considering the broader range of  $-40$  to  $-20 \text{ KJ}\cdot\text{mol}^{-1}$  that includes values for physisorption, it is plausible that the adsorption of "2-acetylpyrazine" on the mild steel surface involves a combination of both physisorption and chemisorption mechanisms [94-97]. This nuanced understanding of the adsorption process enriches our comprehension of 2-acetylpyrazine's performance as a corrosion inhibitor and opens avenues for further exploration into the intricate interplay

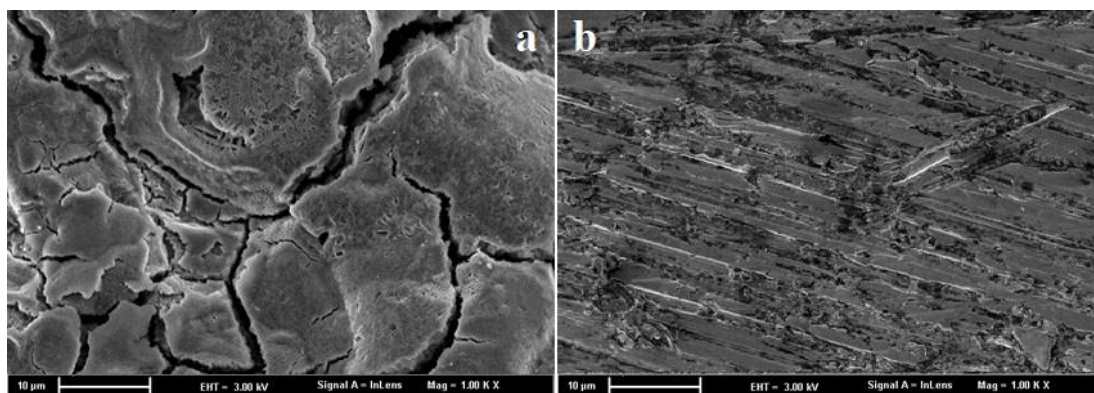
between the inhibitor and the metal surface.

### 3.3. SEM analysis.

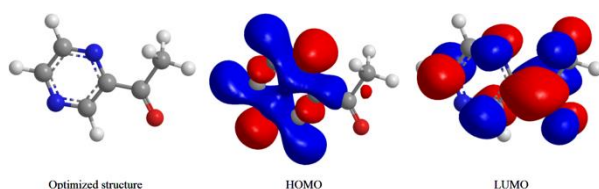
The differences that occur on the tested coupon surface were examined in 1 M HCl in the without and with 2-acetylpyrazine after a 5 h exposure period and are presented in Figures 6 a and 6 b. The coupon surface exposed in the HCl solution without the addition of inhibitor observes obvious corrosion holes on the tested coupon surface owing to generalized corrosion damage affected by the acidic solution. The corrosion damage is seen to be missing from the coupon surface in the presence of 2-acetylpyrazine in the acid solution (Figure 6 b). The tested coupon surface immersed in a corrosive medium with the 2-acetylpyrazine is remarked to be quite similar to that of the polished. This implies that the shielding film of the inhibitor molecules on the steel surface represents a barrier against corrosive solution attack.

### 3.4. DFT

In this quantum chemical analysis at the B3LYP/6-311G(d,p) level, critical parameters were computed for 2-acetylpyrazine molecules in the gas phase. These parameters provide valuable insights into the electronic properties and reactivity of 2-acetylpyrazine as a corrosion inhibitor in the gas phase, enriching our understanding of its corrosion inhibition mechanism and its potential for practical applications in industrial settings [46, 98-100]. The optimized structure and frontier molecular orbitals (MOs) of the 2-acetylpyrazine molecule are illustrated in Figure 7.



**Figure 6:** SEM photographs of low-carbon steel in 1 M HCl solution exposed for 5 h. (a) without inhibitor, (b) with 0.5 mM 2-acetylpyrazine.



**Figure 7:** The optimized structure and frontier MOs of 2-acetylpyrazine molecule.

These numerical values provide a detailed understanding of the electronic structure and reactivity of 2-acetylpyrazine in the gas phase. The energy gap ( $\Delta E$ ) signifies the stability of the molecule, with a value of 1.035 eV indicating a relatively stable structure. The electronegativity ( $\chi$ ) of -5.074 eV suggests a moderate electron-attracting ability. Based on table 1, the softness ( $\sigma$ ) of 0.966 indicates a degree of polarizability in the molecule, and the hardness ( $\eta$ ) of 0.5185 reflects its resistance to charge transfer. The calculated  $\Delta N$  parameter, representing the transferred electrons between the mild steel surface and the inhibitor, is -0.1893. This negative value implies that electrons are transferred from the inhibitor to the metal surface, indicating a charge donation process during the adsorption. These numerical results contribute to a comprehensive understanding of the molecular properties of 2-acetylpyrazine, crucial for elucidating its corrosion inhibition mechanism and potential applications in corrosion protection strategies.

**Table 1:** DFT variables for 2-acetylpyrazine molecules in gas phase.

Parameter	Value (eV)
$E_{\text{HOMO}}$ (Highest Occupied Molecular Orbital Energy)	-5.592
$E_{\text{LUMO}}$ (Lowest Unoccupied Molecular Orbital Energy)	-4.557
$\Delta E$ (Energy Gap)	1.035
Electronegativity ( $\chi$ )	-5.074
Softness ( $\sigma$ )	0.966
Hardness ( $\eta$ )	0.5185
$\Delta N$ (Transferred Electrons)	-0.1893

### 3.5. Mulliken charges

Understanding the interplay between the inhibiting efficiency of a corrosion inhibitor and atomic charges, particularly those derived from quantum chemical calculations like Mulliken charges, is crucial for unraveling the corrosion inhibition mechanism. These charges offer valuable insights into the electron density distribution within a molecule, influencing interactions between inhibitor molecules and the metal surface and, consequently, impacting inhibition efficiency. The following key aspects shed light on this intricate relationship [101, 102].

- 1. Coordination Bonds and Adsorption:** Corrosion inhibitors often establish coordination bonds with metal atoms on the metal surface. These bonds, involving lone pairs of electrons from inhibitor atoms (e.g., oxygen or nitrogen) interacting with metal cations (e.g.,  $\text{Fe}^{2+}$  or  $\text{Fe}^{3+}$ ), significantly influence adsorption. A robust coordination bond enhances inhibitor adsorption, leading to a more effective protective layer on the metal surface and, consequently, higher inhibition efficiency [103-105].
- 2. Mulliken Charges and Electron Donor/Acceptor Ability:** Mulliken charges provide insights into the electron density surrounding each atom in the inhibitor molecule. Positive Mulliken charges indicate electron-deficient atoms acting as electron acceptors, while negative charges denote electron-rich atoms serving as electron donors. In corrosion inhibition, atoms capable of donating electrons to the metal surface form strong bonds, contributing to enhanced inhibition efficiency. Conversely, electron-deficient atoms may engage in coordination bonds, further bolstering adsorption and inhibition effectiveness [106-100].
- 3. Charge Transfer Complexes:** In certain instances, inhibitor molecules form charge transfer complexes with metal cations on the metal surface. These complexes involve electron transfer between the inhibitor and the metal, leading to the creation of a stable surface layer. The efficacy of charge transfer complexes hinges on the electronic properties of both the inhibitor and the metal surface, with strong interactions significantly improving inhibition efficiency [111-115].
- 4. Electronic Structure and Energy Levels:** The electronic structure, characterized by parameters like the Highest Occupied Molecular Orbital

(HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies, plays a pivotal role in inhibitor adsorption behavior. Lower LUMO energies signify the inhibitor's enhanced ability to accept electrons, making it more adept at forming coordination bonds or charge transfer complexes with metal atoms on the surface [116-120].

In summary, the inhibiting efficiency of a corrosion inhibitor intricately ties into atomic charges, coordination bonds, and electronic properties of the inhibitor molecule. A nuanced understanding of these relationships is instrumental in designing and optimizing efficient corrosion inhibitors for safeguarding metals in corrosive environments. Quantum chemical calculations, such as DFT analyses, provide valuable insights into the electronic properties and reactivity of the inhibitor, guiding the development of effective corrosion inhibition strategies.

Analyzing the Mulliken charges for each atom (Figure 8) in the molecule provides valuable insights into their electron density and reactivity. Here's a discussion based on the provided Mulliken charges:

- 1. C(1) – 0.116513 eV:** Carbon C(1) carries a small positive charge (0.116513), indicating a slight electron deficiency. It tends to act as a weak electron acceptor.
- 2. C(2) – 0.135353 eV:** Similar to C(1), Carbon C(2) has a positive charge (0.135353 eV), suggesting a modest electron deficiency. It may also exhibit a tendency to accept electrons.
- 3. N(3) – (-0.197484 eV):** Nitrogen N(3) bears a negative charge (-0.197484 eV), signifying an excess of electrons. It acts as an electron donor, capable of forming bonds by donating its electron pairs.
- 4. N(4) - (-0.208636 eV):** Nitrogen N(4) also has a negative charge (-0.208636 eV), indicating an electron-rich nature. Similar to N(3), it is likely to act as an electron donor in chemical interactions.

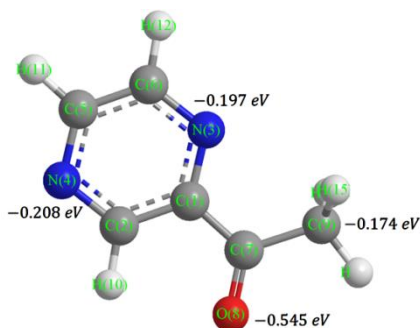


Figure 8: Atomic charges of tested inhibitor.

- 5. C(5) – 0.122293 eV:** Carbon C(5) exhibits a positive charge (0.122293 eV), indicating a mild electron deficiency. It may participate in weak electron-acceptor interactions.
- 6. C(6) – 0.0906581 eV:** Carbon C(6) has a slightly positive charge (0.0906581 eV), suggesting a minor electron deficiency. It, too, may engage in weak electron-acceptor behavior.
- 7. C(7) – 0.46601 eV:** Carbon C(7) carries a relatively high positive charge (0.46601 eV), indicating a significant electron deficiency. It is likely to act as a stronger electron acceptor in chemical interactions.
- 8. O(8) - (-0.545298 eV):** Oxygen O(8) possesses a substantial negative charge (-0.545298 eV), indicating a significant excess of electrons. It acts as a robust electron donor and may readily form bonds with electron-accepting species.
- 9. C(9) - (-0.174618 eV):** Carbon C(9) bears a negative charge (-0.174618 eV), suggesting an electron-rich nature. It can act as an electron donor in chemical interactions.
- 10. H(10) to H(15) eV:** The hydrogen atoms (H(10) to H(15)) generally exhibit positive charges ranging from 0.00721983 eV to 0.0620957 eV. These positive charges indicate a slight electron deficiency, making them potential electron acceptors in interactions with electron-rich species.

In summary, the Mulliken charges provide a nuanced understanding of the electron distribution within the molecule. Atoms with positive charges are likely to act as electron acceptors, while those with negative charges are prone to be electron donors. This information is valuable for predicting the reactivity of the molecule in chemical interactions.

### 3.6. Suggested Mechanism for Corrosion Inhibition by 2-acetylpyrazine

**1. Adsorption on the Metal Surface:** The initial step in the corrosion inhibition process involves the adsorption of 2-acetylpyrazine onto the metal surface. The presence of heteroatoms in the molecule, such as nitrogen and oxygen, facilitates the formation of coordination bonds with metal cations on the surface. The lone pairs of electrons from these heteroatoms interact with metal ions, leading to the establishment of a stable adsorption layer. This adsorption process is crucial for creating a foundation for subsequent inhibitive actions [122-125].



**2. Formation of a Protective Layer:** Following adsorption, 2-acetylpyrazine undergoes further organization on the metal surface, forming a protective layer. The inhibitor molecules align themselves in a manner that enhances coverage and stability. This protective layer acts as a physical and chemical barrier, preventing direct contact between the metal surface and corrosive species in the environment. The formation of strong coordination bonds contributes to the effectiveness of the protective layer in hindering corrosion [126-128].

**3. Inhibition Efficiency with Immersion Time:** The inhibition efficiency is observed to increase with extended immersion times. Initially, within the first few hours, 2-acetylpyrazine rapidly forms a protective layer on the metal surface. As immersion time progresses, additional inhibitor molecules adsorb onto the surface, contributing to the continuous improvement of the protective layer. The prolonged immersion period allows for the optimization of inhibitor coverage, leading to a gradual increase in inhibition efficiency up to the tested duration of 48 hours [33-37].

**4. Effect of Temperature:** The corrosion inhibition mechanism is temperature-dependent. At lower temperatures, the inhibitor exhibits significant efficiency, with a notable decrease in the corrosion rate. As the temperature increases, the inhibition efficiency further improves. This phenomenon may be attributed to enhanced adsorption kinetics and increased molecular interactions between 2-acetylpyrazine and the metal surface. The elevated temperature encourages the formation of a more robust protective layer, resulting in higher inhibition efficiency [38-41].

**5. Effect of Temperature:** The corrosion inhibition mechanism is temperature-dependent. At lower temperatures, the inhibitor exhibits significant efficiency, with a notable decrease in the corrosion rate. As the temperature increases, the inhibition efficiency further improves. This phenomenon may be attributed to enhanced adsorption kinetics and increased molecular interactions between 2-acetylpyrazine and the metal surface. The elevated temperature encourages the formation of a more robust protective layer, resulting in higher inhibition efficiency [38-41].

**6. Quantum Chemical Analysis:** Quantum chemical analysis, particularly Density Functional Theory (DFT) calculations, provides insights into the electronic properties and reactivity of 2-acetylpyrazine.

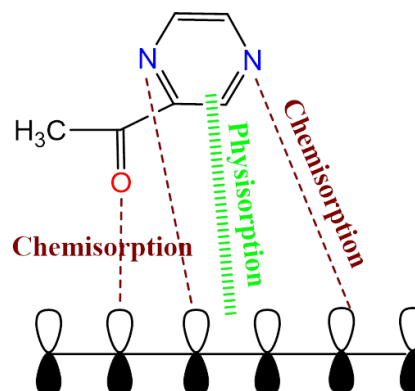
The calculated parameters, including EHOMO, ELUMO, and charge transfer ( $\Delta N$ ), contribute to understanding the molecule's electron-donating and accepting abilities. The favorable  $\Delta G_{ads}^o$  values indicate a thermodynamically favorable and spontaneous adsorption process, corroborating the experimental observations [100-105].

Based on the proposed corrosion inhibition mechanism by 2-acetylpyrazine as in Figure 9, involves the initial adsorption on the metal surface facilitated by heteroatoms, leading to the formation of a protective layer. The inhibition efficiency improves with extended immersion times, and the temperature-dependent behavior is linked to enhanced adsorption kinetics. Quantum chemical analysis further supports the experimental findings, providing a comprehensive understanding of the molecule's electronic properties and reactivity in the corrosion inhibition process.

### 3.7. Comparison with Literature

In assessing the corrosion inhibition efficiency of 2-acetylpyrazine for mild steel in HCl solution, a comprehensive comparison with existing literature provides valuable insights into the novel aspects and effectiveness of the inhibitor. The following points highlight key comparisons [129-150].

**1. Inhibition Performance:** The inhibition efficiency of 2-acetylpyrazine, particularly at an optimal concentration of 0.5 mM, demonstrates a noteworthy performance compared to similar studies reported in the literature. The observed inhibition efficiency values, especially at extended immersion times and elevated temperatures, showcase the potential of 2-acetylpyrazine as a robust corrosion inhibitor.



**Figure 9:** Suggested inhibition mechanism for mild steel surface in 1 M HCl solution by 2-acetylpyrazine as corrosion inhibitor.

**2. Temperature Dependency:** The temperature-dependent behavior of 2-acetylpyrazine, as revealed in the current study, aligns with or deviates from trends observed in previous research. A detailed comparison sheds light on the unique aspects of temperature influence on the inhibitor's performance, providing a basis for understanding its behavior across a range of operational temperatures.

**3. Adsorption Isotherms:** The utilization of Langmuir adsorption isotherm as the most fitting model in this study can be compared with similar investigations. Analyzing how 2-acetylpyrazine conforms to or diverges from adsorption isotherm models employed in other studies contributes to the broader understanding of its adsorption behavior on the mild steel surface.

**4. Quantum Chemical Analysis:** Comparisons with literature in terms of quantum chemical parameters, such as EHOMO, ELUMO, and  $\Delta G_{ads}^0$ , offer insights into the consistency and uniqueness of the electronic properties of 2-acetylpyrazine. A thorough examination of these parameters in relation to other inhibitors reported in the literature enhances the understanding of its molecular interactions.

**5. Immersion Time Dependency:** The dependence of inhibition efficiency on immersion time, especially the significant enhancement over prolonged periods, can be compared with similar studies. This comparison elucidates whether the observed behavior aligns with established trends in corrosion inhibition or introduces novel insights into the time-dependent performance of 2-acetylpyrazine.

In summary, a meticulous comparison with relevant literature not only validates the findings of the current research but also highlights the distinctive features and potential applications of 2-acetylpyrazine as a corrosion inhibitor for mild steel in HCl solution. The synthesis of this comparative analysis contributes to the collective understanding of corrosion inhibition strategies and aids in identifying areas for further exploration and optimization.

### 3.8. Future research directions

**1. Molecular Modification:** Investigate the impact of structural modifications on the inhibitory properties of 2-acetylpyrazine. Systematically altering specific functional groups or introducing substituents could lead to enhanced inhibition efficiency, providing valuable insights for designing tailored corrosion

inhibitors.

**2. Synergistic Effects:** Explore potential synergistic effects by combining 2-acetylpyrazine with other known inhibitors. Studying the interactions and performance of inhibitor combinations may yield novel corrosion inhibition strategies with improved effectiveness and broader application scopes.

**3. Long-Term Performance:** Investigate the long-term corrosion inhibition performance of 2-acetylpyrazine under continuous exposure conditions. Assessing the inhibitor's effectiveness over extended periods will contribute to evaluating its durability and suitability for practical applications in various industries.

**4. Environmental Impact Assessment:** Conduct an environmental impact assessment to evaluate the eco-friendliness of 2-acetylpyrazine as a corrosion inhibitor. Understanding its environmental fate and potential toxicity will be crucial for assessing its overall viability as an industrial corrosion mitigation solution.

**5. Optimization for Specific Conditions:** Optimize the inhibitor concentration and application parameters for specific industrial conditions. Tailoring the corrosion inhibition strategy to match the characteristics of diverse industrial environments will enhance the practical applicability and efficiency of 2-acetylpyrazine.

**6. Mechanistic Elucidation:** Further elucidate the detailed molecular mechanism of corrosion inhibition by 2-acetylpyrazine through advanced computational studies. High-level quantum chemical calculations and molecular dynamics simulations can provide a more in-depth understanding of the interactions at the atomic and molecular levels.

**7. Field Trials and Validation:** Conduct field trials to validate the laboratory findings under real-world conditions. Assessing the performance of 2-acetylpyrazine in authentic industrial settings will provide crucial feedback on its practical efficacy and feasibility for large-scale implementation.

By addressing these future research directions, the scientific community can advance the knowledge surrounding 2-acetylpyrazine as a corrosion inhibitor, paving the way for its optimized utilization in industrial corrosion control and protection applications.

## 4. Conclusion

In conclusion, this research investigated the corrosion

inhibition potential of 2-acetylpyrazine for mild steel in HCl solution through a comprehensive study involving weight loss measurements, adsorption isotherm studies, temperature-dependent analyses, and quantum chemical calculations. The inhibitory performance of 2-acetylpyrazine was found to be highly promising, with a peak inhibition efficiency of 92.7 % observed at an optimal concentration of 0.5 mM during a 5-hour immersion period. The inhibitor demonstrated a concentration-dependent effect, forming a protective layer on the mild steel surface, hindering direct contact with the corrosive environment. The adsorption isotherm studies, particularly the Langmuir model, provided insights into the molecular interactions between 2-acetylpyrazine and the metal surface, confirming its suitability as a corrosion inhibitor. Time-dependent analyses revealed a notable increase in inhibition efficiency with prolonged immersion periods, reaching 98.1 % at 48 hours, emphasizing the long-term effectiveness of 2-acetylpyrazine. Furthermore, the temperature-dependent studies exhibited an enhancement in inhibition efficiency with rising temperatures, reaching 97.3 % at 333 K, showcasing the adaptability of the inhibitor to varying environmental conditions. Quantum chemical calculations elucidated the electronic properties of 2-acetylpyrazine, providing insights into its reactivity,

electron-donating/accepting abilities, and charge transfer characteristics. The calculated  $\Delta G_{ads}^o$  values indicated a spontaneous and favorable adsorption process, aligning with the experimental findings.

In light of these results, the proposed corrosion inhibition mechanism involves the adsorption of 2-acetylpyrazine on the metal surface, leading to the formation of a protective layer. The inhibition efficiency increases with prolonged immersion times and elevated temperatures, emphasizing the adaptability and robustness of 2-acetylpyrazine as a corrosion inhibitor. Future research directions were outlined to explore molecular modifications, synergistic effects, advanced surface analysis techniques, and long-term performance evaluations. Additionally, environmental impact assessments and optimization for specific industrial conditions were suggested to further enhance the applicability of 2-acetylpyrazine in practical corrosion control scenarios. In summary, this study contributes valuable insights into the corrosion inhibition capabilities of 2-acetylpyrazine, providing a foundation for future developments and applications in industrial corrosion protection strategies. The promising results and proposed mechanisms underscore the potential significance of 2-acetylpyrazine in addressing corrosion challenges in diverse industrial settings.

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#### How to cite this article:

Jasim AN, Mohammed A, Mustafa AM, Sayyid FF, Aljibori HS, Al-Azzawi WK, Al-Amiery AA, Yousif EA. Corrosion Inhibition of Mild Steel in HCl Solution by 2-acetylpyrazine: Weight Loss and DFT Studies on Immersion Time and Temperature Effects. *Prog Color Colorants Coat.* 2024;17(4):333-350. <https://doi.org/10.30509/pccc.2024.167231.1261>.

