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# Investigation of the Anticorrosive Efficiency of a Heterocyclic Organic Inhibitor on Mild Steel in Acidic Medium

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## Abstract

Corrosion presents a major challenge for industries like automotive, marine, construction, and oil and gas, as it affects the ability to produce high-quality products while maintaining low maintenance costs. In this study, NT (1-(4-methyl-1-(2-nitrophenyl)-1H-1,2,3-triazol-5-yl) ethanone) which was used as corrosion inhibitor and it was investigated by weight loss (WL), potentiodynamic polarization (PDP) and electrochemical impedance spectroscopy (EIS), measurements. As temperature increases, the inhibitory efficiency (IE) decreases, whereas it improves with higher inhibitor dosage. Weight loss (WL) measurements indicate enhanced adsorption of MNPT on the mild steel surface at elevated inhibitor concentrations, achieving a maximum efficiency of 78.5% at 2ppm and 25 °C. The adsorption behavior of the investigated derivatives on the mild steel surface was best explained by the Langmuir, Temkin, El-Wady, Freundlich adsorption isotherm. The process is spontaneous and exothermic, according to the computed values of the adsorption equilibrium constant ($K_{ads}$) and the standard free energy of adsorption ($\Delta G_{ads}$). NT functions as a mixed-type inhibitor, according to polarization studies.

**Keyword:** Triazole, Potentiodynamic, Polarization, Electrochemical, Impedance, Isotherm.

## 1.Introduction

Mild steel is widely used across various industries because of its good mechanical strength, ease of fabrication, and low cost. However, its application is significantly limited by its high susceptibility to corrosion, particularly in acidic environments encountered during industrial processes such as cleaning, pickling, and oil well acidizing [1]. In many of these operations, acidic solutions are intentionally employed to remove scale deposits and corrosion products from metal surfaces; for instance, metal pickling commonly utilizes acids such as $H_2SO_4$ or HCl [2].

To mitigate excessive metal loss during such treatments, corrosion inhibitors are added, which effectively reduce the rate of metal dissolution in these aggressive environments [2]. Among the various types, organic corrosion inhibitors are especially important, as they typically contain heteroatoms with lone pairs of electrons and π-electrons in conjugated or aromatic systems, enabling strong interaction with metal surfaces. These interactions facilitate adsorption through both physical and chemical mechanisms, leading to the formation of a protective layer that isolates the metal from the corrosive medium [3].

Therefore, the use of corrosion inhibitors is considered an effective approach for protecting mild steel, with organic inhibitors being widely preferred due to their adaptability under different conditions, particularly in acidic media [4]. In this context, organic inhibitors play a crucial role because of their strong ability to form a stable protective film on the steel surface, thereby enhancing corrosion resistance. Recent studies have extensively reported various heterocyclic and macrocyclic compounds, as well as biomolecules and their chemically modified derivatives and composites, as efficient corrosion inhibitors [5,6]. Furthermore, the effectiveness of these inhibitors depends on several factors, including their electronic structure, chemical composition, the presence of specific functional groups, and their adsorption behavior on the steel surface [7,8,9,10,11,12].

(1-(4-methyl-1-(2-nitrophenyl)-1H-1,2,3-triazol-5-yl)ethanone) (NT) was evaluated as a corrosion inhibitor for mild steel in 1N HCl solution. The inhibition efficiency was found to increase with increasing inhibitor concentration. At 25 °C and an optimal concentration of 2 ppm, the inhibitor exhibited high inhibition efficiencies of 91.5% as determined by electrochemical impedance spectroscopy (EIS), 78.5% by weight loss (WL) measurements, and 84.8% using potentiodynamic polarization (PDP) techniques.

## 2.Experimental Work

**2.1 Synthesis:** The compound (1-(4-methyl-1-(2-nitrophenyl)-1H-1,2,3-triazol-5-yl)ethanone) was synthesized by following standard procedure. The synthesized compound confirmed by IR and NMR spectroscopy.

**2.2 Weight loss Method:** Mild Steel coupons measuring 1.0 × 5.0 × 0.5 cm³ with a purity of 99.5% were prepared by thorough polishing, cleaning, and drying prior to the experiments. All chemicals used in the study were of analytical grade. To evaluate the corrosion inhibition performance of the synthesized compounds, weight loss measurements were conducted. The prepared iron specimens were weighed in triplicate before and after immersion in 100 mL of acidic solution for 3 hours, both in the absence and presence of inhibitors at various concentrations. The corrosion rate was determined by calculating the difference between the initial and final masses of the specimens, thereby establishing a correlation between inhibitor concentration and weight loss.

$$\textbf{Inhibitor efficiency (\%)} = W_b - W_i / W_b$$

Where
$W_b$ is the weight loss without inhibitor
$W_i$ is the weight loss with inhibitor

### 2.3 Electrochemical Studies

Electrochemical Impedance Spectroscopy (EIS) and Tafel Polarization studies were carried out using an electrochemical measurement unit (Model Stat, 10 V, 30 mA, IVIUM). EIS measurements were performed at the corrosion potential over a frequency range of 10 kHz to 0.01 Hz with an AC signal amplitude of 10 mV. Subsequently, Tafel polarization measurements were conducted in the potential range of −200 mV to +200 mV with respect to the open circuit potential (OCP) at a scan rate of 1 mV s⁻¹.

The inhibition efficiency (IE%) from potentiodynamic polarization measurements was calculated using the following relation:

$$\mathrm{IE}\ (\%) = [(I_{corr}(\mathrm{blank}) - I_{corr}(\mathrm{inh})) / I_{corr}(\mathrm{blank})] \times 100$$

Where $I_{corr}$(blank) and $I_{corr}$(inh) represent the corrosion current densities in the absence and presence of the inhibitor, respectively.

The Nyquist plots (Z′ vs. Z″) obtained from EIS measurements were analyzed to determine the charge transfer resistance ($R_{ct}$) and double layer capacitance ($C_{dl}$). Tafel polarization curves (E vs. log I) were used to evaluate key electrochemical parameters, including corrosion potential ($E_{corr}$), corrosion current density ($I_{corr}$), and anodic ($b_a$) and cathodic ($b_c$) Tafel slopes.

Similarly, the inhibition efficiency from impedance measurements was determined using:

$$\mathrm{IE}\ (\%) = [(R_{ct}(\mathrm{inh}) - R_{ct}(\mathrm{blank})) / R_{ct}(\mathrm{inh})] \times 100$$

where $R_{ct}$(blank) and $R_{ct}$(inh) correspond to the charge transfer resistance values in the absence and presence of the inhibitor, respectively.

## 3. Results and Discussion

### 3.1 Variation of Inhibition Efficiency of varying Concentrations of NT on Mild Steel in 1N HCl at various time intervals

The inhibition efficiency (IE) of NT for mild steel corrosion in 1 N HCl at different concentrations and immersion times is presented in Table 1. The results clearly demonstrate that the inhibition efficiency is strongly dependent on both inhibitor concentration and exposure time.

**Table. 1 Comparison of IE of Varying Concentrations of NT on Mild Steel in 1N HCl at Various Time Intervals**

| S.No | Concentration (ppm) | 1 h | 3 h | 5 h | 7 h | 24 h |
|---|---|---|---|---|---|---|
| 1 | 0.5 | 69.2 | 69.9 | 56.7 | 53.7 | 51.7 |
| 2 | 1.0 | 72.3 | 71.7 | 57.9 | 54.1 | 52.4 |
| 3 | 1.5 | 76.9 | 74.3 | 63.7 | 58 | 58.8 |
| 4 | 2.0 | 78.5 | 77.9 | 70.8 | 68.9 | 60 |

At lower inhibitor concentration (0.5 ppm), the inhibition efficiency was observed to be 69.2% after 1 h, which slightly increased to 69.9% after 3 h. However, with further increase in immersion time, the efficiency gradually decreased to 56.7%, 53.7%, and 51.7% at 5 h, 7 h, and 24 h, respectively. This trend indicates that although NT initially forms a protective layer on the mild steel surface, the stability of this adsorbed film diminishes with prolonged exposure in the aggressive acidic environment.

A similar pattern was observed at higher concentrations. When the inhibitor concentration was increased to 1.0 ppm, the inhibition efficiency improved to 72.3% at 1 h and 71.7% at 3 h, followed by a gradual decline at longer immersion periods. Further increase in concentration to 1.5 ppm resulted in higher efficiencies of 76.9% at 1 h and 74.3% at 3 h, suggesting enhanced adsorption of inhibitor molecules on the metal surface.

The maximum inhibition efficiency was recorded at 2.0 ppm, where the efficiency reached 78.5% at 1 h and 77.9% at 3 h. Even after extended immersion (24 h), the inhibitor maintained a relatively significant efficiency of 60%, indicating that NT possesses appreciable corrosion protection capability.

The observed improvement in inhibition efficiency with increasing inhibitor concentration can be attributed to the increased surface coverage of NT molecules on the mild steel surface. Higher inhibitor concentration facilitates stronger adsorption and formation of a more compact and stable protective film, which effectively blocks active corrosion sites.

### 3.2 Variation of Corrosion Rate of varying Concentrations of NT on Mild Steel in 1N HCl at various time intervals

The corrosion rate (CR) values obtained for mild steel in the absence and presence of NT at various concentrations and immersion times are shown in Table 2. The data clearly indicate that the corrosion rate of mild steel in the blank solution increases significantly with time, confirming the highly corrosive nature of the acidic medium.

**Table 2. Comparison of CR of Varying Concentrations of NT on Mild Steel in 1N HCl at Various Time Intervals**

| S.No | Concentration (ppm) | 1 h | 3 h | 5 h | 7 h | 24 h |
|---|---|---|---|---|---|---|
| 1 | Blank | 352.2 | 306.1 | 463.2 | 766.7 | 2665.7 |
| 2 | 0.5 | 243.8 | 214 | 262.8 | 411.8 | 1378.9 |
| 3 | 1.0 | 254.6 | 219.4 | 268.2 | 414.5 | 1397.9 |
| 4 | 1.5 | 270.9 | 227.6 | 295.3 | 444.3 | 1568.5 |
| 5 | 2.0 | 276.3 | 238.4 | 327.8 | 528.3 | 1598.3 |

In the absence of inhibitor, the corrosion rate increased from 352.2 at 1 h to 2665.7 at 24 h, indicating severe metal dissolution. This continuous increase in corrosion rate suggests progressive damage to the mild steel surface due to the aggressive attack of hydrochloric acid.

Upon addition of NT, a considerable reduction in corrosion rate was observed at all concentrations and time intervals compared to the blank solution. For instance, at 0.5 ppm, the corrosion rate decreased to 243.8 at 1 h, which is significantly lower than that of the uninhibited system. Similarly, at 1.0 ppm, the corrosion rate remained substantially lower than the blank across all immersion periods.Although corrosion rates at 1.0 ppm and 1.5 ppm are slightly higher compared to some lower concentrations, they remain considerably reduced relative to the blank solution. This indicates that the presence of NT effectively suppresses the corrosion process by limiting metal dissolution.However, it is also evident that the corrosion rate tends to increase with increasing immersion time for all concentrations. This behavior may be attributed to gradual deterioration or partial desorption of the inhibitor molecules from the metal surface over prolonged exposure, which reduces the protective effectiveness of the inhibitor film.

### 3.3 Adsorption Behavior and Inhibition Mechanism

The inhibition performance of NT can be explained based on its adsorption on the mild steel surface. In acidic solutions, corrosion inhibition generally occurs through adsorption of inhibitor molecules onto the metal surface, forming a protective barrier that reduces the interaction between the metal and the corrosive medium.NT molecules likely adsorb onto the mild steel surface through:

- Interaction between the metal surface and heteroatoms present in the inhibitor molecule.
- Possible coordination or electrostatic interactions between the inhibitor and the charged metal surface in acidic medium.
- Formation of a protective adsorbed layer that blocks active corrosion sites.

As the inhibitor concentration increases, the number of inhibitor molecules available for adsorption also increases, leading to improved surface coverage and enhanced corrosion protection. This explains the observed increase in inhibition efficiency with concentration.

The gradual decrease in inhibition efficiency at longer immersion times suggests that the adsorption process may involve a combination of physical and chemical interactions, where partial desorption or weakening of the protective film occurs with time.

### 3.4 Effect of Temperature on Corrosion Rate

Corrosion rate increased with rise in temperature in both blank and inhibited systems. This behaviour is typical of electrochemical reactions, as higher temperature enhances reaction kinetics and diffusion rates.

However, the inhibited system showed comparatively controlled increase in corrosion rate, confirming that the inhibitor remains effective over the studied temperature range.

The slight reduction in inhibition efficiency at higher temperatures may be attributed to partial desorption of inhibitor molecules, consistent with the exothermic nature of adsorption.

### 3.5 Adsorption Isotherms

The adsorption behaviour of NT on the mild steel surface in 1 N HCl was analyzed using Langmuir, Freundlich, and El-Wady adsorption isotherm models at temperatures ranging from 303 to 343 K. The degree of surface coverage (θ), calculated from inhibition efficiency values, was employed to understand the nature of interaction between the inhibitor molecules and the metal surface. The applicability of these isotherms provides valuable insight into the mechanism of corrosion inhibition.

#### 3.5.1 Langmuir Adsorption Isotherm

The Langmuir adsorption isotherm assumes monolayer adsorption of inhibitor molecules on a homogeneous metal surface with no interaction between the adsorbed species. The linear plots of C/θ against inhibitor concentration (C) at different temperatures indicate that the adsorption of NT approximately follows the Langmuir model. The near-linear relationship observed at all studied temperatures suggests that NT molecules adsorb uniformly on the mild steel surface, forming a protective monolayer that isolates the metal from the corrosive environment.

An increase in the C/θ values with rising temperature reflects a decrease in adsorption strength at higher temperatures, which may be attributed to partial desorption of NT molecules from the metal surface. This behaviour suggests that the adsorption process involves predominantly **physisorption**, where electrostatic interactions between protonated NT molecules and the negatively charged metal surface play a significant role. Nevertheless, slight deviations from ideal linearity indicate possible interactions among adsorbed species or surface heterogeneity, which is common in real corrosion systems.

#### 3.5.2 Temkin Adsorption Isotherm

The adsorption behaviour of the inhibitor on the metal surface at various concentrations and temperatures was evaluated using the Temkin adsorption isotherm. The linear plots of surface coverage (θ) against ln C obtained at all studied temperatures confirm that the adsorption process follows the Temkin model, indicating the presence of lateral interactions among adsorbed inhibitor molecules. The positive slope values suggest repulsive interactions between the adsorbed species, likely due to surface crowding or overlapping adsorption sites. It was observed that surface coverage decreased with increasing temperature at a given inhibitor concentration, revealing that adsorption becomes less favorable at elevated temperatures. This trend, together with the decrease in the adsorption equilibrium constant ($K_{ads}$) with temperature, suggests that the adsorption process is predominantly exothermic and mainly governed by physisorption. The strong adsorption at lower temperatures contributes to higher inhibition efficiency through the formation of a protective adsorbed film on the metal surface, while partial desorption at higher temperatures leads to reduced corrosion protection.

#### 3.5.3 Freundlich Adsorption Isotherm

The Freundlich adsorption isotherm is an empirical model that accounts for adsorption on heterogeneous surfaces and the possibility of multilayer adsorption. The linear plots of log θ against log C obtained at different temperatures confirm that NT adsorption also fits well with the Freundlich isotherm. The values of log θ increase with increasing inhibitor concentration, demonstrating enhanced surface coverage due to stronger adsorption of NT molecules.

The Freundlich constant (1/n), inferred from the slope of the plots, being less than unity at all temperatures indicates favorable adsorption of NT on the mild steel surface. The gradual decrease in adsorption intensity with increasing temperature further supports the dominance of physical adsorption. The adherence of the system to the Freundlich isotherm highlights the heterogeneous nature of the metal surface and suggests that NT molecules occupy adsorption sites of varying energies, contributing effectively to corrosion inhibition.

### 3.5.4 El-Wady Adsorption Isotherm

The El-Wady adsorption isotherm considers interactions between adsorbed molecules and provides insight into the degree of surface coverage through $\log(\theta/1-\theta)$ against log C plots. The linearity observed in the El-Wady plots at all investigated temperatures suggests that the adsorption of NT is spontaneous and involves significant interaction between inhibitor molecules and the metal surface.

The positive values of $\log(\theta/1-\theta)$ with increasing concentration confirm progressive surface coverage and strong inhibitor–metal interaction. The decrease in adsorption strength at elevated temperatures indicates reduced stability of the adsorbed layer, again supporting a physisorption-dominated mechanism. The applicability of the El-Wady model further reinforces the conclusion that NT molecules adsorb efficiently on the mild steel surface, forming a protective barrier that retards the corrosion process.

The conformity of NT adsorption to Langmuir, Freundlich, and El-Wady isotherms confirms that corrosion inhibition occurs through adsorption of NT molecules onto the mild steel surface. The results collectively suggest that the adsorption process is spontaneous, favorable, and predominantly physical in nature, with possible contributions from weak chemical interactions. The effectiveness of NT increases with concentration but decreases with temperature, consistent with desorption effects at higher thermal energy. These findings clearly demonstrate the potential of NT as an efficient corrosion inhibitor for mild steel in acidic environments.

### 3.6 Potentiodynamic Polarisation Studies

Potentiodynamic polarization measurements were carried out to evaluate the corrosion inhibition performance of the inhibitor at different concentrations for mild steel in 1 N HCl. The electrochemical parameters such as corrosion potential ($E_{corr}$), corrosion current density ($I_{corr}$), polarization resistance (Rp), Tafel slopes (βa and βc), corrosion rate, and inhibition efficiency were obtained and are summarized in Table 8.

### 3.6.1 Effect of Inhibitor Concentration on Corrosion Current Density

The blank 1N HCl solution exhibited a high corrosion current density of (6.506 A/cm$^2$), indicating severe dissolution of mild steel in the acidic medium. Upon addition of the inhibitor, a marked reduction in $I_{corr}$ was observed with increasing inhibitor concentration from 1.0 to 2.0 ppm.With further increase in inhibitor concentration, $I_{corr}$ decreased significantly, reaching a minimum value of ($9.91 \times 10^{-5}$ A/cm$^2$) at concentration 2.0 ppm. This pronounced decrease in corrosion current density confirms the formation of a protective adsorbed film on the metal surface, which hinders charge transfer reactions.

### 3.6.2 Inhibition Efficiency and Polarization Resistance

The inhibition efficiency increased steadily with inhibitor concentration, attaining a maximum value of 84.8% at concentration 2.0 ppm. This trend is consistent with the corresponding increase in polarization resistance (Rp), which rose from 46.1 Ω for the blank solution to 321.9 Ω at the highest inhibitor concentration. The increase in Rp further supports the effective suppression of the corrosion process due to inhibitor adsorption.

### 3.6.3 Nature of Inhibition Mechanism

The slight shift in corrosion potential ($E_{corr}$) values in the presence of the inhibitor, without significant displacement in either anodic or cathodic direction, indicates that the inhibitor acts as a **mixed-type inhibitor**. The changes observed in both anodic ($\beta_a$) and cathodic ($\beta_c$) Tafel slopes suggest that the inhibitor retards both metal dissolution and hydrogen evolution reactions.

### 3.6.4 Effect of the Corrosion Rate

The corrosion rate decreased dramatically from 2.129 mm y$^{-1}$ for the blank solution to 0.3243 mm y$^{-1}$ at inhibitor concentration 2.0 ppm, reveals the high inhibition efficiency obtained from polarization measurements.

The potentiodynamic polarization results clearly demonstrate that the inhibitor exhibits excellent corrosion inhibition performance for mild steel in 1 N HCl at higher concentrations. The increase in inhibition efficiency, polarization resistance, and simultaneous decrease in corrosion current density and corrosion rate confirm the effective adsorption of inhibitor molecules on the mild steel surface, forming a protective barrier against acidic attack.

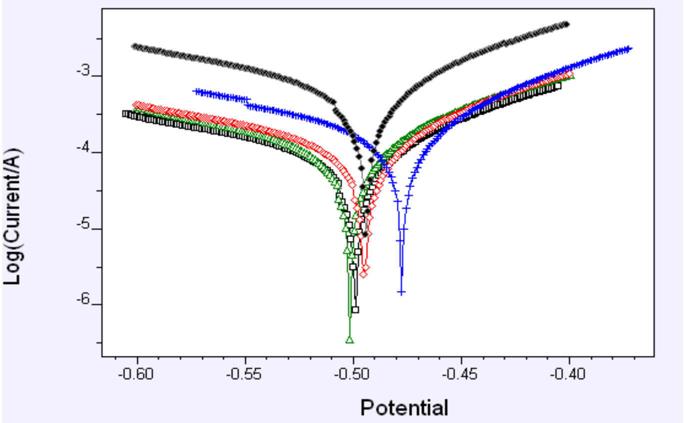


**Fig.1. Tafel Polarization Curves for mild steel corrosion in HCl against various concentrations of NT**

### 3.7. Electrochemical Impedance Studies

### 3.7.1 Effect of inhibitor concentration on inhibition efficiency in 1 N HCl

The corrosion behaviour of the metal in 1 N HCl was evaluated in the absence and presence of varying concentrations of the inhibitor. In the uninhibited (blank) solution, the metal exhibited the highest corrosion rate, confirming the highly aggressive nature of the acidic medium and the rapid dissolution of the metal surface.

**Table 3.**

| Concentration (ppm) | $R_s$ | $R_{ct}$ | $C_{dl}$ | IE % |
|---|---|---|---|---|
| Blank | 6.35 | 12.7 | 0.0000588 | |
| 0.5 | 4.87 | 22.7 | 0.0000429 | 44.1 |
| 1 | 9.21 | 41.7 | 0.0000351 | 69.5 |
| 1.5 | 6.59 | 86.4 | 0.0000311 | 85.3 |
| 2 | 12.6 | 150 | 0.0000299 | 91.5 |

The increase in $R_{ct}$ and the simultaneous decrease in $C_{dl}$ with increasing inhibitor concentration confirm the adsorption of inhibitor molecules on the metal surface and the formation of a protective barrier film.

The inhibition efficiency values calculated from electrochemical impedance spectroscopy clearly demonstrate that the corrosion inhibition performance of the inhibitor increases with increasing concentration. In the uninhibited 1 N HCl solution, the metal exhibits the lowest charge transfer resistance, indicating rapid electrochemical reactions at the metal–solution interface.Upon addition of the inhibitor, a substantial increase in charge transfer resistance is observed, leading to a corresponding rise in inhibition efficiency. At the lowest inhibitor concentration 0.5 ppm, an inhibition efficiency of approximately 44 % is achieved, suggesting partial surface coverage by inhibitor molecules. As the inhibitor concentration increases to 1.0 ppm, the inhibition efficiency increases markedly to about 70 %, reflecting enhanced adsorption and more effective blockage of active corrosion sites.At higher concentrations (1.5 ppm and 2.0 ppm), the inhibition efficiency reaches approximately 85% and 92%, respectively. This significant improvement indicates the formation of a dense and stable protective film on the metal surface, which effectively hinders charge transfer processes. The high inhibition efficiencies obtained at elevated concentrations confirm that the inhibitor acts predominantly through an adsorption-controlled mechanism.Overall, the EIS results validate the weight loss findings and confirm the excellent corrosion inhibition performance of the inhibitor in 1 N HCl. The results demonstrate that the inhibition efficiency of the studied inhibitor in 1 N HCl increases with increasing inhibitor concentration, following a typical adsorption-controlled inhibition mechanism. The concentration-dependent behaviour indicates that corrosion protection is primarily governed by the extent of surface coverage and the formation of an adsorbed protective layer, highlighting the inhibitor's potential applicability for corrosion control in acidic environments.

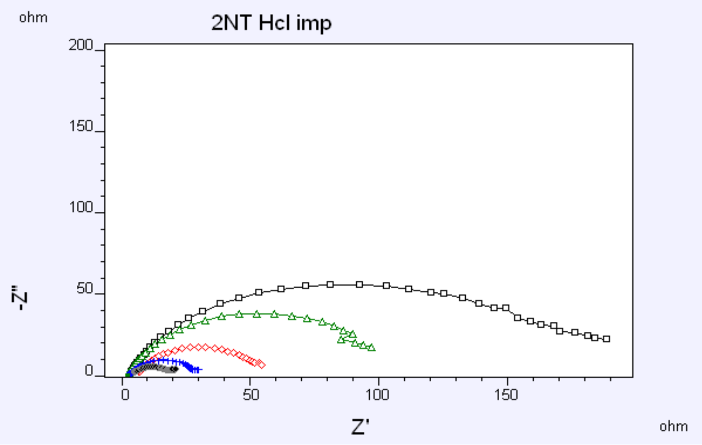


**Figure 6. Nyquist plot for mild steel corrosion in HCl against various concentrations of NT**

The thermodynamic and kinetic evaluation of the investigated inhibitor in 1N HCl medium is discussed below. The study was conducted over the temperature range 303–343 K to understand the adsorption mechanism and temperature dependence of corrosion rate. Thermodynamic parameters such as Gibbs free energy of adsorption ($\Delta G^\circ_{ads}$), enthalpy of adsorption ($\Delta H^\circ_{ads}$), and entropy of adsorption ($\Delta S^\circ_{ads}$) were calculated. In addition, kinetic parameters including activation energy ($E_a$) were determined using Arrhenius relationships.

### 3.8 Thermodynamic Studies

Thermodynamic parameters provide significant insight into the nature, feasibility, and mechanism of adsorption of inhibitor molecules onto the metal surface.

### 3.8.1 Gibbs Free Energy of Adsorption ($\Delta G^\circ_{ads}$)

The Gibbs free energy of adsorption was calculated using the standard thermodynamic relationship:

$$\Delta G^\circ_{ads} = -RT\ln K$$

The obtained $\Delta G^\circ_{ads}$ values show a gradual decrease with increase in temperature. The negative values confirm that the adsorption process is spontaneous in nature.

The magnitude of $\Delta G^\circ_{ads}$ provides information regarding the type of adsorption:

- Values around −20 kJ mol⁻¹ indicate physical adsorption (electrostatic interaction).
- Values around −40 kJ mol⁻¹ or higher indicate chemical adsorption (charge sharing or transfer).

In the present investigation, the $\Delta G^\circ_{ads}$ values fall within the intermediate range, suggesting that the adsorption mechanism involves both physisorption and chemisorption. The decrease in $\Delta G^\circ_{ads}$ at higher temperatures indicates slight weakening of adsorption strength due to increased molecular motion and partial desorption.

Thus, adsorption of inhibitor molecules on the metal surface is spontaneous and temperature dependent.

### 3.8.2 Enthalpy of Adsorption ($\Delta H^\circ_{ads}$)

The enthalpy of adsorption was determined from the slope of the Van't Hoff plot of ln K versus 1/T:

$$\ln K = \frac{-\Delta H^\circ_{ads}}{RT} + \frac{\Delta S^\circ_{ads}}{R}$$

The calculated $\Delta H^\circ_{ads}$ value is negative, confirming that the adsorption process is exothermic. Exothermic adsorption indicates that energy is released when inhibitor molecules attach to the metal surface.

The relatively low magnitude of $\Delta H^\circ_{ads}$ suggests that the adsorption process is predominantly physical in nature. However, the possibility of partial chemisorption through coordination of heteroatoms or $\pi$-electrons cannot be excluded.

The exothermic behaviour further explains the reduction in adsorption efficiency at elevated temperatures, as increased thermal energy facilitates desorption of adsorbed molecules.

### 3.8.3 Entropy of Adsorption ($\Delta S^\circ_{ads}$)

The entropy change was obtained from the intercept of the Van't Hoff plot.

The negative $\Delta S^\circ_{ads}$ value indicates a decrease in randomness at the metal–solution interface during adsorption. This decrease in entropy arises because inhibitor molecules, which are randomly distributed in the bulk solution, become more ordered upon adsorption onto the metal surface.

Formation of an ordered and compact inhibitor layer reduces the degrees of freedom of the adsorbed species. This structured arrangement contributes to effective surface coverage and corrosion protection.

### 3.9 Kinetic Studies

Kinetic parameters were evaluated to understand the effect of temperature and inhibitor concentration on corrosion rate.

### 3.9.1 Activation Energy ($E_a$)

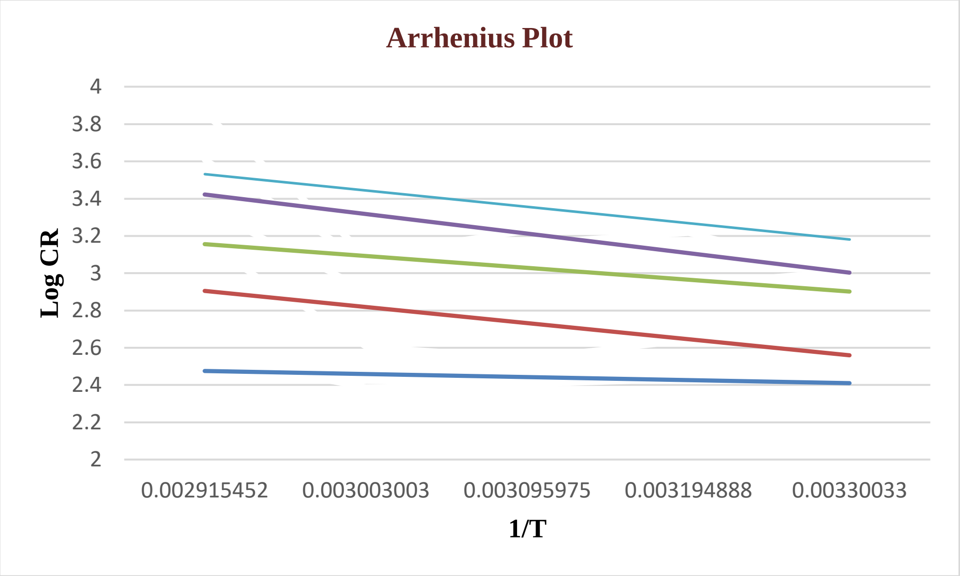
The activation energy was calculated using the Arrhenius equation:

$$\log CR = \log A - \frac{E_a}{2.303RT}$$

The blank solution exhibited the highest activation energy compared to inhibited systems. In the presence of inhibitor, activation energy values changed significantly.

The observed variation in activation energy suggests that adsorption of inhibitor molecules modifies the corrosion reaction pathway. The protective film formed on the metal surface acts as a barrier, thereby altering the energy profile of the corrosion process.

The change in $E_a$ values with inhibitor concentration indicates that surface coverage increases with concentration, leading to improved corrosion resistance.



### 3.10 Mechanism of Corrosion Inhibition

Based on thermodynamic and kinetic findings, the following mechanism is proposed:

1. Inhibitor molecules adsorb onto the metal surface through electrostatic interaction (physisorption).
2. Possible coordination between heteroatoms/π-electrons and vacant metal orbitals contributes to chemisorption.
3. Formation of a compact adsorbed layer blocks active corrosion sites.
4. The protective film reduces direct contact between metal surface and aggressive 1N HCl medium.

The combined thermodynamic and kinetic results confirm a mixed adsorption mechanism involving both physical and chemical interactions.

- Adsorption process is spontaneous (negative $\Delta G^\circ_{ads}$).
- Adsorption is exothermic (negative $\Delta H^\circ_{ads}$).
- Decrease in entropy indicates formation of ordered protective film (negative $\Delta S^\circ_{ads}$).
- Activation energy changes confirm modification of corrosion pathway.
- The inhibitor provides effective corrosion protection in 1N HCl.

These findings confirm that the inhibitor provides effective corrosion protection in 1N HCl medium through adsorption and barrier film formation.

The protective mechanism likely involves both electrostatic interaction and possible coordination between heteroatoms or π-electrons of the inhibitor molecule and vacant d-orbitals of the metal surface, resulting in a stable adsorbed layer

The thermodynamic and kinetic investigations demonstrate that the studied inhibitor effectively reduces corrosion of metal in 1N HCl medium. Adsorption is spontaneous and exothermic, with formation of an organized protective layer at the metal surface. The adsorption mechanism involves both physisorption and chemisorption.

Overall, the inhibitor exhibits appreciable inhibition efficiency across the studied temperature range, making it a promising candidate for acid corrosion protection.

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