Evaluation of corrosion inhibition characteristics of an *N*-propionanilide derivative for mild steel in 1 M HCl: Gravimetrical and computational studies

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Abstract

Due to its low cost, mild steel is frequently employed as a construction material in many industries. Unfortunately, due to the limited corrosion resistance of mild steel, it should be protected with barrier layers to keep it from corrosion in acidic or basic environments. An *N*-propionanilide derivative, namely 3-keto-3-((indolin-2-oneylidene)hydrazinyl)-*N*-propionanilide (KIHP), was studied as a corrosion inhibitor of mild steel in a hydrochloric acid solution at a temperature of 303 K using gravimetrical measurements and density functional theory (DFT) simulation. The findings demonstrate that KIHP performs well as a mild steel corrosion inhibitor in 1 M HCl, with a greater inhibition efficacy of 95.3 percent for gravimetrical analysis at 0.0005 M KIHP concentration. The gravimetrical measurements at various temperatures (303 K to 333 K) were also studied at 5 hours immersion time. It was found that he protection efficacy decreases as the temperature rises. Based on our findings, we believe that KIHP could efficiently inhibit the acidic damage on a mild surface through physical and chemical adsorption. We computed separately the Gibbs free energy parameter. Quantum chemical simulations at the B3LYP/6-31G* level of theory were also applied to compute some electronic properties of molecules in an effort to see if there was a relationship between the inhibitory action and the structure of KIHP molecule.

Received: May 6, 2022. Published: August 2, 2022 doi: 10.17675/2305-6894-2022-11-3-12

Keywords: *mild steel, corrosion rate, weight loss, Langmuir, DFT.*

1. Introduction

Several industries employ corrosion inhibitors to reduce the corrosion rate of metallic surfaces in acid solutions [1]. Acid treatment, cleaning, acid descaling, oil-well acidification, and petrochemical operations are only a few applications for acidic solutions [2]. Hydrochloric acid is one of the most regularly utilized acidic media in metal treatment. The use of inhibitors, especially in acidic media, is among the most common techniques used to prevent metal degradation [3]. Mild steel is commonly employed in acidic media in numerous manufacturing applications, and mild steel corrosion is reported to occur in this environment. Organic inhibitors [4] are among the most efficient ways of preventing corrosion. A large number of scientific investigations have been conducted on mild steel corrosion protection in acid environments [5]. Carbon steel is one of the most popular metals in the business because of its high availability, physicochemical properties, and low cost [6]. Mild steel is widely used in a wide range of applications, including chemical treatment, spatial construction, metal processing, seawater treatment, and petroleum refinery [7]. The introduction of heterocyclic molecules into a corrosive environment might inhibit or control surface corrosion [8]. Heterocyclic organic compounds added to an acid environment (HCl, H_2SO_4, H_3PO_4, or HNO_3) act as corrosion inhibitors by forming a barrier coating on mild steel surface, a process known as the prevention process [9]. Heterocyclic organic molecules are also adsorbed on mild steel surfaces *via* physical and/or chemical adsorption [10]. The charge is distributed or transmitted from heterocyclic organic molecules to a mild steel surface by chemical adsorption, resulting in the formation of coordination covalent bonds. Furthermore, there is electrostatic contact between heterocyclic organic molecules and transition metal elements [11]. Mild steel corrosion inhibitors can comprise heterocyclic organic molecules with coordination sites (particularly heteroatoms like O, N, and S), aromatic rings, and π-electrons [12]. This work aims to investigate the inhibitory effect of KIHP on the corrosion of mild steel in 1 M HCl at 303–333 K using weight loss measurements and the quantum chemical approach. The adsorption mechanism was investigated and explained. The selection of this KIHP (Figure 1) was also affected by its structure, as it is a molecule with many adsorption centers.

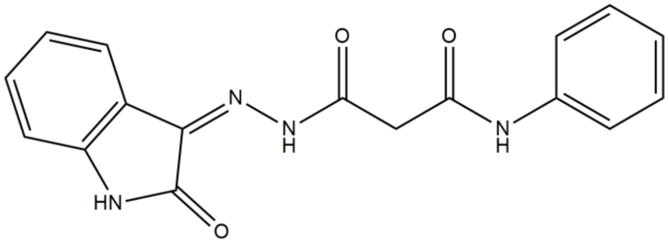

Figure 1. The chemical structure of KIHP.

2.1. Experimental Techniques and Materials

2.1. Materials

2.1.1. Solution

The corrosive solution of 1 M hydrochloric acid was prepared by diluting 37% HCl with distilled water. The concentrations of the investigated inhibitor were varied from 0.0001 to 0.0005 M, with freshly prepared distilled water according to the previous work [13].

2.1.2. Metal Alloy: Mild Steel

The working electrodes were made of mild steel whose elemental analysis in weight percent was 0.210 carbon; 0.380 silicon; 0.090 phosphorus; 0.050 manganese; 0.010 aluminum; 0.050 sulphur; and iron balance. Mild steel coupons with a surface area of 4.0 cm×1.0 cm was polished with various grades of sandpapers. It was rinsed with distilled water, washed with acetone, and dried in an oven. The initial weight of mild steel coupons was measured using an electronic balance.

2.1.3. Weight-Loss Analysis

In the current study, the usual exposure testing approach outlined in NACE TM0169/G31 [14] was obeyed. The gravimetric measurements were conducted in aerated environments. The investigated mild steel coupons were placed in reaction bottles in the absence and in the presence of various inhibitor concentrations in 1 M HCl solution. Mild steel coupons (4.0 cm×2.5 cm×0.5 cm) were suspended in the corrosive environment for various immersion periods (1, 5, 10, 24 and 48 h) in triplicate. The solution temperature was kept at 303 K in a Thermo Scientific precision water bath. The experiments were repeated at different temperatures (303, 313, 323, and 333 K) for 5 hours as immersion time. The tested inhibitor concentrations were 0.0001, 0.0002, 0.0003, 0.0004, and 0.0005 M. The tested coupons were taken after immersion periods and exposed to the ASTM standard G1-03 post-treatment techniques. The average mass loss (g) was utilized to determine the corrosion rate [15] according to the relation (1).

$$C_R(\text{mm/year}) = \frac{87600W}{\rho a t} \tag{1}$$

where C_R is the corrosion rate, W is the average mass loss (g), ρ is the steel density ($\text{g}\cdot\text{cm}^{-3}$), a is the surface area (cm^2), and t is the exposure time (h).

The inhibition efficiency of the tested inhibitor was calculated according to the following equation.

$$\%IE = \frac{w_0 - w}{w_0}\cdot 100 \tag{2}$$

where $\%IE$ is the percent of inhibition efficiency, w_0 is the average mass losses of the tested coupons in 1 M HCl environment in the absence of tested inhibitor, and w is the average mass losses of the tested coupons in 1 M HCl environment in the presence of the tested inhibitor.

2.2. Computational Details

The conventional theory addressing Becke's three-parameter hybrid functional (B3LYP) level using Gaussian 03 series with the 6-31G basis set was used to undertake quantum chemistry computations for the gas phase utilizing density functional theory (DFT) approaches. The ChemOffice application was used to perform all the computations. Relations (3) to (6) were used to compute the physicochemical characteristics [16] including the energy of the highest occupied molecular orbital energy (E_{HOMO}), the energy of the lowest unoccupied molecular orbital energy E_{LUMO}, energy gap $E = E_{\mathrm{HOMO}} - E_{\mathrm{LUMO}}$, chemical hardness (η), chemical softness (σ), and electronegativity (χ).

$$\Delta E = E_{\mathrm{HOMO}} - E_{\mathrm{LUMO}} \tag{3}$$

$$\eta = -\frac{E_{\mathrm{HOMO}} - E_{\mathrm{LUMO}}}{2} \tag{4}$$

$$\sigma = \frac{1}{\eta} \tag{5}$$

$$\chi = -\frac{E_{\mathrm{HOMO}} + E_{\mathrm{LUMO}}}{2} \tag{6}$$

3. Results and Discussion

3.1. Weight Loss Measurements

Figure 2 depicts the rate of corrosion and corrosion inhibition efficiency for mild steel obtained from weight loss measurements in 1.0 M HCl environment with and without the addition of various concentrations of KIHP, the corrosion prevention efficacy was tested at 303 K for various immersion periods [17, 18].

When the concentration of KIHP was raised, the rate of mild steel corrosion fell dramatically whereas the protective efficacy rose, as seen in Figure 2. The larger surface coverage induced by inhibitor molecules adsorbing on the steel surface accounts for the enhanced inhibitory efficiency [19, 20]. The adsorption coating can block active sites, essentially separating the studied specimen from the acid solution. When comparing to the analogous synthetic corrosion inhibitors tested before (Table 1), 3-keto-3-((indolin-2-oneylidene)hydrazinyl)-*N*-propionanilide (KIHP) shows the best performance of corrosion inhibition [21, 22].

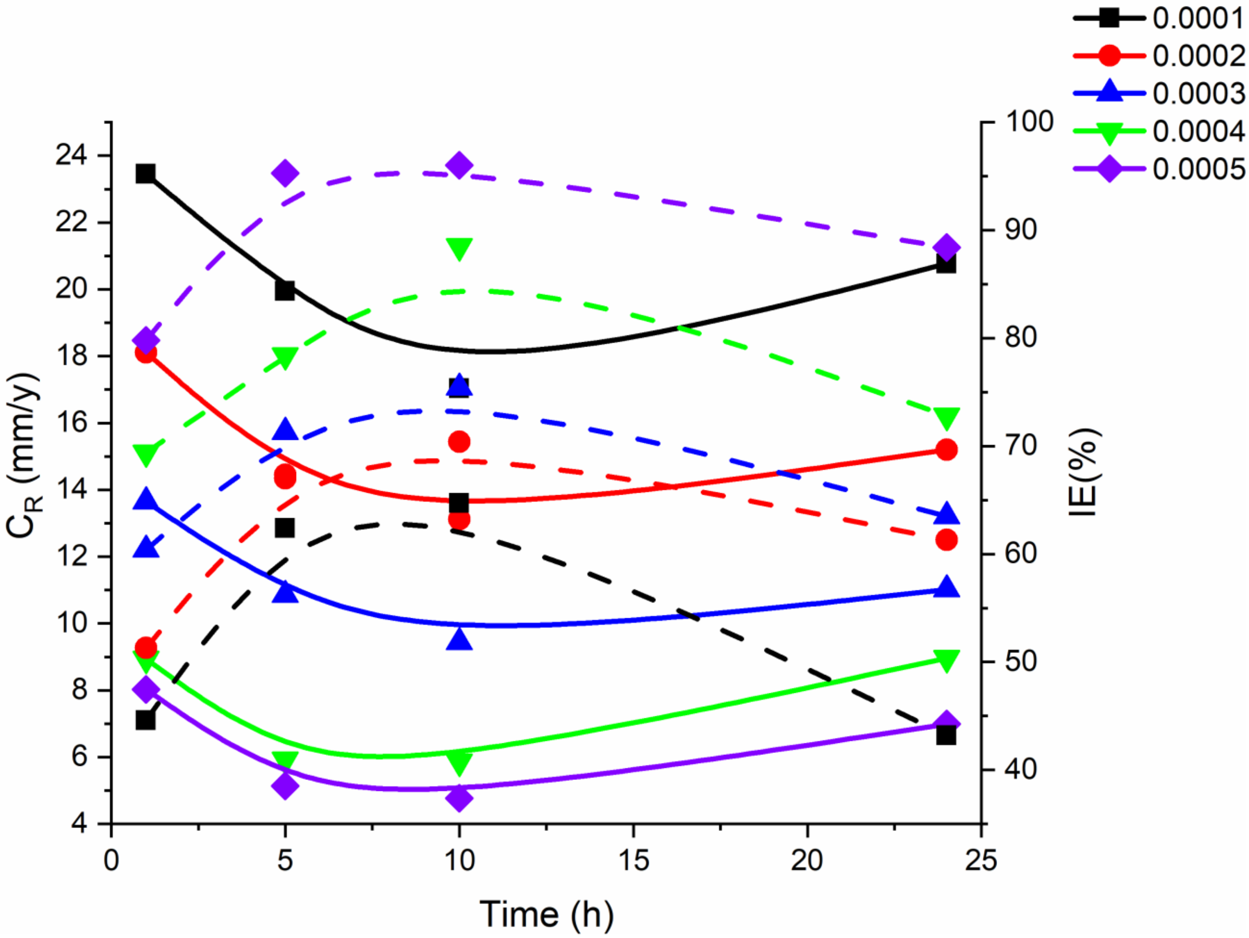

Figure 2. Data on mild steel coupon weight loss in 1.0 M HCl with varied inhibitor concentrations at 303 K and various exposure times.

Table 1. The inhibitory effectiveness of KIHP systematically compared to that of other recently researched synthetic corrosion inhibitors on mild steel in HCl solutions.

No.	Corrosion inhibitor	C (M)	Time (h)	*IE*%	Ref.
1	Current inhibitor (MQT)	0.0005	5	95.3	-
2	N'-(2-(2-Oxomethylpyrrol-1-yl)ethyl)piperidine	0.0005	5	91.9	23
3	2-Amino-4-phenyl-N-benzylidene-5-(1,2,4-triazol-1-yl)thiazole	0.0005	5	98.1	24
4	2-Amino-4-phenylthiazole	0.0005	5	94.7	24
5	1-Amino-2-mercapto-5-(4-(pyrrol-1-yl)phenyl)-1,3,4-triazole	0.0005	5	96.3	25
6	N'-(2-Hydroxybenzylidene)-2-(quinolin-8-yloxy)acetohydrazide	0.0005	5	93.4	26
7	3-(4-Ethyl-5-mercapto-1,2,4-triazol-3-yl)-1-phenylpropanone	0.0005	5	97	27

No.	**Corrosion inhibitor**	**C (M)**	**Time (h)**	***IE*%**	**Ref.**
8	4-Benzyl-1-(4-oxo-4-phenylbutanoyl)thiosemicarbazide	0.0005	5	92.5	28
9	4-Chloro-2-((pyridin-2-ylimino)methyl)phenol	0.0005	5	92.8	29
10	2-N-Phenylamino-5-(3-phenyl-3-oxo-1-propyl)-1,3,4-oxadiazole	0.0005	5	95.1	30
11	4-Ethyl-1-(4-oxo-4-phenylbutanoyl)thiosemicarbazide	0.0005	5	96.1	31
12	4-Pyrrol-1-yl-*n*-(2,5-dimethyl-pyrrol-1-yl)benzoylamine	0.0005	5	95.8	32
13	N'-(1-Phenylethylidene)-4-(1*H*-pyrrol-1-yl)benzohydrazide	0.0005	5	94.5	33
14	5-((4-Fluorobenzylidene)amino)-1,3,4-thiadiazole-2-thiol	0.0005	5	91	34
15	2-(5-Amino-1,3,4-thiadiazol-2-yl)-5-nitrofuran	0.0005	5	83.2	35
16	Terephthalo-hydrazide	0.0005	5	96.4	36
17	Isophthalohydrazide	0.0005	5	97.2	36
18	N-(Naphthalen-1yl)-1-(4-pyridinyl)methanimine	0.0005	5	91.5	37
19	2-Acetylthiophene thiosemicarbazon	0.0005	5	96	38
20	2-Isonicotinoyl-N-phenylhydrazinecarbothioamide	0.0005	5	96.3	39
21	2-Amino-5-(naphthalen-2-ylmethyl)-1,3,4-thiadiazole	0.0005	5	95.1	40
22	5-(4-(1*H*-Pyrrol-1-yl)phenyl)-2-mercapto-1,3,4-oxadiazole	0.0005	5	95	41
23	N-(2,4-Dihydroxytolueneylidene)-4-methylpyridin-2-amine	0.0005	5	93.7	42

The current inhibitor (KIHP) can indeed be comparable to other reported corrosion inhibitors derived from heterocyclic compounds to prevent corrosion of the examined specimen surface in aggressive environments. The majority of heterocyclic chemicals examined exhibit a strong inhibitory impact, as seen in Table 1. KIHP has the strongest inhibitory efficiency among the heterocyclic compounds mentioned in Table 1 [23–28], as well as effectiveness similar to that reported in [29–42]. It has been discovered that increasing the concentration of KIHP reduces the corrosion rate while increasing the inhibitory activity. This could be because as the KIHP concentration grows, the inhibitor’s adsorption coverage on mild steel surfaces increases. The increase in surface coverage owing to inhibitor molecule adsorption on the steel surface may explain the increase in protection performance. By limiting the active sites, the adsorbed layer protects the steel substrate from the corrosive liquid. In comparison to the first heterocyclic inhibitors examined in Table 1, KIHP showed improved corrosion prevention. This phenomenon is linked to the effects of steric hindrance and substituents in inhibitor compounds. When the inhibitor was added to the corrosive media at a concentration of 0.0005 M, the highest inhibitory efficiency was observed. When the concentration was increased to 0.001 M, however, the inhibitory efficiency did not alter considerably.

3.2. Effect of Immersion Time

The inhibition performance can be improved as the concentration and exposure time increased, as per the mass loss results. After 5 hours of immersion, the anticorrosion efficacy at 0.0005 M concentration was found to be around 95%. Based on experimental findings, after 5 hours of exposure, there is no marked increase in anticorrosion efficacy, whereas after 24 hours of exposure, the inhibition efficiency decreases. This is attributable to the researched inhibitor’s desorption from the examined specimen and the specimen's protective layer’s instability [40]. Furthermore, after 48 hours of immersion, there was a considerable decline in inhibition efficacy.

3.3. Effect of Temperature

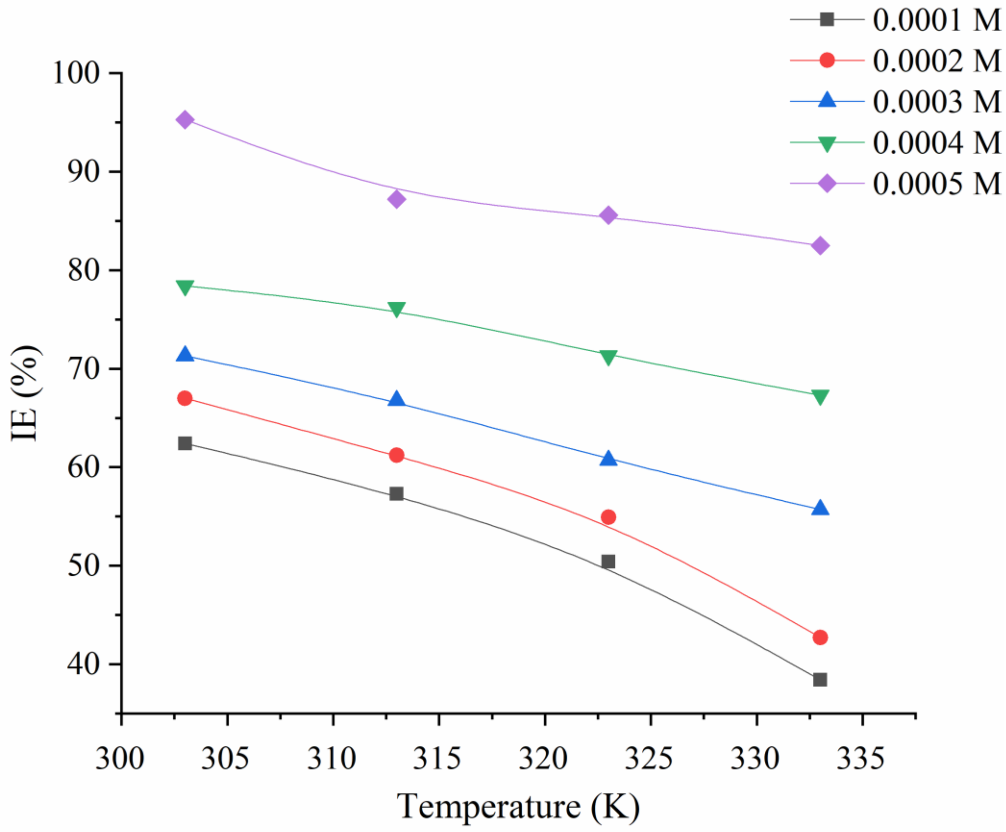

Figure 3. Mass loss analysis results of mild steel specimen in 1.0 M HCl at different temperatures (303–333 K) at various concentrations of the tested inhibitor.

Figure 3 depicts the effect of temperature on corrosion rate and inhibitive effectiveness in 1 M HCl at temperatures ranging from 303 to 333 K in the absence and presence of different inhibitor dosages. When all concentrations were examined, the ideal immersion time (5 hours) was determined based on the actual inhibiting efficiency observed. The preventive efficiency reduced as the temperature increased from 303 to 333 K. The desorption of adsorbed inhibitor molecules on the steel substrates could answer this question. As a consequence of the inhibitor adsorption on the surface of the steel, resistance occurs, and increasing temperature would promote the desorption of inhibitor molecules from the steel substrate [41].

3.4. Adsorption Isotherm

KIHP molecules' ability to be adsorbed on the metal substrate impacts their inhibiting efficiency. As an outcome, understanding the adsorption isotherm is essential, as it offers important information on the inhibitor molecules' interactions with the metal substrate. The corrosion–inhibiting process of mild steel substrates is influenced by the nature and chemical composition of inhibitor molecules, and how they are adsorbed on the surface (physisorption and/or chemisorption) [42]. Various adsorption models were used to estimate the optimal adsorption isotherm for the inhibitor concentration and surface coverage (θ). The equilibrium adsorption of the tested inhibitor in 1 M HCl environment obeys the Langmuir model on metallic surface.

Based on relation (7), θ depends on the concentration of the inhibitor and the equilibrium constant (K_{ads}) and all were determined according to the Langmuir model.

$$\frac{C}{\theta} = \frac{1}{K_{\mathrm{ads}}} + C \qquad (7)$$

When plotting $\frac{C}{\theta}$ *versus* C as seen in Figure 4, the value of the linear correlation coefficient (R^2) was found to be close to one, showing that the adsorption mechanism of the investigated inhibitor molecules in the acid medium on steel substrate follows the Langmuir adsorption model. The $\Delta G^0_{\mathrm{ads}}$ value was calculated using relation (8) [43].

$$\Delta G^0_{\mathrm{ads}} = -2.303RT\log 55.5K_{\mathrm{ads}} \qquad (8)$$

where R is the gas constant, T is the temperature, and 55.5 is the molar concentration of water.

Numerous studies have reported that when $\Delta G^0_{\mathrm{ads}}$ is negative, the inhibitor molecules' adsorption on the metalic substrate occurs spontaneously [44]. The value of $\Delta G^0_{\mathrm{ads}}$ for the investigated inhibitor in this research is $-34.5\ \mathrm{kJ \cdot mol^{-1}}$ (at 303 K), indicating that physisorption and chemisorption mechanisms influence adsorption [45]. The free energy values presented in Table 2 indicate that at all tested temperatures, the adsorption process follows both physisorption and chemisorption mechanisms.

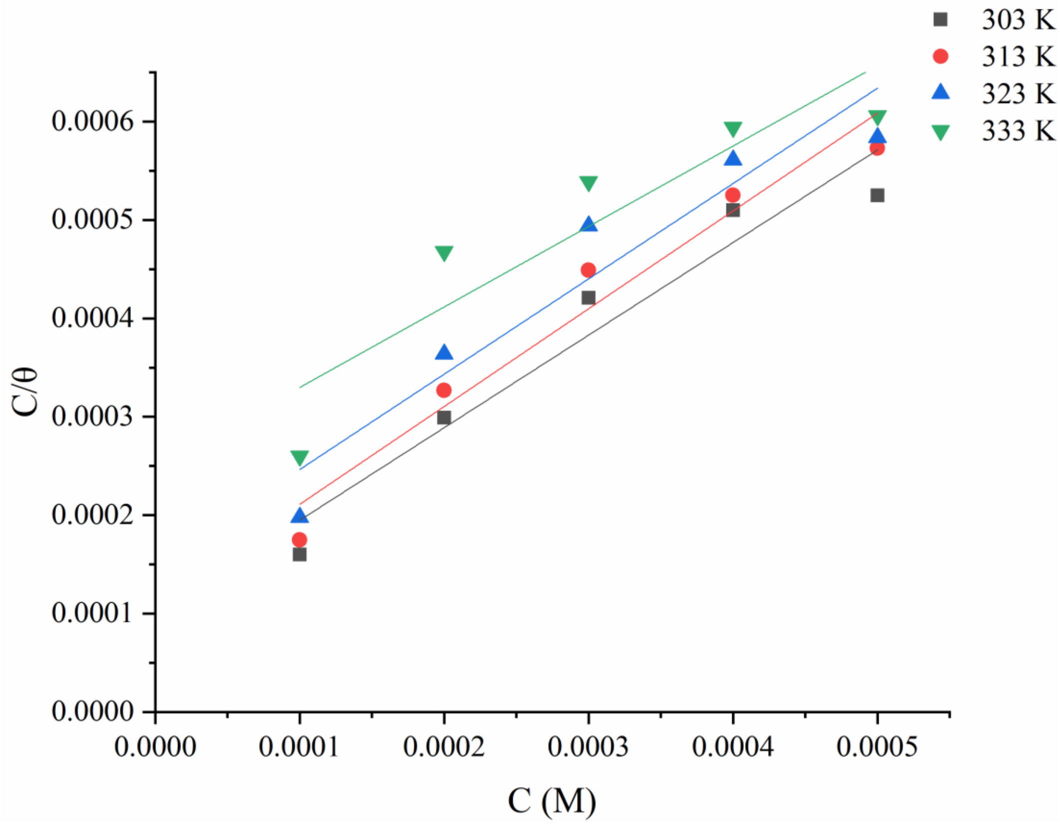

Figure 4. The Langmuir adsorption model for the adsorption of KIHP molecules in 1 M HCl on a mild steel specimen at temperatures ranging from 303 to 333 K.

Table 2. Adsorption parameter (ΔG^0_{ads}) value for the tested inhibitor on mild steel in 1 M HCl based on Langmuir adsorption isotherm.

Temperatures	Adsorption parameter value
303 K	$-34.5\ kJ\cdot mol^{-1}$
313 K	$-34.2\ kJ\cdot mol^{-1}$
323 K	$-33.5\ kJ\cdot mol^{-1}$
333 K	$-32.1\ kJ\cdot mol^{-1}$

3.5. Quantum Chemical Studies

Quantum chemical calculations were performed using the density functional theory using B3LYP at the fundamental set 6-31G*. The suggested quantum values are presented in Table 3. E_{HOMO} and E_{LUMO}, for example, are essential in determining reactive chemical entities. As seen in Figure 5, the ability to donate an electron is typically associated with E_{HOMO}. As a result, an increase in E_{HOMO} indicates a greater willingness to donate electrons to the suitable acceptor with a vacant orbital. E_{HOMO}'s large values facilitate the absorption of protecting particles onto the metal substrate. The inhibitor's protective function was enhanced by increasing the transport process of the adsorbent film [46]. Under both physical and chemical adsorption techniques [47], the obtained quantum chemical research is reliable. The conducted quantum chemistry research proves all physisorption and chemisorption processes, as evidenced by a negative E_{HOMO} and other thermodynamic properties. Because the energy gap is associated to the softness and/or hardness of the inhibitor molecules, earlier research has found that a high value for ΔE indicates that the inhibitor molecules are reactive [48]. A soft molecule with a lower energy gap is much less active than a hard one. In addition to the value of dipole moment (μ), the E value suggests that the investigated inhibitor molecules have a significant inhibitory effectiveness for steel specimen corrosion prevention in 1 M HCl environment.

Many experts believe that donors–acceptor reactions can cause the adsorption of heteroatoms with a significant negative charge on the mild steel surface [49]. Furthermore, a low electronegativity and a low molecular weight facilitate efficient adsorption of tested inhibitor molecules on the mild steel surface, lowering the steel surface's corrosion rate.

Table 3. Electronic properties of KIHP determined by DFT.

Inhibitor	**E_{HOMO}, eV**	**E_{LUMO}, eV**	**ΔE, eV**	**η**	**σ**	**χ**	**μ**
KIHP	–9.004	–4.216	–4.788	2.394	0.4177	6.11	7.0919

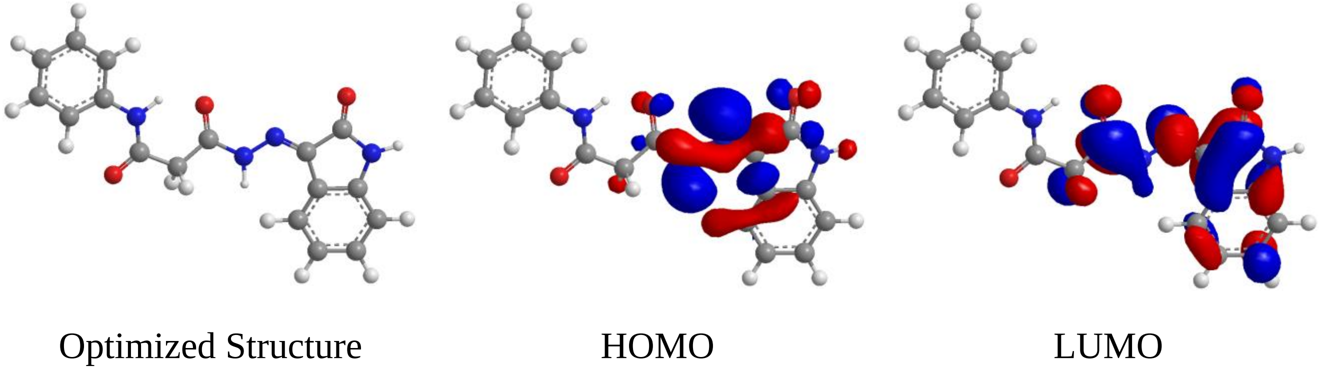

Figure 5. The electronic structures of KIHP.

Conclusions

The study's main findings are as follows:

1. A propionanilide derivative, 3-keto-3-((indolin-2-oneylidene)hydrazinyl)-*N*-propionanilide (KIHP), showed a significant inhibitory activity for steel specimens in 1 M HCl solution.
2. Mass loss studies revealed that an increase in KIHP concentration is accompanied by an increase in protective efficacy and a decrease in corrosion rate.

3. The Langmuir isotherm model was used to explain the adsorption of KIHP molecules on mild steel surfaces.
4. Quantum calculations revealed that the inhibitory impact of KIHP molecules rose as the EHOMO value grew and decreased as the ΔE value decreased. The theoretical conclusions from density function theory computations agreed well with the findings of the mass loss study.
5. Chemical adsorption of KIHP molecules on mild steel surface, as well as van der Waals interactions (physical adsorption) between the inhibitor molecules and the mild steel surface, may be responsible for the adsorption of KIHP molecules on the mild steel surface.

Conflict of Interest

The author declares no conflict of interest.

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