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Inhibition Studies of Aluminium Alloy (2024) Corrosion in Acid Hydrochloride Solution Using an Expired Phenylphrine Drug

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WEIGHT loss method was used to investigate the inhibition and adsorption behavior of phenylephrine drug for aluminum2024 alloy corrosion in 1 M acidic chloride solution at 293-303 Kelvin. Results obtained indicate that phenylephrine act as inhibitor for Al 2024 alloy in molar hydrochloric acid solution. Increasing both phenylephrine concentration and temperature lead to increase the inhibition efficiency, which is indicating the chemisorption mechanism. The adsorption of the phenylephrine onto the Al 2024 alloy surface follow Langmuir adsorption isotherm model. The mechanism of inhibition was additionally proved by the activation parameters results that obtained from the experimental data. SEM image shows a smoothed surface of Al 2024 alloy in the presence of phenylephrine in acidic solution. Quantum chemical calculation was used to correlate inhibition efficiencies data of phenylephrine with its electronic structural parameters. Theoretical calculations support the experimental results and elucidate working mechanisms.

Keywords: Weight loss, Phenylephrine, Aluminum alloy, Acid hydrochloride.

Introduction

Aluminum and its alloys have superior electrical with thermal conductivities and for this reason they are used in verified employments and newly in the manufacture of integrated circuits [1, 2]. So, study of its corrosion inhibition is of high significance. hydrochloric acid is vastly used as pickling acid, so this medium promoted a great important of aluminum research [3-5]. The molecular structure of the inhibitory molecules is fundamentally influence on the inhibition efficiency of an inhibitor [5, 6]. Organic compounds containing sulphur, oxygen, nitrogen, and phosphorus in their functional groups are the most notable inhibitors for corrosion studies [7–11]. The adsorption of these compounds on the metal surfaces was suggested to be the inhibitory mechanism, through the lone pairs of electron, of the organic functional groups [12]. Moreover, current research was directed to identify cheap and environmentally safe corrosion inhibitors, so a well number of drugs are known to have most of these qualities [13,14]. Recently, drug compounds were used in wide range as inhibitors due to the presence of hetero atoms like nitrogen, sulphur, oxygen and ð- bond in their structure and because of their safe use, high solubility in water and high molecular size, as a result the use of drug compounds provide excellent inhibition potential for corrosion. Some of the azo-sulpha and anti-malarial drugs were reported as good corrosion inhibitors **[**15,16**].** Many researchers have studied the use of drugs Specifically antibacterial as corrosion inhibitors [17]. For example, Eddy and Ebenso [17] investigated on Corrosion Inhibition and Adsorption Characteristics of Tarivid on Mild Steel in H_2SO_4 using thermometric and gasometric methods. Their finding showed that tarivid drug inhibits the deterioration of mild steel in the acid environment (H_2SO_4). The inhibition efficiency of tarivid was established to increase in values as its concentration increased however; it decreased as the temperature increases. The mechanism of physical adsorption was proposed from the acquired kinetic and thermodynamic factors. Also, Langmuir isotherm adsorption model was followed. Abdallah [18] studied the

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effect of Rhodanine azo-sulpha drugs as corrosion inhibitors on the corrosion of 304 stainless steel in HCl environment using gravimetric and potentiodynamic methods. Parallel adsorption technique was used for the inhibition process on the steel surface because of the presence of multiactive center within the molecules of the inhibitor. Solmaz et al. [19] have shown that Rhodanine is a good corrosion inhibitor for low carbon steel in hydrochloric acid. They used electrochemical techniques for the corrosion findings. The effect of a number of antibiotic drugs, like; spectinomycin, paromomycin and streptomycin on the corrosion performance of zinc metal in hydrochloric acid environment was studied by [20], using some electrochemical and gravimetric techniques. The percentage of inhibition efficiency was discovered to be increasing as the concentration of drug increases but decreases with temperature. It has been discovered that majority of the drugs used display vital roles in biological reactions due to their antibacterial, anticonvulsant, antidiabetic, and other properties [21,22]. Phenylephrine [23] is an antibiotic drug. It's present in the formulations of several vasopressin medicines, in eye- washes, in medicines for relief of congestion, and in syrups .It's a crystalline white or pale yellow salt that is fairly soluble in water.

The aims of this study is to examine the inhibition possibility of aluminum alloy (2024) corrosion in molar hydrochloric acid solution using phenylephrine drug by weight loss and computational methods. The temperature effect on the corrosion rate was studied in the extent of temperatures from 293 to 303 K. The adsorption thermodynamic parameters, such as enthalpy of adsorption, $\Delta H_{ads.}$, entropy change of adsorption, $\Delta S_{ads.}$, and adsorption of free energy change, $\Delta G_{ads.}$, were determied.

Experimental

Inhibitor

The IUPAC nomenclature of Phenylephrine drug is Benzene- methanol,3- hydroxy-α[(methylamino)methyl]-hydrochloride (R)[24], and it's molecular formula ($C_9H_{10}O_2N$) and weight of molecular structure of 368 g/mol. The chemical and optimized structures are shown in Scheme 1.

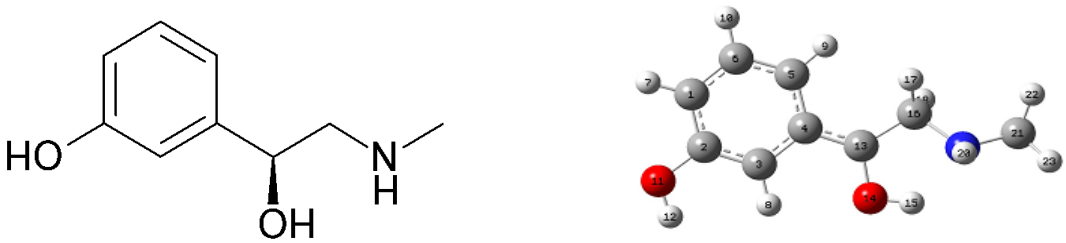
The Capsules of phenylephrine was obtained from Samarra Drugs Industry (SDI) with a purity exceeding 99% under the trade name "phenylephrine hydrochloride". Different drug concentrations were prepared by dissolving appropriate weights of the phenylphrine in 50 ml of 1M HCl solution.

Corrosion medium

The aggressive 1 M HCl solution to be prepared by diluting the analar grade of 37% HCl with distilled water. The concentration of the drug solutions (inhibitor) ranges from (100 ppm) to (500 ppm) were prepared and used.

Aluminum alloy (2024) Specimen

Al2024 alloy have the following chemical compositions as (wt%) (Cr 0.1%), (Mn 0.3-0.9%), (Zn 0.25%), (Si 0.5%), (Fe 0.5%), (Cu 3.8-4.9%), (Mg 1.2-1.8%) and balance Al. Circular shape samples of Al2024 alloys were mechanically cut with dimensions of 2.5 cm diameter and 0.5 mm thickness was used in this study. Prior to each experiment, the test specimens were polished with emery silicon carbide paper in different grades (320, 500, 1000, 2400, 4000) with diamond product sprays that contain ethanol with different size of the diamond particles (1µm, 3µm, 6µm, 9µm), then washed with acetone and finally rinsed with distilled water and keep in a desiccator for further use.



Scheme 1. Chemical and optimized Structure of Phenylephrine drug .

Weight Loss Experiment

Weight loss experiments were done under total immersion using 200 mL capacity beakers containing 100 mL 1M HCl solutions at 293–303 K maintained at thermostat with an accuracy of ±0.01 °C. The Al2024 alloy specimens were weighed and immersed in the beaker with the help of another smaller beaker with a capacity of 10 ml. The specimens were recaptured at half hour interval gradually for three hours, washed thoroughly in distilled water, dried with acetone, and then weighed again. The losses in weight , in mg, was taken as the difference in the weight of the Al2024 alloy specimens before and after flooding in different test solutions.

The corrosion rate (C_R) was determined using the following equation[25]:

$$C_R \text{ (mg/cm}^2 \text{ h)} = (w / A\, t) \quad \text{.....(1)}$$

where (w) is the average losses of weight for Al2024 alloy , the represents the surface area of an alloy, (t) is the flooding period in hour , (d) is the density of aluminum which is in g cm^{-3}. inhibition efficiency (IE%) obtained by using the relation[25]

$$IE\% = (1- C_R /C_R^{o}) \text{ x}100 \quad \text{.....(2)}$$

C_R and C_R^{o} are respectively, the corrosion rate of Al2024 alloy specimen in the absence and presence of different concentrations of Phenylphrine as well as, in different temperatures of 293, 298 and 303 K. An expression of (1- C_R / C_R^{o}) was used to determine the surface coverage (θ) of aluminum alloy (2024) by inhibitor molecules.

Computational Details

Gaussian 03 software were used for quantum chemical calculations. The Phenylphrine structure has been used as the performer one for theoretical studies. Density Functional Theory (DFT) was provided the Phenylphrine optimized structures which involve the Backe's three Parameter hybride functional and Lee-Yang-Paar Correlation functional (B3LYP) with 6–31G basis set. The evaluated parameters were: energy (TE), the highest filled molecular orbital energy (E_{HOMO}), the lowest unfilled molecular orbital energy (E_{LUMO}), the energy gap between E_{LUMO} and E_{HOMO} (ΔEgap), dipole moment (μ), The number of electrons transferred from the molecule to the surface (ΔN).

Results and Discussion

Weight Loss Method

Effect of Inhibitor concentration

The inhibitive effect of Phenylphrine addition at various concentrations on the Al2024 alloy corrosion in (1 M) HCl at varying temperatures at the range of 293 to 303 K were studied chemically using weight loss measurements. The obtained parameters from this study such as the corrosion rate (C_R) and protection efficiency (PE %) are tabulated in Table 1. The C_R values of Al2024 alloy in 1 M HCl decreases, while the PE values increases as increasing the concentrations of an inhibitor in 1 M HCl solution. At 500 ppm concentration, Phenylphrine exhibit maximum PE of 83.92%, which represent satisfactory inhibition ability. This behavior can be attributed to the adsorption and the coverage of the studied inhibitor on Al2024 alloy surface.

TABLE 1.Corrosion rate (C_R), Inhibition Efficiency (IE%) and Surface Coverage (θ) of Al2024 alloy corrosion in 1M HCl solution in the absence and presence of various concentrations of Phenylphrein drug at 3 hour immersion and at various temperatures in the range 293-303 K.

Inhibitor conc./ ppm	C_R (mg/cm².h)			IE %		
	293	298	303	293	298	303
Blank	0.698	1.324	1.437	-	-	-
100	0.327	0.503	0.469	53.17	58.23	74.32
200	0.269	0.412	0.462	61.48	64.35	74.81
300	0.267	0.286	0.3101	61.76	78.39	78.43
400	0.224	0.273	0.279	67.92	79.83	80.58
500	0.194	0.2256	0.231	72.22	82.96	83.92

The data obtained regarding the corrosion rate of Al2024 alloy in 1M HCl without and with varying concentrations of phenylphrine drug indicates that the rate of corrosion was decreased with the various concentrations of phenylphrine with the smallest quantity given at 500 ppm of phenylphrine that used at all temperatures that studied. Further examination in the table showed that the rate of corrosion of Al2024 alloy when the phenylephrine was presence increases as the temperature increases.

Figure 1 a, b and c are respectively, represent a plots of weight loss versus immersion time for Al2024 alloy in (1 M) HCl solution when the various concentrations of phenylphrine drug absence or presence at (293) to (303) K. It is clear from the plots that the weight loss of 2024 alloy in the different test media increases with time and decreases with increasing phenylphrine concentration. The non linearity of the weight loss curves plot may be indicates that the corrosion process of Al2024 alloy is heterogeneous and involving many steps. On the other hand, plots show that loss of weight for the 2024 alloy when addition of phenylphrine was depended on the concentration, that the loss of weight decrease as concentration of phenylphrine increase.

Inspection of temperature dependence of inhibition efficiency in the presence of inhibitor gives some insight into the possible mechanism of inhibitor adsorption [26]. Inhibition efficiency increase with increasing in temperature is may be attributed to the indicative with formation of adsorbed chemical layer, while inhibition efficiency decrease with an increase in temperature is revealed to mechanism of physical adsorption [26,27]. The inhibition efficiency was found to increase with increase in temperature as shown in figure 3. This trend in inhibition efficiency with temperature obtained suggesting chemical adsorption of the phenylphrine molecules on the Al2024 alloy surface.

Temperature Effect on Corrosion Rate

For corrosion reaction that in which corrosion rate increases with an increase in temperature, kinetics parameters were calculated by using Arrhenius equation [28].

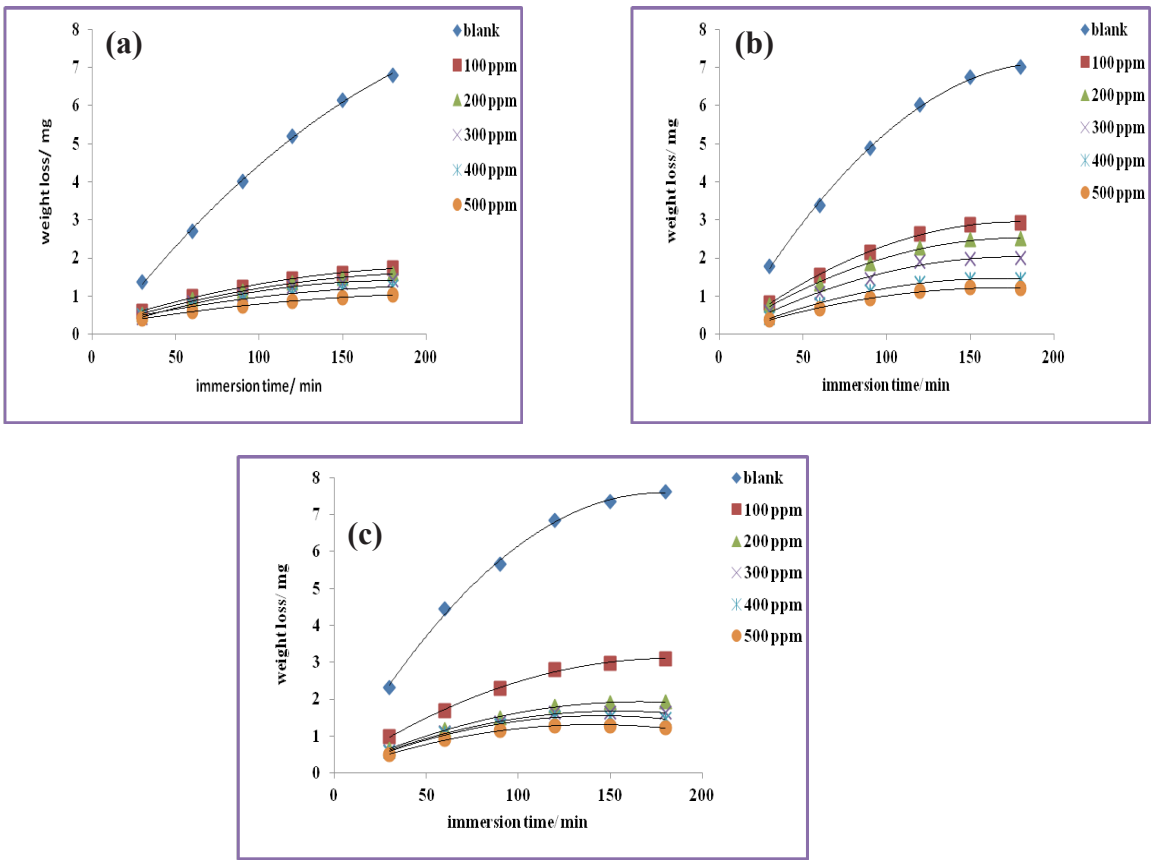


Fig.1.Weight loss versus immersion time for Al2024 alloy corrosion in 1 M HCl in the absence and presence of different concentrations of phenylphrine drug at (a) 293 (b) 298 and (c) 303 K.

$$\log C_R = \log A - E_a/RT \quad .....(3)$$

where C_R is corrosion rate, A and Ea are the pre-exponential factor and energy of activation of the corrosion process respectively, R is constant of the gas in Joule and T the absolute temperature. A plot of ($\log C_R$) versus (1/T) for Al2024 alloy corrosion at (1 M) HCl if the various concentrations of phenylphrine is absence and presence that shown in Figure 4, linear relations were given. The E_a values were then tabulated at the table 3. From the data tabulated in the table, it is obviously seen that the E_a values were greater than 20 kJ mol^{-1} in the absence and presence of the inhibitor compoun, indicating that the corrosion reaction is surface controlled [29], E_a in the presence of inhibitors is lower than that in the uninhibited solution, this indicate that the corrosion reaction of 2024 alloy is inhibited by chemical adsorption of phenylephrine molecules on alloy surface [30]. Lower values of E_a when the inhibitor is presence can be accumulated with decreasing the double layer thickness which impairs the E_a of the corrosion reaction [31]. It is an indication of a strong inhibitive effect of inhibitors by increasing energy barrier for the corrosion reaction, this emphasize that the chemical nature of the phenylephrine molecules adsorbed on the surface of Al2024 alloy [32]. Moreover, the values of E_a Confirm the electrostatic nature of the absorbing inhibitor on the surface of Al2024 alloy. Again, the observed decrease in activation energy phenomenon, E_a, at the highest efficiency of the inhibitor may arise from the transformation from a net corrosion reaction from that on the exposed surface to one that involves adsorbing locations [33].

Entropy of activation, ΔS* and enthalpy of activation, ΔH* were obtained from the Arrhenius transition state equation [34].

$$\log (C_R/T) = \log (R/Nh) + \log (\Delta S^*/2.303R) - \log(\Delta H^*/2.303R\ T) \quad ..... (4)$$

where N is the Avogadro's number, h is the Planck's constant. A plot of log (CR/T) as a function for (1/T) was made for Al2024 alloy in (1 M) of HCl in the absence and presence of vary concentrations of phenylphrine. From drawing straight lines are found, the slope is -ΔH* /R and the intercept is (logR/Nh + ΔS*/2.303R) from which the ΔH* and ΔS* values are computed and put them in table 4. If ΔH* have positive sign denote the endothermic nature of the corrosion process suggesting that the dissolution of 2024 alloy is decelerate and slaw. Also, lower values of ΔH* in the presence of phenylephrine molecules indicate that the inhibition efficiencies increase with increase in temperature [35]. On the other hands, the large negative value of ΔS* in the presence of inhibitor revealed that the formation of activated complex is the rate determining step, rather than the dissociation step. In the presence of the inhibitor, the values of ΔS* decreases and is generally interpreted as an increase in order as the reactants are converted to the activated complex [36]. It was also observed that small amount addition of phenylephrine to the acidic solution change the ΔS* (without presence of inhibitor) to a less negative values which reduces the corrosion rates. This observation can considered as indirect guide to support the proposed inhibition mechanism.

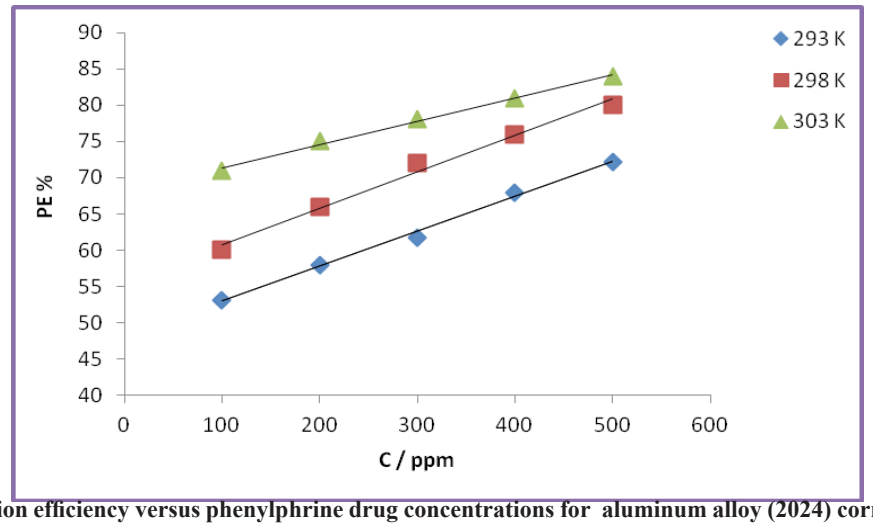


Fig. 2.Protection efficiency versus phenylphrine drug concentrations for aluminum alloy (2024) corrosion in (1 M HCl) in various temperatures at the range 293-303 K.

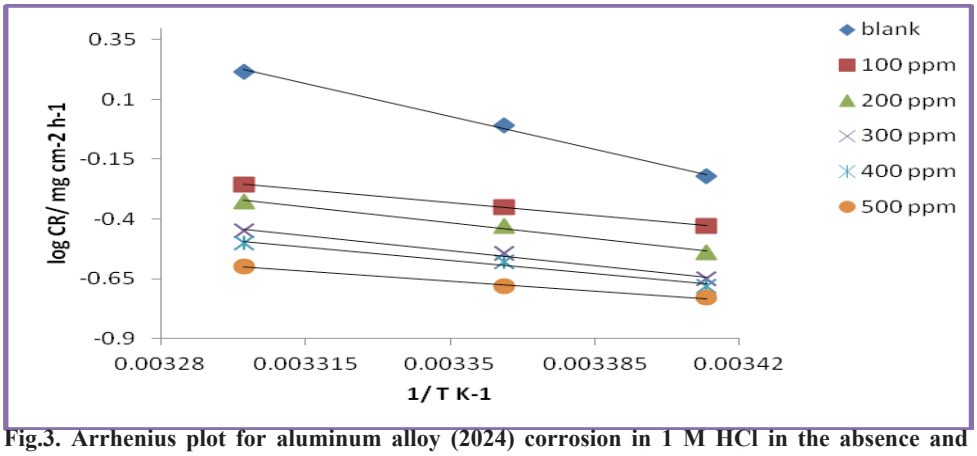


Fig.3. Arrhenius plot for aluminum alloy (2024) corrosion in 1 M HCl in the absence and presence of different concentrations of phenylphrine drug.

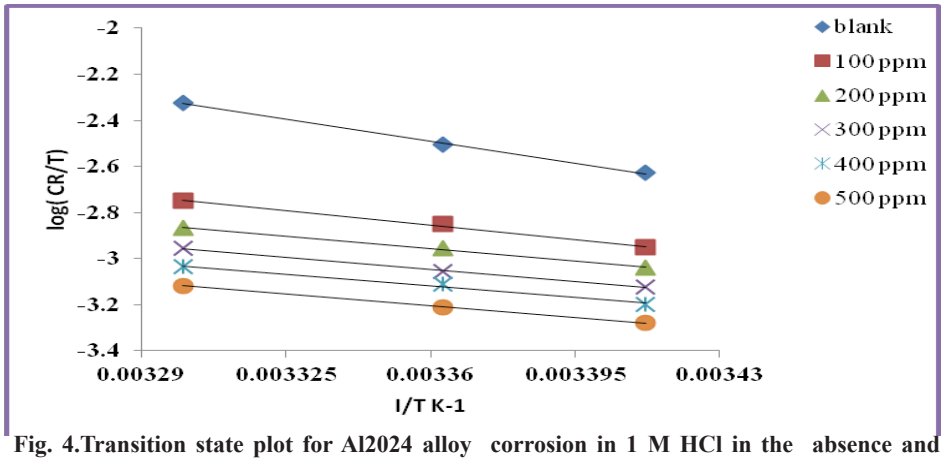


Fig. 4.Transition state plot for Al2024 alloy corrosion in 1 M HCl in the absence and presence of various concentrations of phenylphrine drug.

TABLE 2. Activation energy (E_a), Pre-exponential factor (A), activation enthalpy (ΔH^*), and the entropy of activation (ΔS^*) of Al2024 alloy corrosion in (1 M) hydrochloric solution with the presence or not presence of varies concentrations of phenylpherine drug at range of temperatures from 293 K To 313 K .

Inh. Conc. (ppm)	E_a (kJ.mol^{-1})	A$10^{25}\times$ (molecules.cm^{-2}.s^{-1})	ΔH^* (kJ.mol^{-1})	$-\Delta S^*$ (J.K^{-1}.mol^{-1})
-	32.47	3.713	22.67	69.81
100	16.80	2.693	14.93	136.66
200	15.78	2.571	13.46	154.89
300	14.73	2.433	12.74	155.56
400	13.23	2.250	12.59	158.54
500	13.02	1.698	12.07	163.84

Langmuir isotherm analysis

In order to investigate the adsorption behavior of the Phenylephrine drug on Al2024 alloy surface, Langmuir isotherm was applied on the experimental data. The best fit obtained for results supposes that the surface of Al2024 alloy contains a constant number of sites of adsorption and every site carried one adsorbed sort [37]. Langmuir isotherm suggests that each site holds one adsorbed species and can be represented by Equation

$$K_{ads.} = \theta / [C (1-\theta)] , \quad \ldots\ldots (5)$$

The equilibrium adsorption constant ($K_{ads.}$) and the Gibbs free energy at standard circumstances (ΔG^{o}_{ads}) for adsorption values which, respectively, obtained by using the following relations,

$$\Delta G^{o}_{ads} = -RT \ln (55.5\ K_{ads.}) \quad \ldots\ldots (6)$$

where 55.5 represents the concentration of water in solution. A plot of concentration of phenylphrine (C) versus C/θ data leads to a longitudinal line for R^2 quantity that is almost equal to one as showed in Figure 6.This suggested that adsorption of phenylephrine drug obeyed Langmuir isotherm. The adsorption parameters were presented in table 5. It is seen from the table that the $K_{ads.}$ values increases with increasing temperature showed that phenylephrine compound was chemically reacted with surface of the Al2024 alloy. It is also know that when the ΔG^{o}_{ads} values reached (-20) kJ mol^{-1} propose temporarily adsorption that called physical adsorption then reach (-40) kJ mol^{-1} propose permanent adsorption that is called chemical adsorption. The average quantities of ΔG^{o}_{ads} to phenylephrine drug is (-31.53) kJ mol^{-1}, denoted that the inhibitor when adsorbed on the surface of Al 2024 alloy to became general a chemical adsorption [38].

A $\Delta S_{ads.}$ and $\Delta H_{ads.}$ values were determined, respectively by a slope and linear plot of intercept of $\Delta G_{ads.}$ against different temperatures (T) for the corrosion of Al2024 alloy in 1 M HCl as shown in figure 7, and data obtained are put in table5. The values of $\Delta H_{ads.}$ Are positive indicates the adsorption process is an endothermic one. Generally; for endothermic process, by considering the value of ΔH_{ads} in order to differentiated between chemical and physical adsorption . For physical adsorption process, the enthalpy of adsorption is lower than (41) kJ mol^{-1} while that for chemical adsorption approaches 100 kJ mol^{-1} [39]. $\Delta H_{ads.}$ value of phenylephrine is 81.42 kJ mol^{-1} indicate a chemical adsorption of this inhibitor on alloy surface. The adsorption of inhibitor molecules is accompanied by positive values of $\Delta S_{ads.}$.

Mechanism of corrosion and inhibition

The mechanism of aluminum and its alloys corrosion in hydrochloric acid medium was explained based on the proposed mechanism. Due to this mechanism, the anodic and cathodic reactions can be expressed as:

$$Al_{(s)} \qquad Al^{3+} + 3e \qquad \text{(oxidation)}$$

$$2H^{+} + 2e \qquad H_{2\,(g)} \qquad \text{(reduction)}$$

The overall electrochemical reaction is

$$2Al + 6H^{+} \qquad 2Al^{+3} + 3H_{2\,(g)}$$

The chemisorbed hydrogen atoms produce from cathode reaction when selecting the electron which be free in the oxidation reaction, $H^{+} + e = H_{adsorbed}$ in corrosion of aluminum in hydrochloric acid. In similar acidic media, chemisorbed hydrogen atoms that appear on the aluminum roof are interacts with adsorbed hydrogen atom to obtain hydrogen gas on the roof of aluminum. Small amount of the unreacted adsorbed hydrogen atoms will still uncombined; So, this quantity does not effect on the process. Conformable data gave it for the rates of corrosion that calculated from the method of weight loss which shown in Table 1.

It is well known [40] provided that an inhibitor can effect on the rate of corrosion of metals in a corrosive medium if it is capable to effect on the kinetics of dissolution or change electrochemical behavior position. This behavior is occurring when the inhibitor formed as thin film at a surface of the metal by the processes of adsorption. The formation of this film is usually resulted by adsorption for anionic inhibitors at positive locations produced at aluminum roof which resulting by resealed of electrons at the oxidation process. The protective coating film will separate a metal of aluminum from the medium which corrosive and, keeps more aluminum atoms from departure the metal roof to the medium which decreased the rate of corrosion. As a result, the oxidation interaction may be regarded as the rate-determining step in the corrosion reaction.

Khairou and El-Sayed [41] found that a rate of corrosion decreases when the inhibitor molecules contained hydroxyl groups, as these groups have

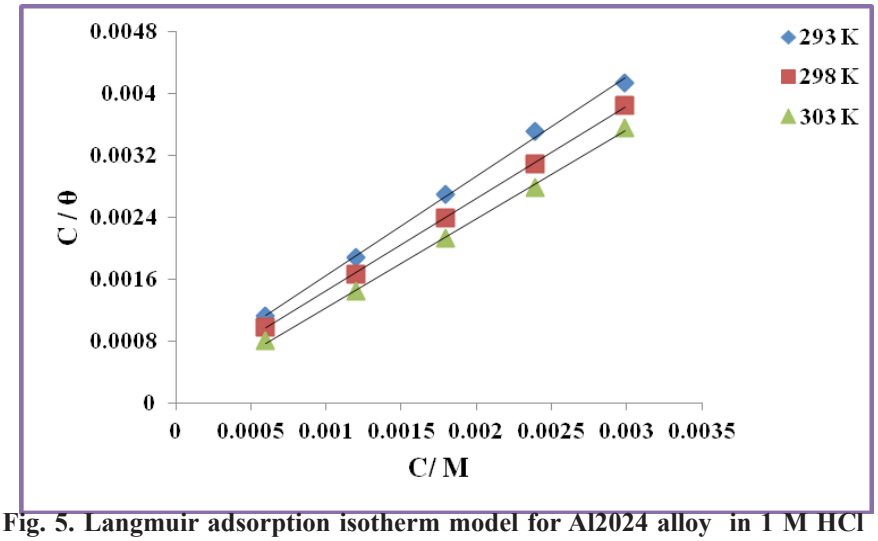


Fig. 5. Langmuir adsorption isotherm model for Al2024 alloy in 1 M HCl containing phenylephrine at different temperatures in the range 293-303 K.

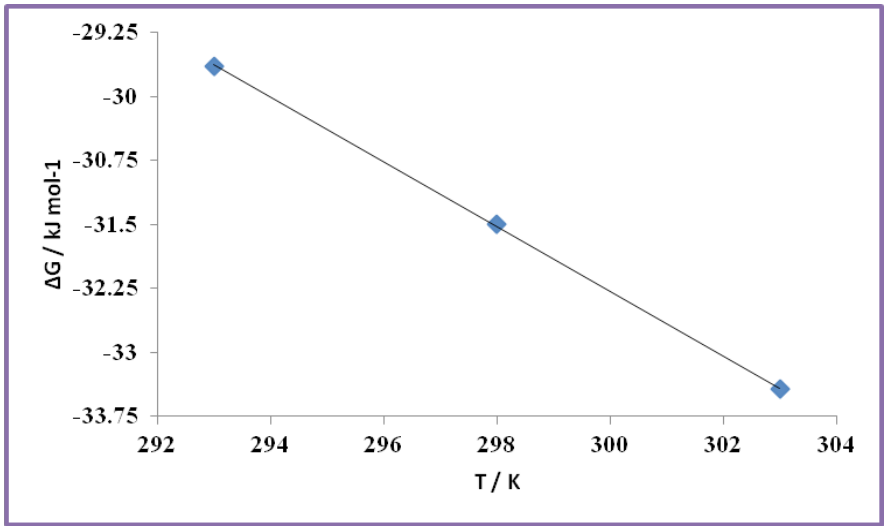


Fig. 6. Gibbs free energy of adsorption versus temperature for Al2024 alloy in 1 M HCl containing phenylephrine drug.

TABLE 3. Thermodynamic parameters for adsorption of the Phenylephrine drug on the surface of Al2024 alloy in 1M HCl solution.

T (K)	R^2	K_{ads} (M^{-1})	$-\Delta G_{ads}$ ($kJ.mol^{-1}$)	ΔH_{ads} ($kJ.mol^{-1}$)	ΔS_{ads} ($J.K^{-1}.mol^{-1}$)
293	0.9997	3468.80	29.64	81.42	379.00
298	0.9997	6604.72	31.74		
303	0.9998	11061.95	33.57		

the ability to form a connection bridge between the inhibitor molecules and the surface of the metal as shown in figure 7. In addition, lone-pairs of electrons that presence on the oxygen atoms of the hydroxyl groups of the phenylphrine may lower an inhibitor reaction and the positive locations which formed at aluminum roof.

Computational results

The calculation of quantum chemical has potential application in designing and subsequent development of many organic corrosion inhibitors in the field of corrosion inhibition chemistry [42]. To study the relationship between the molecular structure of inhibitors and their ability to inhibit corrosion, the density function theory is used [43]. Chemical parameters, which include a higher energy full orbital with electrons (E_{HOMO}). the lower energy of the orbit is not full with electrons (E_{LUMO}) , the energy difference between them, hardness(S) , absolute electronegativity (χ) as well as the number of electrons transferred and dipolar moment (μ)determined in the table No. The chemical reactivity of phenylphrine molecules has a significant relationship with the energy of molecular orbitals of this compound, which contains an occupied higher molecular energy E_{HOMO} and lower of unoccupied molecular orbital energy E_{LUMO}. E_{HOMO} refers to the ability of the organic compound to donate an electrons where the high value of it indicates a high ability to give electrons while E_{LUMO} indicates the ability of the compound to accept electrons and therefore the ability of compounds increases with increase E_{HOMO} and decrease of E_{LUMO}, and ΔE [44]. In this work, the results obtained indicate that the compound is a good inhibitor. The dipole moment of the molecule is a good parameter to describe the polarity [45]. Thus, inhibitor with higher dipole moment value refers to large ability of it to be adsorbed on the metal surface [46]. The estimated value of the dipole moment of phenylphrine is 3.0546 Debye and this value is more than the dipole moment of water (1.88 D). The number of electrons that transferred from the inhibitor molecules to the metal surface is defined by ΔN which shows the inhibition efficiency[47]. Depending to researchers [48], if the estimated value of Δ*N* is lower than 3.6, so this indicates that the inhibition efficiency increase with increasing the ability of electron donating of the inhibitor molecules to the surface of a metal. The value of Δ*N* is -0.017025 as shown in Table 4, this indicates that the phenylephrine molecules is electron donors to the surface of the (2024) aluminum alloy which is an acceptor. The obtained data from theoretical quantum chemical calculations relieves good evidence to the obtained experimental results by weight loss technique.

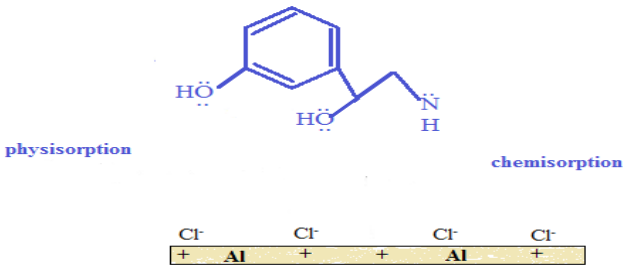
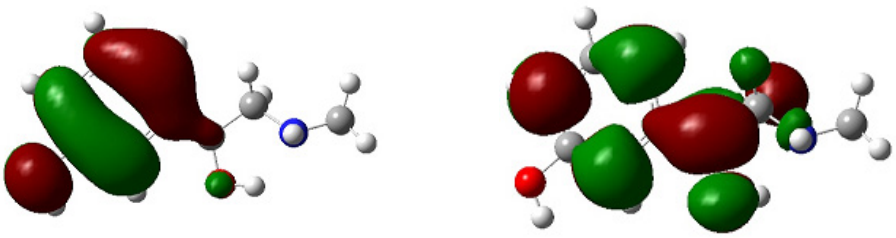


Fig. 7. A proposed adsorption mechanism of phenylephrine drug on aluminum alloy (2024).



HOMO structure LUMO structure

Fig. 8.Frontier molecule orbital density distributions of the inhibitor.

TABLE 4.The parameters of quantum chemical Calculated for inhibitor compound

parameters	Inhibitor compound
E_{HOMO} (eV)	-6.0993
E_{LUMO} (eV)	-0.1170
$\Delta E_{LUMO-HOMO}$ (eV)	5.9823
dipole moment (μ)	3.0546
$E_I = - E_{HOMO}$	6.0993
$E_A = - E_{LUMO}$	0.1170
η	2.99115
S	0.33432
χ	3.10815
W	0.49139
ΔN	-0.017025

Conclusion

Based on the results obtained from this study, the following conclusions obtained

- Various concentrations of phenylephrine drug were used successfully as corrosion inhibitors for Al 2024 alloy in HCl solution at different temperatures in the range 293-313 K.
- Corrosion current density data were decreased significantly with increasing of the phenylephrine drug concentration and increase with increasing studied temperature.
- The inhibition efficiencies of this inhibitor increase with increasing both concentration and temperature indicating chemical adsorption mechanism of drug molecules on aluminum surface.
- The kinetic results confirmed the chemical adsorption of phenylephrine drug on aluminum surface.
- Adsorbed phenylephrine drug molecules on the surface of Al2024 alloy obey Langmuir isotherm adsorption.
- A good agreement was obtained between theoretically calculated parameters and experimentally determined inhibition efficiencies for corrosion process of phenylephrine drug in HCl solution by using density function theory.

References

1. Burleigh T.D., Smith A.T., Evaluation of Natural Oxides on Aluminum in Neutral Borate Electrolyte technical papers, *J. Electrochem. Soc*.,139, 2799-2805(1992)
2. Lee E. J.Pyun S.J, The effect of oxide chemistry on the passivity of aluminium surfaces, *Corros . Sci.,* 37, 157-168, (1995).
3. Shyamala M., Arulanantham A., Ocimum sanctum (Tulasi) as Corrosion Inhibitor on Mild Steel in Hydrochloric Acid", *Nature environment and PollutionTech*., 7,415-422 (2008).
4. Ehteram, N., Potential of aqueous extract of Hibiscus sabdariffa leaves for inhibiting the corrosion of aluminum in alkaline Solutions, *J. Apple. Electrochem*, 39 .1465-1475, (2009).
5. Abiola K.O., Otaigbe J.O.E., Kio O.J., *Gossipium hirsutum* L. extracts as green corrosion inhibitor for aluminum in NaOH solution, *Corros. Sci*., 51,1879-1881(2009).
6. Ashassi-Sorkhabi H. , Nabavi-Amri S. A., Corrosion inhibition of carbon steel in petroleum/ water mixtures by Ncontaining compounds, *Acta Chimica Slovenica*, 47, 4, 507–517(2000).
7. Ouali I. El, Hammouti B., Aouniti A., Thermodynamic characterisation of steel corrosion in HCl in the presence of 2-phenylthieno (3, 2-b) quinoxaline, *Journal of Materials and Environmental Science*, vol. 1, 1, 1–8 (2010).
8. Sachin H. P., Khan M. H. M., Bhujangaiah N. S., Surface modification of mild steel by orthophenylenediamine and its corrosion study, *International Journal of Electrochemical Science*, 4(1), 134–143 (2009).
9. Umoren S. A., Eduok U. M., Oguzie E. E., Corrosion inhibition of mild steel in 1M H2SO4 by polyvinyl pyrrolidone and synergistic iodide additives,*Portugaliae Electrochimica Acta,* 26, 533–546 (2008).
10. Kumar A., Corrosion inhibition of mild steel in hydrochloric acid by Sodium Lauryl Sulfate (SLS), *E-Journal of Chemistry*, 5(2), 275–280 (2008).
11. Maayta A. K., Fares M.M., Al-Shawabkeh A. F., Influence of linear alkylbenzene sulphonate on corrosion of iron in presence of magnetic field: kinetic and thermodynamic parameters, *International Journal of Corrosion*, 20 (1), 9-18 (2010).
12. Niamien P. M., Trokourey A., Sissouma D., Copper corrosion inhibition in 1M HNO3 by 2-thiobenzyl benzimidazole:adsorption and chemical modeling of inhibition efficiency, *International Journal of Research in Chemistry and Environment*, 2(4), 204–214 (2012).

13. Ofoegbu S. U. , Ofoegbu P. U., Corrosion inhibition of mild steel in 0.1M hydrochloric acid media by chloroquine diphosphate, *ARPN Journal of Engineering and Applied Sciences*, 7(3), 272–276 (2012).

14. Kumar S. H., Karthikeyan S., Inhibition of mild steel corrosion in hydrochloric acid solution by cloxacillin drug, *Journal ofMaterials and Environmental Science*, 3 (5), 925–934 (2012).

15. Fouda A.S., Mostafa H.A., Mostafa H.A.,Elabbasy H.M.,Antibacterial drugs as inhibitors for corrosion of stainless steeltype304in HCl solution, *Journal of applied electrochemistry*, 40 (1), 163-173 (2010).

16. Bhat J. I.,Vijaya D.P.Alva;Meclizine hydrochloride as potential non-toxic corrosion inhibitor formild steel in hydrochloric acidmedium, *Archives of Applied Science research*, 3(1), 343-356 (2011).

17. Eddy NO, Ebenso EE. Corrosion inhibition and adsorption characteristics of tarivid on mi[ld steel in H2SO4E-Journal of Chemistry, 7(1), 442-448 (2010).

18. Abdallah M. Rhodanine azosulpha drugs as corrosion inhibitors for corrosion of 304 stainless steel in hydrochloric acid solution, *Corrosion Science,* 44(4), 717-728 (2002).

19. Solmaz R, Kardas G, Yazici B, Erbil M. Inhibition effect of rhodanine for corrosion of mild steel in hydrochloric acid solution, *Protection of Metals*, 41(6), 581-585 (2005).

20. Abdallah M, Zaafarany BA, Jahdaly AL. Corrosion inhibition of zinc in hydrochloric acid using some antibiotic drugs, *Journal of Materials and Environmental Science,* 7(4), 1107-1118 (2016).

21. Abood HA. The study of the inhibitory properties of Omeprazole on the corrosion of Aluminum 6063 in alkaline media, *Basrah Journal of Science*, 28, 74-93 (2011).

22. Uma K, Rekha S. Investigation and inhibition of aluminium corrosion in methane sulphonic acid solution by organic compound, *Journal of Chemical and Pharmaceutical Research*, 7(4), 165-169 (2015).

23. United States Pharmacopeia Drug Information (USP DI) Drug Information for the Health Care Professional, 15th Ed., Vol. I, J.A. Halperin (Ed.), United States Pharmacopeial Convention, Inc., Rockville, MD, Part II, 2235–2239 (1995).

24. Maryadele, JO Neil; The Merck Index, 13th edition, Merck Research Lab publishers, White House Station. NJ. USA,7370, 4571(2001).

25. Lodha S. R., *Pharmaceutical Reviews*, 6 (2008).

26. peter C. Okafor, Eno E. Ebenso and Udofot J. Ekpe ,Azadirachta Indica Extracts as Corrosion Inhibitor for Mild steel in Acid Medium, *Int.J.Electrochem. Sci*., 5 , 978-993 (2010).

27. Salman T.A.,Zinad D. S, Jaber Sh. H., AL-Ghezi M., Mahal A., Takriff M. S., Al-Amiery A., Effect of 1,3,4-Thiadiazole Scaffold on the corrosion Inhibition of Mild Steel in Acidic Medium:An Experimental and Computational Study*, J. Bio. Tribo. Corro*.,, 5:48, 1-11 (2019).

28. Zarrouk1 A., Warad I., Hammouti B., Kinetic Parameters of Activation , *Int. J. Electrochem. Sci.,* 5, 1516 – 1526, (2010).

29. Herrag L., Hammouti B.,Elkadiri S., Aouniti A., Jama C., Vezin H., Bentiss F., Adsorption properties and inhibition of mild steel corrosion in hydrochloric solution by some newly synthesized diamine derivatives: Experimental and theoretical investigations, *Corros. Sci*., 52, 3042–3051, (2010).

30. Popova A., Sokolova E., Raicheva S., Christov M., AC and DC study of the temperature effect on mild steel corrosion in acid media in the presence of benzimidazole derivatives, *Corros. Sci.,* 45, 33-58, (2003).

31. Solomon M. M., Umoren S.A., Udosoro I.I., Udoh A.P., Inhibitive and adsorption behaviour of carboxymethyl cellulose on mild steel corrosion in sulphuric acid solution‖, *Corros. Sci*., 52, 1317-1325, (2010).

32. Umoren S. A., Solomon M.M., Udousoro I.I., Udoh A.P., Synergistic and antagonistic effects between halide ions and carboxymethyl cellulose for the corrosion inhibition of mild steel in sulphuric acid solution, *Cellulose*, 17, 635-648, (2010).

33. Noor, E.A., Potential of Aqueous Extract of Hibiscus Sabdariffa Leaves for Inhibiting the Corrosion of Aluminum in Alkaline Solutions, *J. Appl. Electrochem*. 39, 1465–147 (2009).

34. Cheyad M. S. , Salman T.A., Characterization and Study the Inhibition Activity of Pomegranate Peel Extract for a-Brass corrosion in H_2SO_4 Solution, *Orient. J. Chem*., 33 (3), 1241-1251 (2017).

35. Guan N. M., Xueming I., Fei I., Synergistic inhibition between ophenanthroline and chloride ion on cold rolled steel corrosion in phosphoric acid, *Mater. Chem. Phys*., 86, 59-68, (2004).

36. El Ouali I.,Hammouti B., Aouniti A., Ramli Y., Azougagh M., Essassi E. M., Bouachrine M., Thermodynamic characterisation of steel corrosion in HCl in the presence of 2-phenylthieno (3, 2-b) quinoxaline *J. Mater. Envir. Sci*., 1, 1-8, (2010).

37. Singh P., Quraishi M.A., Ebenso E.E., Thiourea-formaldehyde polymer a new and effective corrosion inhibitor for mild steel in hydrochloric acid solution. *Int J Electrochem Sci,* 9, 4900–4912 (2014).

38. Singh P., Ebenso E.E., Olasunkanmi L.O., Obot I.B., Quraishi M.A. ,Electrochemical, theoretical, and surface morphological studies of corrosion inhibition effect of green naphthyridine derivatives on mild steel in hydrochloric acid. *J Phys Chem C*, 120, 3408–3419 (2016).

39. Badiea A. M., Mohana K. N., Effect of temperature and fluid velocity on corrosion mechanism of low carbon steel in presence of 2-hydrazino-4,7-dimethylbenzothiazole in industrial water medium, *Corros. Sci.,* 51, 2231-2241, (2009).

40. McCafferty, E. *Corrosion Control by Coating*; Leidheiser, H., Jr., d.; Science Press: Princeton, NJ, USA, 1979.

41. Khairou, K.S.; El-Sayed, A. Inhibition Effect of Some Polymers on The Corrosion of Cadmium in A Hydrochloric Acid Solution. *J. Appl. Polym. Sci*, *88*, 866–871 (2003).

42. Leila B.**,** Djahida H., Djamila A., Saida M., Salah Ch., Inhibitive properties and quantum chemical calculations of a new synthesized Schiff base 1-[(3hydroxyphenylamino)methylene]-naphtalen-2-one for XC48in hydrochloric acid solution*, Int. J. Electrochem. Sci.*, 13, 6734-6755 (2018) .

43. Bahram M.J., Hosseini S.M.A., Pilvar P., Experimental and theoretical investigation of organic compounds as inhibitors for mild steel corrosion in sulphuric acid medium, *Corrosion Science*, 52, 2793-2803 (2010).

44. Aytac A., Bilgic S., Gece G., Ancin N., Oztas S.G., Experimental and theoretical study of the inhibition effects of some Schiff bases as corrosion inhibitors of aluminium in HCl, *Materials and Corrosion*, 63 (8) 729-734(2012).

45. Ebenso E. E., Isabirye D. A., Eddy N. O., Adsorption and quatum chemical studies on the inhibition potentials of some thiosemicarbazides for the corrosion of mild steel in acidic medium, *Int. J. Mol. Sci*., 11(6) 2473-2498 (2010).

46. Ahamad I., Khan S., Ansari K.R., Quraishi M.A., Primaquine: A pharmaceutically active compound as corrosion inhibitor for mild steel in hydrochloric acid solution, *Journal of Chemical and Pharmaceutical Research*, 3(2), 703-717 (2011).

47. Khaled K.F., corrosion control of copper in nitric acid solutions using some amino acids-a combined experimental and theoretical study, *Corrosion Science*, 52 (10), 3225-3234 (2010).

48. Lukovits I., Kálmán E., Zucchi F., corrosion inhibitors-correlation between electronic structure and efficiency *, Corrosion*, 57 (1) 3-8 (2001).

دراسة امتزاز و تثبيط دواء الفنيلفرين على تاكل سبيكة الالمنيوم (2024) في محلول حامض الهيدروكلوريك

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تم استخدام طريقة فقدان الوزن للتحقيق في سلوك تثبيط وامتصاص عقار فينيليفرين لتآكل سبيكة الألومنيوم 2024 في محلول واحد مولاري من حامض الهيدروكلوريك في مدى الدرجات الحرارية 303-293 كلفن. تشير النتائج التي تم الحصول عليها إلى أن فينيلفرين يعمل كمثبط تاكل لسبيكة الالمنيوم 2024 في محلول حمض الهيدروكلوريك المولاري. تؤدي زيادة تركيز الفينيلفرين ودرجة الحرارة إلى زيادة كفاءة تثبيط ، 2024 مما يدل على آلية الامتزاز الكيميائي. يتبع امتزاز الفينيلفرين على سطح سبيكة الالمنيوم نموذج لانكماير ايزوثيرم. تم إثبات آلية تثبيط من خلال نتائج دوال التنشيط التي تم الحصول عليها 2024 من البيانات التجريبية. تُظهر صورة المجهر الالكتروني الماسح سطحًا ناعمًا لسبيكة الالمنيوم في وجود الفينيلفرين في المحلول الحامضي. تم استخدام الحساب الكيميائي الكمي لربط بيانات كفاءة تثبيط الفينيلفرين مع الدوال التركيبية الإلكترونية. تدعم الحسابات النظرية النتائج التجريبية وتوضح آليات العمل.