

Research Article

Computational and Experimental Evaluation of Inhibition Potential of a New Ecologically Friendly Inhibitor Leaves of Date Palm (*Phoenix dactylifera* L.) for Aluminium Corrosion in an Acidic Media

Oraas Adnan Hatem 

Department of Chemistry, College of Science, University of AL-Qadisiyah, Iraq

Correspondence should be addressed to Oraas Adnan Hatem; oraas.adnan@qu.edu.iq

Received 6 June 2022; Revised 13 July 2022; Accepted 15 July 2022; Published 4 August 2022

Academic Editor: Michael J. Schütze

Copyright © 2022 Oraas Adnan Hatem. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

PDL (*Phoenix dactylifera* leaves) is widely spread in Iraq and is known to be rich in phytochemicals as flavonoids, saponins, tannins, glycosides, oils, and lipids. The effect of PDL extract in reducing the corrosion of Aluminium in 1 M HCl solution using a weight loss technique, and computational chemistry calculations were investigated in this study. The study carried out at different temperatures (20, 30, 40, and 50) in the presence of plant extract and the absence of extract. A number of parameters were included to be detected in this study according to the density functional theory (DFT)/P3LYP/6-311G, including the highest occupied molecular orbital EHOMO, the lowest unoccupied molecular orbital ELUMO, energy gap ΔE , softness S , hardness η , dipole moment μ , electronegativity χ , electrophilicity ω , inhibitor-metal interaction energy $\Delta\psi$, and electrons transferred fraction ΔN . Two adsorption isotherms were used to explain inhibitor adsorption behavior. Two adsorption isotherms were used to explain inhibitor adsorption behavior, the Freundlich adsorption isotherm and the Langmuir adsorption isotherm, the Freundlich adsorption isotherm was discovered to be followed by the inhibitor with correlation coefficient values ranging from 0.98 to 0.94 with temperature increased from 20 to 50 degrees Celsius. The adsorption mechanism includes a physical adsorption process. The results showed that with the increment of the inhibitors concentration, there was an improvement of the inhibition efficiency. The most outstanding inhibitor efficiency was 97.7% at 10 mL/L inhibitor concentration.

1. Introduction

Numerous studies have been conducted on Aluminium and its alloys due to its high technological value and wide range of industrial applications, notably in the aerospace and domestic industries. Aluminium and its alloys, on the other hand, are reactive and prone to corrosion. Aluminium is dependent on the creation of a compact, firmly adhering, and continuous passive oxide coating when exposed to air or aqueous solutions. This is what gives Aluminium its corrosion resistance in most situations. When the metal is exposed to strong acids or bases, this amphoteric surface layer drastically deteriorates [1]. Aluminium metal has the ability to form a thin, stable oxide layer on its surface, but when aggressive media, such HCl, are pres-

ent, this stable layer is disrupted, and the metal starts to corrode [2]. In the industry, numerous compounds are used as corrosion inhibitors to eliminate or minimize metal corrosion in acidic environments. Because of their toxicity and high cost, it is critical to producing inhibitors that are both environmentally friendly and less expensive [3]. Plants, for example, include a wide range of chemical compounds (alkaloids, steroids, amino acids, tannins, and flavonoids), the majority of which are known to have inhibitory properties. The corrosion attitude of aluminium has been explored in acidic media. Iron corrosion has been successfully inhibited by adding halide salt to an H₂SO₄ solution containing an organic inhibitor [4, 5]. Concerns regarding chemical inhibitors' toxicity, which may hurt living things and contaminate the environment, have been

TABLE 1: Aluminium coupon composition as evaluated by OES.

Element	Al	Si	Fe	Cu	Mn	Mg	Cr	Ni	Zn	Ti	Ga	V
Weight %	99.85	0.049	0.068	0.004	0.002	0.001	0.003	0.002	0.005	0.002	0.008	0.006



FIGURE 1: Phoenix dactylifera leaves and powder.

attributed. Plant extracts have become popular as corrosion inhibitors because they are friendly to the environment, widely available, and environmentally sustainable sources of various inhibitors. A significant amount of naturally produced compounds is found in plant extracts that could be extracted using simple, inexpensive methods [6].

Plant extracts were employed in order to avoid metal corrosion in acidic and alkaline settings. These extracts degrade biologically and clear heavy metals and other potentially hazardous materials [7–9].

This study used weight loss measurements to explore the inhibitive performance of Phoenix dactylifera leaves extract in preventing aluminium corrosion in 1 M hydrochloric acid. The goal of this study is to learn more about the function of the functional groups of the inhibitors used in the adsorption process and the effect of the medium's nature on the corrosion mechanism.

2. Methodology

2.1. Specimen Preparation. The purity of the aluminium which is used in the experiment is 99.85 percent. The aluminium sheets were cut into $3 \times 3 \times 1$ cm for each coupon (coupon exposed area = 4.65 square inch). A 3-mm diameter hole was bored on the upper edge to suspend each coupon in the corrosive environment. The coupons were cleaned and degreased, after being washed in 100 percent ethanol, sprayed in acetone, and left to dry. The dehydrated coupons were maintained in a dry desiccators until they were needed. This experiment employed analytical grade chemicals.

The composition of the Aluminium has been determined by (optical emission spectroscopy OES).

The result is depicted in Table 1.

2.2. Preparation of Corrosive Solution. 1 M HCl solutions were produced by diluting the (37% HCl) solution with deionized water. Before each experience, the test solutions were made fresh by mixing the extract immediately into the corrosion solution.

2.3. Preparation of Phoenix dactylifera Leaves PDL Extract. Phoenix dactylifera leaves are a common, inexpensive, and readily available plant in Iraq. To avoid any decrement in the concentration of corrosive solution after adding a particular amount of inhibitor solution, PDL was extracted in an acidic solution with the same concentration as the corrosive solution. PDL leaves were collected in the month of October, and they were rinsed with distilled water, cut into small pieces, and sun-dried. The dried samples were crushed with an electric blender. The extract is made by refluxing 10 gm of powder in 100 mL of 1 M HCl for 4 hours at 40°C and then filtering carefully as shown in Figure 1.

2.4. Weight Loss Measurement. For weight loss measures, aluminium specimens were employed. After being cleaned and dried, the specimens were plunged in a 1 M HCl solution with or without an inhibitor for 3 hr and then washed, dried, and weighed. Experiments were performed at different concentrations of inhibitor (2, 4, 6, 8, and 10 mL/L) and at varying temperatures (20, 30, 40, and 50°C) to calculate the amount of weight lost. The corrosion rate was determined using the following relationship [10] based on the change in weight of specimens.

$$\rho = \frac{KW}{DAT}, \quad (1)$$

where ρ is the corrosion rate in mpy, K is the rate constant

TABLE 2: Effect of inhibitor concentration and temperature on the corrosion behavior of aluminium in hydrochloric acid in the absence and presence of PDL extract as a corrosion inhibitor.

EXP	Concentration of inhibitor/(mL/L)	Temperature/C°	C_R /mpy	θ (surface coverage)	% IE
1		20	1.861	0	0
2		30	5.168	0	0
3	0	40	17.365	0	0
4		50	24.994	0	0
5		20	1.447	0.222	22.222
6		30	3.928	0.240	24.000
7	2	40	11.370	0.345	34.524
8		50	13.189	0.472	47.229
9		20	1.034	0.444	44.444
10		30	2.274	0.560	56.000
11	4	40	4.341	0.750	75.000
12		50	6.022	0.759	75.906
13		20	0.620	0.666	66.667
14		30	1.447	0.720	72.000
15	6	40	3.308	0.809	80.952
16		50	4.465	0.821	82.134
17		20	0.207	0.889	88.889
18		30	0.558	0.892	89.200
19	8	40	1.240	0.929	92.857
20		50	1.474	0.941	94.103
21		20	0.145	0.922	92.222
22		30	0.310	0.940	94.000
23	10	40	0.827	0.952	95.238
24		50	0.724	0.971	97.105

equal to 534 mpy, W is the weight loss, D is the material density, T is the time of the exposure, and A is the coupon exposed area.

3. Result and Discussion

3.1. *The Inhibition Efficiency: The Inhibitor Efficiency Was Determined Using the Formula below [11].*

$$IE = \left(1 - \frac{\rho_{inh}}{\rho_{plank}} \right) \times 100\%, \quad (2)$$

where ρ_{plank} is the weight reduction in the absence of inhibitor and ρ_{inh} is the weight reduction in the presence of inhibitor. The surface coverage degree θ for different inhibitor concentrations is obtained with the given equation

$$\theta = \frac{IE}{100}, \quad (3)$$

where θ is the surface coverage degree and IE is the inhibitor efficiency. At various temperatures and inhibitor concentrations, the corrosion and inhibitor efficiency rates are evaluated, and the results are compiled in Table 2 and Figures 2

and 3. The rate of corrosion tends to increase as the temperature increases and reduces with the inhibitor concentration increment.

3.2. *Temperature's Effect: Thermodynamic Studies.* Temperature affects the rate of nearly all chemical reactions and increases the speed of corrosion and effectiveness of inhibition. The corrosion rate of aluminium in an acidic medium increases with increasing temperature. The Arrhenius equation, in which the rate of corrosion reaction is connected with temperature, can be used to express this effect:

$$\ln C_R = \ln A - \frac{E_a}{RT}, \quad (4)$$

where E_a is the activation energy, A is the frequency factor, R is the universal gas constant, and T is the temperature in Kelvin.

$$\ln \left[\frac{C_R}{T} \right] = \ln \frac{R}{Nh} + \left[\frac{\Delta S}{R} \right] - \left[\frac{\Delta H}{RT} \right]. \quad (5)$$

We may plot $\ln (C_R/T)$ versus $1/T$ using Equation (5), the straight line slope is $(-\Delta H/R)$, and the intercept is

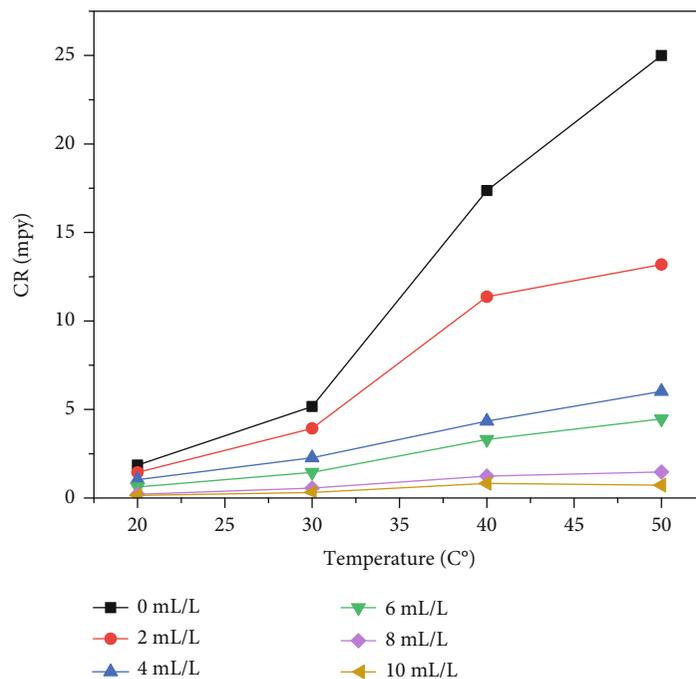


FIGURE 2: Temperature's effect on corrosion rate of aluminium after immersion in 1 M hydrochloric acid for 3 hr at different concentrations of inhibitor.

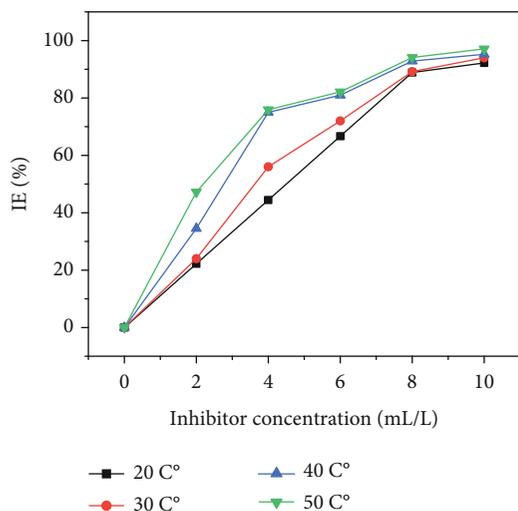


FIGURE 3: The impact of temperature on inhibitive efficiency of PDL extract for aluminium corrosion in 1 M hydrochloric acid.

$(\Delta S/R + \ln R/Nh)$, from which ΔH and ΔS can be determined (Figures 4 and 5 and Table 3).

Table 3 shows that the enthalpy of activation values for PDL extract were all negative, indicating that the aluminium corrosion process is exothermic. Additionally, the activation entropies were negative, showing that the activation complex represented association steps and that the reaction was both spontaneous and available.

3.3. Adsorption of Inhibitor and Isotherm

3.3.1. *Langmuir Adsorption Isotherm.* Many examples of strong adsorption do not suit the Langmuir isotherm model, which is a set of uniform adsorption sites. This isotherm is expressed mathematically as [12]:

$$\frac{C_i}{\theta} = \frac{1}{K_L} + C_i, \quad (6)$$

where K_L is the equilibrium constant (L/mL), K_L represents the adsorption degree (a higher value of K_L shows that the inhibitor is heavily adsorbed on the surface of the metal), and C_i represents the inhibitor concentration (mL/L) (Figure 6 and Table 4).

$$K_L = \frac{1}{55.5} \exp\left(-\frac{\Delta G_{\text{ads}}^{\circ}}{RT}\right), \quad (7)$$

where ΔG° is the standard adsorption free energy (kJ mol^{-1}). C_i/θ versus C_i can be plotted according to Equation (5). The values of K_L are constructed using the intercept. With increasing temperature, the calculated behavior of the equilibrium constant of adsorption (K_L) decreased.

In general, negative values of ΔG_{ads} larger than 40 kJ mol^{-1} suggest chemical adsorption, whereas negative values of less than 20 kJ mol^{-1} imply physical adsorption [13]. According to the data result, ΔG_{ads} values are negative and are less than -20 kJ mol^{-1} . This suggests that the inhibitor's spontaneous adsorption on the metal surface supports the physical adsorption process.

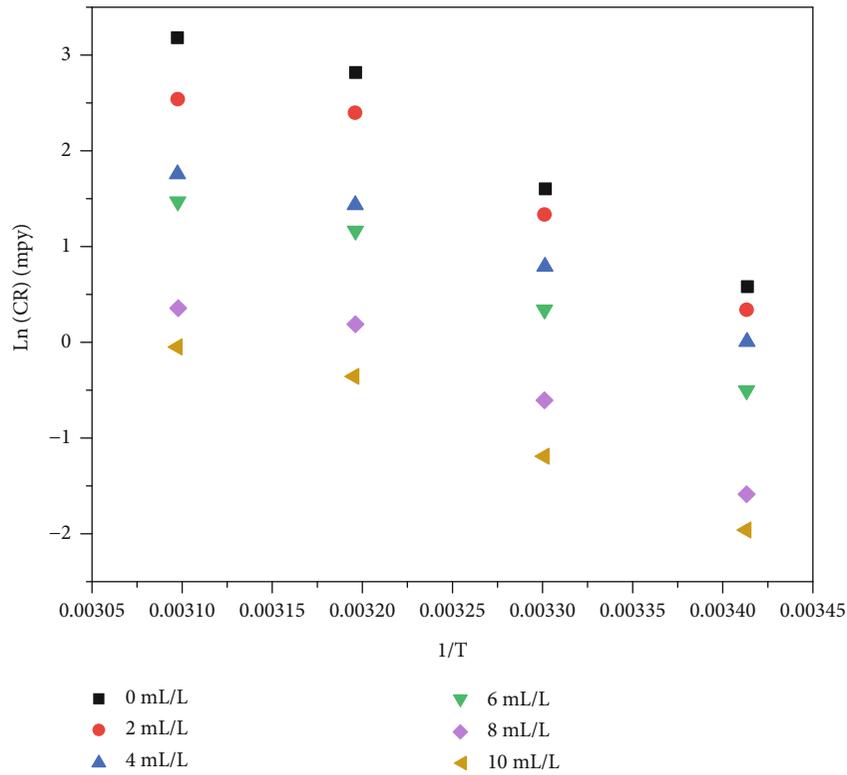


FIGURE 4: Arrhenius plot of aluminium corrosion in 1 M hydrochloric acid, including varying temperatures and concentrations of PDL extract.

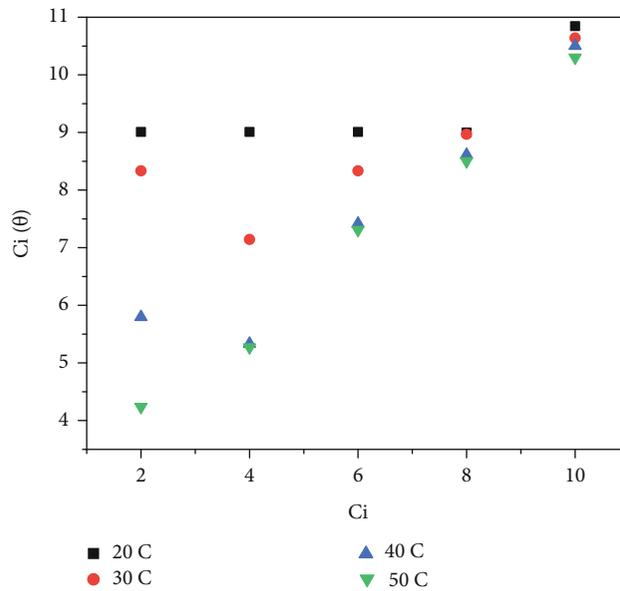


FIGURE 5: Langmuir adsorption isotherm of PDL extract for aluminium corrosion in 1 M hydrochloric acid at different temperatures.

3.3.2. *Freundlich Adsorption Isotherm.* The equation can represent this isotherm is:

$$\theta = K_F C_i^n, \tag{8}$$

where K_F (Freundlich constant) and n are constants for a particular system at a specific temperature. This isotherm

can be expressed as follows [14]:

$$\ln \theta = \ln(K_F C_i^{1/n}), \tag{9}$$

$$\ln \theta = \ln K_F + 1/n \ln C_i. \tag{10}$$

We can plot $\ln \theta$ against $\ln C_i$ using Equation (10),

TABLE 3: Enthalpy, entropy, and activation energy of the Aluminium corrosion reaction with different concentrations of PDL extract.

Inhibitor concentration (mL/L)	E_a	R^2	$-\Delta H_{KJ/mol}$	$-\Delta S_{KJ/mol}$
0	1181.861	0.969	68.582	0.633
2	1065.673	0.940	58.363	0.592
4	743.082	0.978	44.331	0.547
6	852.530	0.972	50.790	0.568
8	945.872	0.941	50.476	0.552
10	909.914	0.975	43.574	0.524

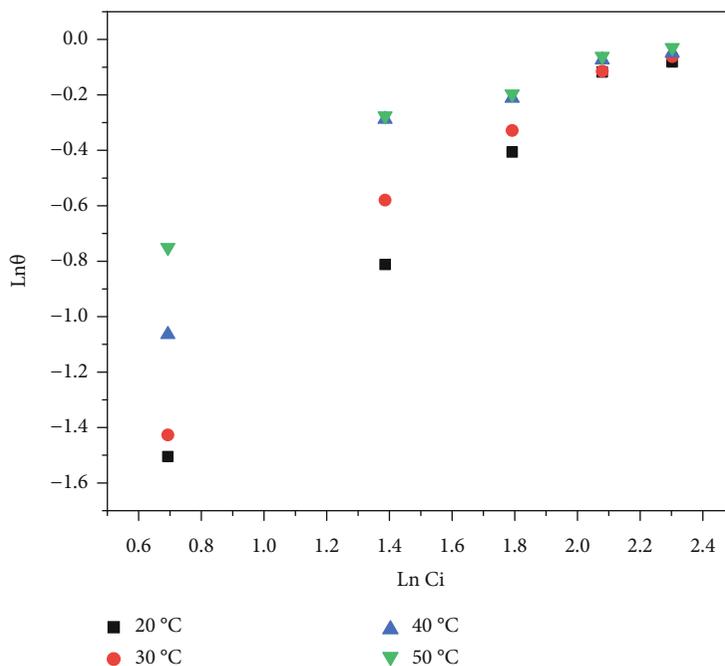


FIGURE 6: Freundlich adsorption isotherm of PDL extract for aluminium corrosion in (1 M HCl) at different temperatures.

TABLE 4: Langmuir equilibrium constant, standard adsorption free energy and correlation coefficient for Langmuir adsorption isotherm of the PDL extract inhibitor for aluminium corrosion at different temperatures.

Temperature °C	K_L	$\Delta G_{ads}^{o} KJ/mol$	R^2
20	0.120	-4.620	0.495
30	0.148	-5.302	0.635
40	0.268	-7.025	0.902
50	0.397	-8.304	0.991

TABLE 5: Freundlich parameters for Freundlich adsorption isotherm of the PDL extract inhibitor for aluminium corrosion at different temperatures.

Temperature °C	K_F	$1/n$	R^2
20	-2.11	0.925	0.986
30	-1.92	0.856	0.959
40	-1.36	0.619	0.888
50	-0.997	0.444	0.946

where the intercept and slope reveal the values of K_F and $1/n$, respectively. The corrosion inhibition behavior of PDL tends to be more compatible with Freundlich isotherm (Figure 6 and Table 5).

The value of $1/n$ is employed to express the ease of adsorption. Usually, when $0 < 1/n < 1$, adsorption is believed to be easy, and it considers to be moderated when $1/n = 1$ and difficult if $1/n > 1$ [15]. According to the result in Table 5, the adsorption of PDL inhibitor on the surface of aluminium is thought to be an easy process.

The phytochemical analysis PDL leaves extract resulted in the identification of three main components, oleanolic acid, vanillyl alcohol, and β sitosterol 3-O- β -D-glucoside in addition to minor constituents, fatty acids, lutein, and sucrose [16] which is expected to be adsorbed on the surface of aluminium resulting in inhibition of corrosion and reduction in the corrosion rate.

Vanillyl alcohol was chosen as a model for theoretical study due to its high percentage in the PDL extract and the simplicity of its chemical composition.

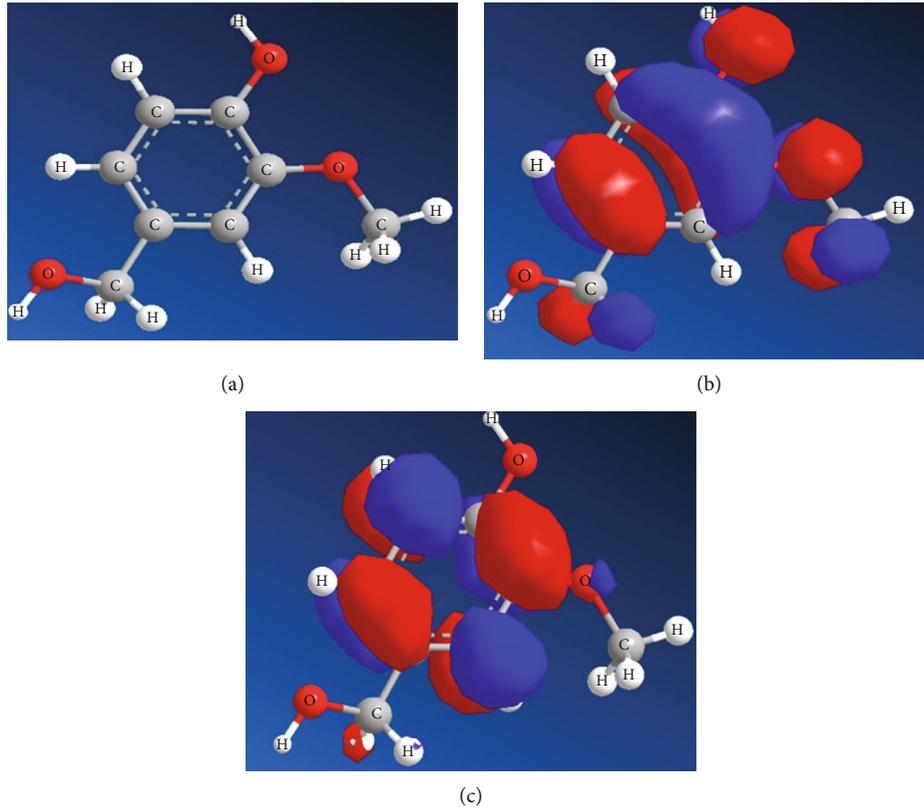


FIGURE 7: (a) Optimized structure of vanillyl alcohol according to DFT, (b) HOMO, and (c) LUMO.

TABLE 6: Quantum chemical parameters for Vanillyl Alcohol obtained by DFT/B3LYP/6-311G (d,p) level.

Inhibitor molecule	E_{HOMO}	E_{LUMO}	ΔE	IE	EA	η	χ	μ	S	ω	ΔN	$\Delta \psi$
PDL	-11.26	-0.29	10.97	11.26	0.29	5.49	5.78	3.71	0.09	1.25	-0.14	0.1

3.4. Computational Study. The theoretical characteristics of the inhibitor compound were calculated employing the density functional theory DFT/B3LYP. The base set 6-311G(d,p) was employed in all computations. A computational study has been conducted with Gaussian 07 software. E_{HOMO} , E_{LUMO} (Figure 7), energy gap ΔE , μ , S , η , ω , χ , $\Delta \psi$ inhibitor-metal interaction energy, and electrons transferred fraction (ΔN) have been calculated (Table 6) employing Equations (11)–(16):

$$\text{IE (Ionization potential)} = E_{N-1} - E_N, \quad (11)$$

$$\text{EA (Electron affinity)} = E_N - E_{N+1}. \quad (12)$$

At the optimized geometry, the neutral molecule has the optimal energy E_N , and E_{N+1} and E_{N-1} are single point (SP) energies of the neutral, anionic, and cationic forms of the multiple electron system (N).

$$\chi = -\mu = -\left[\frac{\partial E}{\partial N}\right]_{v(r)} = \frac{1}{2}(\text{IP} + \text{EA}), \quad (13)$$

$$\eta = \frac{1}{2} \left[\frac{\partial^2 E}{\partial N^2} \right]_{v(r)} = \frac{1}{2} \left[\frac{\partial \mu}{\partial N} \right]_{v(r)} = \frac{1}{2}(\text{IP} - \text{EA}), \quad (14)$$

$$S = \frac{1}{2\eta}, \quad (15)$$

$$\omega = \frac{\mu^2}{2\eta}, \quad (16)$$

where the relative values of χ and η have been utilized, and the electron transfer fraction (N) from the inhibitor to the surface of the metal has been calculated as seen as [17]:

$$\Delta N = \frac{\chi_{\text{metal}} - \chi_{\text{inhibitor}}}{2(\eta_{\text{metal}} + \eta_{\text{inhibitor}})}, \quad (17)$$

where χ_{metal} , $\chi_{\text{inhibitor}}$, and η_{metal} and $\eta_{\text{inhibitor}}$ indicate the species' absolute electronegativity and hardness; differences in electronegativity drive electron transport. The summation of the hardness parameters serves as resistance [18]. In this research, $\eta_{\text{Al}} = 0$, whereas the theoretical aluminium work function, $\text{Al } \phi = 4.28 \text{ eV}$, was utilized instead χ of Al [19].

So, Equation (10) can be rewritten as:

$$\Delta N = \frac{\phi_{Al} - \chi_{inhibitor}}{2\eta_{inhibitor}} \quad (18)$$

Another significant factor measured, the initial inhibitor-metal interaction energy ($\Delta\psi$), developed by Kokalj and Kovačević, is used in this work [20]. The initial interaction energy of inhibitor-metal $\Delta\psi$ has been computed as follows:

$$\Delta\psi = \frac{(\chi_{metal} - \chi_{inhibitor})^2}{4(\eta_{metal} + \eta_{inhibitor})}, \quad (19)$$

which can be written as:

$$\Delta\psi = \frac{(\chi_{metal} - \chi_{inhibitor})^2}{4\eta_{inhibitor}}. \quad (20)$$

The lower the value of χ for inhibitor, the less the molecule electron grip and the greater the tendency to release electrons during intermolecular interactions [21]. The corrosion inhibitor had a negative ΔN value, indicating that it supplied electrons to the surface of the metal [22]. The increase in the number of electrons donated to the surface of the metal increases the efficiency of inhibition [23–25]. The inhibitor compounds' capacity to absorb on the surface of Aluminium is linked to HOMO and LUMO [26, 27]. HOMO refers to the capacity to donate electrons, whereas the capability to accept electrons is referred to as LUMO. An energy gap with low values is a crucial indicator of the significant efficacy of the inhibitor due to the low energy required to remove electrons from an occupied orbital [28]. The dipole moment (μ) was another quantum parameter that turned out to be essential for corrosion inhibition effectiveness. More specifically, bond polarity and electron distribution are important [29]. EHOMO and ELUMO are related to the softness and hardness, respectively [28]. Vanillyl alcohol has the lowest hardness value of any inhibitor, 5.49. (eV).

A corrosion inhibitor with a low hardness value is expected to have a high inhibitory effectiveness [16]. Adsorption occurs where a molecule has a high softness value for easy electron transport [30].

4. Conclusion

The result shows that PDL acid extract is an excellent and efficient inhibitor of Aluminium corrosion in hydrochloric acid media, and as extract concentration increases, the efficiency of the inhibition increases. The adsorption of different concentrations of plant extract on the surface of Aluminium in 1 M HCl acid obeyed the Freundlich adsorption isotherm. The values of standard free energy of adsorption show that the inhibitor adsorption on the Aluminium surface proceeded via physisorption.

The fact that the free energy of adsorption has a negative sign suggests that the inhibitors' adsorption on the Aluminium surface occurred in a spontaneous process.

Data Availability

The data are deposited in a repository.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

This study is self-funded.

References

- [1] T. Hurlen, H. H. Lian, O. S. Ødegard, and T. V. Valand, "Corrosion and passive behaviour of aluminium in weakly acid solution," *Electrochimica Acta*, vol. 29, no. 5, pp. 579–585, 1984.
- [2] O. Sanni, A. P. I. Popoola, and O. S. I. Fayomi, "Oil as corrosion inhibitor for aluminium alloy in aggressive environment," *Materials Science and Engineering*, vol. 391, article 012004, 2018.
- [3] E. E. Oguzie, "Inhibition of acid corrosion of mild steel by *Telfaria occidentalis* extract," *Pigment & Resin Technology*, vol. 34, pp. 321–326, 2005.
- [4] G. Y. Elewady, I. A. El-Said, and A. S. Fouda, "Effect of anions on the corrosion inhibition of aluminium in HCl using ethyl trimethyl ammonium bromide as cationic inhibitor," *International Journal of Electrochemical Science*, vol. 3, pp. 644–655, 2008.
- [5] A. M. Abdel-Gaber, E. Khamis, H. Abo-EIDahab, and A. Sh, "Inhibition of aluminium corrosion in alkaline solutions using natural compound," *Materials Chemistry and Physics*, vol. 109, no. 2-3, pp. 297–305, 2008.
- [6] O. K. Abiola, N. C. Oforika, E. E. Ebenso, and N. M. Nwinuka, "Eco-friendly corrosion inhibitors: the inhibitive action of *Delonix Regia* extract for the corrosion of aluminium in acidic media," *Anti-Corrosion Methods and Materials*, vol. 54, pp. 219–224, 2007.
- [7] M. Kliškić, J. Radošević, S. Gudić, and V. Katalinić, "Aqueous extract of *Rosmarinus officinalis* L. as inhibitor of Al–Mg alloy corrosion in chloride solution," *Journal of Applied Electrochemistry*, vol. 30, pp. 823–830, 2000.
- [8] S. A. Umoren and E. E. Ebenso, "Studies of anit-corrosion effect of *Raphiahookeri* exudates gum-halide mixtures for aluminium corrosion in acidic medium," *Pigment & Resin Technology*, vol. 37, pp. 173–182, 2008.
- [9] W. D. Callister, *Materials Science and Engineering: An Introduction*, John Wiley and Sons Inc., New York, 2003.
- [10] E. E. Oguzie, "Evaluation of the inhibitive effect of some plant extracts on the acid corrosion of mild steel," *Corrosion Science*, vol. 50, pp. 2993–2998, 2008.
- [11] I. A. Adejoro, F. K. Ojo, and S. K. Obafemi, "Corrosion inhibition potentials of ampicillin for mild steel in hydrochloric acid solution," *Journal of Taibah University for Science*, vol. 9, no. 2, pp. 196–202, 2015.
- [12] K. H. Hassan, A. A. Khadom, and N. H. Kurshed, "Citrus aurantium leaves extracts as a sustainable corrosion inhibitor of mild steel in sulfuric acid," *South African Journal of Chemical Engineering*, vol. 22, pp. 1–5, 2016.
- [13] R. Saratha, D. Saranya, H. N. Meenakshi, and R. Shyamala, "Enhanced corrosion resistance of *Tecomastans* extract on

- the mild steel in 0.5 M H₂SO₄ solution,” *International Journal of Current Research*, vol. 2, pp. 92–96, 2011.
- [14] I. Lukovit, E. Kalman, and F. Zucchi, “Corrosion inhibitors—correlation between electronic structure and efficiency,” *Corrosion*, vol. 57, pp. 3–8, 2001.
- [15] B. N. Oza and R. S. Sinha, “Thermometric study of corrosion behavior of high strength Al–Mg alloy in phosphoric acid in presence of halides,” *Transactions of the SAEST (Society for Advancement of Electrochemical Science and Technology)*, vol. 17, no. 1, pp. 281–285, 1982.
- [16] R. K. Suleiman, W. Iali, B. El Ali, and S. A. Umoren, “New constituents from the leaves of date palm (*Phoenix dactylifera* L.) of Saudi origin,” *Molecules*, vol. 26, article 4192, 2021.
- [17] A. Lesar and I. Milošev, “Density functional study of the corrosion inhibition properties of 1,2,4-triazole and its amino derivatives,” *Chemical Physics Letters*, vol. 483, pp. 198–203, 2009.
- [18] A. Kokalj and N. Kovacevic, “On the consistent use of electrophilicity index and HSAB-based electron transfer and its associated change of energy parameters,” *Chemical Physics Letters*, vol. 507, pp. 181–184, 2011.
- [19] K. Khanari and M. Finšgar, “Organic corrosion inhibitors for aluminium and its alloys in acid solutions: A review,” *RSC Advances*, vol. 6, pp. 62833–62857, 2016.
- [20] T. V. Kumar, J. Makangara, C. Laxmikanth, and N. S. Babu, “Computational studies for inhibitory action of 2-mercapto-1-methylimidazole tautomers on steel using of density functional theory method (DFT),” *International Journal of Computational and Theoretical Chemistry*, vol. 4, pp. 1–6, 2016.
- [21] N. A. Wazzan and F. M. Mahgoub, “DFT calculations for corrosion inhibition of ferrous alloys by pyrazolopyrimidine derivatives,” *Open Journal of Physical Chemistry*, vol. 4, pp. 6–14, 2014.
- [22] M. M. Mohamed Abdelahi, H. Elmsellem, M. Benchidmi et al., “A DFT and molecular dynamics study on inhibitory action of indazole derivative on corrosion of mild steel,” *Journal of Materials and Environmental Sciences*, vol. 8, pp. 1860–1876, 2017.
- [23] N. Anusuya, P. Sounthari, J. Saranya, K. Parameswari, and S. Chitra, “Corrosion inhibition effect of hydroxypyrazoline derivatives on mild steel in sulphuric acid solution together with quantum chemical studies,” *Journal of Materials and Environmental Sciences*, vol. 6, pp. 1606–1623, 2015.
- [24] A. Y. Issa, K. S. Rida, A. Q. Salam, and A. A. Al-Amiery, “Acetamidocoumarin as a based eco-friendly corrosion inhibitor,” *International Journal of ChemTech Research*, vol. 9, pp. 39–47, 2016.
- [25] H. J. Habeeb, H. M. Luaibi, T. A. Abdullah, R. M. Dakhil, A. A. H. Kadhum, and A. A. Al-Amiery, “Case study on thermal impact of novel corrosion inhibitor on mild steel,” *Case Studies in Thermal Engineering*, vol. 12, pp. 64–68, 2018.
- [26] H. Ashassi-Sorkhabi, B. Shaabani, and D. Seifzadeh, “Effect of some pyrimidinic Schiff bases on the corrosion of mild steel in hydrochloric acid solution,” *Electrochimica Acta*, vol. 50, pp. 3446–3452, 2005.
- [27] M. Filali, E. M. El Hadrami, A. Ben-tama et al., “3,6-Di(pyridin-2-yl) pyridazine derivatives as original and new corrosion inhibitors in support of mild steel: experimental studies and DFT investigational,” *International Journal of Corrosion and Scale Inhibition*, vol. 8, no. 1, pp. 93–109, 2019.
- [28] T. Arslan, F. Kandemirli, E. E. Ebenso, I. Love, and H. Alemu, “Quantum chemical studies on the corrosion inhibition of some sulphonamides on mild steel in acidic medium,” *Corrosion Science*, vol. 51, pp. 35–37, 2009.
- [29] R. Javaherdashti, “How corrosion affects industry and life,” *Anti-Corrosion Methods and Materials*, vol. 47, no. 1, pp. 30–34, 2000.
- [30] M. M. Antonijevic and M. B. Petrovic, “Copper corrosion inhibitors. A review,” *International Journal of Electrochemical Science*, vol. 3, pp. 1–28, 2008.