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Experimental Aspect and Theoretical Modelling of Aluminium Inhibition Corrosion by Vitamins B1, B3 and B6 in Chloric Acid Solution

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Abstract: Metal corrosion phenomenon is an important topic in many industries because of its consequences on industrial equipment. The purpose of this study was to investigate the inhibition potential of three vitamins on aluminum corrosion in 1M HCl using experimental and theoretical techniques. So, the inhibitive effect of three vitamins that are vitamin B1, B3 and B6 on aluminium corrosion in 1M hydrochloric acid solution was studied by gravimetric techniques and quantum chemical method based on density functional theory (DFT). Gravimetric proved that these compounds are excellent inhibitors in tested solution. Vitamins adsorption on aluminium surface obeys to modified Langmuir model or Villamil model. Thermodynamic adsorption parameters were determined and discussed. Kinetic study of aluminum dissolution in absence or presence of each inhibitor indicates that the addition of each vitamin in corrosive solution does not change dissolution reaction order which is zero order. Finally, it was found that quantum chemical and experimental calculations correlate and indicated that inhibition effect of investigated molecules is strongly related to E_{HOMO}, E_{LUMO}, and energy gap (ΔE).

Keywords: Vitamins, Aluminium, Gravimetric, Hydrochloric Acid, Density Functional Theory

1. Introduction

Physic-chemical interactions between a metallic material and its environment can lead to its corrosion. This corrosion is a chemical reaction involving electrons transfer from a metal to an external electron acceptor, which results in the release of metal ions into the surrounding environment and leads to metal dissolution. This process goes through a series of oxidation and reduction reactions of chemical species [1]. Thus, the metal loses its physical and chemical properties and becomes unusable in many areas. Corrosion is based on the principles of thermodynamics and electrochemical kinetics. Thermodynamic approach predicts the possibility or not of corrosion reaction, while kinetic approach permits to evaluate the elementary reactions rate and consequently global corrosion rate. There are several corrosion forms which are: generalized corrosion, pitting corrosion, crevice corrosion, microbial corrosion, stress corrosion and intergranular corrosion. These different forms of corrosion that metals undergo contribute to economic losses in industrial sector and are a source of contamination and environmental pollution.

Aluminium is a metal that is widely used in aerospace, automotive, food handling, construction, heat exchange and electrical transmission [2]. This massive use is due to its numerous physicochemical properties that are low density, high ductility, high thermal and electrical conductivity, good corrosion resistance attractive appearance, and low toxicity [3].

Despite its many physicochemical properties and

applications, aluminium is not immune to corrosion during acid pickling [4, 5]. These operations of pickling and cleaning in acid medium which favored aluminium dissolution challenged the researchers to develop protection methods to reduce dissolution phenomenon [6-8]. Among these methods of protection, we have corrosion inhibitors. It has been found that some organic substances containing polar functions with nitrogen atoms, sulfur atoms and / or oxygen in the conjugate system have been reported to have good properties of aluminium corrosion inhibition in acidic and alkaline solutions [8-11]. Indeed it has been recognized that the use of organic inhibitors, especially therapeutic organic inhibitors of plant origin is viable and very beneficial as they are essentially non-toxic, environmentally benign, readily available, renewable and inexpensive [12-15].

Through DFT based quantum chemical studies, the inhibition performances of some organic molecules have been explained. These performances are favored by the presence of polar functions with N, S, O atoms as well as conjugated double bonds or aromatic rings in the molecular structures of these organic compounds, which are the main adsorption centers and facilitate electronic exchanges [16-20].

This study aims to investigate the thermodynamic, kinetic and theoretical aspects of vitamins B1, B3 and B6 of aluminium corrosion inhibition in 1M hydrochloric acid solution.

2. Experimental

2.1. Studied Compounds

Molecular structures of studied compounds are given by figure 1.

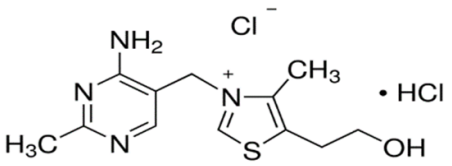
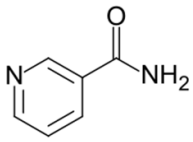
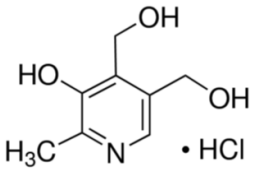
	Vitamin B1 or 3-((4-Amino-2-methyl-5-pyrimidinyl) methyl)-5-(2-hydroxyethyl)-4-methylthiazolium chloride hydrochloride	Vitamin B3 or pyridine-3-carboxamide	Vitamin B6 or 4,5-Bis (hydroxymethyl)-2-methyl-3-pyridinol, hydrochloride
Name			
Formula	$C_{12}H_{18}Cl_2N_4OS$	$C_6H_6N_2O$	$C_8H_{12}ClNO_3$
Molecular structures			

Figure 1. *Molecular structure of vitamins B1, B3 and B6.*

2.2. Gravimetric Method

In this gravimetric or weight loss method, aluminium coupons of 99.5% purity in rod form measuring 10 mm in length and 2 mm in diameter were successively polished with fine grade emery papers with grit sizes ranging from 150 to 600, cleaned with acetone, washed with bidistilled water, oven dried (ASTEL) and weighed. Each sample was completely immersed in 50ml of 1M HCl solution and placed in a thermostatic bath (Frigitherm) maintained at temperatures of 298K, 303K, 308K, 313K, 318K and 323K. The procedures were conducted with and without different concentrations of each inhibitor. After 1h, aluminium coupons were removed from the test solution. They were scrubbed under running water with a bristle brush and then dried and reweighed. The mass loss was taken as the difference in mass of the coupon before and after immersion, determined by an analytical balance from KERN & SOHN GmbH (accuracy: ±0.1 mg). The test was carried out in triplicate to ensure the reliability of result and average value of the mass loss was reported.

Corrosion rate (W), the rate of surface coverage (θ) and the inhibition efficiency (IE) were calculated according to the equation below:

$$w = \frac{\Delta m}{S_e.t} = \frac{m_0 - m}{S_e.t} \quad (1)$$

$$\theta = \frac{w_0 - w}{w_0} \quad (2)$$

$$IE(\%) = \frac{W_0 - W}{W_0} * 100 \quad (3)$$

Δm: is mass loss (g); m_0 and m are respectively the mass (g) before and after immersion in solution test; t: immersion time (h); Se: total surface of aluminium coupon (cm^2); w_0 and w; are respectively the corrosion rates of aluminium in absence and presence of each molecule.

Kinetic model was used from the experimental data to evaluate the order of aluminum dissolution reaction in HCl 1M with or without the studied compounds:

$$\text{Zero order: } mo - m = kt \quad (4)$$

$$\text{First order: } \ln\left(\frac{m_0}{m}\right) = kt \quad (5)$$

$$\text{Second order: } \frac{1}{m} - \frac{1}{m_0} = kt \quad (6)$$

2.3. Theoretical Approach

Quantum chemical calculations based on density functional theory (DFT) have been used to understand the organic molecules studied reactivity. These calculations were performed with full geometric optimizations using Gaussian 09W software [21]. The optimization geometry of the molecules was performed by functional B3LYP at 6-31G (d) basis level [22, 23]. The calculated quantum chemical

parameters are: E_{HOMO} (Highest Occupied Molecular Orbital Energy), E_{LUMO} (Lowest Unoccupied Molecular Orbital Energy), energy gap (ΔE), dipole moment (μ), electronegativity (χ), hardness (η), softness (S), electrophylicity index (ω), electron affinity (A), ionization energy (I) and the fraction of electron transferred (ΔN).

3. Results and Discussion

3.1. Gravimetric Analysis

Figures 2, 3 and 4 show respectively the inhibition efficiency evolution as a function of the vitamins B1, B3, B6 concentration and corrosive medium temperature.

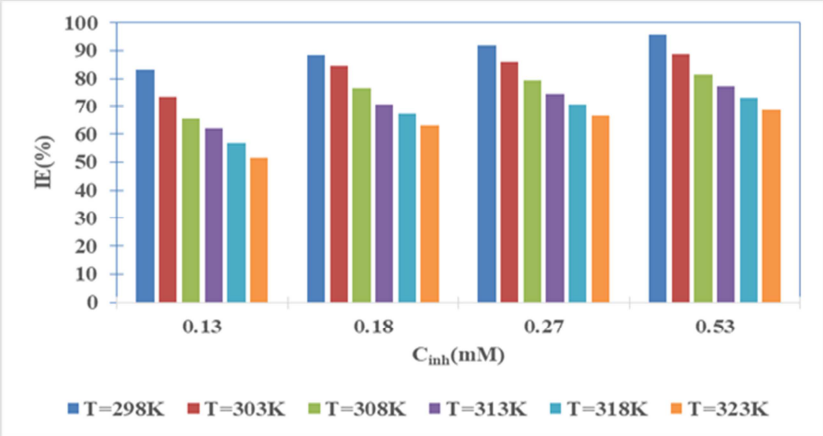


Figure 2. *Inhibition efficiency versus concentration for different temperatures of vitamin B1.*

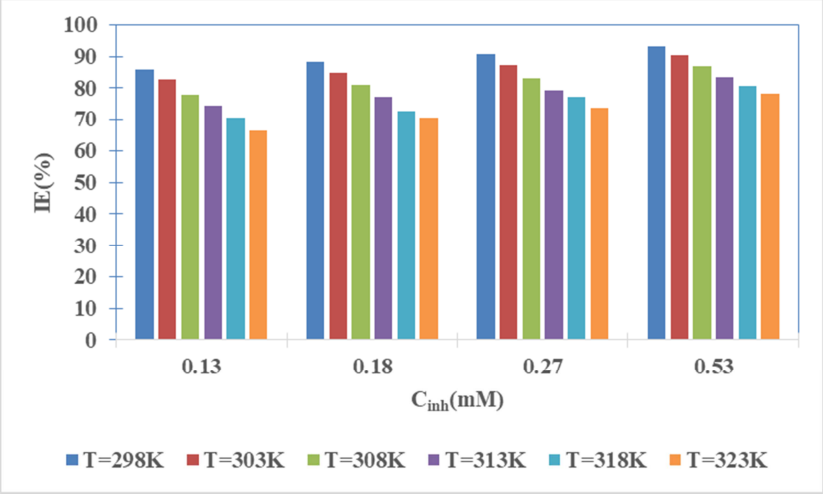


Figure 3. *Inhibition efficiency versus concentration for different temperatures of vitamin B3.*

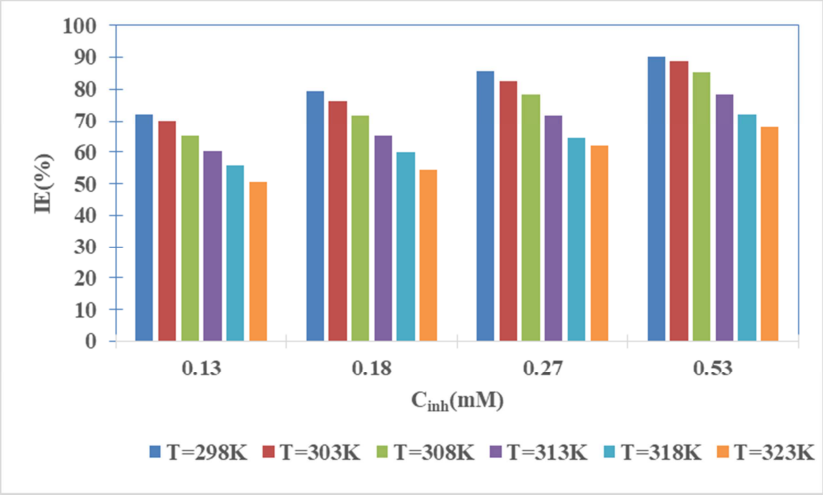


Figure 4. *Inhibition efficiency versus concentration for different temperatures of vitamin B6.*

Figures 2, 3 and 4 examination clearly shows that the studied molecules inhibition efficiency increases when inhibitor concentration increases and decreases when the temperature increases. These observations reveal on the one hand that the corrosion inhibition process of aluminium is due to the studied molecules adsorption on metal surface and this adsorption becomes important when inhibitor concentration inhibitor increases and on other hand to the increase of the solubility of protective film including inhibitors and corrosion products initially precipitated on metal surface, exposing progressively this surface to the aggressive solution attacks when temperature increases. Experimental values report that vitamin B1 is more effective than vitamin B3 and more than vitamin B6.

3.2. Adsorption and Thermodynamic Parameters Evaluation

Four isotherm models which are Temkin isotherm, Langmuir isotherm, El-Awady isotherm and Freundlich isotherm have been tested to determine which is suitable for molecules. It emerges Langmuir isotherm is the most appropriate to apply to experimental values because this one has coefficients of determination which tend more towards the unit than the other isotherms. The expression of this model is [24]:

$$\frac{C_{inh}}{\theta} = \frac{1}{K_{ads}} + C_{inh} \quad (7)$$

Table 1. *Adsorption thermodynamic parameters of studied molecules.*

vitamin	T (K)	Equation	R^2	K_{ads} (M^{-1})	ΔG^0_{ads} ($kJmol^{-1}$)	ΔH^0_{ads} ($kJmol^{-1}$)	ΔS^0_{ads} ($Jmol^{-1}K^{-1}$)
B1	298	$C_{inh}/\theta = 1.0265C_{inh} + 0.0267$	0.9999	37453	-36.2	-18.67	60.0
	303	$C_{inh}/\theta = 1.677C_{inh} + 0.280$	0.9995	35714	-36.5		
	308	$C_{inh}/\theta = 1.091C_{inh} + 0.0333$	0.9999	30030	-36.6		
	313	$C_{inh}/\theta = 1.1401C_{inh} + 0.0339$	0.9996	29498	-37.3		
	318	$C_{inh}/\theta = 1.2884C_{inh} + 0.0400$	0.9998	25000	-37.4		
	323	$C_{inh}/\theta = 1.364C_{inh} + 0.0460$	0.9994	21739	-37.6		
B3	298	$C_{inh}/\theta = 1.052C_{inh} + 0.0157$	0.999	67006	-37.5	-31.34	20.0
	303	$C_{inh}/\theta = 1.055C_{inh} + 0.0187$	1.000	56417	-37.7		
	308	$C_{inh}/\theta = 1.110C_{inh} + 0.0232$	1.000	47845	-37.9		
	313	$C_{inh}/\theta = 1.147C_{inh} + 0.0277$	0.999	41408	-38.1		
	318	$C_{inh}/\theta = 1.176C_{inh} + 0.0336$	0.999	35000	-38.3		
	323	$C_{inh}/\theta = 1.206C_{inh} + 0.0399$	0.999	30226	-38.4		
B6	298	$C_{inh}/\theta = 1.0235C_{inh} + 0.0434$	0.9996	23041	-34.9	-23.38	38.0
	303	$C_{inh}/\theta = 1.0303C_{inh} + 0.0509$	0.9999	19646	-35.1		
	308	$C_{inh}/\theta = 1.0522C_{inh} + 0.0622$	1.0000	16077	-35.3		
	313	$C_{inh}/\theta = 1.1494C_{inh} + 0.0672$	1.0000	14881	-35.4		
	318	$C_{inh}/\theta = 1.2486C_{inh} + 0.0752$	0.9995	13298	-35.7		
	323	$C_{inh}/\theta = 1.2951C_{inh} + 0.0915$	0.9993	10929	-35.8		

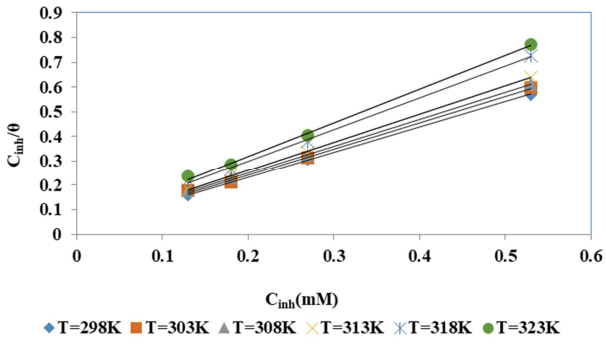


Figure 5. *Langmuir's adsorption isotherm plots of vitamin B1.*

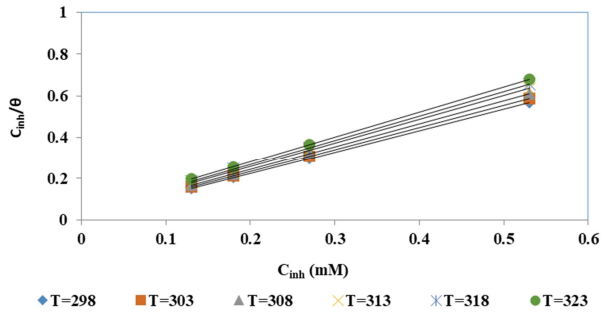


Figure 6. *Langmuir's adsorption isotherm plots of vitamin B3.*

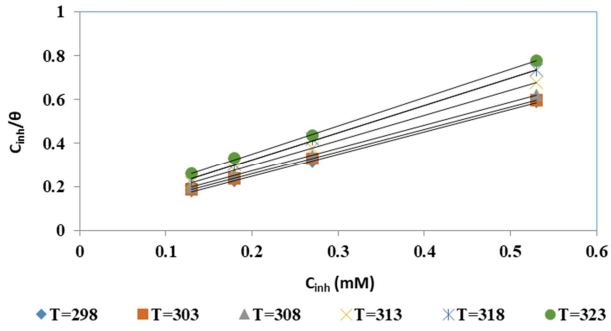


Figure 7. *Langmuir's adsorption isotherm plots of vitamin B6.*

Figures 5, 6 and 7 illustrate respectively the representations of this model for vitamins B1, B2 and B3. Table 1 shows Langmuir isotherm parameters values and the thermodynamic adsorption parameters.

The lines obtained have determination coefficients (R^2) close to unity and slopes greater than unity, it appears then that modified Langmuir isotherm or Villamil model is the most appropriate to study this adsorption. The expression of this model is reflected as follows [25]:

$$\frac{C_{inh}}{\theta} = \frac{n}{K_{ads}} + nC_{inh} \quad (8)$$

Thus the standard free energy of adsorption (ΔG^0_{ads}) and the adsorption enthalpy (ΔH^0_{ads}) and the adsorption entropy (ΔS^0_{ads}) can be determined from the following expressions:

$$\Delta G^0_{ads} = -RTln(55.5\ K_{ads}) \quad (9)$$

$$\Delta G^0_{ads} = \Delta H^0_{ads} - T\Delta S^0_{ads} \quad (10)$$

For determining the variation of adsorption enthalpy and adsorption entropy, we use the plot of ΔG^0_{ads} versus temperature.

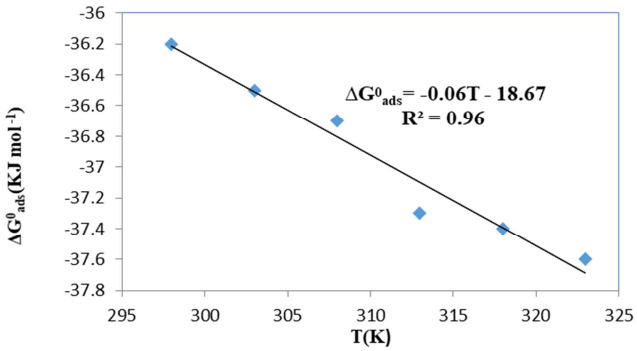


Figure 8. *ΔG^0_{ads} versus temperature of vitamin B1.*

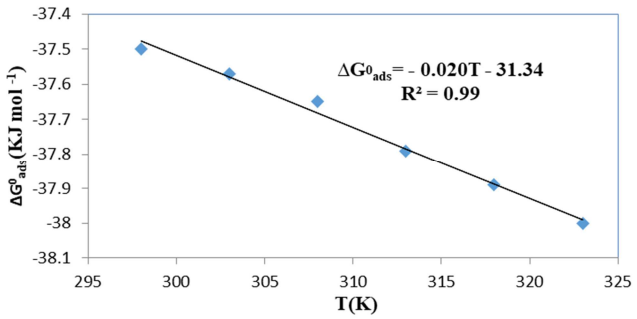


Figure 9. *ΔG^0_{ads} versus temperature of vitamin B3.*

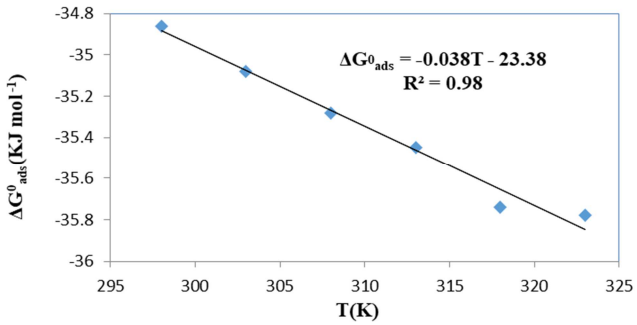


Figure 10. *ΔG^0_{ads} versus temperature of vitamin B6.*

Referring to Table 1, standard free energy of adsorption (ΔG^0_{ads}) values are negative for all compounds studied, which suggests that adsorption is spontaneous and the adsorbed layer is stable [26]. Thus the inhibitors used can protect aluminium at the indicated temperatures. Adsorption enthalpy (ΔH^0_{ads}) values are negative, indicating an exothermic process and these values also indicate the physical adsorption predominance [27]. Adsorption entropy (ΔS^0_{ads}) values are positive, reflecting the increase in disorder during the adsorption phenomenon of each molecule on aluminium surface [28].

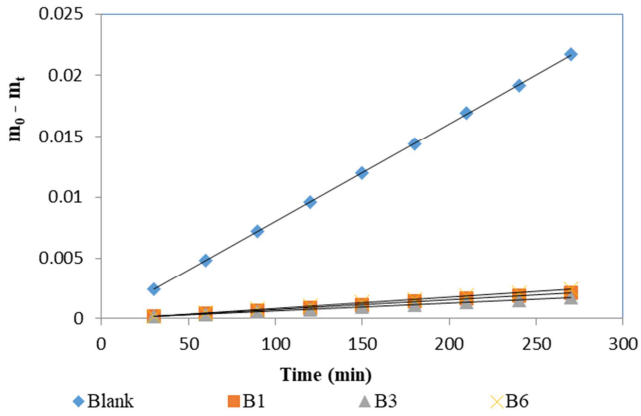


Figure 11. *Zero order kinetic model of aluminum dissolution.*

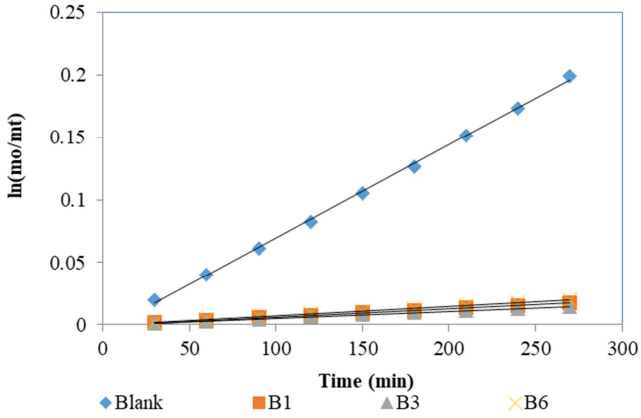


Figure 12. *First order kinetic model of aluminum dissolution.*

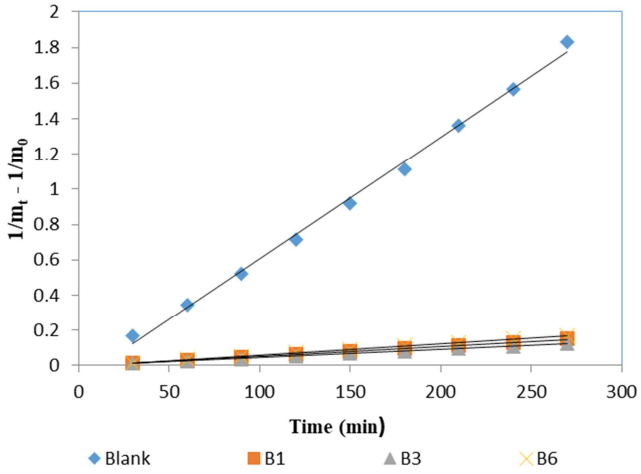


Figure 13. *Second order kinetic model of aluminum dissolution.*

3.3. Assessment of Kinetic Aspect

To determine the aluminum dissolution reaction order in HCl solution in absence and presence of each compound, we studied sample mass evolution over time. For studying zero order, first order and second order kinetic of aluminium dissolution in corrosive solution in absence (blank) and presence of each vitamin B1, B3 and B6 (0.53mM at 298K)

we have plotted m_o-m_t, $\ln(m_0/m_t)$ and $1/m_t$ -$1/m_0$ as a function of immersion time respectively. These representations are shown in Figures 11, 12 and 13.

Table 2 shows the slopes, coefficients of determination (R^2) and intercepts of the lines obtained for different orders studied. For slopes, units are: zero order ($g.mn^{-1}$), first order (mn^{-1}) and second order ($g^{-1}.mn^{-1}$); for the intercepts: zero order (g), first order (no unit) and second order (g^{-1}).

Table 2. *Kinetic parameters of the different orders studied.*

Kinetic order	Inhibitor	Slope	R^2	Intercept
Zero order	blank	0.00008	0.99997	0.00003
	B1	0.000008	0.99992	0.00007
	B3	0.000007	0.99993	0.00005
	B6	0.000009	0.99997	0.00008
First order	blank	0.000743	0.99902	0.00483
	B1	0.000055	0.99970	0.00042
	B3	0.000068	0.99980	0.00061
	B6	0.000077	0.99995	0.00069
Second order	blank	0.006885	0.99653	0.08466
	B1	0.000566	0.99964	0.00555
	B3	0.000461	0.99943	0.00380
	B6	0.000650	0.99988	0.00643

The analysis of lines parameters obtained during kinetic study of aluminium dissolution in inhibitor absence (blank) shows that the regression coefficients (R^2) of kinetic models of zero order and first order are very close to unity. However, the zero order kinetic model has an intercept of 0.00003 against 0.00483 for the first order kinetic model, so we can conclude that aluminium reaction dissolution in the inhibitors absence in 1M HCl is zero order reaction.

In the presence of each molecule used (vitamin B1, B3 and B6), the kinetic models of second order have the high intercepts. Therefore, aluminium reaction dissolution in the presence of each inhibitor in 1M HCl cannot be of second order. The intercepts for zero order model are the lowest and tend towards zero to those obtained with the first model order. It appears in this case that the order of aluminium dissolution reaction in the presence of each molecule (vitamin B1, B3 and B6) is zero order reaction.

Finally, the therapeutic molecules (vitamin B1, B3 and B6) reduces considerably aluminium corrosion in 1M HCl but does not change the dissolution reaction order in corrosive solution. Knowing that the rate constants for kinetic model of zero order for vitamin B3 is 0.007 $g.min^{-1}$, vitamin B1 is 0.008 $g.min^{-1}$ and for vitamin B6 is 0.009 $g.min^{-1}$, we deduce that vitamin B1 and vitamin B3 have a high inhibiting power compared to B6. This result is consistent with the result obtained during the gravimetric tests.

Aluminum dissolution reaction in HCl solution in the absence and presence of each compound is zero order, the half-reaction time ($t_{1/2}$) were calculated using the equation:

$$t_{1/2} = \frac{m_0}{2k} \qquad (11)$$

Where $(m_0 = 0.1207g)$ is initial mass and k (slope) is corrosion rate constant. The results obtained are listed in table 3.

Table 3. *Value of the half-reaction time in presence or absence of inhibitors.*

Half -time	Blank	B1	B3	B6
$t_{1/2}$ (min)	754.38	8621.43	7543.75	6705.55

To determine the energy amount that must be supplied to the reaction medium to initiate the chemical reaction, activation energy for each molecule was calculated from Arrhenius law expressed as follows :

$$E_a = \frac{RT_1T_2}{T_2-T_1} ln\left(\frac{k_{T_2}}{k_{T_1}}\right) \qquad (12)$$

Where k_{T_1} and k_{T_2} are respectively constant rates, slopes of straight lines obtained for kinetic of zero order at two temperatures T_1= 298K and T_2= 318K.

In this context, study kinetic was performed with a concentration of 0.53 M for each vitamin (vitamin B1, B3 and B6) at temperatures of 298 K and 318 K.

Figures 11 and 14 show respectively mass loss versus time at temperatures of 298K and 318K.

Vitamins B1, B3 and B6 activation energies are listed in Table 4.

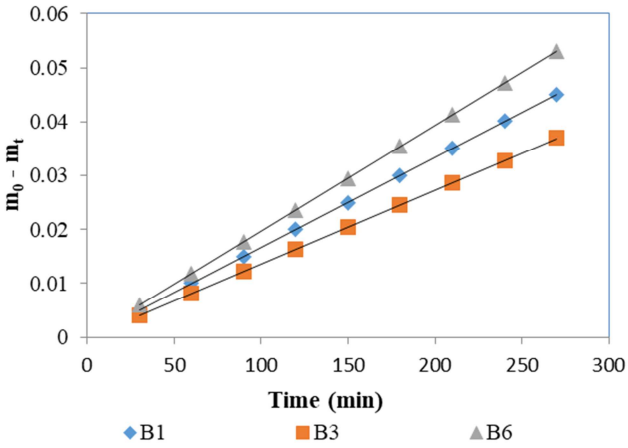


Figure 14. *Mass loss versus time of zero order kinetic at T = 318K.*

Table 4. *Corrosion rate and activation energy.*

Vitamins	Constant rate $k.10^{-6}(g.min^{-1})$		activation energy $(kJ.mol^{-1})$
	298K	318K	298K-318K
B1	8	167	119.8
B3	7	137	117.2
B6	9	197	121.7

3.4. Theoretical Correlation

The geometries of studied molecules are fully optimized at B3LYP/6-31G (d) level of theory. The final geometries are presented by figures 15.

The values of different chemical parameters calculated from the DFT at B3LYP/6-31G (d) are in Table 5.

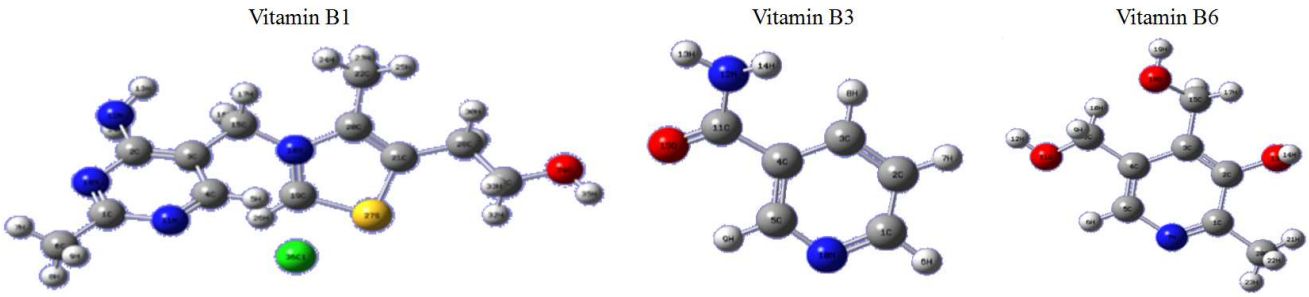


Figure 15. *Optimized structure of studied molecules.*

Table 5. *Quantum chemical parameters of molecules investigated.*

Quantum chemical parameters	Vitamin B1	Vitamin B3	Vitamin B6
E_{HOMO} (eV)	-5.838	-6.853	-6.114
E_{LUMO} (eV)	-1.681	-1.374	-0.648
ΔE (eV)	4.157	5.479	5.466
μ (Debye)	7.551	4.8891	2.1459
$I = -E_{HOMO}$ (eV)	5.838	6.853	6.114
$A = -E_{LUMO}$ (eV)	1.681	1.374	0.648
$\chi = -\mu_p = \frac{I+A}{2}$ (eV)	3.759	4.1135	3.381
$\eta = \frac{I-A}{2}$ (eV)	2.078	2.7395	2.733
$S = \frac{1}{\eta}$ $(eV)^{-1}$	0.481	0.365	0.366
$\Delta N = \frac{\chi_{Al}-\chi_{inh}}{2(\eta_{Al}+\eta_{inh})}$	0.125	0.030	0.164
$\omega = \frac{\mu_P^2}{2\eta} = \frac{(I+A)^2}{4(I-A)}$	3.399	3.088	2.091
E_T (Ha)	-1620.10	-416.985	-591.86

HOMO and LUMO energies are used to explain the inhibition properties and to indicate inhibitors adsorption centers [29]. Indeed the higher LUMO energy level of a molecule, more it tends to offer molecules to unoccupied orbitals of metal and higher inhibition efficiency. In our study, E_{HOMO} values of studied molecules are high, which indicate that they can give electrons to aluminium, hence the great inhibition efficiencies obtained experimentally. Vitamin B1 having the highest value of E_{HOMO} is the best inhibitor, which corresponds well to experimental observations. While low values of LUMO energy indicate that molecule is capable of receiving electrons from metal [30]. Referring to literature [31, 32], E_{LUMO} values obtained with the studied molecules are low therefore, these compounds are likely to receive electrons from aluminium. The calculations also show that vitamin B1 has the lowest E_{LUMO} value, so it has the highest capacity to interact with aluminium surface, which is in agreement with gravimetric tests.

Inhibitors reactivity depends on energy gap (ΔE) value. In fact if energy gap is low, the inhibitor adsorption on metal surface increases, and finally the inhibition efficiency increases [33, 34]. Energy gap values for vitamins B1, B2 and B3 are 4.157eV, 5.479eV and 5.66eV respectively. Comparing these values with that of aluminium which oscillates between 1.518eV and 6.12eV, it is apparent that it is easier to remove an electron from HOMO orbital of each molecule to migrate it to metal LUMO. However, our theoretical results show that there is a good correlation between ΔE and inhibition efficiency variation, it results that vitamin B1 with the lowest ΔE value has the best inhibition potential.

According to literature, dipole moment (μ) low values of the compounds could favour their adsorption on metal surface [35], while some authors affirm that high values of an organic compound dipole moment ensure a good inhibition efficiency [36, 37]. In this case, there is no consensus concerning the correlation between dipole moment and inhibition efficiency (IE).

Electronegativity (χ) values of studied inhibitors is lower than those of aluminium (χ_{Al} = 4.28 eV, $\eta_{Al} = 0$ [38]) showing that aluminium has the best electron attraction capacity. This leads to a positive value of fraction electrons transferred (ΔN) of each vitamin, indicating a possible movement of electrons from each inhibitor to aluminium. These observations justify that the good performance of these molecules is related to electron transfer from these compounds to the metal.

According to previous studies [39, 40], the three molecules studied have high values of softness (S) and low values of hardness (η) which favors their ability to interact with aluminium surface thus reducing its oxidation.

The high values of electrophilicity index (ω) of different molecules express their electrophilic character and thus showing a possible transfer of electrons from metal to inhibitors [41].

Total energy (E_T) values of all molecules studied are negative, revealing that charge transfer to a molecule, followed by electron donation back from the molecule, are energetically favored [42]. In this context, adsorption of inhibitors to metal surface can occur spontaneously. Similar results have been obtained in literature [43].

4. Conclusion

Gravimetric tests showed that vitamins B1, B2 and B3 can significantly reduce aluminium corrosion in 1M HCl. It was found that inhibition efficiency increases with increasing concentration of inhibitors but decreases with increasing temperature suggesting physical adsorption. The adsorption process occurs according to Villamil isotherm. The thermodynamic adsorption parameters were determined. These findings show that each vitamin adsorption is spontaneous, exothermic with an increase in disorder. The kinetic study reveals that aluminium dissolution reaction in absence and presence of each molecule is zero order. It appears clearly that inhibitors contribution does not influence

the reaction order. Half-reaction time and energy to initiate the dissolution reaction were determined. Quantum chemical calculations revealed good inhibiting abilities of the studied molecules. These abilities are due to an electron exchange between aluminium and these therapeutic molecules. Moreover, vitamin B1 is the best inhibitor of aluminium corrosion in 1M HCl among vitamins studied. Finally, experimental and theoretical results are coherent.

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