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Thiamine Hydrochloride as Copper Corrosion Inhibitor in 1M HNO_3

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Abstract

3-((4-Amino-2-methyl-5-pyrimidinyl) methyl)-5-(2-hydroxyethyl)-4-methylthiazolium chloride hydrochloride also known as Thiamine hydrochloride (Vitamin B1 hydrochloride) was used as copper corrosion inhibitor in 1.0M HNO_3 solution. The study was performed using weight loss and Density Functional Theory (DFT) methods. Copper dissolution was found to be temperature and Thiamine concentration dependent. The thermodynamic functions related to the adsorption of the molecule on the copper surface and that of the metal dissolution were determined. The results show a spontaneous adsorption and an endothermic dissolution processes. Adsorption models, including Langmuir, El-Awady and Flory-Huggins isotherms were examined. The Dubinin Raduskhevich isotherm was used to distinguish between physisorption and chemisorption. Furthermore, the global and local reactivity parameters of the molecule were analysed. Experimental and theoretical results were found to be in good agreement.

Keywords: Copper Corrosion Inhibition; Thiamine Hydrochloride; Weigh Loss Method; DFT Method; Global and Local Descriptors.

1. Introduction

Copper [1-3] is widely applied in many industries and applications (industrial equipment, electricity and electronics, communications, pipelines for domestic and industrial water utilities, etc.) due to its excellent electrical and mechanical properties and low prices. Thus corrosion of copper and its inhibition in aggressive media, particularly in presence of chloride ions [4-7], have attracted the attention of many researchers.

One of the most important methods in copper protection against corrosion [8-10] is the use of organic inhibitors containing polar groups, including nitrogen, sulfur and oxygen. Nowadays, heterocyclic compounds with polar functional groups and conjugated double bonds are frequently used for copper corrosion inhibition. The inhibiting action of these organic compounds [11-13] is usually attributed to their interactions with the copper surface via adsorption which depends on the nature of the copper/solution interface.

Recently, the effectiveness of an inhibitor molecule [14-16] has been related to its spatial as well as electronic structure. Quantum chemical methods are ideal tools for investigating these parameters and are able to provide insight into the inhibitor-surface interaction. A variety of chemical concepts which are now widely used as descriptors of chemical reactivity, e.g., electronegativity [17], hardness or softness [18], etc., appear within DFT. The Fukui function [19] and the local softness [20] measure the local electron density/population displacements corresponding to the inflow of single electron. They have been successfully performed [21, 22] to link the corrosion inhibition efficiency with molecular orbital (MO) energy levels for many organic compounds.

Vitamins, including vitamin B-12 [23], Riboflavin [24], vitamins B1 and C [25] have been used as mild steel corrosion inhibition in different acidic media. Though vitamin E [26] has been used for copper protection in acidic media, very few studies using vitamins as copper corrosion inhibitors have been reported in the literature.

The objective of the present paper is to study the behavior of Thiamine (vitamin B1) by analyzing its inhibition efficiency both on the experimental and theoretical points of views. Theoretical parameters such as the energy of the highest occupied molecular orbital (E_{HOMO}), the energy of lowest unoccupied molecular orbital (E_{LUMO}), the energy gap

(ΔE) between E_{LUMO} and E_{HOMO}, the dipole moment (μ), the ionization energy (I), the electron affinity (A), the electronegativity (χ), the global hardness(η), the global softness(S), the electrophilicity index(ω), the fraction of electrons transferred (ΔN) are determined and analyzed. The local reactivity has been analyzed through the Fukui indices, since they indicate the reactive regions in the form of nucleophilic and electrophilic behavior of each atom in the molecule.

2. Experimental

2.1 Copper Specimens

The copper specimens were in form of rod measuring 10 mm in length and 2.2 mm of diameter; they were cut in commercial copper of purity 95%.

2.2 The Studied Molecule

The structure of Thiamine hydrochloride (Formula: $C_{12}H_{17}ClN_4OS.HCl$) is given in Fig.1.

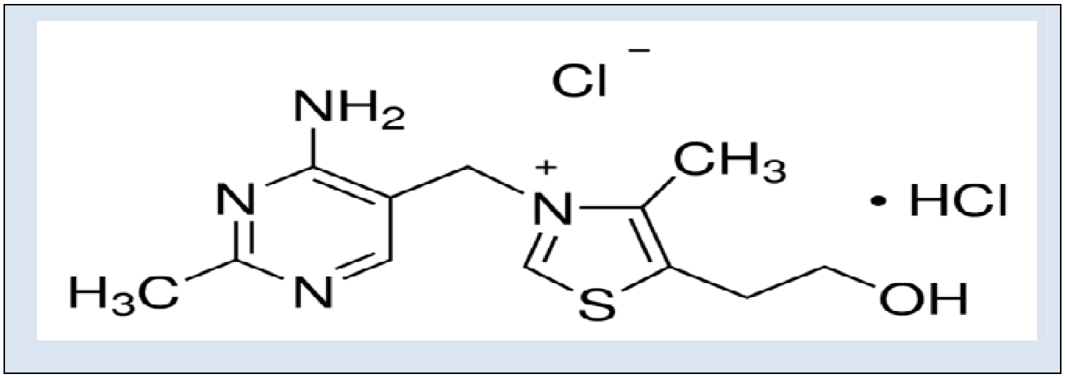


Fig. 1: Molecular structure of Thiamine hydrochloride

2.3 Solutions

Analytical grade 68% nitric acid solution from SUVCHEM Laboratory chemical was used to prepare the corrosive aqueous solution. The solution was prepared by dilution of the commercial nitric acid solution using double distilled water. The blank was a 1M HNO_3 solution. Solutions of Thiamine hydrochloride of analytical grade from Sinopharm Chemical Reagent Co, Ltd with concentrations in the range of 0.13 mM to 0.53 mM were prepared.

2.4 Mass loss Method

The mass loss method [27, 28] is the most widely used method of inhibition assessment. The simplicity and reliability of the measurement offered by mass loss method [29, 30] is such that the technique forms the baseline method of measurement in many corrosion monitoring programs. The samples were polished successively with fine grade emery papers, cleaned with acetone, washed with double distilled water and dried in moisture free desiccator. Tests were conducted under total immersion conditions of the polished copper specimen in 50 mL of 1.0M nitric acid solutions without and with different concentrations of Thiamine hydrochloride. Tests solutions were maintained at (308-328K). All tests were made in aerated solutions (Nitric acid solutions without and with Thiamine in presence of chloride ions) and were run triplicate to guarantee the reliability of the results. To determine the mass loss at the end of the test, the samples were retrieved from the tests solutions after 1 hour immersion time. The corrosion rate (W) was calculated according to the equation below:

$$W = \frac{m_1 - m_2}{St} \qquad (1)$$

Where m_1 and m_2 are respectively the mass (in g) before and after immersion in the test solution, S is the total surface of the sample (in cm^2) and t is the immersion time (in h). The inhibition efficiency IE (%) was then calculated using the following relation:

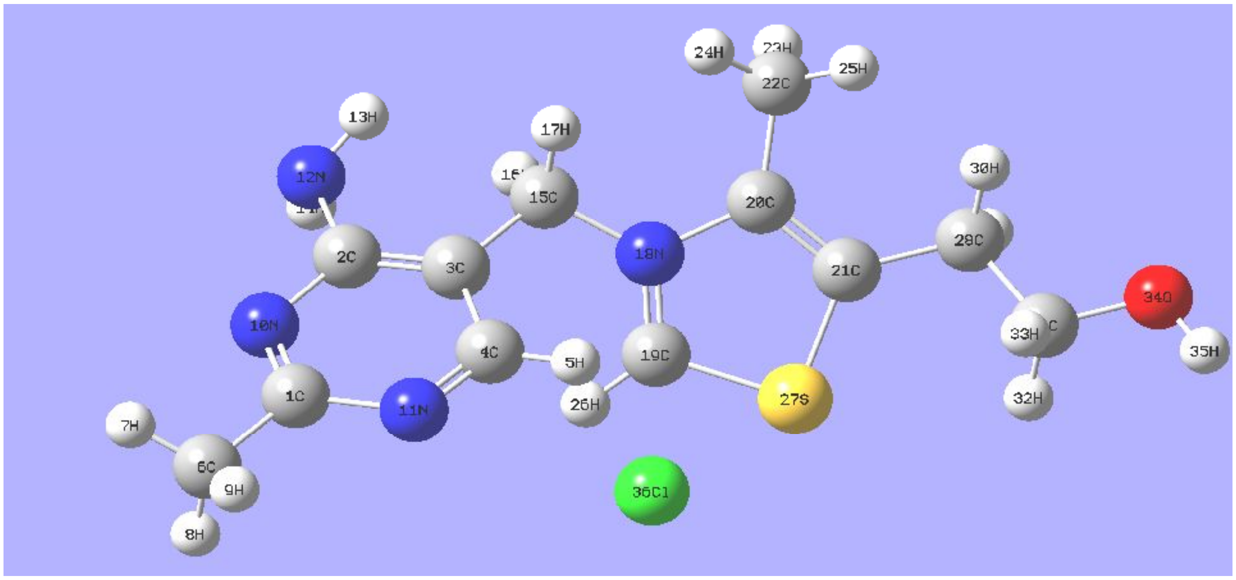
$$IE(\%) = \frac{w_0 - w}{w_0} \times 100 \qquad (2)$$

In this equation, w_0 and w are respectively the corrosion rates of copper in the absence and the presence of the tested compounds.

2.5 Computational Method

In order to explore the theoretical-experimental consistency, quantum chemical calculations were performed in gas phase using Gaussian 03 software package [31]. Complete geometrical optimization of Thiamine chloride was performed using density functional theory (DFT) with Becke's three parameter exchange functional along with the Lee-Yang-Parr nonlocal correlation functional (B3LYP) [32, 33]. The calculations were based on 6-31 G (d) basis set [34]. Fig.2 presents the optimized structure of Thiamine chloride.

Fig. 2: Optimized Structure of Thiamine chloride Calculated by B3LYP/6-31 G (d)



2.6 Theoretical Background

2.6.1 Global Parameters

The basic relationship of density functional theory of chemical reactivity [35] links the chemical potential (μ_p) with the first derivative of energy with respect to the number of electrons, and therefore with the negative of the electronegativity:

$$\mu_p = \left(\frac{\partial E}{\partial N}\right)_{v(r)} = -\chi \tag{3}$$

Where μ_p is the chemical potential, E is the total energy, N is the number of electrons, and $v(r)$ is the external potential of the system.

Hardness (η) [36] has been defined within the DFT as the second derivative of the energy with respect to N as $v(r)$, property which measures both the stability and reactivity of the system:

$$\eta = \left(\frac{\partial^2 E}{\partial N^2}\right)_{v(r)} \tag{4}$$

According to Koopman's Theorem [37], ionisation potential (*I*) and electron affinity (A) are defined as follow:

$$I = -E_{HOMO} \tag{5}$$

$$A = -E_{LUMO} \tag{6}$$

The electronegativity which is the measure of the power of an atom or group of atoms to attract electrons towards itself can be estimated using the equation:

$$\chi = \frac{I+A}{2} \tag{7}$$

Chemical hardness (η) [36] which measures the resistance of an atom to a charge transfer is given by:

$$\eta = \frac{I-A}{2} \tag{8}$$

Chemical softness (S) [36] is the measure of the capacity of an atom or group of atoms to receive electrons. It is estimated by the above equation:

$$S = \frac{1}{\eta} \tag{9}$$

For a reaction of two systems with different electronegativities [37], the electronic flow will occur from the system with lower value (inhibitor) towards that of higher value (metallic surface) until the chemical potential are equal. The fraction of electrons transferred ΔN from the inhibitor molecule to the metal was calculated according to Pearson electronegativity scale [37]:

$$\Delta N = \frac{\chi_{Cu}-\chi_{inh}}{2(\eta_{Cu}+\eta_{inh})} \tag{10}$$

Where χ_{Cu} and χ_{inh} are respectively the absolute electronegativity of copper and that of the inhibitor, whereas η_{Cu} and η_{inh} denote respectively hardness of copper and that of the inhibitor. In our study, we use a theoretical value of $\chi_{Cu} = 4.98$ eV [38] and $\eta_{Cu} = 0$, assuming that for a metallic bulk, $I = A$ [39] because they are softer than neutral metallic atoms.

The electrophilicity index (ω) is the descriptor of reactivity that expresses [40] a measure of energy lowering due to maximal electron flow between donor and acceptor. This parameter is defined as follows:

$$\omega = \frac{\mu_P^2}{2\eta} \tag{11}$$

Local Parameters

The local selectivity of a corrosion inhibitor [41] is generally assessed using Fukui functions. Their values are used to identify which atoms in the inhibitor are more prone to undergo an electrophilic or nucleophilic attack. The change in electron density [42] is the nucleophilic $f^+(r)$ and electrophilic $f^-(r)$ Fukui functions, which can be determined using the finite difference approximation:

$$f_k^+ = q_k(N+1) - q_k(N) \tag{12}$$

$$f_k^- = q_k(N) - q_k(N-1) \tag{13}$$

Where $q_k(N+1)$, $q_k(N)$ and $q_k(N-1)$ are the electronic population of atom k in $(N+1)$, N and $(N-1)$ electrons systems. Condensed softness indices of reactivity can be estimated as follows:

$$s_k^\alpha(r) = \left(\frac{\partial\rho(r)}{\partial N}\right)_{v(r)}^\alpha \left(\frac{\partial N}{\partial\mu}\right)_{v(r)} = f_k^\alpha(r)S \tag{14}$$

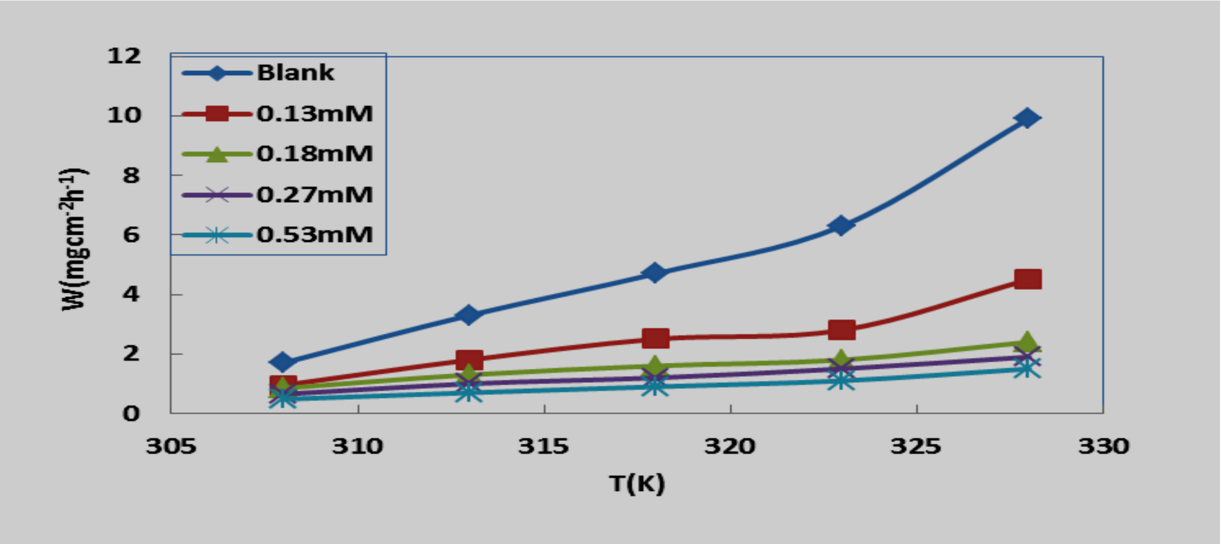
Where $\alpha = +$ or $-$

3. Results and Discussion

3.1 Mass Loss Measurement

Fig.3 gives the representation of corrosion rate versus temperature for different concentrations in Thiamine.

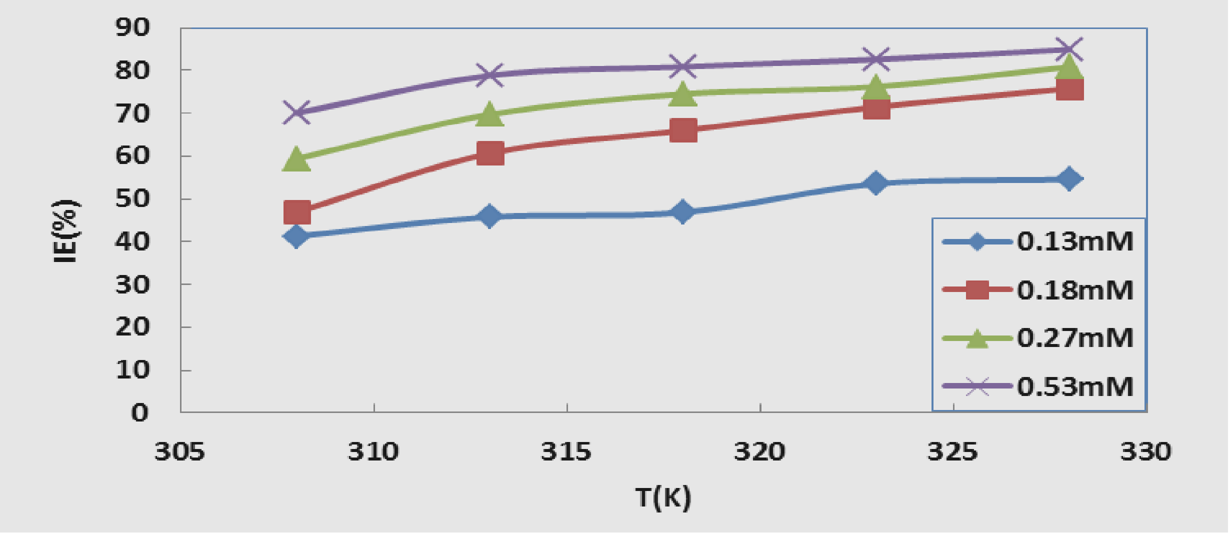
Fig. 3: Corrosion Rate Versus Temperature for Copper Corrosion in 1M HNO_3



It can be seen that for all the range of temperature, corrosion rate increases with increasing temperature. However, the rise in Thiamine concentration affects the evolution of the corrosion rate which decreases when the concentration increases.

Examining the plots of the inhibition efficiency IE (%) versus temperature for different concentrations (fig.4), one can infers that temperature favours the protection ability of the studied compound. The above observations enable us to state that the increase in temperature leads to an increase in adsorption process of Thiamine chloride on the metal surface, and therefore an increase in the metal surface covered by the compound. The highest efficiency attained for 0.53 mM and T = 328 K is 84.85% showing the good inhibitory effect of Thiamine at elevated temperature.

Fig. 4: Inhibition Efficiency Versus Temperature for Different Concentration in Thiamine



3.2 Adsorption Parameters

Attemps were made to fit values of θ to three isotherms including Langmuir, El-Awady and Flory-Huggins. The best fit was obtained with Langmuir adsorption model written in the rearranged form:

$$\frac{C_{inh}}{\theta} = \frac{1}{K_{ads}} + C_{inh} \qquad (15)$$

With:

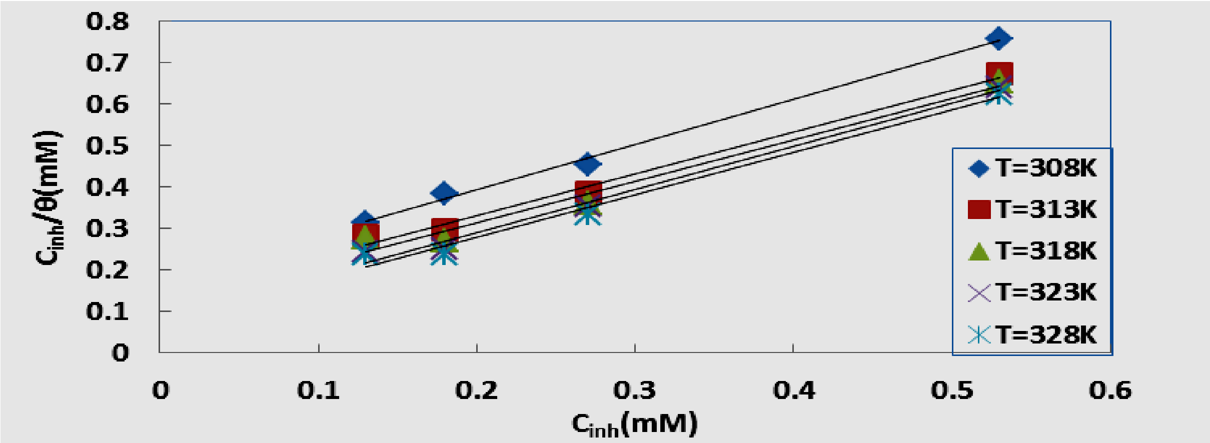
$$K_{ads} = \frac{1}{55.5} exp\left(\frac{-\Delta G^0_{ads}}{RT}\right) \tag{16}$$

Where C_{inh} is the concentration of the inhibitor, K_{ads} is the adsorption equilibrium constant, θ is the surface coverage and ΔG^0_{ads} is the change in standard free adsorption enthalpy. The relationship between (C_{inh}/θ) and C_{inh} is linear at all temperatures studied (fig. 5) with slopes nearly equal to unity.

To determine the change in adsorption enthalpy and change in adsorption entropy, we have used the equation which relates the two quantities and the change in free adsorption enthalpy:

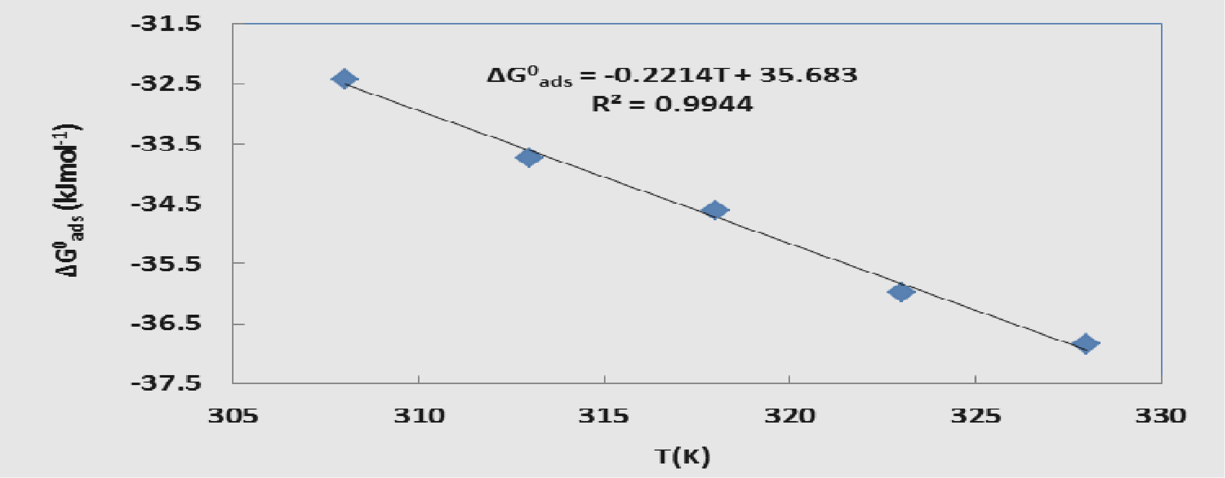
$$\Delta G^0_{ads} = \Delta H^0_{ads} - T\Delta S^0_{ads} \tag{17}$$

Fig. 5: Plots of (C_{inh}/θ) versus C_{inh} for Various Temperatures



Plotting ΔG^0_{ads} versus temperature leads to $(-\Delta S^0_{ads})$ and (ΔH^0_{ads}), which are respectively the slope and the intercept of the obtained straight lines (fig.6).

Fig. 6: Change in Free Enthalpy Versus Temperature



All the adsorption parameters are collected in Table 1.

The adsorption parameters gathered in Table 1 enables us to clarify the interaction between the organic compound and the metallic surface. In general, two kinds of adsorption can be considered (physical adsorption or chemisorption) and sometimes the both.

The negative values of ΔG^{0}_{ads} [43] indicate a spontaneous adsorption process. Usually, the adsorption [44] is regarded as physisorption if the value of change in free adsorption enthalpy is upper or equal to -20 $kJmol^{-1}$ and the chemisorption is pronounced when the value of ΔG^{0}_{ads} is lower or equal to -40 $kJmol^{-1}$.

Table 1: Parameters of the Adsorption of Thiamine Chloride on Copper Surface in 1M HNO_3

T(K)	$K_{ads}(\times 10^{3} M^{-1})$	$\Delta G^{0}_{ads}(kJ\ mol^{-1})$	$\Delta H^{0}_{ads}(kJ\ mol^{-1})$	$\Delta S^{0}_{ads}(J\ mol^{-1}K^{-1})$
308	5.724	-32.43		
313	7.722	-33.74		
318	8.772	-34.61	35.68	221.4
323	11.947	-35.99	35.68	221.4
328	13.315	-36.84		

In our case ΔG^{0}_{ads} values range from -36.84 to -32.43, showing that both physisorption and chemisorption exist. However, chemisorption is favoured by increasing temperature. The positive values of ΔH^{0}_{ads} indicate that the adsorption of the inhibitor is an endothermic process. Literature [45] pointed out that an exothermic process signifies either physisorption or chemisorption while an endothermic process is associated to chemisorption. The positive values of ΔS^{0}_{ads} denote a disorder, probably due to desorption of water molecules.

To distinguish between physisorption and chemisorption, experimental data were fitted to Dubinin-Radushkevich isotherm. This model [46, 47] has been recently used to explain the mechanism of corrosion inhibition onto a metal surface in acidic solution. The model [48] is based on the following equation:

$$ln\theta = ln\theta_{max} - a\delta^{2} \qquad (18)$$

Where θ_{max} is the maximum surface coverage and δ is the Polanyi potential which is given by:

$$\delta = RT\ln\left(1 + \frac{1}{C_{inh}}\right) \qquad (19)$$

In this equation, R is the universal gas constant, T is the thermodynamic temperature and C_{inh} is the concentration in $g\ L^{-1}$ of the inhibitor. Fig. 7 gives the plot of $ln\theta$ versus δ^{2}. The parameters of the model are gathered in table 2.

Fig. 7: Dubinin-Radushkevich Isotherms for Thiamine Chloride Adsorption on Copper in 1M HNO_3

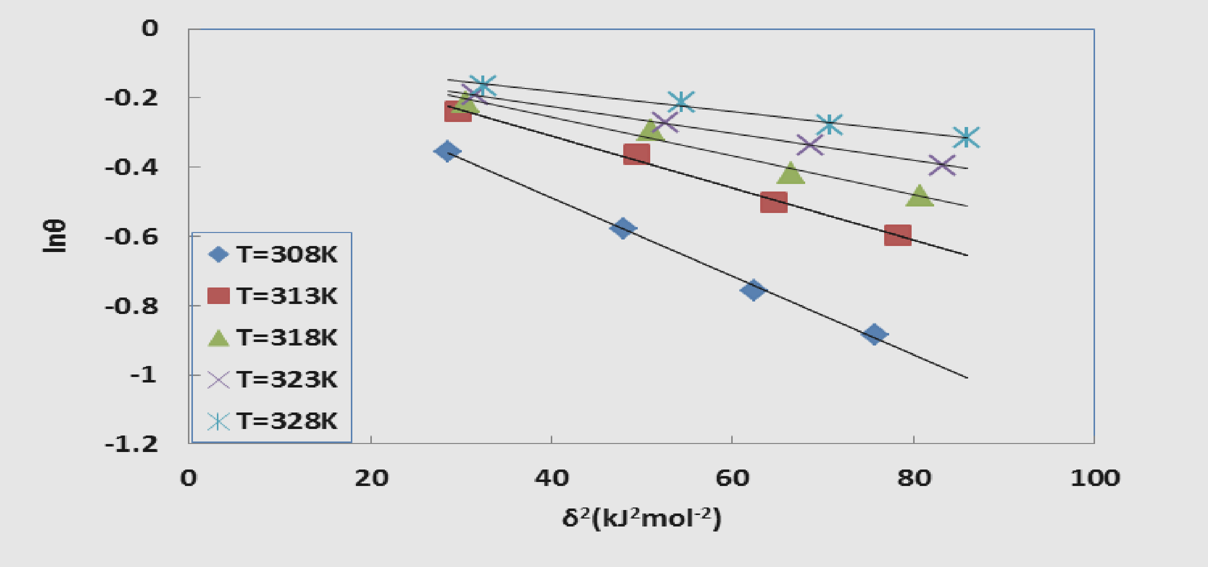


Table 2: Dubinin-Radushkevich Isotherms Parameters

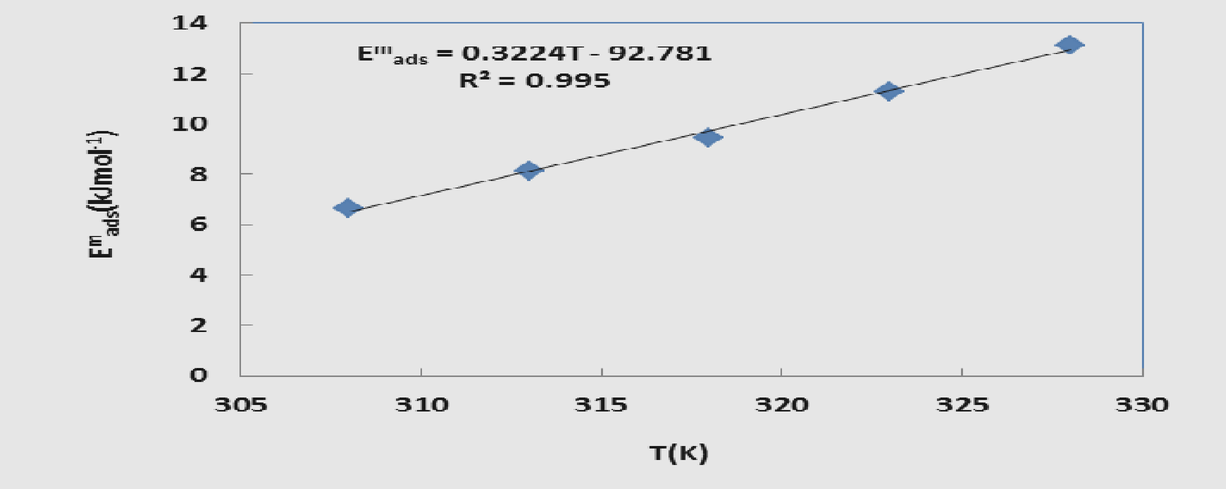
T(K)	R^2	a (kJ^{-2} mol^2)	E_m (kJ mol^{-1})
308	0.998	0.0113	6.65
313	0.986	0.0075	8.16
318	0.965	0.0056	9.45
323	0.999	0.0039	11.32
328	0.976	0.0029	13.13

The values of the constant a are obtained from the slope of the straight lines; this parameter is related to E_m, the adsorption energy which is the transfer energy of 1 mol of adsorbate from infinity (bulk solution) to the surface of the adsorbent. E_m is defined as:

$$E_m = \frac{1}{\sqrt{2a}} \tag{20}$$

The magnitude of E_m gives information about the type of adsorption. E_m values less than 8 kJ mol^{-1}[48] indicate physical adsorption. Plotting E_m versus temperature leads to the determination of the domains in which we have physisorption and that of chemisorption.

Fig. 8: Mean Adsorption Energy Versus Temperature



Analysing the results, one can see that we have both physisorption and chemisorption (physisorption for $T \leq 312.56\ K$ and chemisorption for $T > 312.56\ K$).

3.3 Kinetic and thermodynamic consideration

Arrhenius equation provides a mathematical dependency between the corrosion rate and temperature as follows:

$$logW = logA - \frac{E_a}{2.303RT} \tag{21}$$

Where W is the corrosion rate, A is the Arrhenius pre-exponential constant, R is the molar gas constant, T is the absolute temperature and E_a is the activation energy. A plot of $logW$ against $1/T$ produces straight lines (figure 9) with slope as $(-E_a/2.303RT)$ and intercept as $logA$. Activation parameters calculated from the plot are displayed in Table 3.

Fig. 9: Arrhenius Plot for Different Concentration of Thiamine in 1M HNO_3

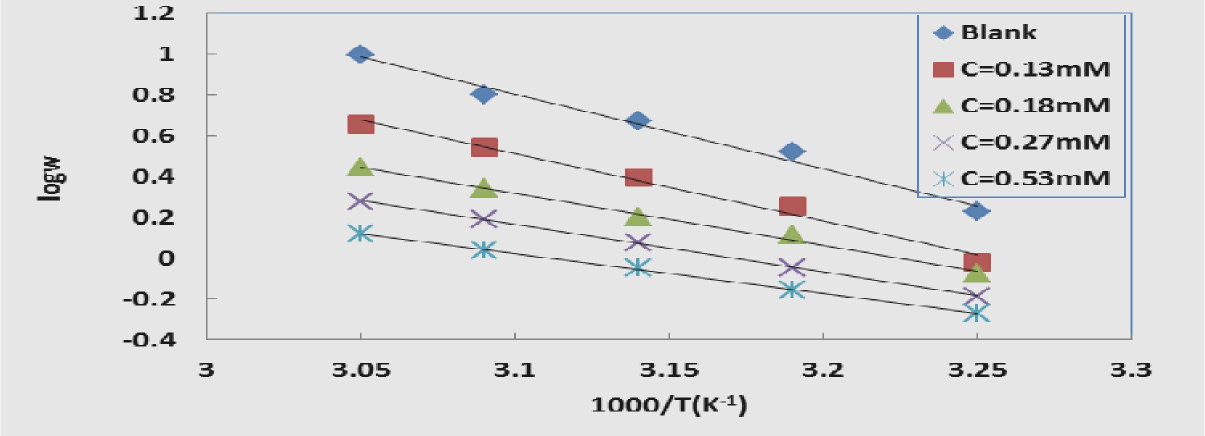


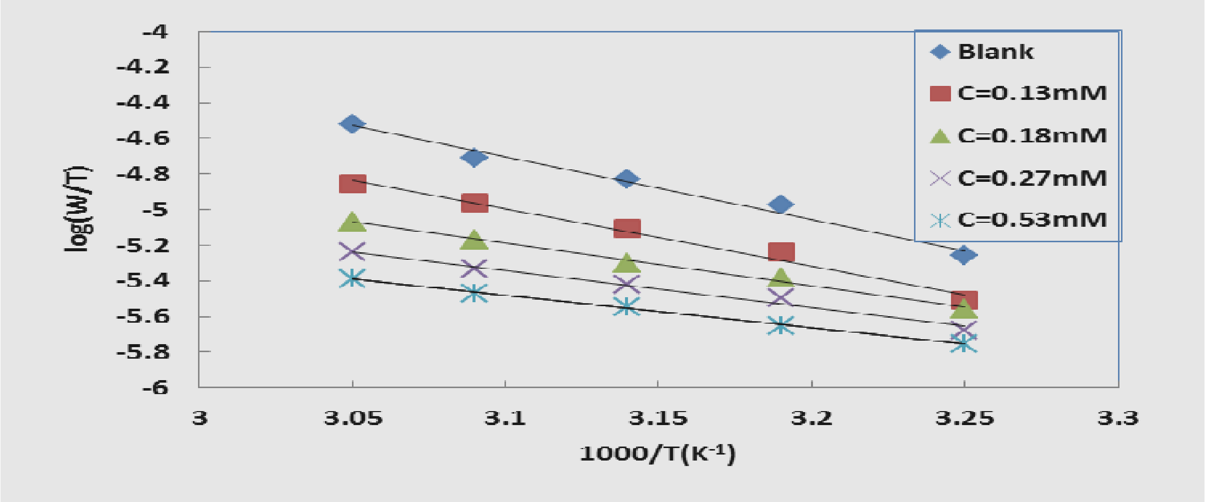
Table 3: Copper Corrosion Activation Parameters in 1M HNO_3 With or Without Thiamine			
	$E_a(kJmol^{-1})$	$\Delta H_a^*(kJmol^{-1}$	$\Delta S_a^*\ (Jmol^{-1}K^{-1})$
Blank	69.5	63.9	-80.3
0.13mM	63.2	58.6	-103.2
0.18mM	48.2	43.8	*-154.9*
0.27mM	44.6	38.2	-175.8
0.53mM	37.5	33.3	-194.4

The transition state equation (22) afforded thermodynamic parameters (Table 3) such as enthalpy change ΔH_a^* and entropy change ΔS_a^* from the plot of $\log(W/T)$ versus $1/T$ shown in fig. 10.

$$\log\left(\frac{W}{T}\right) = log\left(\frac{R}{Nh}\right) + \frac{\Delta S_a^*}{2.303R} - \frac{\Delta H_a^*}{2.303RT} \qquad (22)$$

Where N is the Avogadro's number and h is the Planck's constant. The enthalpy change was calculated from the slope $(-\Delta H_a^*/2.303R)$ while the entropy change was calculated from the intercept $\{log(R/Nh) + \Delta S_a^*/2.303R\}$ of the plots (fig.10).

Fig. 10: Transition State Plots for Different Concentrations of Thiamine Chloride in 1 M HNO_3



The literature [49] states that physical adsorption is associated with, E_a values of the inhibited solution larger than that of the free acid solution. In our work, the uninhibited solution is associated with E_a value, higher than that of the inhibited solutions, confirming the predominance of chemisorption. ΔH_a^* has a positive sign, denoting an endothermic activation process. ΔS_a^* is negative, showing [50] that the activated complex in the rate determining step represents an association rather than a dissociation.

3.4 Quantum Chemical Computation Details

According to the frontier molecular orbital (FMO) theory of chemical reactivity, transition of electron is due to interaction between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of reacting species. E_{HOMO} [51] measures the tendency towards the donation of electron by a molecule whereas E_{LUMO} indicates the ability of the molecule to accept electrons. The binding ability of the inhibitor to the metal surface [51] increases with increasing of the HOMO and decreasing of the LUMO energy values. The calculated quantum chemical and reactivity parameters are collected in table 4.

Table 4: Chemical Properties of Thiamine Chloride

Descriptor	Value	Descriptor	Value
E_{HOMO} (eV)	-5.838	χ (eV)	3.759
E_{LUMO} (eV)	-1.681	η (eV)	2.078
ΔE (eV)	4.157	S (eV) $^{-1}$	0.481
μ (D)	7.551	ΔN	0.294
I (eV)	5.838	ω	3.399
A(eV)	1.681	E_N (a.u)	-1620.1

The inhibitor does not only donate electron to the unoccupied d orbital of the metal ion but can also accept electron from the d orbital of the metal, leading to the formation of a feedback bond. The highest value of E_{HOMO} -5.838 eV of Thiamine chloride could explain its good inhibition efficiency (84.85 % at C_{inh} = 0.53 mM and T = 328 K).

The energy gap ($\Delta E = E_{LUMO} - E_{HOMO}$) is an important parameter as a function of reactivity of the inhibitor molecule towards the adsorption on the metallic surface. Lower values of the energy gap [52] will render good inhibition efficiency, because the energy to remove an electron from the last occupied orbital will be low. In our case, the low value of ΔE (4.157 eV) when compared with that of many molecules [52-54] in the literature could explained the good inhibition efficiency of Thiamine chloride.

The dipole moment (μ in Debye) is another important electronic parameter that results from the non-uniform distribution of charges on the atoms in the molecule. According to some authors, a high value of the dipole moment [55] probably leads to an important adsorption of the chemical compound on the metal surface. However, many other authors [56] state that low values of dipole moment favour the adsorption process. So in general [57], there is no significant relationship between the dipole moment and the inhibition efficiency.

Ionization energy is a fundamental descriptor of the chemical reactivity of molecules that deals with their stability or their inertness. High ionization energies [58] indicate a high stability of the system while low values denote high reactivity. In our case, the low ionization energy (5.838 eV) of the molecule could explain its high inhibition efficiency.

Absolute hardness and softness also measure molecular stability and reactivity. The chemical hardness fundamentally signifies the resistance towards the deformation or polarization of electron cloud of a system under a small perturbation of the chemical reaction. A hard molecule [59] has a large energy gap and a soft molecule a small energy gap. In our work, Thiamine chloride has a small hardness value (2.078 eV) and a high value of softness (0.481 $(eV)^{-1}$) compared with many molecules in the literature. These results confirm those obtained with the earlier mentioned descriptors.

The number (ΔN) of electrons transferred was also calculated and the obtained value (0.294) shows according to the literature [60] that the inhibition efficiency results from electrons donation.

The absolute electrophilicity index was also calculated. According to the definition, this index measures the propensity of chemical species to accept electrons. A high value of electrophilicity index [40] describes a good electrophile while a small value of electrophilicity index denotes a good nucleophile. This reactivity index measures the stabilization in energy when the system acquires an additional electronic charge from the environment. The obtained value (ω = 3.399) shows that the inhibitor is an electrophile molecule: it can receive electrons.

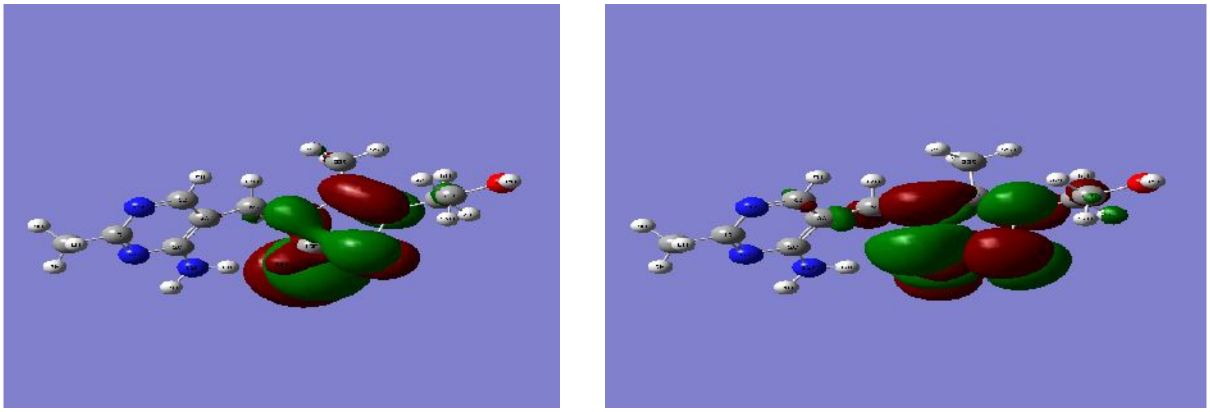
Many authors [55] state that the more negatively charged an heteroatom is, the more it can be adsorbed on the metal surface through the donor-acceptor type reaction. All the probable adsorption centers are tabulated in table 5.

Table 5: Charges of Some Selected Atoms, Condensed Fukui Functions and Softness Indices

Atom N°	$q_k(N+1)$	$q_k(N)$	$q_k(N-1)$	f_k^+	f_k^-	s_k^+	s_k^-
C(4)	-0.006136	0.046681	0.033312	-0.052817	0.013369	-0.025405	0.006430
C(6)	-0.491046	-0.492772	-0.494366	0.001726	0.001594	0.000830	0.000767
N(10)	-0.516521	-0.454785	-0.423397	-0.061736	-0.031388	-0.029695	-0.015098
N(11)	-0.505536	-0.431301	-0.410874	-0.074235	-0.020427	-0.035707	-0.009825
N(12)	-0.773559	-0.746893	-0.725373	-0.026666	-0.021520	-0.012826	-0.010351
C(15)	-0.185571	-0.189986	-0.201024	0.004415	0.020038	0.002124	0.009638
N(18)	-0.386513	-0.395075	-0.378924	**0.008562**	-0.016151	**0.004118**	-0.007769
C(19)	-0.265980	-0.209397	-0.244739	-0.056503	**0.035342**	-0.027216	**0.016999**
C(21)	-0.216508	-0.203055	-0.205165	-0.013453	0.002110	-0.006471	0.001015
C(22)	-0.511443	-0.509308	-0.512267	-0.002135	0.002959	-0.001027	0.001423
C(28)	-0.299981	-0.307698	-0.317959	0.007717	0.010261	0.003712	0.004935
C(31)	-0.048740	-0.042157	-0.043918	-0.000717	0.001761	-0.000345	0.000847
O(34)	-0.649627	-0.637871	-0.619648	-0.016796	-0.021516	-0.008079	-0.001035
Cl (36)	-0.356127	-0.266797	-0.015007	-0.089330	-0.251790	-0.042968	-0.121111

The frontier molecular orbitals HOMO and LUMO are given in fig. 11.

Fig. 11: HOMO (left) and LUMO (right) Diagrams of Thiamine Chloride using B3LYP/6-31G (d)



Analyzing figure 11, one can observed that HOMO and LUMO densities are concentrated in nearly the same region, around the following atoms C (19), N (18), C (28), C (21), Cl (36) and S (27). Fukui functions compute local reactivity indices that make possible the rationalization of the molecular reactivity. The condensed Fukui function and local softness indices allow distinguishing each part of the molecule on the basis of distinct chemical behaviors due to different functional groups. The preferred site for nucleophilic attack is the atom in the molecule where the value of f_k^+ is maximum and it is associated with the LUMO region while the site for electrophilic attack is controlled by the values of f_k^- which is associated with the HOMO region. Fukui function depicted in table 5, implies that atom N (18) is the preferred site for nucleophilic attack, as this site has the highest value f_k^+. The atom C (19) is the preferred site for electrophilic attack since this atom has the highest value of Fukui function f_k^-.

4. Conclusions

The following conclusions can be drawn from this study:

1. The Inhibition efficiency of thiamine chloride is temperature and concentration dependent;
2. Thiamine chloride adsorbs on copper according to the Langmuir adsorption isotherm;
3. Adsorption and activation thermodynamic functions indicate a spontaneous chemisorption process;
4. Global reactivity parameters confirm the good inhibition efficiency of the molecule;
5. Local reactivity parameters allow determining the probable electrophilic and nucleophilic attacks sites.

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