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Research Article

Copper Corrosion Inhibition by Cefuroxime Drug in 1M Nitric Acid

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Abstract

The copper corrosion inhibition in one molar nitric acid by cefuroxime drug is studied through weight loss and quantum chemical methods based on DFT (B3LYP/6-31G (d, p). The results show that the studied drug is a good inhibitor which adsorbs spontaneously on copper via Langmuir modified isotherm. The thermodynamic adsorption and activation parameters indicate a predominant physisorption process and an endothermic dissolution process. Quantum chemical calculations at B3LYP level with 6-31G (d, p) basis set lead to molecular descriptors such as E_{HOMO} (energy of the highest occupied molecular orbital), E_{LUMO} (energy of the lowest unoccupied molecular orbital), ΔE (energy gap) and μ (dipole moment). The global reactivity descriptors such as χ (electronegativity), η (hardness), S (softness) and ω (electrophilicity index) were derived using Koopman's theorem and analyzed. The local reactivity parameters, including Fukui functions $f(\vec{r})$ and local softness $s(\vec{r})$ were determined and discussed. Experimental and theoretical results were found to be in good agreement.

Keywords: Copper corrosion inhibition, cefuroxime, weight loss, adsorption, DFT, Fukui functions

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Introduction

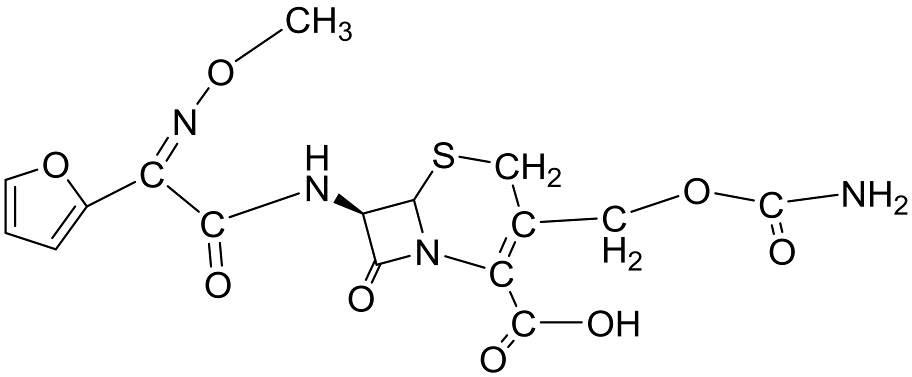
The environmental, economical and safety consequences of metals corrosion are enormous and their chemical protection has been deeply investigated [1]. Copper and its alloys [2] are often used in many applications in modern chemistry. Copper is a relatively noble metal, however, it undergoes corrosion when being in contact with acidic solutions, especially in the presence of oxygen or other oxidants [3]. Several research methods on inhibition of its corrosion have been reported and it has been established that the use of inhibitors is one of the best methods for the prevention of the corrosion of copper in acidic medium [4]. Organic compounds, which can donate electrons to unoccupied d orbital of the metal surface to form coordinate covalent bonds, and can also accept free electrons from the metal surface by using their anti-bonding orbital to form feedback bonds, constitute excellent corrosion inhibitors [5]. A number of heterocyclic compounds containing nitrogen, oxygen, and sulfur either in the aromatic or long chain carbon system have been reported to be effective inhibitors [6, 7].

Recently, several studies have been carried out on the inhibition of corrosion of metals by drugs due to environmental constraints [8, 9]. Cefuroxime (**Scheme 1**) is the commercial name of (6R, 7R) -3 - {[(aminocarbonyl) oxy] methyl} -7 - {[(2Z) -2- (furan-2-yl) -2- (methoxyimino) acetyl] amino} -8-oxo acid -5-thia-1-azabicyclo [4.2.0] oct-2-ene-2-carboxylic acid, an antibiotic drug which is easily available, environmentally friendly and nontoxic. In view of these favorable characteristic properties, Cefuroxime drug was chosen for the corrosion studies. In order to support experimental studies, quantum chemistry calculations are used to study reaction mechanisms and to interpret the experimental results. To get insight into chemical reactivity and selectivity of organic compounds, authors use DFT parameters including global parameters such as electronegativity χ [10], hardness η [11], softness S, electrophilicity index ω [12] and local parameters as condensed Fukui functions $f(\vec{r})$ [13] and condensed local softness $s(\vec{r})$ [14]. The aim of the present paper is to evaluate the inhibitive properties of cefuroxime drug against copper corrosion in 1 M HNO_3, by analyzing both experimental data and theoretical parameters.

Experimental

Copper specimen

The samples of copper used in this study were in the form of rods with 10 mm as length and 2.2 mm as diameter which were cut in commercial copper of purity 95%.



Scheme 1 Chemical structure of cefuroxime

Reagents

Cefuroxime of analytical grade with $C_{16}H_{16}N_4O_8S$ as formula and acetone of purity 99.5% were purchased from Sigma-Aldrich Chemicals. Commercial nitric acid of purity 65% was purchased from Pan Reac AppliChem.

Solution preparation

1M HNO_3 solutions without or with different concentrations of Cefuroxime ranging from 0.05 to 5 mM were then prepared.

Weight loss method

Before each measurement, the copper samples were mechanically abraded with different grade emery papers (1/0, 2/0, 3/0, 4/0, 5/0, and 6/0). The specimens were washed thoroughly with double distilled water, degreased and rinsed with acetone and dried in a moisture-free desiccator. Weight loss measurements conducted in a beaker of 100 mL capacity containing 50 mL of the test solution. The immersion time for weight loss was 1h at a given temperature. In order to get good reproducible data, parallel triplicate experiments were performed accurately and the average weight loss was used to calculate the corrosion rate (W), the degree of surface coverage (ϴ) and the inhibition efficiency (IE) using Equation 1-3 respectively:

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

$$\theta = \frac{W_0 - W}{W_0} \quad (2)$$

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

where W_0 and W are the corrosion rate without and with inhibitor respectively, m_1 and m_2 are the weight before and after immersion in the corrosive aqueous solution respectively, S is the total surface of the aluminum specimen and t is the immersion time.

Quantum Chemical Calculations

The quantum chemical calculations have been performed with Gaussian-09 series of program package [15]. In our calculation we have used Becke's three parameter exchange functional [16] along with the Lee-Yang–Parr nonlocal correlation functional (B3LYP) [17] using 6-31G (d, p) basis set. Quantum chemical methods also have been proved to be a very powerful tool for studying inhibition of corrosion of the metals [18]. Density functional theory (DFT) has been quite successful in providing theoretical basis for popular qualitative chemical concepts like energy of highest occupied molecular orbital (E_{HOMO}) and the lowest unoccupied molecular orbital (E_{LUMO}), energy gap (ΔE), total electronic energy (E) of the molecule through global reactivity parameters such as chemical hardness (η), global softness (S), fraction of electrons transferred (ΔN), electrophilicity index(ω) and local ones such as Fukui function ($f(\vec{r})$) and local softness ($s(\vec{r})$).

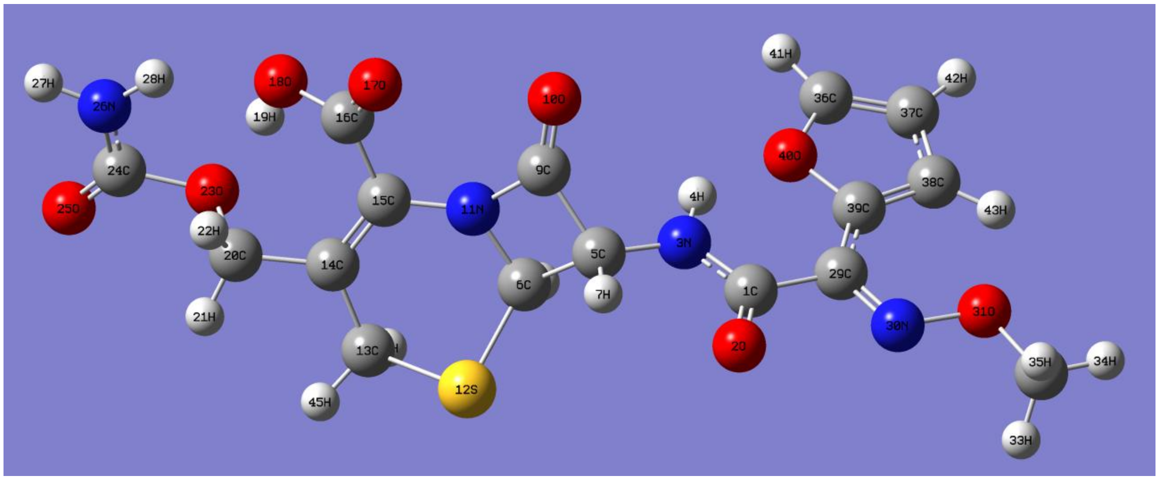


Figure 1 Optimized structure of cefuroxime by B3LYP/6-31G (d, p)

For N-electrons system with total energy E, the electronegativity is given by Equation 4:

$$\chi = -\mu_P = -\left(\frac{\partial E}{\partial N}\right)_{v(\overrightarrow{r})} \tag{4}$$

Where μ_P and $v(\overrightarrow{r})$ are the chemical and external potentials respectively. The chemical hardness η which is defined as the second derivative of E with respect to N is then given by Equation 5:

$$\eta = \left(\frac{\partial^2 E}{\partial N^2}\right)_{v(\overrightarrow{r})} \tag{5}$$

The global softness S is the inverse of the global hardness as seen in Equation 6:

$$S = \frac{1}{\eta} \tag{6}$$

According to Koopman's theorem [19], the ionization potential *I* can be approximated as the negative of the highest occupied molecular orbital (HOMO) energy:

$$I = -E_{HOMO} \tag{7}$$

The negative of the lowest unoccupied molecular orbital (LUMO) energy is related to the electron affinity *A*:

$$A = -E_{LUMO} \tag{8}$$

The electronegativity was obtained using the ionization energy *I* and the electron affinity *A* as given in Equation 9:

$$\chi = \frac{I+A}{2} \tag{9}$$

The hardness which is the reciprocal of the electronegativity was obtained by Equation 10:

$$\eta = \frac{I-A}{2} \tag{10}$$

When the organic molecule is in contact with the metal, electrons flow from the system with lower electronegativity to that of higher electronegativity until the chemical potential becomes equal. The fraction of electrons transferred, ΔN, was estimated according to Pearson [20]:

$$\Delta N = \frac{\chi_{Cu}-\chi_{inh}}{2(\eta_{Cu}+\eta_{inh})} \tag{11}$$

In this study, we used theoretical values of $\chi_{Cu}$and η_{Cu} (η_{Cu}= 4.98 eV [12] and η_{Cu}= 0 [21]).
The global electrophilicity index, introduced by Parr [12] is given by Equation (12):

$$\omega = \frac{\chi^2}{2\eta} \tag{12}$$

The local selectivity of a corrosion inhibitor [22] 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 [23] is the nucleophilic and electrophilic Fukui functions, which are defined as:

$$f(\overrightarrow{r}) = \left(\frac{\partial\rho(\overrightarrow{r})}{\partial N}\right)_{v(\overrightarrow{r})} \tag{13}$$

where N and $\rho(\overrightarrow{r})$ are the number of electrons and the electron density at position $\vec{r}$ of the chemical species respectively. After taking care of the discontinuities in $f(\overrightarrow{r})$ versus N plot, the "condensed-to –atom" approximations of $f(\overrightarrow{r})$, when multiplied by global softness (S) [24] provide local softness values given by Equation 14-15 respectively:

$$s_k^+(\vec{r}) = [q_k(N+1) - q_k(N)]S = f_k^+S \tag{14}$$
$$s_k^-(\vec{r}) = [q_k(N) - q_k(N-1)]S = f_k^-S \tag{15}$$

In these equations$q_k(N+1)$, $q_k(N)$ and $q_k(N-1)$ represent the condensed electronic populations on atom "k" for anionic, neutral and cationic systems respectively. Therefore, $s_k^+(\vec{r})$ and $s_k^-(\vec{r})$ represent the condensed local softness values of atom "k" towards nucleophilic and electrophilic attacks.

Results and discussion

Effect of concentration and temperature

The corrosion rate curves of copper without and with the addition of cefuroxime in 1M HNO_3 at different temperatures are presented in **Figure 2**. These curves show that corrosion rate of copper in the studied medium, increases with increasing temperature. But this evolution is moderated when the concentration of the studied inhibitor increases, revealing the effectiveness of the molecule as a corrosion inhibitor for copper in 1 M HNO_3. These results could be interpreted as the formation of a film barrier which isolates the metal from its aggressive environment.

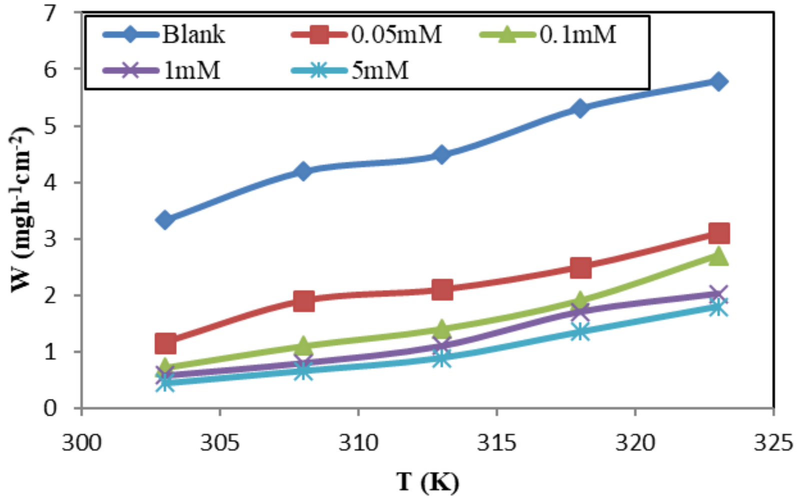


Figure 2 Evolution of corrosion rate with temperature for different concentrations of cefuroxime

As shown in **Figure 3**, the inhibition efficiency decreases with the rise in temperature for the concentration range studied. It has been reported [25] that the decrease in inhibition efficiency with increase in temperature indicates that the process of adsorption of the inhibitor on the corroding metal surface is physical adsorption.

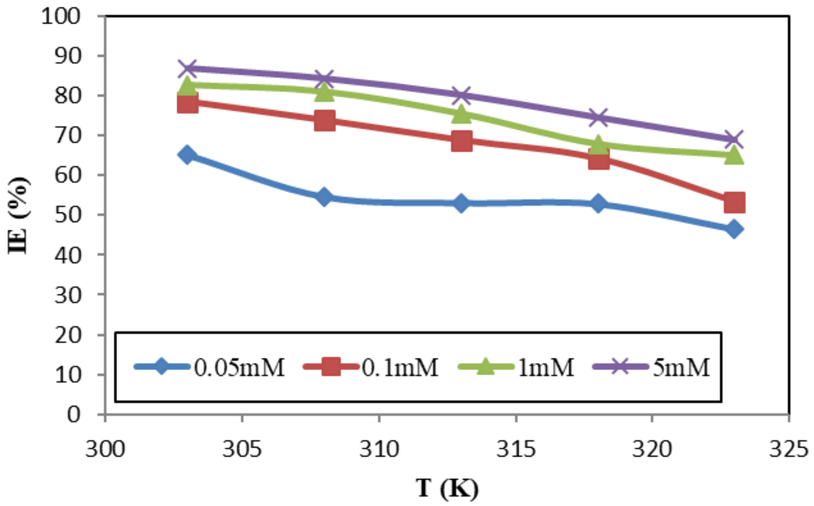


Figure 3 Inhibition efficiency versus temperature for different concentrations of cefuroxime

Adsorption isotherms

The adsorption isotherms study gives knowledge about the interaction of inhibitors on the metal surface. The adsorption isotherms tested in this work are the models of Langmuir, Temkin and Flory-Huggins. By fitting the degree of surface coverage (Ɵ) and the inhibitor concentration (C_{inh}) (**Figure 4**), the best adsorption isotherm obtained graphically is Langmuir adsorption isotherm with the mean value of $R^2 = 0.999$.

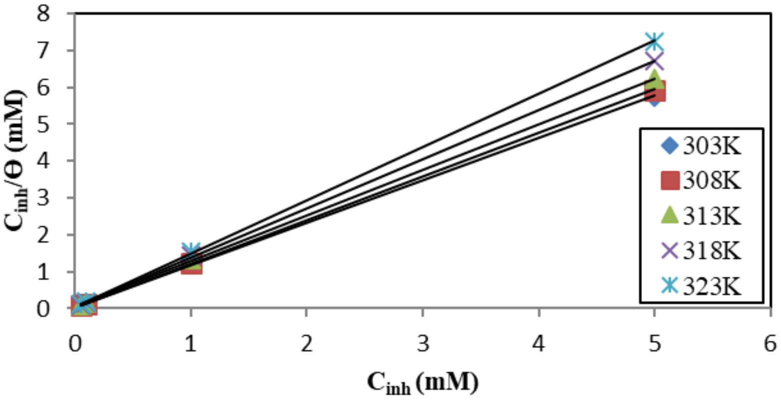


Figure 4 Langmuir adsorption isotherm for cefuroxime on copper surface in 1M HNO_3

The slopes of the straight lines are different from unity, what suggests [26] interactions between adsorbed species on copper surface as well as changes in the values of Gibbs energy with increasing surface coverage. The results reveal a slight deviation from ideal conditions (all the adsorption sites are equivalent) assumed in the Langmuir adsorption model. Therefore, a modified Langmuir equation [27] must be considered. This equation, which takes into account the deviation from the ideal conditions, is given through Equation 16:

$$\frac{C_{inh}}{\theta} = \frac{n}{K_{ads}} + nC_{inh} \quad (16)$$

where *n* is the slope of the straight line corresponding to the Langmuir isotherm (see n values in **Table 1**). The values of adsorption equilibrium constant K_{ads} were obtained from the intercepts of the straight lines on the C_{inh}/θ–axis. K_{ads} is related [28] to the standard free adsorption energy ΔG^0_{ads} according to Equation 17:

$$\Delta G^0_{ads} = -RTln(55.5K_{ads}) \quad (17)$$

where 55.5 is the concentration of water in the solution in $mol.L^{-1}$, R is the perfect gas constant and T is the absolute temperature. The calculated values of ΔG^0_{ads} are summarized in **Table 2**.

Table 1 Regression parameters of Langmuir isotherm

T(K)	Correlation coefficient	Slope	Intercept
303	0.9999	1.1475	0.0298
308	1	1.1810	0.0337
313	0.9999	1.2408	0.0434
318	0.9998	1.3341	0.0495
323	0.9999	1.4416	0.0552

Table 2 Thermodynamic parameters for the adsorption of cefuroxime on copper surface at different temperatures

T(K)	K_{ads}(M^{-1})	$\Delta G^0_{ads}(kJ\ mol^{-1})$	$\Delta H^0_{ads}(kJ\ mol^{-1})$	$\Delta S^0_{ads}(J\ mol^{-1}K^{-1})$
303	33557.05	–36.35	–25.899	34.70
308	29673.59	–36.64		
313	23041.47	–36.57		
318	20202.02	–36.81		
323	18115.94	–37.1		

Generally, values of ΔG^0_{ads} around –20 kJ mol^{-1} are consistent in proving spontaneous adsorption at the interface with electrostatic interactions between the charged molecules and the charged metal (physical adsorption) whereas those more negative than –40 kJ mol^{-1} involves charge sharing or transfer from the inhibitor's molecule to the metal surface leading to the formation of a donor-acceptor bond (chemical adsorption) [29, 30]. In the present study, the values of ΔG^0_{ads} are within the range of –37.10 to –36.35 kJ mol^{-1} indicating both chemisorptions and physisorption. The change in standard adsorption enthalpy ΔH^0_{ads} and the change in standard adsorption entropy ΔS^0_{ads} are calculated using Equation 18:

$$\Delta G^0_{ads} = \Delta H^0_{ads} - T\Delta S^0_{ads} \qquad (18)$$

The plot of ΔG^0_{ads} versus T (**Figure 5**) leads to the determination of ΔH^0_{ads} and ΔS^0_{ads} as regression parameters with ΔH^0_{ads} as the intercept and ΔS^0_{ads} as the negative of the slope of the straight line obtained.

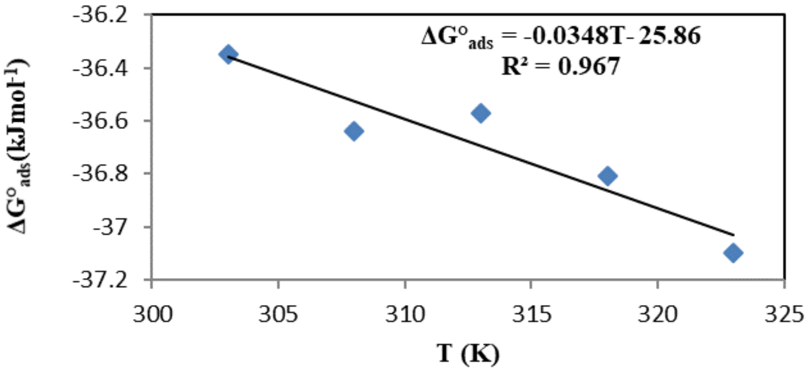


Figure 5 $\Delta G°_{ads}$ versus *T* for the adsorption of cefuroxime on copper in 1M HNO_3

In this study, ΔH^0_{ads} is negative, showing an exothermic process. The literature [31] stated that an exothermic process means either physisorption or chemisorptions. Therefore this result confirms that the process of adsorption is both physisorption and chemisorption. The change in adsorption entropy (ΔS^0_{ads}) is positive, meaning that disorder increases during the adsorption process. This situation can be explained by desorption of water molecules replaced by the inhibitor.

Effect of temperature

The effect of temperature on the corrosion of copper in HNO_3 containing various concentrations of cefuroxime was investigated using the Arrhenius law (Equation 19):

$$logW = logA - \frac{E_a}{2.303RT} \qquad (19)$$

where $E_a$is the apparent activation energy, T is the absolute temperature, A is the preexponential factor. The linear regression plot of $logW$ versus $^1/_T$ (**Figure 6**) has ($-\frac{E_a}{2.303R}$) as slope.

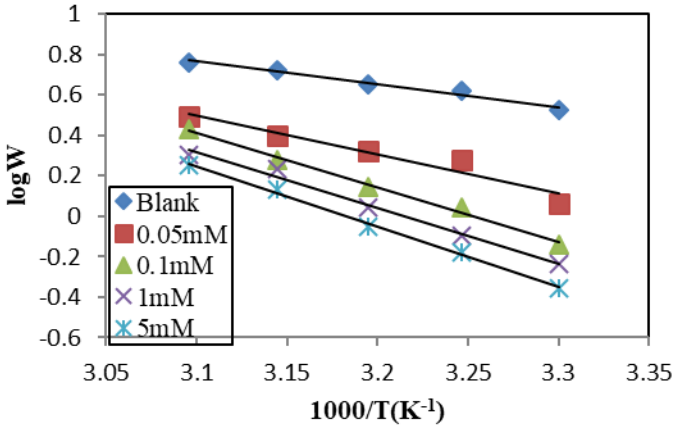


Figure 6 Arrhenius plots for Copper corrosion in 1M HNO_3 solutions without and with cefuroxime

The effect of the temperature on the corrosion process can also be investigated by determining the change in activation enthalpy ΔH_a^* and the change in activation entropy ΔS_a^* using the transition state equation (Equation 20):

$$log\left(\frac{W}{T}\right) = [log(\frac{R}{\aleph h}) + \frac{\Delta S_a^*}{2.303R}] - \frac{\Delta H_a^*}{2.303RT} \qquad (20)$$

where h is the Planck's constant and $\aleph$ is the Avogadro number. The transition state plots of (*W/T*) versus (1/*T*) are given in **Figure 7**. The transition plots were used to determined ΔS_a^* and ΔH_a^* from respectively the intercepts $[log(\frac{R}{\aleph h}) + \frac{\Delta S_a^*}{2.303R}]$ and the slopes$(-\frac{\Delta H_a^*}{2.303RT})$. The obtained values are displayed in **Table 3**.

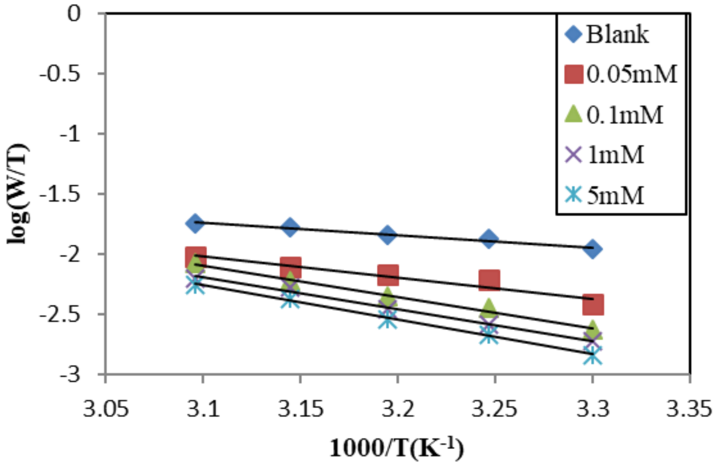


Figure 7 Transition state plots for copper corrosion in 1M HNO_3 with or without cefuroxime

It is clear from Table 3 that Ea in the inhibited solutions are higher than that obtained for the blank, indicating that the corrosion reaction of copper is inhibited by the studied compound [32], hence supports the phenomenon of physical adsorption [33]. Higher values of Ea in the presence of inhibitor can be correlated with increasing thickness of the double layer which enhances the Ea of the corrosion process [34]. It is also an indication of a strong inhibitive action of cefuroxime drug by increasing energy barrier for the corrosion process, emphasizing the electrostatic character of the inhibitor's adsorption on the copper surface (physisorption) [35]. The positive sign of change in activation enthalpy reveals an endothermic dissolution process and therefore a slow dissolution of copper [36] in the presence of the studied drug. The change in activation entropy is negative and it increases when the inhibitor concentration increases, probably due to desorption of the adsorbed species. Similar observation has been reported [37] in the literature.

Table 3 Activation parameters for copper corrosion without and with cefuroxime in 1M HNO_3

	E_a (kJmol^{-1})	ΔH_a^*(kJmol^{-1})	ΔS_a^*(Jmol^{-1}K^{-1})
Blank	21.87	19.24	-170.86
0.05mM	36.57	33.93	-130.53
0.1mM	51.91	49.25	-84.61
1mM	52.90	50.23	-83.41
5mM	57.50	54.83	-70.43

Quantum chemical calculations

Global reactivity

The calculated molecular descriptors are displayed in **Table 4**. From Table 4, it is obvious that the high inhibition efficiency value of cefuroxime can be explained by its high value of E_{HOMO} (-6.4841 eV) when considering the values reported in the literature [38-40]. This high value indicates the tendency to donate electrons to empty molecular orbital of copper ions (C*u*2+: [*Ar*] 3*d*^{9}) [41]. 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 feed- back bond [42]. The low value of E_{LUMO} (-1.9359 eV) compared to that reported in the literature [38, 43] indicates its ability to accept electrons. 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. As ΔE decreases, the reactivity of the molecule increases leading to increase in the inhibition efficiency of the molecule. Lower values of the energy difference will render good inhibition efficiency, because the energy to remove an electron from the last occupied orbital will be low [44]. In our case, the low value of energy gap (ΔE = 4.5482 eV) could explain the high inhibition efficiency value (IE (%) = 88.79 for C_{inh} = 5 mM at T = 303 K). The density HOMO and LUMO diagrams are shown in **Figure 8**.

Table 4 Values of some molecular descriptors

Descriptor	Value	Descriptor	Value
E_{HOMO} (eV)	–6.4841	I (eV)	6.4841
E_{LUMO} (eV)	–1.9359	A (eV)	1.9359
ΔE (eV)	4.5482	μ(Debye)	4.9152
ΔN	0.1693	Ƞ (eV)	2.2741
S (eV)$^{-1}$	0.4397	ωμ	3.8969
χ(eV)	4.2100	TE (a.u)	–1828.3297

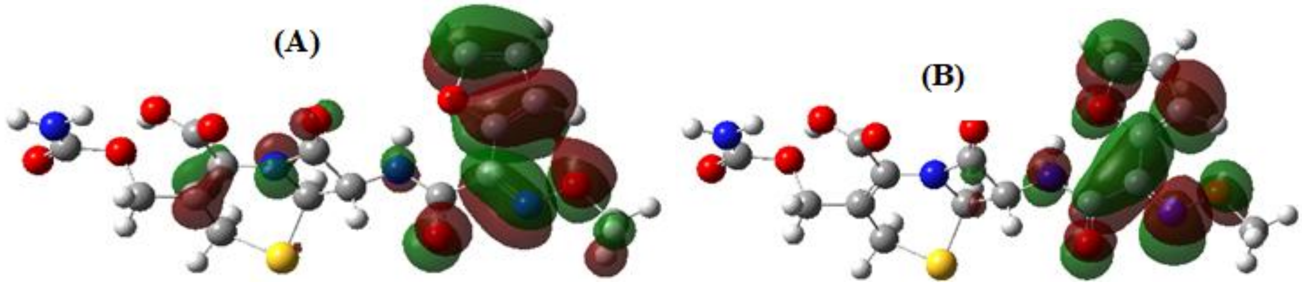


Figure 8 HOMO (A) and LUMO (B) by B3LYP 6-31G (d, p)

As presented in Figure 8A&B, the density HOMO is distributed almost throughout the molecule whereas the density LUMO is distributed only from the five-membered ring to the antibiotic function.

According to the literature [45], the obtained value of the dipole moment (4.9152D) is high implying the compound's effectiveness as corrosion inhibitor. Ionization energy is a fundamental descriptor of the chemical reactivity of molecules that deals with their stability or their inertness. High ionization energies [46] indicate a high stability of the system while low values denote high reactivity. In our case, the low ionization energy (6.4841 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 has a large energy gap and a soft molecule a small energy gap [47]. In the present work, Cefuroxime has a small hardness value (2.2741 eV) and a high value of softness (0.4397 $(eV)^{-1}$) 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 (0.1693) shows according to the literature [48] 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 [12] 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 = 3.8969) shows that the inhibitor is an electrophile molecule: it can receive electrons.

Local reactivity

Fukui functions compute local reactivity indices that makes possible to rationalize the reactivity of individual molecular orbital contributions. The condensed Fukui function and local softness indices allow one distinguish each part of the molecule on the basis of its distinct chemical behavior due to the different substituted functional group. 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 energy while the site for electrophilic attack is controlled by the values of f_k^- which is associated with the HOMO energy. The local softness contains the information similar to those condensed Fukui function plus additional information about the total molecular softness. A high value of s_k^+ indicates high nucleophilicity and the high value of s_k^- indicates high electrophilicity. The Fukui and softness indices values for Cefuroxime drug calculated with B3LYP/6-31G (d, p) are displayed in **Table 5**.

Table 5 Charges of some selected atoms, condensed Fukui functions and local softness indices

Atom	**q_k(N+1)**	**q_k(N)**	**q_k(N-1)**	**f_k^+**	**f_k^-**	**s_k^+**	**s_k^-**
1C	0.745	0.739	0.747	0.006	-0.008	0.003	-0.004
2O	-0.505	-0.492	-0.465	-0.013	-0.027	-0.006	-0.012
3N	-0.748	-0.759	-0.760	0.011	0.001	0.005	0.000
5C	-0.157	-0.142	-0.112	-0.015	-0.030	-0.007	-0.013
6C	-0.233	-0.215	-0.274	-0.018	**0.059**	-0.008	**0.026**
9C	0.682	0.698	0.682	-0.016	0.016	-0.007	0.007
10O	-0.464	-0.429	-0.359	-0.035	-0.070	-0.015	-0.031
11N	-0.698	-0.754	-0.675	0.056	-0.079	0.025	-0.035
12S	-0.381	0.321	0.426	-0.702	-0.105	-0.309	-0.046
13C	-0.353	-0.657	-0.646	**0.304**	-0.011	**0.134**	-0.005
14C	-0.091	0.019	0.040	-0.110	-0.021	-0.048	-0.009
15C	0.240	0.277	0.310	-0.037	-0.033	-0.016	-0.015
16C	0.619	0.662	0.706	-0.043	-0.044	-0.019	-0.019
17O	-0.484	-0.439	-0.423	-0.045	-0.016	-0.020	-0.007
18O	-0.575	-0.608	-0.580	0.033	-0.028	0.015	-0.012
20C	-0.191	-0.242	-0.230	0.051	-0.012	0.022	-0.005
23O	-0.521	-0.493	-0.504	-0.028	0.011	-0.012	0.005
24C	0.835	0.809	0.974	0.026	-0.165	0.011	-0.073
25O	-0.544	-0.463	-0.550	-0.081	0.087	-0.036	0.038
26N	-0.795	-0.771	-0.761	-0.024	-0.010	-0.011	-0.004
29C	0.149	0.149	0.148	0.000	0.001	0.000	0.000
30N	-0.279	-0.270	-0.238	-0.009	-0.032	-0.004	-0.014
31O	-0.378	-0.369	-0.347	-0.009	-0.022	-0.004	-0.010
32C	-0.297	-0.307	-0.326	0.010	0.019	0.004	0.008
36C	0.108	0.107	0.124	0.001	-0.017	0.000	-0.007
37C	-0.266	-0.260	-0.246	-0.006	-0.014	-0.003	-0.006
38C	-0.177	-0.169	-0.150	-0.008	-0.019	-0.004	-0.008
39C	0.325	0.326	0.342	-0.001	-0.016	0.000	-0.007
40O	-0.525	-0.536	-0.537	0.011	0.001	0.005	0.000

The analysis of **Table 5** shows that according to the Fukui theory of reactivity, C (13) is the nucleophilic attacks center when C (6) is the electrophilic attacks center.

Conclusion

The following conclusions can be drawn from this study:

- Inhibition efficiency is temperature and concentration dependent;
- Cefuroxime drug adsorbs on copper surface according to modified Langmuir adsorption isotherm;
- Adsorption thermodynamic functions and activation parameters indicate a spontaneous adsorption process and predominant physisorption;
- Global reactivity parameters explain the good inhibition efficiency of cefuroxime;
- Fukui functions and local softness indices show the nucleophilic and electrophilic attacks sites in the molecule.

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