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Effect of Orphenadrine Citrate Drug on Corrosion of 316L Stainless Steel in Hydrochloric Acid

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Abstract

The use of varied quantities of orphenadrine to protect stainless steel against corrosion in an acidic media at 298 K has been investigated. It was observed that when the drug's concentration is increased, the drug's speed of corrosion lowers. The data of inhibition efficiency (percent IE) in the presence of orphenadrine drug and corrosion resistance showed that the highest protection efficiency was achieved with the best concentration, and that the corrosion rate decreased with increasing orphenadrine drug concentrations, making it a good inhibitor for stainless steel in an acidic environment. The theoretical investigation proved the efficiency of the drug for inhibition, as the drug is absorbed on the surface of the stainless steel by the active groups in the drug, using the hyperchem-8.07 software to compute the molecular orbital energies.

Keywords: Corrosion inhibitors, Stainless Steel (316L), Orphenadrine citrate drug, Theoretical Studies

تأثير دواء السترات أورفينادرين على تآكل (316L)الفولاذ المقاوم للصدأ في حامض الهيدروكلوريك

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الخلاصة

استخدام عقار الأورفينادرين بتراكيزات مختلفة لحماية الفولاذ المقاوم للصدأ من التآكل في وسط الحامضي عند 298 كلفن. وقد وجد أن سرعة التآكل تتناقص مع وجود الدواء مع زيادة تركيزه . كانت نتائج كفاءة التثبيط IE % ومقاومة التاكل بجود عقار الأورفينادرين في اعلى كفاءة حماية وافضل تركيز ، وتناقص معدل التآكل مع زيادة تركيز عقار الأورفينادرين المثبط الجيد للفولاذ المقاوم للصدأ في الوسط الحامضية. باستخدام برنامج hyperchem−8.07 لحساب الطاقات المدارية الجزيئية ، أظهرت الدراسة النظرية فعالية الدواء للتثبيط ، حيث يتم امتصاص الدواء على سطح الفولاذ المقاوم للصدأ بواسطة المجموعات الفعالة في الدواء.

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1. Introduction

Corrosion is the deterioration or shattering of minerals and metals, which has an impact on the country's development [1]. This is comparable to the danger of natural calamities such as earthquakes and floods, although corrosion can be controlled [2,3]. Plastics, organic particles, and polymers as protective coatings for metal surfaces, as well as organic and organic inhibitors for catholic and anode protection [4], are some of the approaches used to protect metals from corrosion. Active inhibitors are heterocyclic compounds that contain oxygen, sulfur and nitrogen, either with long chain or aromatic carbon compounds. These inhibitors contain functional groups such as (-NH2, -OR, -SR, -C = C, -NR2, -OH) and have p-electron systems. Tetracycline, ampicillin, penicillin G, methocarbamol, ampiclox, cloxacillin, orphenadrine, azithromycin, and other medications are used to prevent metal corrosion because they contain electrons of functional groups that enable their absorption on the metal's surface [5]. The role of inhibitors is to prevent or reduce metal corrosion by increasing the metal' resistance to corrosion, reducing the spread of substances that interact on the surface of the metal and reduce or increase the cathodic or anode reactions, as well as the inhibitor increases the absorption of ions or particles on the surface of the metal [6,7]. Orphenadrine citrate is used to treat lower back pain and headache because it is an N-methyl-D-aspartate receptor antagonist. Urinary retention, blurred vision, dry mouth, and confusion result from side effects of orphenadrine use, which is partly related to the anticholinergic process [8].
Previous study has shown that employing inhibitors in an acidic solution can regulate or minimize stainless steel corrosion. There are a variety of corrosion inhibitors that are better suited to industrial demands. Inhibitor compounds' inhibition efficacy is primarily determined by the composition and chemical characteristics of the inhibitor produced on the metal surface. Corrosion is prevented by inhibitors adsorbing on the metal surface through polar atoms. SiO2 [9], ZrO2 [10], nanomaterials, and chemical derivatives as 1,3-Thiazolidin-5-one Derivatives [11] are examples of inhibitors. The effect of Orphenadrine at various concentrations on the corrosion of stainless steel in an acidic environment at 298K and Theoretical Studies using the hyperchem-8 software were explored in this research. The higher the concentration of the medication, the better at suppressing corrosion.

2.Material and Method

2.1. Material

2.1.1. Stainless steel: Table 1 shows the chemical composition of the stainless steel metal used as a sample to study corrosion, the chemical composition device was X-ray fluorescence.

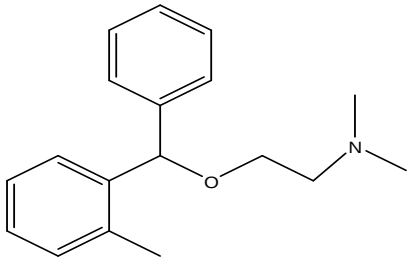
Table 1-composition of Stainless steel:

Grade	C (Max)	Mn (Max)	P (Max)	S (Max)	Si (Max)	Cr	Ni	Mo	Nitrogen (Max)
316	0.028	2.00	0.045	0.030	0.75	16.00-18.00	10.00-14.00	2.00-3.00	0.10

2.2.1. Hydrochloric acid of Test Solution : (0.2M HCl) supplier from BDH, the solution was prepared by adding 16.70 ml of HCl to one liter of distilled water.

2.2.2. Inhibitor

The Orphenadrine citrate drug inhibitor in different concentration (10,100,200,300and 400 ppm) used for testing the corrosion protection for Stainless Steel in acid media. Orphenadrine citrate drug has chemical name:- N-(4-Hydroxyphenyl) acetamide.



N,*N*-dimethyl-2-(phenyl(*o*-tolyl)methoxy)ethanamine

Chemical Formula: $C_{18}H_{23}NO$
Exact Mass: 269.18
Molecular Weight: 269.38
m/z: 269.18 (100.0%), 270.18 (19.8%), 271.18 (2.1%)
Elemental Analysis: C, 80.26; H, 8.61; N, 5.20; O, 5.94

2.2.3. Metal preparations: Utilize wire-cutting technology to cut stainless steel with a diameter of 2.5 cm and a thickness of 2 mm in a circular motion, as it utilizes silicon carbide sheets of various sizes (100, 260, 320, 600, 800, and 1200) to flatten and polish the metal's surface. The corrosion of stainless-steel metal in acidic medium and at a temperature of 298 K, in the presence and absence of an inhibitor (**Orphenadrine citrate** in various concentrations) was studied using electrochemical measurements. The corrosion voltage and current are determined for the presence and absence of the inhibitor using the corrosion cell, which consists of three electrodes. The corrosion cell is built of pyrex and has a one-liter capacity. It is made up of two external containers for water flow from the cooling device and to keep the temperature constant at 298 Kelvin, as well as an interior container that houses the cell's three poles. The working electrode potential is determined using the reference electrode which corresponds to the reference potential .The reference electrode is composed of two inner vessels that consist of silver, silver chloride, potassium chloride, and the outer vessel that is filled with a prepared acid solution of 0.2 M hydrochloric acid as the voltage of the reference electrode is defined and accurate. The auxiliary electrode is made of high purity platinum metal, its length is 10 cm. The working electrode that connects to the composite stainless steel which consists of a metal wire of 20 cm in length, Figure-1. shows measurements of the polarization.

Figure 1- Complete system set up for polarization measurements

3. RESULTS AND DISCUSSION

3.1. Inhibition efficiency

Fig. 2. shows a diagram of the various drug concentrations against an efficiency of inhibition of corrosion of stainless steel in an acidic medium at 298 K. The explanation for this is because the drug's inhibitory efficiency at the maximum concentration has improved due to the stainless steel's enhanced capacity to absorb the drug, and the efficiency has remained consistent [12,13]. The corrosion current density is utilized before and after inhibition to compute the ratio of inhibition efficiency.

$$IE\% = \left\{\frac{(icorr)i - icorr}{(icorr)i}100\right\} \quad \ldots\ldots\ldots 1$$

Where, $(icorr)i$ and $(icorr)$are corrosion current density in inhibited and uninhibited medium, respectively [14].

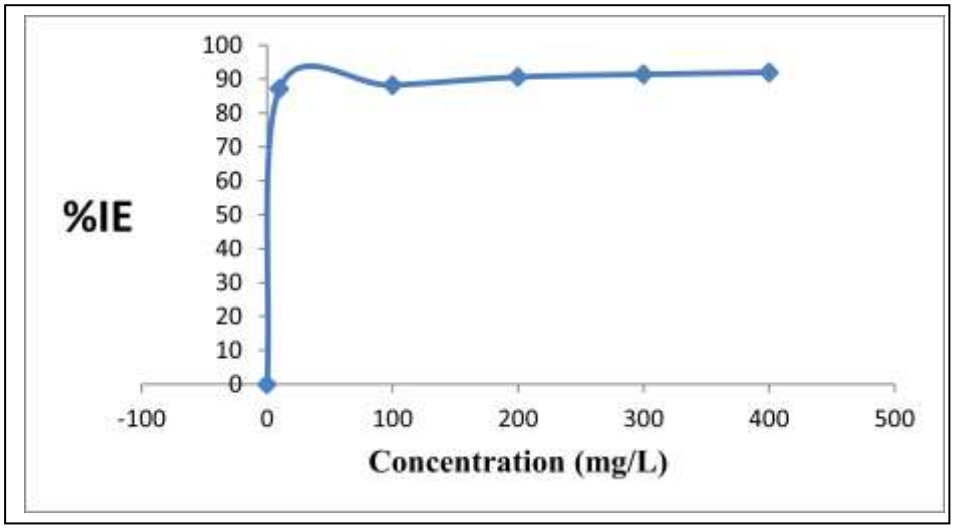


Figure 2-Inhibition efficiency (%IE) of stainless-steel metal at different concentration of drug at 298 K.

3.2-Potentiodynamic polarization curves

Fig. 3. shows the polarizing behavior of the stainless-steel metal in an acidic medium at 298 K and in the presence of the drug. The inhibitor is in the form of organic molecules that inhibit the corrosion of the stainless steel

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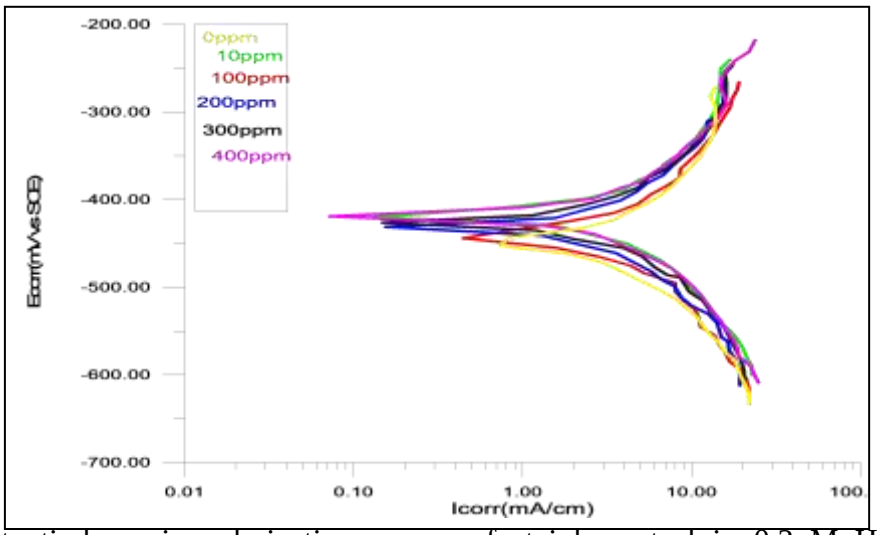


Figure 3-Potentiodynamic polarization curves of stainless steel in 0.2 M HCl with and without inhibitor concentrations at 298 K.

Table 2-Parameters of Potentiodynamic polarization curves of the stainless steel with and without inhibitor solutions at 298 K.

Conse. of inhibitor(ppm)	Icorr (mA/cm2)	-Ecorr (mV)	ba (mV.dec^{-1})	-bc (mV.dec^{-1})	P.L (mm.y-1)	W.L g/(m^2.d)	%IE	θ	Rp/ Ω.cm2
0	10.70	466.5	359.7	246.1	2350	104	0	0	5.929
10	1.37	417.5	295	345.4	344	15.3	87.19	0.8719	50.42
100	1.26	440	380.9	281.6	317	14.1	88.22	0.8822	55.79
200	1	430.8	346.3	208.6	280	12.5	90.65	0.9065	56.52
300	0.916	424.4	322.6	292.7	230	10.2	91.43	0.9143	72.74
400	0.855	415.2	344.3	267.4	214	9.54	92.00	0.9200	76.43

When the inhibitor (Orphenadrine citrate medication) was introduced, the corrosion current values in the acid medium decreased significantly, as shown in Table 2. and Fig. 4. Furthermore, changes in the corrosion potential values, as well as changes in the anode Tafel curve (Ba) and the cathodic tafel curve (Bc), are minor and barely detectable. In summary, the results demonstrate that adding an inhibitor largely prevents hydrogen from forming and regulates anodic dissolution without affecting the corrosion process [15]. These chemicals are mixed type inhibitors, according to the results [16]. The basic function of inhibitors is to prevent active sites from forming on the metal's surface, reducing anodic dissolution and disrupting hydrogen gas release. They can also screen the covered part of the electrode and therefore protect it from the action of the corrosion medium [17]. The values E(corr) not effect on the addition of increasing concentrations of drug [18].

3.3. Adsorption Isotherm

Many factors influence the adsorption process. Adsorption is characterized as a chemical process in which the adsorbent material interacts with the adsorbent material, or as a physical process involving a mild reaction. To determine the adsorption equations, the degree of surface coverage (θ) of different concentrations was used, which is illustrated in Equation 2[19]

$$C/\theta = \left\{\frac{1}{K} + Cinh\right\} \ldots\ldots\ldots 2$$

The plots of (C/ θ) against concentrations of Orphenadrine citrate drug for the at 298 K were straight lines [20], this indicates that the process is an adsorption process of the drug by the metal in 0.2 M of hydrochloric acid [21] as shown in Fig. 4.

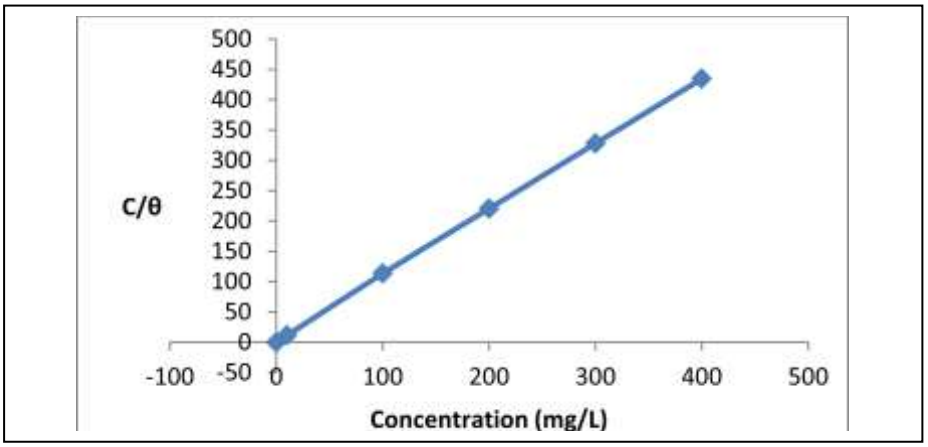


Figure 4-The degree of surface coverage (C/*θ*) of stainless steel metal at different concentration of drug at 298 K.

3.4. Polarization resistance (Rp)

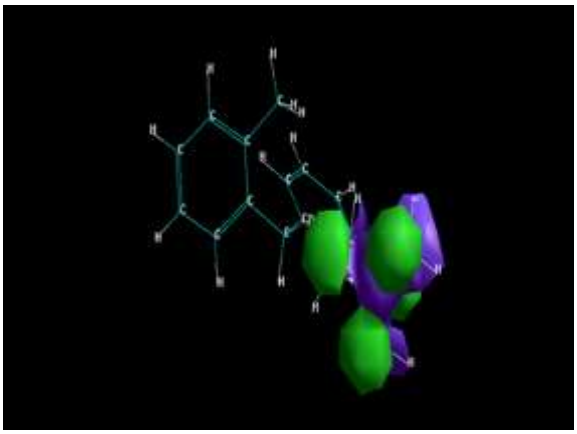
Equation 3 indicates the polarization resistance [22]

$$Rp = \frac{ba\ bc}{2.303\ (ba + bc)icorr} \quad \ldots\ldots\ldots\ldots 3$$

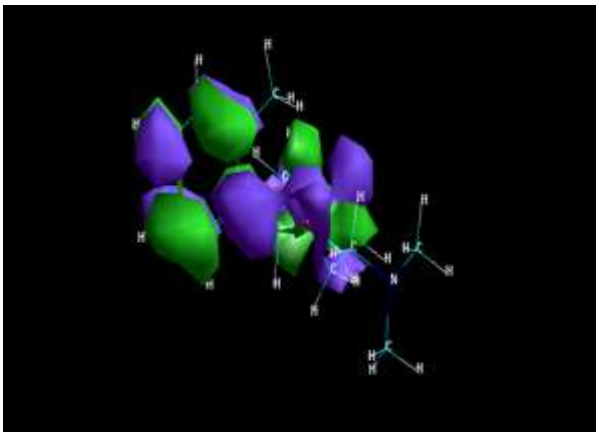
Table 2 shows the polarization resistance, where we note that the increase in inhibitor concentration increases with it the polarization resistance, and therefore the stainless steel is more resistant to corrosion [23,24], because the drug is less conductive than stainless steel, so the surface of the metal is completely covered with the drug [25].

3.5. Theoretical Calculations

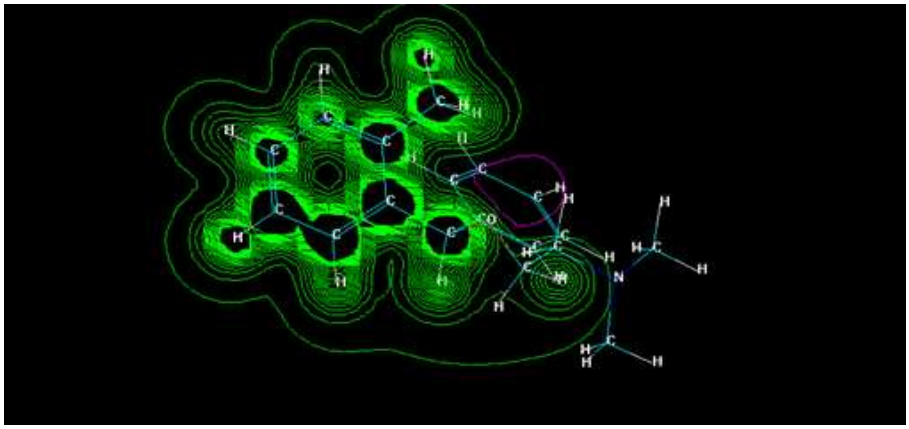
In Theoretical, study molecular mechanics are used for calculations of minimum energy, PM3 method explains the semi-empirical and Hyperchem program [26]. Energies EHOMO, ELUMO, energy gap (, (ΔE) between the participating HOMO and LUMO calculate optimized molecular structures [27,28]. Because the last occupied orbital is small, an electron will be removed from orbital, the drug has polarity, and thus the dipole moment of the drug increases with increasing inhibition efficiency [29]. Because the last occupied orbital is small, an electron will be removed from orbital, the drug has polarity, and thus the dipole moment of the drug increases with increasing inhibition efficiency. Because the stainless-steel metal has an electrical charge on its surface and the medication possesses electric moments, there is an electrostatic interaction between the electric field and the drug [30-32]. This is show in Figure-(5and6),and Table(3).



Homo Sites



Lumo Sites



Electrostatic potential Sites

Figure 5-Homo,Lumo and Electrostatic potential Sites as 2D & 3D Counters for the Drug.

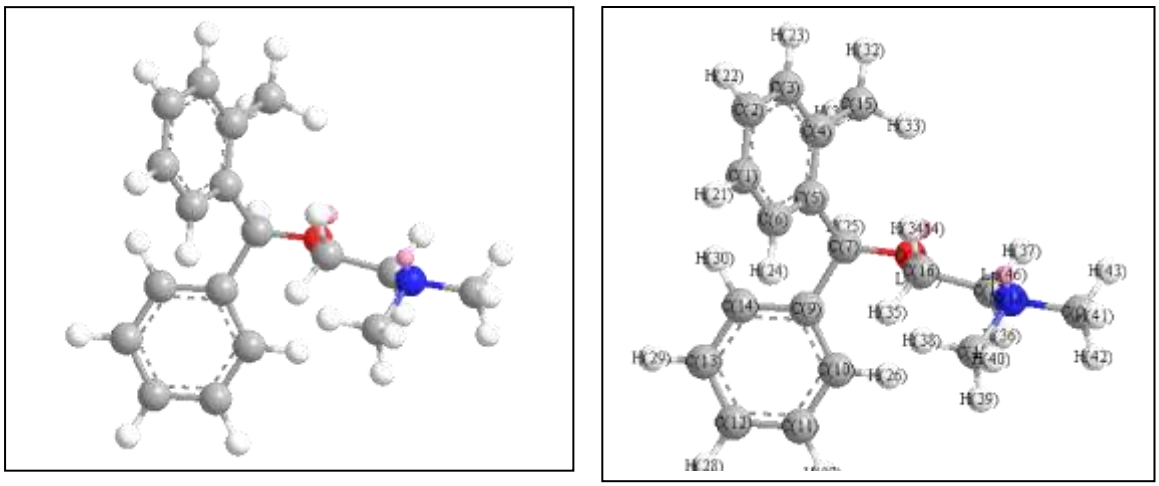


Figure 6-The optimized structure (down) and HOMO (center) and LUMO (high) distribution for molecules.

Table 3-Quantum chemical parameters for drug

Compd. No.	ΔE_{tot}	ΔH^{o}_{f}	ΔE_{b}	E_{Homo}	E_{Lumo}	Dipole moment
	-67855.33	4.15	-4442.77	- 9.180616	0.2634013	0.6602

3.6. FT-IR Spectra

The FTIR spectrum of drug compound reveals a stretching vibration band at C-H (aromatic ring), C=C(aromatic ring) , C-H (aliphatic group),R-O-R(ether group), (3048, 1594, 2962, 1181) cm^{-1}groups stretching vibrations respectively, see Fig. 7 and Table.4 and Fig. 8 explain Vibration stretching bond of drug mode of (C=C), aliphatic (CH), ether(CO)[33].

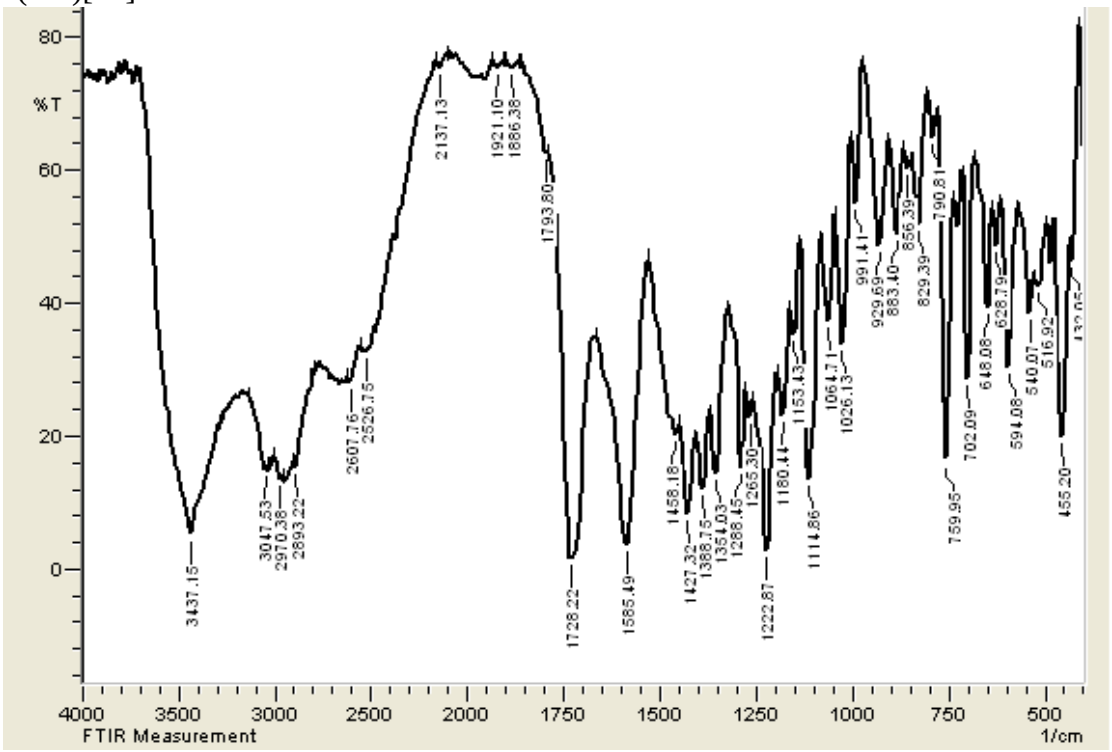
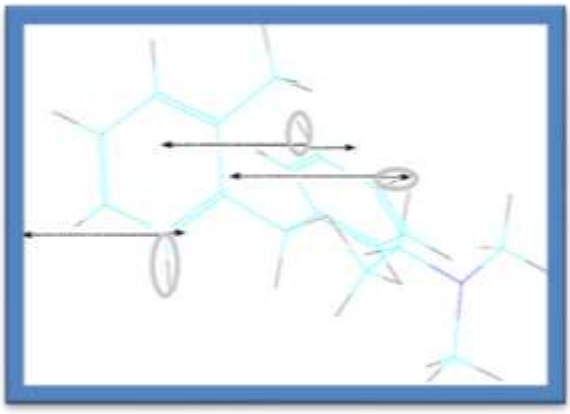


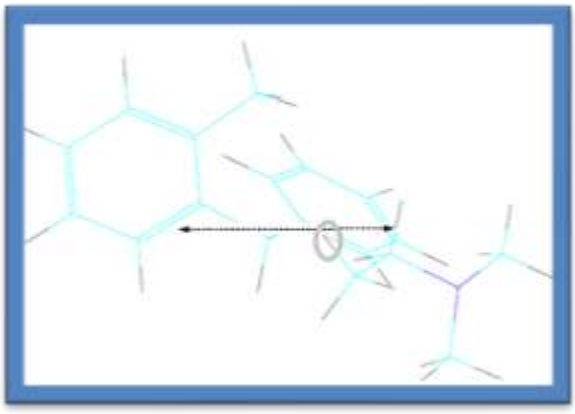
Figure 7 -IR of Orphenadrine citrate drug inhibitor

Table 4-Comparison of theoretical and experimental Frequency for drug.

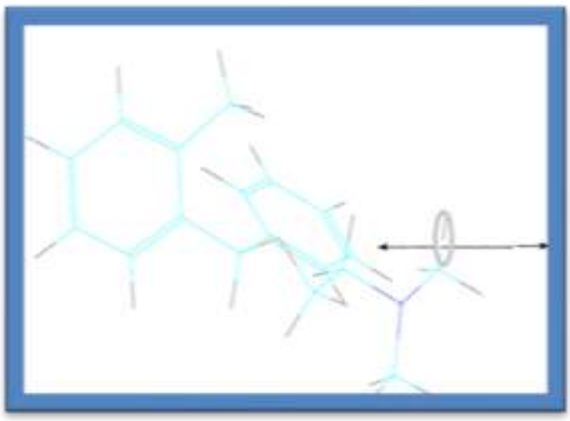
Comp. NO.		Frequency		Intensity
		Theoretical	experimental	
1	C-H (aromatic ring)	3048	3047	3.74212
	C=C(aromatic ring)	1594	1585	1.13956
	C-H (aliphatic group)	2962	2970	1.79535
	R-O-R (Ether group)	1181	1180	2.42710



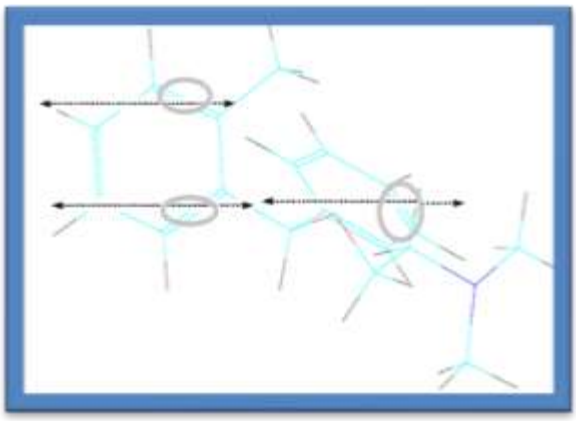
Vibration stretching mode of aromatic (CH)



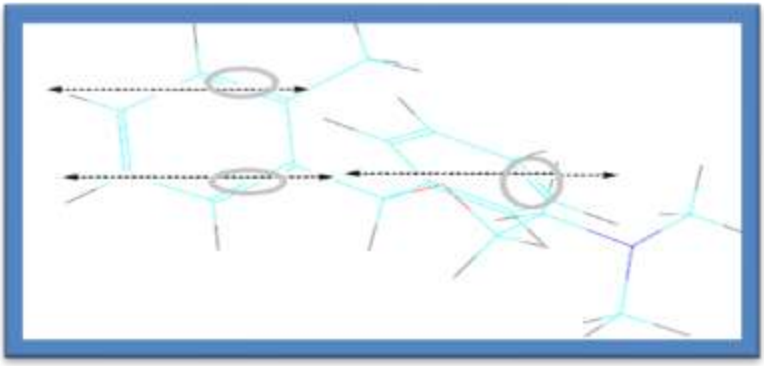
Vibration stretching mode of ether(CO)



Vibration stretching mode of aliphatic (CH)



Vibration stretching mode of (C=C)



Vibration stretching mode of aromatic (CH)

Figure 8-explain Vibration stretching bond of drug (mode of (C=C), aliphatic (CH), ether(CO).

4.Conclusions

This work describes the corrosion inhibition of 316L Stainless Steel by Orphenadrine citrate drug. Experimental results from potenciodynamic measurements are subjected to theoretical calculations. The results of the inhibition efficiency showed that the use of Orphenadrine citrate for corrosion inhibition in the aqueous acidic media, can decrease the corrosion from 10.70to 0.916 (mA/cm2), also the inhibition efficiency reaches 92.00%, due to, the adsorption of inhibitor from solution attachment to surface of 316L Stainless Steel in acid solution. The work includes a theoretical study using molecular mechanics and semi-empirical calculations by the program of hyperchem 8.07 (PM3)& (DFT), the heat of formation (ΔH˚f),total energy(ΔEb) and optimized structural geometries were calculated at 298K, vibration spectra for Orphenadrine citrate was calculated and then compared with the experimental value.

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