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Experimental and Theoretical Study of Neomycin Sulfate as Corrosion Protection for Titanium in Acid Media

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Abstract:

The experimental and theoretical methods were studied for inhibition of the corrosion titanium in HCl by using neomycin sulfate drug. The results of neomycin sulfate drug had good corrosion protection for titanium in hydrochloric acid and the inhibition efficiency (%IE) increasing with increasing concentration of drug because the neomycin sulfate drug had adsorption from acid solution on surface of titanium metal. The program of hyperchem-8.07 was used for theoretical study of the drug by molecular mechanics and semi-empirical calculations. Quantum chemical was studied drug absorption and electron transferred from the drug to the Titanium metal, also inhibition potentials of drug attachment with the (LUMO-HOMO) energy gap, dipole moment (μ) of the molecules and electrostatic potentials.

Key words: Corrosion inhibitors, Neomycin sulfate, Theoretical Studies, Titanium metal.

Introduction:

Corrosion is the deterioration of metals due to their reaction with a corrosive element in their surroundings, such as chlorine, fluorine, carbon dioxide, oxygen, etc. Damages due to corrosion in terms of economic aspects include repair and maintenance costs, loss of materials, damage to equipment, a decrease in efficiency, and loss of useful or productive life. Furthermore, corrosion damages have other social effects, such as safety impacts (cause of fire, explosions, release of toxic products), health impacts (personal injuries, pollution due to contamination of toxic products), the depletion of resources, etc(1). The inorganic compounds have chromate,nitrites and compounds have hetro atoms (O, P, S, N), π bonds were most effective and efficient (2). Compounds containing both nitrogen and chloro atoms can provide excellent inhibition, compared with compounds containing only nitrogen or chloro atom(3). Heterocyclic compounds such as antibiotic (pharmaceutical drugs) can provide excellent inhibition. These molecules depend mainly on certain physical properties of the inhibitor molecule such as functional groups, steric factors, electron density at the donor atom and electronic structure of the molecules (4,5). A few researchers have reported the use of antibacterial drugs as corrosion inhibitors because of presence of oxygen, nitrogen and sulphur in their structures as active centers, high solubility in water, high molecular size, non-toxic(environmentally friendly)corrosion inhibitors, important in biological reactions and drugs that can be easily produced and purified (6-7). The use of neomycin sulphate as an antimicrobial agent and antibacterial agent has a long history(8).The neomycin sulphate and chitosan used as for wound healing activity show synergistic activity, they were used as epidermal proliferation and possessed antibacterial properties against Staphylococcus aureus, Pseudomonas aeruginosa and Escherichia coli.(9). The cathodic protection system and aqueous media can be calculated corrosivity from corrosion protection and electrical conductivity, properties electrolytes solutions estimated from conductivity. Dilute aqueous concentration is electrical conductivity solution (10). Regarding the adsorption of the inhibitor on the metal surface, two types of interactions are responsible. One is physical adsorption which involves electrostatic force between ionic charges or dipoles of the adsorbed species and electric charge at metal/solution interface. Other is chemical adsorption, which involves charge sharing or charge transfer from inhibitor molecules to the metal surface to form coordinated types of bonds (11). The selection of appropriate inhibitors mainly depends on the type of acid, its concentration, and temperature. In this study, the corrosion inhibition of titanium in 0.25N HCl solution using neomycin drug, the results obtained from the electrochemical measurements are associated with IR spectra and the quantum chemical studies, as support for the confirmation of experimental data.

Material and Method

Material

Titanium metal

Titanium metal was used as test specimen have the following composition in Table 1.

Table 1. Composition of Titanium metal.

Si%	Fe%	Cu%	Mn%	Mg%	Cr%	Zn%	V%	Ti %
< 0.25	< 0.40	< 0.05	< 0.05	< 0.05	< 0.05	< 0.05	< 0.03	98.09

Acid Media :(0.25M HCl) hydrochloric acid is Supplier from BDH .

Inhibitor

The inhibitor used for testing the corrosion protection of the metal is neomycin sulfate drug

Neomycin sulfate drug

5-amino-2(aminomethyl)-6-(3,5-diamino-2-(3-amino-6(aminomethyl) 4,5mdihydroxytetrahydro-2H-pyran-2-yloxy)-6-hydroxycyclohexyioxy)-4-hydroxy-2 (hydroxymethyl)tetrahydrofuran-3-yloxy)tetrhydro-2H-pyran-3,4-diol sulfate**.** Different concentrations of neomycin sulfate drug (10,100,200,300 and 400 mg/L) prepared dissolving different amounts of the inhibitor in HCl solution as show in Fig.1.

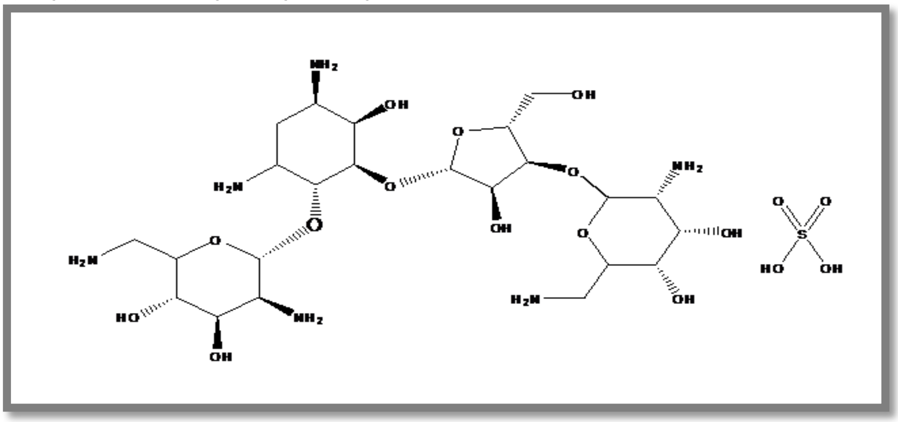

Figure 1. The chemical Structure of neomycin sulfate drug.

Method

The titanium metal (2×2 cm^2) size surface was washed with water and acetone respectively, after that it was dried via air dryer and kept into desiccators. The current study of corrosion was done in 25 C^0 by using polarization measurements. Different concentrations of the drug were used directly in HCl solution. The current and potential of corrosion were calculated in the absence and presence of the drug by using a corrosion cell that consists of three electrodes. Corrosion cell made of Pyrex with (1L) capacity consists of two vessels, internal and external vessel. Chiller device was used to make the temperature of water which flows through the external vessel constant at 25 C^0. Three electrodes and thermostat are replaced in the internal vessel, reference electrodes is used to determine the working electrode potential according to the potential of reference. The potential of reference electrode is well known and accurate, and it is combined of two tubes, the inner tube contains Agcl,Ag,Kcl. The outer tube is filled with the prepared solution (0.25M HCl).The reference electrode is replaced at the distance 2mm working electrode. The auxiliary electrode consists of high purity platinum metal. Its length is 10 cm and the working electrode is the studying and testing subject which potential will be measured this electrode is formed from 20 cm length metallic wire and connected to the mounted specimen(titanium metal) as show in Fig. 2.

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Figure 2. Set up the corrosion cell and three electrodes

Results and Discussion:

The effect of concentration drug on corrosion rate. Figure 3 and Table 2 show the inhibition efficiency (%IE) of titanium metal increasing in high concentration (400 ppm) of drug while the less in low concentration (10 ppm), due to titanium metal in hydrochloric acid bears positive charge, therefore, the drug was attached with the titanium and the corrosive media surface bears negatively charged ions (12).

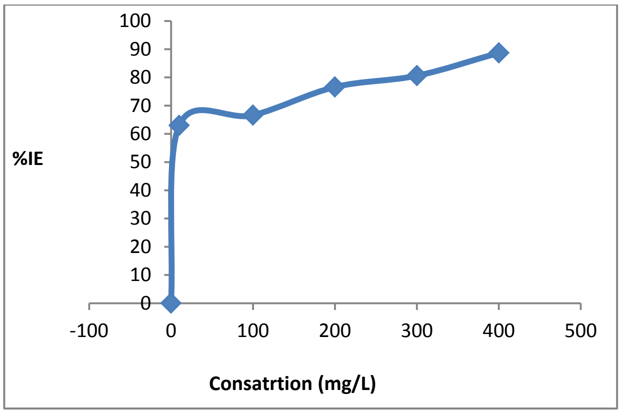

Figure 3. Inhibition efficiency (%IE) of titanium metal at different concentration of drug at 25 C^0

Table 2. Values of inhibition efficiency (%IE) of titanium metal with different concentration of drug at 25 C^0.

Concentration (mg/L)	%IE
0	0
10	63
100	66.6
200	76.6
300	80.6
400	88.7

Polarization Measurements

Figure 4 shows the polarization curves for titanium various concentrations of the drug in 0.25 M hydrochloric acid. While, the values of polarization measurements corrosion potential (Ecorr), corrosion current density (icorr), tafel slopes (ba ,bc), and calculated inhibition efficiency (IE%), corresponding with electrochemical parameters are displayed in Table 3. It is apparent that neomycin sulfate drug in solution caused a shift in the corrosion potential towards more negative values well as reduced the cathodic and anodic current densities, with a more pronounced cathodic effect. Titanium protection in presence neomycin sulfate drug leads to significant changes of corrosion potential in the positive direction as well as a huge reduction of cathodic and anodic current densities. Percentage of corrosion inhibition was calculated according to equation (1)(13). Both cathodic (βc) and anodic Tafel lines (βa) are parallel and are shifted to more negative and positive direction, respectively by adding inhibitors. This is indicating that the mechanism of the corrosion reaction does not change and the corrosion reaction is inhibited by simple adsorption mode. The irregular trends of βa and βc values indicate the involvement of more than one type of species adsorbed on the metal surface (14).

$$IE\% = (icorr)_i - icorr / (icorr)_i \times 100 \ldots\ldots..(1)$$

where $(icorr)_i$ represent the value of the corrosion current densities for Titanium, icorr the value of the corrosion current densities for Titanium in the presence neomycin sulfate drug.

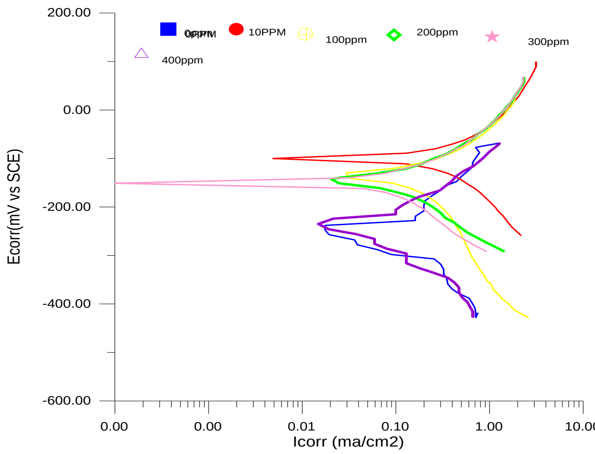

Figure 4. Tafel line of titanium metal with and without addition drug in 0.25N HCl .

Table 3. Values of potentiodynamic polarization curves for titanium metal with and without addition drug in 0.25N HCl.

Conc. of drug(mg/L)	Icorr (mA/cm^2)	-Ecorr(mV)	-bc	ba	%IE	θ
0	254.18	271.7	373.3	306.1	0	0
10	94.12	102.1	53.6	53.4	63	0.63
100	81.97	140.2	98.1	76.6	66.6	0.666
200	59.40	146.6	84.7	70.7	76.6	0.766
300	49.32	147.1	60.7	58.6	80.6	0.806
400	28.80	149.2	56.4	48.9	88.7	0.8867

When increasing concentration of neomycin sulfate drug the current density increases, indicating the high concentration of the drug increased inhibition efficiency. In acidic solution the anodic process of corrosion is the passage of metal ions from the solid metal to the solution, and the principal cathodic process is the discharge of hydrogen ions to produce hydrogen molecules or reduction of oxygen. The corrosion potential values slightly shifted to more negative values, indicating that the addition of Neomycin sulfate drug reduces both anodic dissolution and cathodic reduction (15).

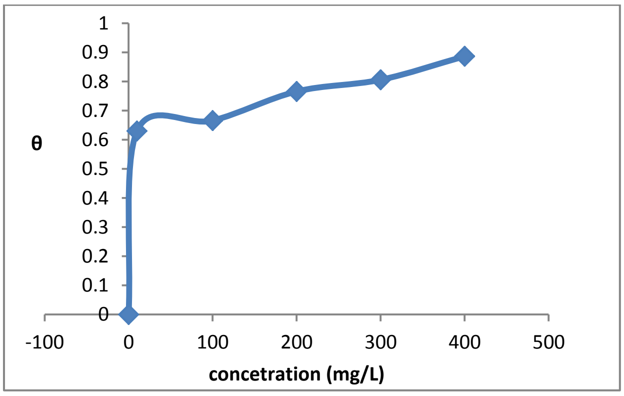

Figure 5. Surface coverage (θ) of titanium metal at different concentration of drug at 25 C^0.

Adsorption Isotherm

The surface coverage (θ) values were increased with increasing concentration of inhibitor neomycin sulfate drug due to the adsorption of inhibitor from solution attachment to surface of titanium metal in acid solution (16) as shown in Table 3 and Fig. 5. The surface coverage (θ) values can be calculated from equation (17):

$\theta = (1 - K / Ko)$ …………………………..(1)

where θ = Surface coverage area, Ko = corrosion rate without coating equal current density for titanium metal in absence neomycin sulfate drug , K = corrosion rate with coating equal current density for titanium metal in a presence neomycin sulfate drug.

Computational Study

The quantum chemical properties such as total energy, E_{HOMO} (highest occupied molecular orbital energy), E_{LUMO} (lowest unoccupied molecular orbital energy), energy gap (ΔE_{gap}), dipole moment (μ), hardness (η), softness (S), the absolute electronegativity (χ), the electrophilicity index (ω), ionization energy (I) and electron affinity (A) were performed using Density Functional Theory (DFT) as shown Table4, the optimized geometry and schematic diagrams of the HOMO(highest occupied molecular orbital energy), E_{LUMO} (lowest unoccupied molecular orbital energy) and the electrostatic potential of Neomycin sulfate as shown in Fig.6.

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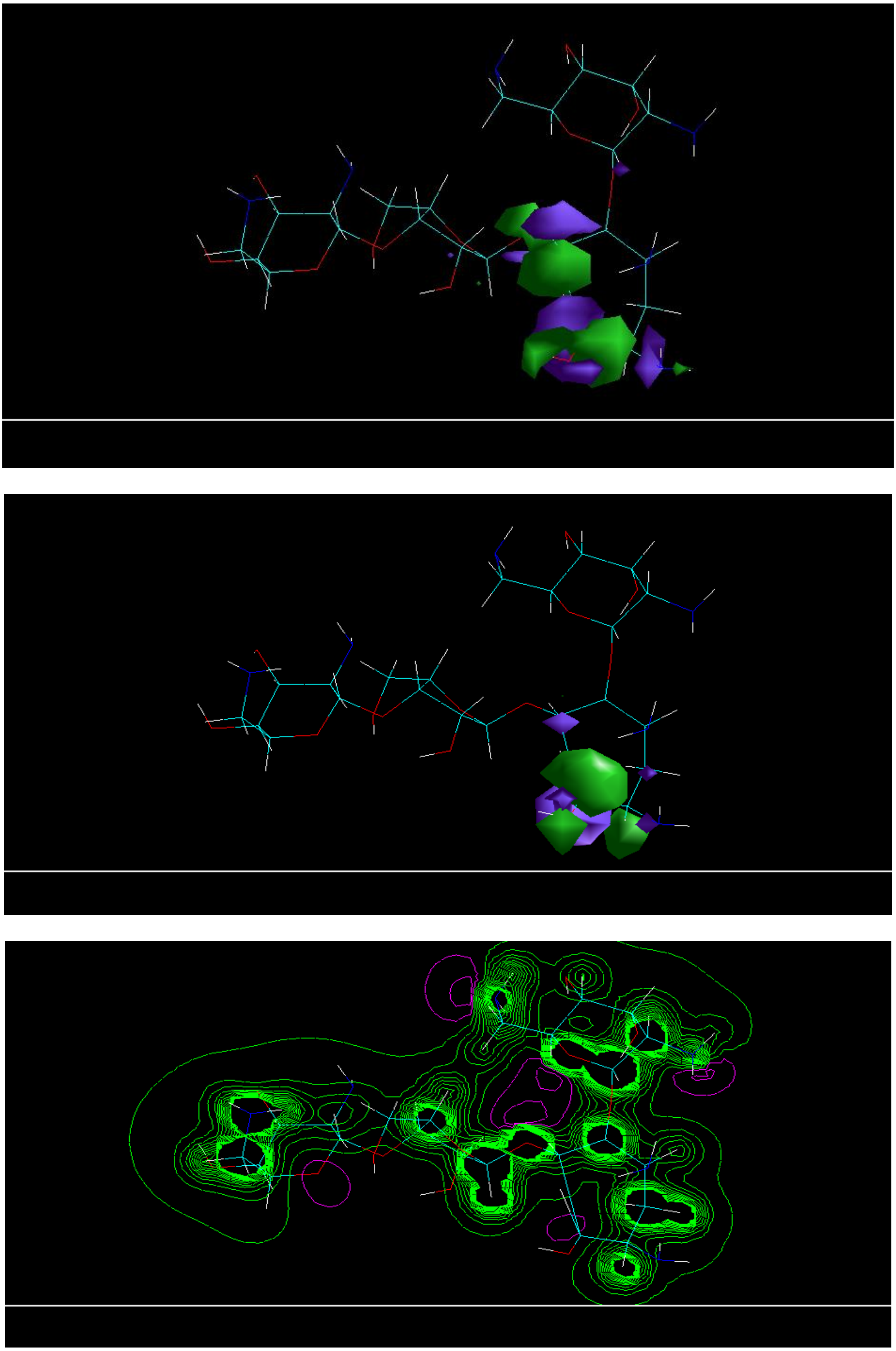

Figure 6. Optimized geometry and schematic diagrams of the HOMO, LUMO, and the electrostatic potential of Neomycin sulfate.

The changing energy (ΔE) explains that Neomycin sulfate drug molecule was absorbed on Ti surface, due to adsorption on the Ti surface with increasing of inhibition efficiency electron, therefore, transfer molecular orbital E_{HOMO} (highest occupied molecular orbital energy) and E_{LUMO} (lowest unoccupied molecular orbital energy). Transfer electrons to unoccupied orbital of the Ti surface and gain free electrons from the Ti therefore the neomycin sulfate drug good corrosion inhibitor .It can be seen that all results for quantum chemical (Theoretical measurements) parameters validate our experimental data(18).

Table 4. Quantum chemical parameters for Neomycin sulfate calculated using program of hyperchem-8.07

Parameters	Data
Total Energy (eV)	-189682.14
ΔE_b	-8266.38
ΔH^o_f	-486.95
E_{HOMO} (eV)	- 9.03993
E_{LUMO} (eV)	-0.19003
Δ**E_{gap}** (eV)	8.84989
μ (Debye)	-8.9133
I (eV)	9.03993
A (eV)	0.19003
η (eV)	8.8499
ω (eV)	1.2033
χ (eV)	4.61498
S $(eV)^{-1}$	0.11299

FT-IR Spectra:

The FTIR spectrum of drug compound revealed a stretching vibration band at OH (carboxylic group), NH_2 (amine group), and R-O-R (ether group), (3406, 3147, and 1126) cm^{-1} groups respectively, as shown in Fig. 7 and Table 5.

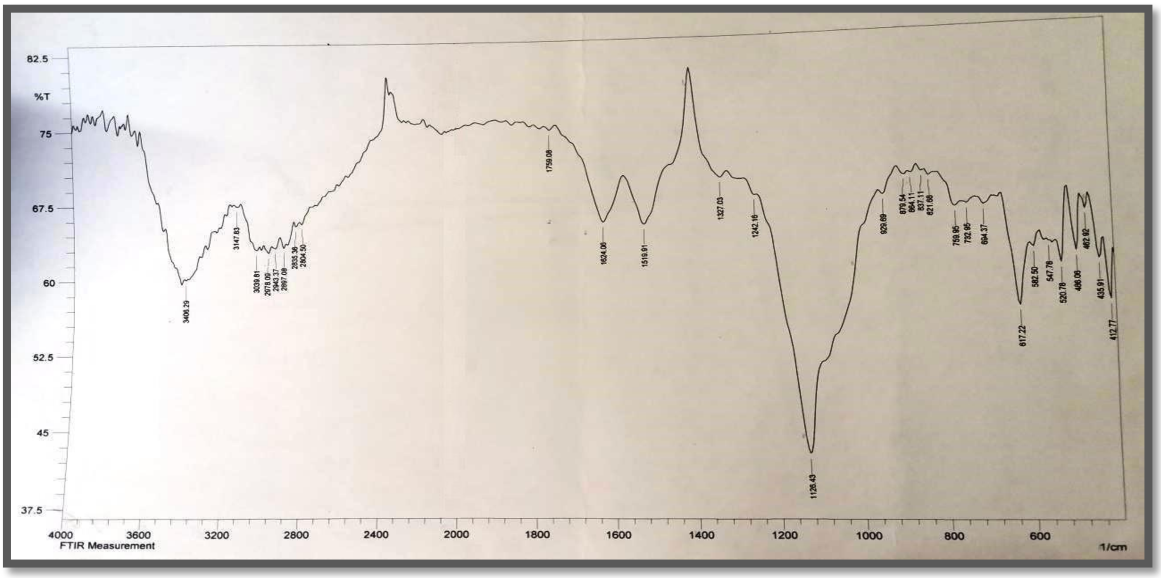

Figure 7. FTIR spectrum of Neomycin sulfate.

The results are close between the theoretical and experimental Frequency as displayed in Table 5.

Table 5. A Comparison between Experimental and Theoretical Vibrational Frequencies of Neomycin sulfate (cm^{-1})

ν O-H (carboxylic group)	*ν* N-H (amine group)	*ν* R-O-R (ether group)
*3406	*3147	*1126
**3386	**3348	**1124
***0.5906	***-6.0035	***0.17

*: Experimental frequency.
**: Theoretical frequency.
***: Error % due to main difference in the experimental measurements and theoretical treatments of vibrational spectrum.

The program of hyperchem-8.07 was used for theoretical study and calculate bond length and dihedral angles of the Neomycin sulfate as shown in Table 6,7.

Table 6. bond length of Neomycin sulfate.

Bond	Actual (A°)	Optimal(A°)	Bond	Actual (A°)	Optimal(A°)
N(47)-Lp(36)	0.6	0.5983	O(26)-Lp(18)	0.6	0.5999
O(46)-Lp(35)	0.6	0.5967	N(27)-Lp(20)	0.6	0.6003
O(46)-Lp(34)	0.6	0.599	O(5)-Lp(4)	0.6	0.5989
O(45)-Lp(33)	0.6	0.6009	O(5)-Lp(3)	0.6	0.5983
O(45)-Lp(32)	0.6	0.5995	O(4)-Lp(2)	0.6	0.5988
N(44)-Lp(31)	0.6	0.6004	O(4)-Lp(1)	0.6	0.5986
O(38)-Lp(30)	0.6	0.5973	N(47)-H(95)	1.035	1.0351
O(38)-Lp(29)	0.6	0.5999	N(47)-H(94)	1.035	1.0346
O(36)-Lp(28)	0.6	0.6013	O(46)-H(93)	0.961	0.9639
O(36)-Lp(27)	0.6	0.6005	O(45)-H(92)	0.961	0.9617
O(34)-Lp(26)	0.6	0.5971	N(44)-H(91)	1.035	1.0359
O(34)-Lp(25)	0.6	0.5999	N(44)-H(90)	1.035	1.0346
O(33)-Lp(24)	0.6	0.6	C(43)-H(89)	1.113	1.1142
O(33)-Lp(23)	0.6	0.601	C(43)-H(88)	1.113	1.1148
O(32)-Lp(22)	0.6	0.5981	C(42)-H(87)	1.113	1.1174
O(32)-Lp(21)	0.6	0.6013	C(41)-H(86)	1.111	1.1153
O(22)-Lp(13)	0.6	0.5984	C(40)-H(85)	1.111	1.1152
O(16)-Lp(12)	0.6	0.6004	C(39)-H(84)	1.111	1.1175
O(16)-Lp(11)	0.6	0.6006	C(37)-H(83)	1.109	1.1116
O(15)-Lp(10)	0.6	0.6009	O(36)-H(82)	0.961	0.9618
O(15)-Lp(9)	0.6	0.6004	C(35)-H(81)	1.111	1.1074
O(14)-Lp(8)	0.6	0.6004	C(35)-H(80)	1.111	1.1084
O(14)-Lp(7)	0.6	0.6003	O(33)-H(79)	0.961	0.962
N(13)-Lp(6)	0.6	0.599	C(31)-H(78)	1.111	1.1168
N(12)-Lp(5)	0.6	0.5983	C(30)-H(77)	1.111	1.1145
O(25)-Lp(17)	0.6	0.5998	C(29)-H(76)	1.111	1.1122
O(25)-Lp(16)	0.6	0.5979	C(28)-H(75)	1.109	1.1078
N(24)-Lp(15)	0.6	0.5969	N(27)-H(74)	1.035	1.0345
O(22)-Lp(14)	0.6	0.6001	N(27)-H(73)	1.035	1.0349
O(26)-Lp(19)	0.6	0.601	O(26)-H(72)	0.961	0.9603
O(25)-H(71)	0.961	0.9602	C(18)-O(25)	1.401	1.4084
N(24)-H(70)	1.035	1.0351	C(21)-O(16)	1.391	1.4108
N(24)-H(69)	1.035	1.0348	C(8)-O(16)	1.382	1.4068
C(23)-H(68)	1.113	1.1147	C(30)-O(34)	1.382	1.4016
C(23)-H(66)	1.113	1.1156	C(29)-O(33)	1.401	1.4093
C(21)-H(66)	1.109	1.1098	C(19)-O(26)	1.401	1.4083
C(20)-H(65)	1.113	1.1172	C(20)-N(27)	1.468	1.4706
C(19)-H(64)	1.111	1.1151	C(9)-O(15)	1.382	1.4032
C(18)-H(63)	1.111	1.1156	C(10)-O(14)	1.401	1.4092
C(17)-H(62)	1.111	1.118	C(11)-N(13)	1.468	1.4739
O(14)-H(61)	0.961	0.9605	C(43)-N(44)	1.468	1.4732
N(13)-H(60)	1.035	1.035	C(39)-C(43)	1.514	1.5294
N(13)-H(59)	1.035	1.0344	C(42)-C(37)	1.505	1.5205
N(12)-H(58)	1.035	1.0348	C(41)-C(42)	1.514	1.5252
N(12)-H(57)	1.035	1.0353	C(40)-C(41)	1.505	1.5182
C(11)-H(56)	1.113	1.1171	C(39)-C(40)	1.505	1.5215
C(10)-H(55)	1.111	1.1139	O(38)-C(39)	1.382	1.3989
C(9)-H(54)	1.111	1.1161	C(37)-O(38)	1.391	1.4094
C(8)-H(53)	1.111	1.1136	O(34)-C(37)	1.391	1.4108
C(7)-H(52)	1.113	1.1175	C(35)-O(36)	1.408	1.4146
C(6)-H(51)	1.113	1.115	O(32)-C(28)	1.391	1.4112
C(6)-H(50)	1.113	1.1158	C(31)-O(32)	1.382	1.4061
O(5)-H(49)	0.942	0.9403	C(30)-C(31)	1.505	1.5243
O(4)-H(48)	0.942	0.9393	C(29)-C(30)	1.505	1.5164
C(40)-O(45)	1.401	1.4103	C(28)-C(29)	1.496	1.5068
C(41)-O(46)	1.401	1.408	C(23)-N(24)	1.468	1.471
C(42)-N(47)	1.468	1.4728	C(17)-C(23)	1.514	1.532
C(31)-C(35)	1.505	1.5203	O(22)-C(17)	1.382	1.4017
C(28)-O(15)	1.391	1.4131	C(21)-O(22)	1.391	1.4093
C(20)-C(21)	1.505	1.5199	C(8)-C(9)	1.505	1.5352
C(19)-C(20)	1.514	1.5224	C(7)-C(8)	1.514	1.5342
C(18)-C(19)	1.505	1.5192	C(6)-C(7)	1.523	1.5316
C(17)-C(18)	1.505	1.5269	S(1)-O(5)	-------	1.6609
C(7)-N(12)	1.468	1.475	S(1)-O(4)	-------	1.6651
C(11)-C(6)	1.523	1.5314	S(1)-O(3)	1.45	1.4516
C(10)-C(11)	1.514	1.526			
C(9)-C(10)	1.505	1.5319			

Table 7. Dihedral angles of Neomycin sulfate.

Bond	Actual (deg.)	Optimal(deg.)	Bond	Actual (deg.)	Optimal(deg.)
H(95)-N(47)-H(94)	104.5	109.4418	H(85)-C(40)-C(39)	109.39	109.4821
H(95)-N(47)-C(42)	…….	109.4418	O(45)-C(40)-C(41)	107.7	109.4505
H(94)-N(47)-C(42)	…….	109.5	O(45)-C(40)-C(39)	107.7	109.4505
H(93)-O(46)-C(41)	106.9	120	C(41)-C(40)-C(39)	109.51	109.4653
H(92)-O(45)-C(40)	106.9	120	H(84)-C(39)-C(43)	109.39	108.2168
H(91)-N(44)-H(90)	104.5	109.4418	H(84)-C(39)-C(40)	109.39	110.6249
H(91)-N(44)-C(43)	…….	109.4418	H(84)-C(39)-O(38)	106.7	110.6249
H(90)-N(44)-C(43)	…….	109.5	C(43)-C(39)-C(40)	109.51	109.9389
H(89)-C(43)-H(88)	109.4	109.52	C(43)-C(39)-O(38)	107.7	109.9389
H(89)-C(43)-N(44)	…….	109.4618	C(40)-C(39)-O(38)	107.7	107.5
H(89)-C(43)-C(39)	109.41	109.4618	C(39)-O(38)-C(37)	106.8	106.8
H(88)-C(43)-N(44)	…….	109.4418	H(83)-C(37)-C(42)	109.39	110.6249
H(88)-C(43)-C(39)	109.41	109.4418	H(83)-C(37)-O(38)	106.7	110.6249
N(44)-C(43)-C(39)	109.5	109.5	H(83)-C(37)-O(34)	106.7	108.2168
H(87)-C(42)-N(47)	108.8	109.5	C(42)-C(37)-O(38)	107.7	107.5
H(87)-C(42)-C(37)	109.39	109.4793	C(42)-C(37)-O(34)	107.7	109.9389
H(87)-C(42)-C(41)	109.39	109.4793	O(38)-C(37)-O(34)	97	109.9389
N(47)-C(42)-C(37)	108.8	109.4493	H(82)-O(36)-C(35)	106.9	120
N(47)-C(42)-C(41)	108.8	109.4493	H(81)-C(35)-H(80)	109.4	109.52
C(37)-C(42)-C(41)	109.51	109.47	H(81)-C(35)-C(31)	109.41	109.4618
H(86)-C(41)-O(46)	106.7	109.5117	H(81)-C(35)-O(36)	106.7	109.4618
H(86)-C(41)-C(42)	109.39	109.4691	H(80)-C(35)-C(31)	109.41	109.4418
H(86)-C(41)-C(40)	109.39	109.4691	H(80)-C(35)-O(36)	106.7	109.4418
O(46)-C(41)-C(42)	107.7	109.4449	C(31)-C(35)-O(36)	107.4	109.5
O(46)-C(41)-C(40)	107.7	109.4449	C(30)-O(34)-C(37)	106.8	120
C(42)-C(41)-C(40)	109.51	109.4876	H(79)-O(33)-C(29)	106.9	120
H(85)-C(40)-O(45)	106.7	109.4969	C(28)-O(32)-C(31)	106.8	104
H(85)-C(40)-C(41)	109.39	109.4821	H(78)-C(31)-C(35)	109.39	107.6898
H(78)-C(31)-O(32)	106.7	111.1087	H(68)-C(23)-N(24)	109.41	109.4618
H(78)-C(31)-C(30)	109.39	111.1087	H(68)-C(23)-C(17)		109.4618
C(35)-C(31)-O(32)	107.7	110.1452	H(67)-C(23)-N(24)	109.41	109.4418
C(35)-C(31)-C(30)	109.51	110.1452	H(67)-C(23)-C(17)	109.5	109.4418
O(32)-C(31)-C(30)	107.7	106.6645	N(24)-C(23)-C(17)	106.8	109.5
H(77)-C(30)-O(34)	106.7	105.0228	C(17)-O(22)-C(21)	106.7	106.8
H(77)-C(30)-C(31)	109.39	113.6867	H(66)-C(21)-O(16)	106.7	108.275
H(77)-C(30)-C(29)	109.39	113.6867	H(66)-C(21)-O(22)	109.39	110.572
O(34)-C(30)-C(31)	107.7	111.24	H(66)-C(21)-C(20)	97	110.572
O(34)-C(30)-C(29)	107.7	111.24	O(16)-C(21)-O(22)	107.7	109.9164
C(31)-C(30)-C(29)	109.51	102.1698	O(16)-C(21)-C(20)	107.7	109.9164
H(76)-C(29)-O(33)	106.7	106.0753	O(22)-C(21)-C(20)	108.8	107.5913
H(76)-C(29)-C(30)	109.39	112.6423	H(65)-C(20)-N(27)	109.39	109.3517
H(76)-C(29)-C(28)	109.39	112.6423	H(65)-C(20)-C(21)	109.39	109.6095
O(33)-C(29)-C(30)	107.7	110.7973	H(65)-C(20)-C(19)	108.8	109.6095
O(33)-C(29)-C(28)	107.7	110.7973	N(27)-C(20)-C(21)	108.8	109.505
C(30)-C(29)-C(28)	109.51	104	N(27)-C(20)-C(19)	109.51	109.505
H(75)-C(28)-O(15)	106.7	106.0753	C(21)-C(20)-C(19)	106.7	109.2467
H(75)-C(28)-O(32)	106.7	112.6423	H(64)-C(19)-O(26)	109.39	109.5
H(75)-C(28)-C(29)	109.39	112.6423	H(64)-C(19)-C(20)	109.39	109.4793
O(15)-C(28)-O(32)	97	110.7973	H(64)-C(19)-C(18)	107.7	109.4793
O(15)-C(28)-C(29)	107.7	110.7973	O(26)-C(19)-C(20)	107.7	109.4493
O(32)-C(28)-C(29)	107.7	104	O(26)-C(19)-C(18)	109.51	109.4493
H(74)-N(27)-H(73)	104.5	109.4418	C(20)-C(19)-C(18)	106.7	109.47
H(74)-N(27)-C(20)	…….	109.4418	H(63)-C(18)-O(25)	109.39	109.5
H(73)-N(27)-C(20)	106.9	109.5	H(63)-C(18)-C(19)	109.39	109.4793
H(72)-O(26)-C(19)	106.9	120	H(63)-C(18)-C(17)	107.7	109.4793
H(71)-O(25)-C(18)	104.5	120	O(25)-C(18)-C(19)	107.7	109.4493
H(70)-N(24)-H(69)	…….	109.4418	O(25)-C(18)-C(17)	109.51	109.4493
H(70)-N(24)-C(23)	…….	109.4418	C(19)-C(18)-C(17)	109.39	109.47
H(69)-N(24)-C(23)	109.4	109.5	H(62)-C(17)-C(23)	106.7	108.2168
H(68)-C(23)-H(67)	…….	109.52	H(62)-C(17)-O(22)	109.39	110.6249

Conclusions:

This work describes the corrosion inhibition of titanium by Neomycin sulfate drug. Experimental results from potenciodynamic measurements are subjected to theoretical calculations. The results of the inhibition efficiency showed that the use of Neomycin sulfate drug for corrosion inhibition in the aqueous acidic media, can decrease the corrosion from 254.18 to 28 (mA/cm^2), also the inhibition efficiency reaches 88.7%, due to, the adsorption of inhibitor from solution attachment to surface of titanium metal 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(ΔE_b) and optimized structural geometries were calculated at 298K and the bond length, vibration spectra for Neomycin sulfate drug was calculated and then compared with the experimental value(19).

Authors' declaration:

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are mine ours. Besides, the Figures and images, which are not mine ours, have been given the permission for re-publication attached with the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee in University of Baghdad.

References

1. Dana HA, Mohamad EH, Muammer K, Muataz AA. A Review on the Corrosion Behaviour of Nanocoatings on Metallic Substrates. Materials. 2019; 12(2):210.
2. Tambi R, Stefano R, Lucien B. Corrosion Inhibition Action of Sulfamethoxazole for Brass in Acidic Media. Int. J. Electrochem. Sci. 2016; 11: 6819 – 6829.
3. Abboud Y, Abourriche A, Berrada M, Charrouf M, Bennamara A, Al Himidi N. et al. 2,3-Quinoxalinedione as a novel corrosion inhibitor for mild steel in 1 M HCl. Mater. Chem.phy. 2007; 1(105): 1-5.
4. Khaled KF, Hackerman N. Investigation of the inhibitive effect of ortho-substituted anilines on corrosion of iron in 1 M HCl solutions. Electrochim. Acta. 2003;48(19):2715-2723.
5. Popova A, Raicheva S, Sokolova E. Adsorption and inhibitive properties of benzimidazole derivatives in acid carbon steel corrosion. Corros.Sci.2004; 46(6):1333-1350.
6. Nnabuk OE, Stanislav RS, Eno EE. Fluoroquinolones as Corrosion Inhibitors for Mild Steel in Acidic Medium; Experimental and Theoretical Studies.Studies. Int. J. Electrochem. Sci. 2010; 5:1127 – 1150.
7. Samide A, Tutunaru B, Negrila C. Corrosion inhibition of carbon steel in hydrochloric acid solution using a sulfa drug. Chem. Biochem. Eng. 2011; 25 (3):299–308.
8. Anjali DV, Gowrav MP, Atul S, Riyaz AM. A study of chitosan nanofibers containing neomycin sulphate for wound healing activity. Der Pharmacia Lettre. 2016 ;8 (11) :128-139.
9. Karthikeya S. Drugs/Antibiotics as potential corrosion inhibitors for Metals- A Review. IJCRGG. 2016; 9 (6) : 251-259.
10. Adnan M, Irfan T. Review on Cathodic Protection System Modelling. B&H Electr.Eng. 2017; 11:81-91.
11. Ehteram AN, Aisha HM. Thermodynamic study of metal corrosion and inhibitor adsorption processes in carbon steel/1-methyl-4[4′(-X)-styryl pyridinium iodides/hydrochloric acid systems. Mater.Chem.Phys..2008; 110(1):145-154.
12. Saed AA, Abdulkareem MA. Anticorrosion behavior of deposited nanostructured polythiophene on stainless steel carbon steel and aluminum in sea water. IJOER. 2016; 2(3) :1-7.
13. Ladislav V, Senka G, David G, Ivana S, Ivana I, Maja K ,et al. Corrosion Protection of Copper in Sodium Chloride Solution using Propolis. Int. J. Electrochem. Sci. 2018; 13 :2102 – 2117.
14. Fouda AS, Elmorsi MA, Fayed TA, Hassan AF, Soltan M. Corrosion Inhibitors Based on Antibiotic Derivatives for Protection of Carbon steel Corrosion in Hydrochloric Acid Solutions . IJAR. 2014; 2 (4):788-807.
15. Adriana S, Bogdan T, Aurelian D , Petru I , Ana-CV, Cristian T . Electrochemical and Theoretical Study of Metronidazole Drug as Inhibitor for Copper Corrosion in Hydrochloric Acid Solution. Int. J. Electrochem. Sci. 2016; 11 : 5520 – 5534.
16. Ambrish S, Eno. EE , Quraishi MA. Theoretical and Electrochemical Studies of Metformin as Corrosion Inhibitor for Mild Steel in Hydrochloric Acid Solution. Int. J. Electrochem. Sci. 2012 ; 7: 4766 – 4779.
17. Adriana S, Gabriela EI , Bogdan T , Roxana G, Cristian T, Cezar S. Inhibitory Properties of Neomycin Thin Film Formed on Carbon Steel in Sulfuric Acid Solution Electrochemical and AFM Investigation. Coatings. 2017; 7(11):181.
18. Fouda AS, Rashwan SM, Kamel M , Badawy AA. Unused Meropenem Drug as Corrosion Inhibitor for Copper in Acidic Medium; Experimental and Theoretical Studies. Int. J. Electrochem. Sci. 2016; 11:9745 – 9761.
19. Valbone M, Fetah IP. Experimental and Theoretical Studies on Corrosion Inhibition of Niobium and Tantalum Surfaces by Carboxylated Graphene Oxide. Materials .2018;11(6) :893.

الدراسة النظرية والعملية لحمايه التيتانيوم من التاكل بوساطه دواء كبريتات النيومايسين في الوسط الحامضي

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الخلاصة:
تم دراسة الطرق التجريبية والنظرية لتثبيط التآكل لمعدن التيتانيوم في الوسط الحامضي باستخدام حامض الهيدروكلوريك بوساطه عقار كبريتات النيومايسين. وكان للدواء (كبريتات النيومايسين) نتائج جيدة بحماية التآكل لمعدن التيتانيوم في محلول الحامض وكفاءة تثبيط تزداد مع زيادة تركيز الدواء، ويعود السبب الى امتزاز دواء كبريتات النيومايسين على سطح معدن التيتانيوم في الوسط الحامضي. استخدم برنامج hyperchem-8.07 للدراسة النظرية لعقاركبريتات النيومايسين بوساطة الميكانيكية الجزيئية والحسابات شبه التجريبية .كيمياء الكم استخدمة لدراسة امتزاز العقار وانتقال الالكترون من العقار الى معدن التيتانيوم ، كذلك جهد العقار المثبط للتاكل مرتبط (HOMOاعلى طاقة مدارية جزية مشغولة –اوطا طاقة مدارية جزية غير مشغولةLUMO)،عزم ثنائي القطب للجزيئات والجهود الكتروستاتيكية .

الكلمات المفتاحية: الدراسة النظرية، تثبيط التاكل، معدن التيتانيوم، نيومايسين .