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Experimental and Computational Study of Corrosion Potentials of Penicillin G

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Abstract: Inhibition and adsorption potentials of penicillin G for the corrosion of mild steel in solutions of HCl have been investigated using experimental and quantum chemical approaches. The experimental study was carried out using gravimetric and Fourier transform infrared spectroscopy methods of monitoring corrosion while the quantum chemical study was carried out using quantum chemical approaches. The results obtained showed that various concentrations of penicillin G inhibited the corrosion of mild steel in solutions of HCl through the mechanism of physiosorption. The adsorption of penicillin G on mild steel surface was found to be exothermic and spontaneous and fitted the Langmuir Adsorption Model. DFT study has been used to identify the site for electrophillic and nucleophillic attack and the molecular orbital diagram of penicillin G has been drawn using Extended Huckel Method.

Key words: Inhibitor, potentials, corrosion, physiosorption and penicillin G, molecular

INTRODUCTION

Corrosion is a primary means by which metals deteriorate and is therefore a major industrial problem. The degradation occurs when metals come in contact with moisture, acids, bases, salts, aggressive metal polishes and other liquid chemicals. Other agents of corrosion are gaseous materials like acid vapours, formaldehyde gas and sulphur containing and ammonia gases. When metals are exposed to corrosion agents within an electrical circuit, they give up electrons to become positively charged ions.

Corrosion of mild steel is a major problem in some industries including the oil and fertilizer industries (Bentiss *et al*., 2007). This is because in these industries, there are some processes (such as scaling and etching, etc.) that necessitate contact between mild steel and aggressive medium such as acid, alkaline and salt solutions (Ashassi-Sorkhabi *et al*., 2005). In view of the problems created by mild steel corrosion, several researches on the methods of inhibition of its corrosion have been reported and it has been established that the use of inhibitors is one of the best methods of the prevention of the corrosion of mild steel in acidic medium (Odiongenyi *et al*., 2009; Gopi *et al*., 2009). The choice of inhibitors for the corrosion of metals depends on the ability of the inhibitor to be synthesised from cheap raw materials and for the inhibitor to be environmentally friendly. Most inhibitors are organic compounds that contain heteroatoms (S, N, O, P) or those that have long carbon chains or aromatic ring systems. Among the compounds investigated and found to be good inhibitors are some drugs (Achary *et al*., 2008; Hosseini and Azimi, 2009). Some researchers generally agree that drugs are inhibitors that can researchers favourably with green corrosion inhibitors and that most drugs can bes synthesised from natural products. The choice of some drugs as corrosion inhibitors is based on the following:

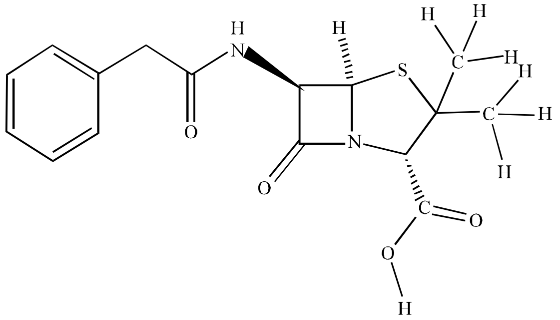

Fig. 1: Chemical structure of penicilline G (2S, 5R, 6R)-3, 3-dimethly-7-oxo-6-(2-phenylacetamido)-4-thia-1-azabicyclo [3.2.0] heptane-2-carboxylic acid (Pen G)

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drug molecules containing oxygen, nitrogen and sulphur as active centres; drugs that are reportedly environmentally friendly and important in biological reactions and drugs that can be easily produced and purified. In this study penicillin G shall be used for the inhibition of the corrosion of mild steel in HCl (Fig. 1).

MATERIALS AND METHODS

Materials used for the study were mild steel sheet ofcomposition as determined by quotiometric method, wt (%): Mn (0.6), P (0.36), C (0.15), Si (0.03) and 98.86% Fe. The sheet was mechanically pressed cut into different coupons, each of dimension, 5×4×0.11 cm. Each coupon was degreased by washing with ethanol, cleaned with acetone and allowed to dry in the air before preservation in a desiccator. All reagents used for the study were of analar grade and double distilled water was used for their preparation. The concentration of HCl used for weight loss studies was 0.1 M.

Gravimetric method: In the gravimetric experiment, a previously weighed mild steel coupon was completely immersed in 250 mL of the test solution in an open beaker. The beaker was covered with aluminium foil and inserted into a water bath maintained at 303 K. After every 24 h, the corrosion product was removed by washing each coupon (withdrawn from the test solution) in a solution containing 50% NaOH and 100 g dm^{-3} of zinc dust. The washed coupon was rinsed in acetone and dried in the air and to constant weight.

The experiment was repeated at 333 K. In each case, the difference in weight for a period of 168 h was taken as the total weight loss.

From the average weight loss (mean of three replicate analyses) results, the inhibition efficiency (I%) of the inhibitor, the degree of surface coverage (θ) and the Corrosion Rate of mild steel (CR) were calculated using Eq. 1-3, respectively:

$$I\% = (1 - W_1/W_2)\times 100 \quad (1)$$

$$\theta = 1 - W_1/W_2 \quad (2)$$

$$CR = \Delta W/At \quad (3)$$

Where:

W_1 and W_2 = The weight losses (g) for mild steel in the presence and absence of the inhibitor

θ = The degree of surface coverage of the inhibitor, $\Delta W = W_2 - W_1$

A = The area of the mild steel coupon (cm^2)

t = The period of immersion (in hours)

W = The weight loss of mild steel after time, t

RESULTS AND DISCUSSION

In Table 1, the inhibition efficiencies penicillin G obtained from Gravimetric Method are presented. From the results obtained, it is evident that the inhibition efficiencies of the inhibitors increase with increase in concentration of the inhibitors but decrease with increasing temperature. These also suggest that the inhibitors are adsorption inhibitors and that the mechanism of adsorption favours physical adsorption (Yurt *et al*., 2005).

Figure 2 shows the plots of weight loss with time in different concentrations of HCl solutions and Fig. 3 shows the plot of weight loss with time in different concentrations of penicillin G.

Table 1: Inhibition efficiencies for various concentrations of penicillin G for the corrosion of mild steel in 0.1M HCl

Cg L^{-1}	At 303 K	At 333 K
0.1	89.40	68.36
0.2	90.73	73.05
0.3	91.66	76.43
0.4	92.56	78.02
0.5	93.19	80.01

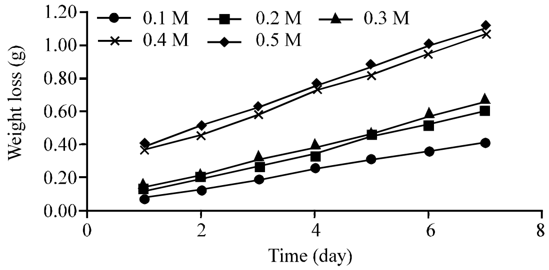

Fig. 2: Variation of weight loss with time for the corrosion of mild steel in various concentrations of HCl

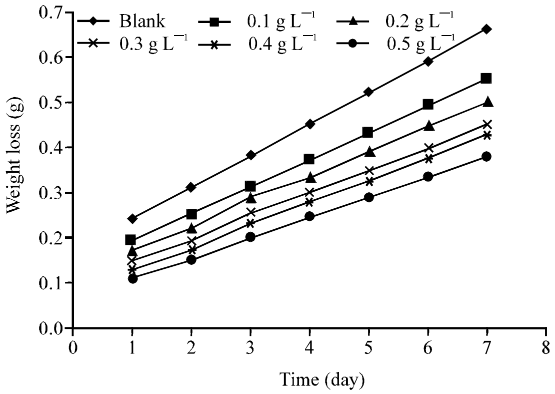

Fig. 3: Variation of weight loss with time for the corrosion of mild steel in 0.1 M HCl containing various concentrations of penicillin G

Effect of temperature: The effect of temperature on the corrosion of mild steel in HCl in the absence and presence of various concentrations of penicillin G was assessed from the Arrhenius equation which can be represented as Eq. 4 (Oguzie *et al.*, 2007):

$$CR = A\exp(-E_a/RT) \tag{4}$$

Where:

CR = The rate of corrosion of mild steel
A = The Arrhenius or pre-exponential constant
E_a = The activation energy
R = The universal gas constant
T = The temperature

The logarithm of both sides of Eq. 4 yields Eq. 5:

$$\log CR = \log A - E_a/2.303RT \tag{5}$$

If the corrosion rates of mild steel at temperatures T_1 (303 K) and T_2 (333 K) are CR_1 and CR_2 then substitutions into Eq. 5 yields Eq. 6:

$$\log\frac{CR_2}{CR_1} = \frac{E_a}{2.303R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right) \tag{6}$$

The activation energies calculated from Eq. 6 are shown in Table 2. From the results obtained, it can be seen that the activation energies are below the threshold value of 80 kJ mol^{-1} expected for the mechanism of chemical adsorption.

Therefore, the adsorption of penicillin G on mild steel surface is consistent with the mechanism of charge transfer from the inhibitor's molecule to the charged metal surface which supports physiosorption mechanism (Eddy, 2009a).

Thermodynamic and adsorption considerations: The heat of adsorption of penicillin G on mild steel surface was calculated using Eq. 7 (Eddy, 2009b):

$$Q_{ads} = 2.303R\left[\log\left(\frac{\theta_2}{1-\theta_2}\right) - \log\left(\frac{\theta_1}{1-\theta_1}\right)\right] x \left(\frac{T_1 x T_2}{T_2 - T_1}\right) kJmol^{-1} \tag{7}$$

Where, Q_{ads} is the heat of adsorption, R is the universal gas constant, θ_1 and θ_2 are the degrees of surface coverage of the inhibitors at temperatures T_1 and T_2, respectively. From the calculated values of Q_{ads} (Table 2), it can be deduced that the adsorption of the inhibitors on mild steel surface is exothermic. Also, since the reactions were carried out at constant pressure calculated values of Q_{ads} are expected to be approximately equal to the enthalpy change. The adsorption characteristics of penicillin G were also studied by fitting data obtained for the degree of surface coverage of the inhibitors into different adsorption isotherms such as Langmuir, Temkin and Freundlich adsorption isotherms etc. The test revealed that the adsorption characteristics of the compounds are best described by the Langmuir adsorption isotherm which can be expressed as according to Eq. 8:

Table 2: Activation energy and heat of adsorption for the adsorption of penicillin G on mild steel surface

Cg L^{-1}	Ea (kJ mol^{-1})	Qads (kJ mol^{-1})
0.1	37.16	-65.39
0.2	37.44	-68.79
0.3	38.21	-66.88
0.4	38.02	-64.35
0.5	38.41	-69.87

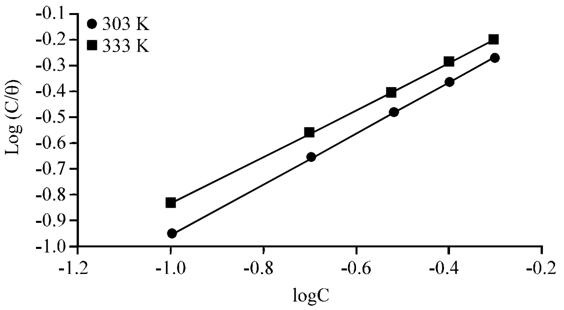

Fig. 4: Langmuir isotherms for the adsorption of penicillin G on mild steel surface

$$\theta = \frac{K_{ads}C}{1 + K_{ads}C}$$

Where:

C = The concentration of the inhibitor in the bulk electrolyte
θ = The degree of surface coverage of the inhibitor
K_{ads} = The equilibrium adsorption constant

Transformation of Eq. 8 yields Eq. 9:

$$\log(C/\theta) = \log C - \log K_{ads} \tag{9}$$

From Eq. 9 plots of log (C/θ) versus logC should yield straight lines provided the assumptions establishing the Langmuir adsorption isotherm are valid. Figure 4 shows the Langmuir isotherms for the adsorption of penicillin G on mild steel surface, respectively. The adsorption parameters deduced from the isotherms are shown in Table 3. From the results obtained, it can be

Table 3: Langmuir adsorption parameters for the adsorption of Penicillin G on mild steel surface

Parameters	At 303 K	At 333 K
Slope	0.9743	0.9743
log K_{ads}	0.0236	0.0236
R2	1.0000	1.0000
ΔG^0 ($kJmol^{-1}$)	-10.2300	-10.2300

Fourier Transform Infrared (FTIR) spectra

Table 4: Peaks, intensity and assignments of IR adsorption by penicillin G and mild steel corrosion product (containing penicillin G as an inhibitor)

Penicillin G			Corrosion product		
Peak (cm^{-1})	Intensity	Assignments	Peak (cm^{-1})	Intensity	Assignments
1172.76	44.224	C-O stretch	1112.96	16.079	C-O stretch
1271.13	23.568	C-O stretch			
1396.51	37.531	C=C stretch			
1454.38	47.497	Aromatic C=C			
1604.83	15.909	Aromatic C=O	1647.26	45.0294	C=O stretch
1778.43	28.779	C=O stretch			
2974.33	51.812	C-H stretch			
3225.09	42.995	Acid O-H			
3340.82	42.046	N-H stretch			
3487.42	45.447	-OH stretch	3473.91	30.0645	-OH stretch

seen that the slopes and R^2 values for the Langmuir plots are very close to unity indicating the adsorption data very much fit the Langmuir adsorption model. The equilibrium adsorption constant of adsorption obtained from the intercept of the Langmuir adsorption isotherms is related to the standard free energy of adsorption according to the Eq. 10 (Odiongenyi *et al.*, 2009):

$$\Delta G^0_{ads} = -2.303RT \log (55.5 K_{ads}) \quad (10)$$

Calculated vales of the free energy are also shown in Table 3. From the results obtained, the free energies are negatively less than the threshold value of -40 kJ mol^{-1} required for the mechanism of chemical adsorption. Generally, values of ΔG^0_{ads} between 0 and -20 kJ mol^{-1} are consistent with the mechanism of charge transfer from charged inhibitor's molecules to charged metal surface. Therefore, the adsorption of penicillin G on mild steel surface is spontaneous with a mechanism of physical adsorption (Eddy and Mamza, 2009). Figure 5 shows the FTIR spectrum of the corrosion of mild steel product in the absence of an inhibitor.

Figure 6 shows the FTIR spectra of pure samples of penicillin G. The wavelengths and peaks of IR adsorption by penicillin G are shown in Table 4. Figure 7 shows the FTIR spectrum of the mild steel corrosion product containing 0.5 g L^{-1} of penicillin G. The peaks and frequencies of IR adsorption are also shown in Table 4. With penicillin G as an inhibitor, it was found that the C-O stretch at 1172.76 cm^{-1} shifted to 1112.96 cm^{-1}, the aromatic C = O stretch at 1604.83 shifted to 1647.26 cm^{-1} and the -OH stretch at 3487.42 cm^{-1} shifted to 3473.91 cm^{-1}.

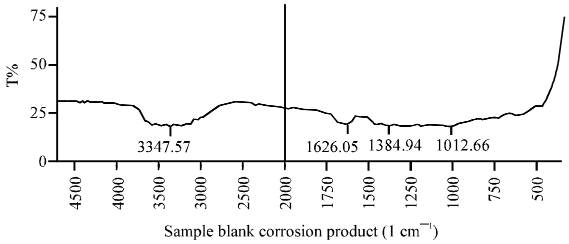

Fig. 5: FTIR spectrum of the corrosion product of mild steel in the absence of inhibitor

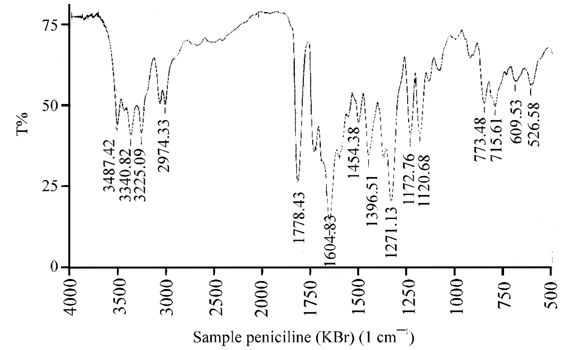

Fig. 6: FTIR spectrum of pure sample of penicillin G

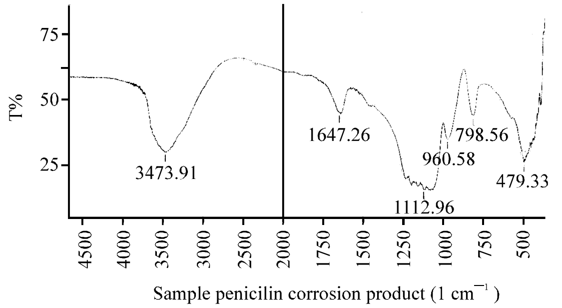

Fig. 7: FTIR spectrum of corrosion product of mild steel in the presence of 0.5 g L^{-1} of penicillin G

These shifts also suggest that there is interaction between penicillin G and the metal surface. Also, the absence of C-O stretch (at 1271.13 cm^{-1}), C = C stretch (at 1396.51 cm^{-1}), the aromatic C = C stretch (at 1454.38 cm^{-1}), the C = O stretch (at 1778.43 cm^{-1}), the C-H stretch (at 2974.33 cm^{-1}), the acid -OH stretch (at 3225.09 cm^{-1}) and the N-H stretch (3340.82 cm^{-1}) reveals that these bonds might have been used in the adsorption of the inhibitor's molecules on the surface of mild steel (Eddy, 2010).

Density Functional Theory (DFT): DFT is based on the principle that the energy of a molecule can be determined from the electron density instead of a wave function. The DFT based on the Hohnenberg-Kohn theorems has been found to be a strong tool for the modelling and development of conceptual issues on chemical reactivity (Wang *et al*., 2007). In corrosion study, DFT has also been found to be a powerful tool that can be used for the prediction of the sites for electrophilic and nucleophilic attacks (Fuentealba *et al*., 2000). The Fukui function provides an avenue for analysing the local selectivity of a corrosion inhibitor. The Fukui function can be defined as Eq. 11.

Table 5: Calculated Muliken charges and Fukui functions for penicillin G using B3-YLP exchange correlation

Sites	q_N	q_{N-1}	q_{N+1}	f^+	f^-
C (1)	-4.0000	1.4563	-1.0172	2.9828	-5.4563
C (2)	-4.0000	1.6168	-1.0283	2.9717	-5.6168
C (3)	-4.0000	2.3846	-1.0333	2.9667	-6.3846
C (4)	-4.0000	2.8810	-1.0699	2.9301	-6.8810
C (5)	-4.0000	2.8525	-0.9381	3.0619	-6.8525
C (6)	-4.0000	0.2244	-1.0219	2.9781	-4.2244
C (7)	-4.0000	1.2125	-2.2080	1.7921	-5.2125
C (8)	-3.0001	-3.0395	0.9035	3.9037	0.0394
N (9)	-2.0000	4.2045	-1.9750	0.0250	-6.2045
O (10)	-3.7229	-3.9998	4.0205	7.7434	0.2769
C (11)	3.7296	-3.9995	3.3083	-0.4214	7.7291
C (12)	4.9941	-3.0615	-1.5632	-6.5574	8.0556
N (13)	3.9958	-3.9997	3.6881	-0.3077	7.9955
C (14)	-0.0215	-1.9998	3.7125	3.7340	1.9784
S (15)	4.0275	-3.1605	-0.2505	-4.2780	7.1881
C (16)	3.9962	2.6294	-1.7442	-5.7404	1.3668
C (17)	4.0078	4.0015	-3.9774	-7.9851	0.0062
C (18)	6.0073	5.9992	-1.9992	-8.0065	0.0082
O (19)	6.0005	6.0003	-1.9987	-7.9993	0.0002
O (20)	0.0631	-2.0000	4.9908	4.9277	2.0631
O (21)	3.9930	-1.9881	-0.3699	-4.3629	5.9812
C (22)	3.9929	-2.9039	-0.3346	-4.3275	6.8968

Table 6: Calculated Muliken charges and Fukui functions for penicillin G using EDF1 exchange correlation

Sites	q_N	q_{N-1}	q_{N+1}	f^+	f^-
C (1)	-4.0000	3.9954	3.9967	7.9967	-7.9954
C (2)	-4.0000	3.9965	3.9965	7.9965	-7.9965
C (3)	-4.0000	3.9942	3.9967	7.9967	-7.9942
C (4)	-4.0000	6.0231	3.9968	7.9968	-10.0231
C (5)	-4.0000	6.0022	3.9977	7.9977	-10.0022
C (6)	-4.0000	4.9982	3.9967	7.9967	-8.9982
C (7)	-4.0000	3.9917	3.9942	7.9942	-7.9917
C (8)	-4.0000	3.9917	3.9993	7.9994	-7.9917
N (9)	-3.0002	3.2407	5.1615	8.1617	-6.2409
O (10)	-2.0000	6.0009	6.0010	8.0010	-8.0010
C (11)	-3.7341	-4.0807	-3.2224	0.5118	0.3466
C (12)	3.7361	-4.0012	-3.9983	-7.7344	7.7373
N (13)	-0.0300	-2.0004	-3.0000	-2.9700	1.9705
C (14)	4.0277	-4.0000	-4.0000	-8.0277	8.0277
S (15)	3.9960	-4.0000	-4.0000	-7.9960	7.9960
C (16)	4.0076	-4.0000	-4.0000	-8.0076	8.0076
C (17)	6.0279	-2.0000	-2.0000	-8.0279	8.0279
C (18)	6.0006	-2.0000	-2.0000	-8.0006	8.0006
O (19)	0.0708	-2.0000	-1.9999	-2.0707	2.0708
O (20)	3.9928	-4.0000	-4.0000	-7.9928	7.9928
O (21)	3.9927	-4.0000	-4.0000	-7.9927	7.9927

$$f(r) = [(\delta\Upsilon/\delta v(r))]_N \tag{11}$$

where, v (r) is the external potential and the functional derivative must be taken at constant number of electrons. Assuming $[\delta TE/\delta N]_v$ and $[\delta TE/\delta v(r)]_N$ are exact differentials then the Maxwell relations between the derivatives can be written as Eq. 12.

$$f(r) = [(\delta\rho(r)/\delta N)]_v \tag{12}$$

According to Fuentealba *et al*. (2000), Eq. 12 is the most standard presentation of the Fukui function. Owing to the discontinuity of the chemical potential at integer N, the derivative will be different if taken from the right or the left hand side. Therefore three different forms of Fukui functions (f^+, f^0 and f^-) are possible. These correspond to the situation when N increases from N to N+1 (f^+) and when N decreases from N to N-1 (f^-). f^+ is associated with the LUMO and measures the reactivity towards a donor reagent while f^- is associated with the HOMO and measures the reactivity toward an acceptor reagent. However, the average of both (f^0) measures reactivity towards a radical. However, in this research, the finite difference approximation was used to calculate the Fukui functions for electrophilic and nucleophilic Fukui function from Eq. 13 and 14:

$$f^+ = (\delta\rho(r)/\delta N)^+_\upsilon = q_{(N+1)} - q_{(N)} \tag{13}$$

$$f^- = (\delta\rho(r)/\delta N)^-_\upsilon = q_{(N)} - q_{(N-1)} \tag{14}$$

where, ρ, $q_{(N+1)}$, $q_{(N)}$ and $q_{(N-1)}$ are the density of electron and the Mulliken/Lowdin charge of the atom with N+1, N and N-1 electrons. Since, there is similarity sbetween the Fukui function and the frontier molecular orbitals, it is expected that the site for nucleophilic attack is the site where the value of f^+ is maximum while the site for electrophillic attack is controlled by the values of f^- (Table 5-8).

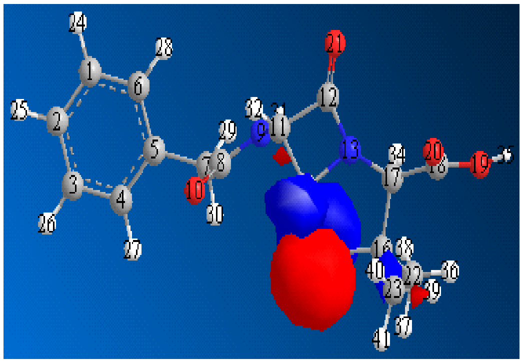

Fig. 8: Lumo diagram of penicillin G

Table 7: Calculated Muliken charges and Fukui functions for penicillin G using B3-PW91 exchange correlation

Sites	q_N	q_{N-1}	q_{N+1}	f^+	f^-
C (1)	-4.0000	2.2367	-1.0259	2.9741	-6.2367
C (2)	-4.0000	1.5773	-1.0366	2.9634	-5.5773
C (3)	-4.0000	2.6876	-1.0407	2.9593	-6.6876
C (4)	-4.0000	3.4568	-1.0762	2.9238	-7.4568
C (5)	-4.0000	3.9909	-0.9405	3.0595	-7.9909
C (6)	-4.0000	3.4559	-1.0305	2.9695	-7.4559
C (7)	-4.0000	3.0169	-0.1620	3.8380	-7.0169
C (8)	-4.0000	0.3425	-2.2098	1.7903	-4.3425
N (9)	-3.0001	-3.0347	0.8741	3.8742	0.0345
O (10)	-2.0000	3.8303	-1.9742	0.0258	-5.8303
C (11)	-3.7251	-3.9999	4.0206	7.7457	0.2748
C (12)	3.7278	-3.9996	3.2756	-0.4523	7.7274
N (13)	4.9943	-3.0482	-1.5418	-6.5360	8.0425
C (14)	3.9897	-3.9998	3.6748	-0.3149	7.9895
S (15)	-0.0207	-2.0001	3.6901	3.7107	1.9795
C (16)	4.0274	-3.8431	-0.2533	-4.2807	7.8705
C (17)	3.9962	1.7320	-1.7171	-5.7133	2.2641
C (18)	4.0078	4.0032	-3.9761	-7.9839	0.0046
O (19)	6.0032	5.9992	-1.9991	-8.0023	0.0040
O (20)	6.0005	6.0003	-1.9986	-7.9992	0.0003
O (21)	0.0671	-2.0000	4.9216	4.8545	2.0671
C (22)	3.9930	-3.5851	-0.3729	-4.3659	7.5781
C (23)	3.9929	-3.6297	-0.3303	-4.3232	7.6225

Table 8: Calculated Muliken charges and Fukui functions for penicillin G using Becke 97 exchange correlation

Sites	q_N	q_{N-1}	q_{N+1}	f^+	f^-
C(1)	-4.0000	3.9841	-1.0250	2.9750	-7.9841
C(2)	-4.0000	3.9923	-1.0388	2.9612	-7.9923
C(3)	-4.0000	3.9930	-1.0513	2.9487	-7.9930
C(4)	-4.0000	3.9835	-1.0923	2.9077	-7.9835
C(5)	-4.0000	6.0998	-0.9606	3.0394	-10.0998
C(6)	-4.0000	6.0068	-1.0302	2.9698	-10.0068
C(7)	-4.0000	3.9813	-0.1978	3.8023	-7.9813
C(8)	-4.0000	3.9882	-2.2203	1.7797	-7.9882
N(9)	-3.0001	5.3054	0.8456	3.8458	-8.3056
O(10)	-2.0000	6.0127	-1.9742	0.0258	-8.0127
C(11)	-3.7238	-4.5532	4.0220	7.7458	0.8294
C(12)	3.7279	-4.0001	3.2848	-0.4431	7.7280
N(13)	4.9942	-3.0003	-1.5228	-6.5170	7.9945
C(14)	3.9919	-3.9979	3.6832	-0.3088	7.9898
S(15)	-0.0202	-2.0043	3.7394	3.7596	1.9840
C(16)	4.0275	-4.0000	-0.2182	-4.2457	8.0275
C(17)	3.9917	-4.0000	-1.6834	-5.6751	7.9917
C(18)	4.0078	-4.0000	-3.9757	-7.9834	8.0078
O(19)	6.0056	-2.0000	-1.9991	-8.0048	8.0056
O(20)	6.0005	-2.0000	-3.9757	-9.9762	8.0005
O(21)	0.0660	-2.0000	4.9507	4.8847	2.0660
C(22)	3.9930	-4.0000	-0.3337	-4.3268	7.9930
C(23)	3.9929	-4.0000	-0.3117	-4.3046	7.9929

In the penicillin G molecule, several sites are eminent for nucleophilic and electrophilic attacks. These sites include O10, N9, C11 and C11 while the corresponding sites for electrophilic attack are C12, N13, C17 and C16. The site favoured depends on the energy associated with the adsorption and also on the orientation of the molecule. The information revealed by Fukui analysis is also manifested in the HOMO and LUMO molecular orbitals of the penicillin compounds (Fig. 8 and 9).

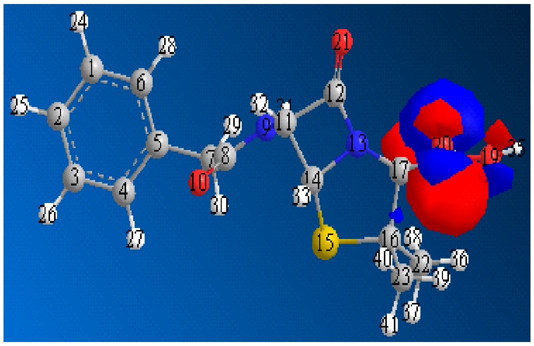

Fig. 9: Homo diagram of penicillin G

CONCLUSION

Penicillin G is a good adsorption inhibitor for the corrosion of mild steel in HCl solutions. The adsorption of the inhibitor on the mild steel surface is exothermic, spontaneous and is consistent with the Langmuir adsorption model. The mechanism of adsorption of the inhibitor on the mild steel is consistent with the mechanism of charge transfer from the inhibitor to the metal surface which indicates physiosorption. The sites for nucleophilic and electrophilic attacks on the Penicillin G molecule are on the (C11) and (C12) bonds, respectively.

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