Experimental and Quantum Chemical Studies on the Corrosion Inhibition Potentials of *Xylopia aethiopica* extracts

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Abstract: Root and root bark extracts of *Xylopia aethiopica* (XE) have been evaluated as corrosion inhibitors for mild steel in aerated 0.1 M HCl and H_2SO_4 solutions by gravimetric method. The inhibition efficiency increases with increase in inhibitor concentrations. Adsorption mechanisms for the adsorptions of XE extracts' molecules were predicted using the following adsorption isotherms (Langmuir, Freundlich, Temkin and El-Awady) by linear regression. With the aid of Chi-square (X^2) statistic, the best fitted adsorption isotherms were selected. Physisorption mechanisms have been proposed for the extracts in the studied acidic media. Quantum chemical calculations gave some electronic properties of the molecules of XE extracts so as to ascertain any correlation(s) between the corrosion inhibition and molecular structures.

Keywords: Quantum Chemical calculation, Xylopia aethiopica, corrosion inhibition

1.0 Introduction

Mild steel and its alloys have proved to be strategically important materials and have extensive uses in fertilizer, oil and metallurgical industries. Engineering systems depend upon corrosion protection for their reliability, performance and safety. However, the applications of steel in industrial acid cleaning, acid pickling, acid descaling and oil well acidizing, involve contacts between acidic media and steel which cause the metal to corrode [1].

The use of corrosion inhibitors had been shown to be the most effective and efficient practical way of preventing metal corrosion. The toxicity of most synthetic corrosion inhibitors have brought severe criticisms against their uses because they pose environmental hazards, therefore, the use of natural products of plant origin as corrosion inhibitors at present is encouraged because they are eco-friendly. Most of the efficient corrosion inhibitors contain nitrogen, oxygen, sulphur, double and triple bonds. The availabilities of lone pairs of electrons and π bonds existing in their molecules have been reported to inhibit metal corrosion in acidic media by adsorption on metal surfaces via these sites. These inhibition abilities of corrosion inhibitors have been shown to depend on [2, 3]: (i) the chemical structure of the compound, (ii) the surface charge of the metal, and (iii) the type of interactions between the inhibitor molecules and the metal surface.

In corrosion inhibition studies, many methods of investigation have been employed and they include: gasometric [4], electrochemical impedance spectroscopy [5, 6, 7], weight loss [8, 9, 10, 11, 12], polarization [13, 14], UV/visible spectrophotometric [15], and so on. These aforementioned techniques involve the measurements of change in hydrogen gas evolved, change in spectrum/graph generated due to change in electrical current of electrolytes, change in weight loss of metal, change in corrosion reaction temperature, change in electrical resistance of an electrolyte (majorly) due to accumulation of gaseous molecules on the electrode, change in the shape of spectrum and wavelength of absorption maxima respectively. The use of any of the mentioned techniques depends on the economic buoyancy of the researcher. In any case, results obtained from any of these techniques are valid and reliable. However, the weight loss method of monitoring corrosion rate is useful because of its simple application and reliability.

Quantum chemical calculation is usually used to study the correlations between the corrosion inhibition and molecular properties of inhibitors. Recently, Density Functional Theory (DFT) has become an attractive theoretical method because basic parameters for even huge complex molecules at low cost. Also, the application of DFT now extends to explanation of some empirical molecular properties such as corrosion inhibition with quantum mechanics. Therefore, DFT is a very powerful technique to probe the inhibitor/surface interaction and to analyze experimental data [2].

The need for a cheap, renewable, easily available and eco-friendly source of material as corrosion inhibitor has therefore attracted us to investigate the mild steel corrosion inhibition properties of *Xylopia aethiopica* in acidic media.

2.0 Experimental

2.1 Materials preparation

The sheet of mild steel used has the following composition (%): C 0.05; Mn 0.6; P 0.36; Si 0.3; balance Fe. The mild steel sheet was mechanically press-cut into coupons of dimension 5 × 2 × 0.04 cm. These coupons were used as supplied without further polishing. However, surface treatments of the coupons involve degreasing in absolute ethanol and drying in acetone. The treated coupons were then stored in a moisture-free desiccator before their use in corrosion studies.

Samples of *X. aethiopica* were obtained from Abia State in the South eastern part of Nigeria. Samples of the *X. aethiopica* root and root bark were dried, ground to powder and soaked in a solution of ethanol for 48 h. After 48 h, the samples were cooled and filtered. The filtrates were further subjected to evaporation at 352 K in order to leave the sample free of the ethanol. The stock solutions of the extract so obtained were used in preparing different concentrations of the extract by dissolving 0.1, 0.2, 0.3, 0.4 and 0.5 g of the extract in 1 L of 0.1 M HCl and H_2SO_4 respectively.

2.2 Weight loss determination

Gravimetric experiments were carried out as earlier reported [10-12]. The maximum duration of tests was 24 h at 30 °C in aerated solutions. At the end of the tests, the coupons were scrubbed with bristle brush under running water in order to remove the corrosion product, dried and re-weighed. The tests were performed in triplicate to guarantee the reliability of the results and the mean value of the weight loss is reported. The reproducibility of the experiment was very high (>98%). The differences in weight of the coupons were taken as the weight loss, which was used to compute the corrosion rate given by [10-12]:

Corrosion rate $$(C_{corr}) = \frac{\Delta m}{At} \qquad 1$$

where Δm is the mass loss, A is the total area of the specimen and t is the corrosion time.

The inhibition efficiencies (%I) of inhibitors, were calculated using [10-12]:

$$\%I = \frac{C_1 - C_2}{C_1} \times 100 \qquad 2$$

where C_1 and C_0 are the corrosion rates for mid steel in the presence and absence of inhibitor respectively in HCl/H_2SO_4 solution at the same temperature. The degree of surface coverage (θ), is given by the equation [10-12]:

$$\theta = {\%I}/{100} \qquad 3$$

2.3 Computational Details

2.3.1 Statistical analyses

2.3.1.1 Chi-Square Statistics

Experimental and calculated values of θ were compared using chi-square statistic according to equation 4 [16]:

$$\chi^2 = \Sigma \frac{(\theta_{\exp} - \theta_{cal})^2}{\theta_{cal}} \qquad 4$$

where $\theta_{\exp}$ and θ_{cal} are experimental and theoretical/calculated surface coverage values respectively, and χ^2 is chi-square statistic.

2.3.1.2 Factorial Analyses

The effects of three factors, namely: (i) type of acid, (ii) extract type, and (iii) inhibitor concentration on inhibition efficiency were investigated and the data were statistically analysed using Statistical Package for the Social Sciences (SPSS) version 16.

2.3.2 Quantum chemical calculations

Computational modeling of the electronic and adsorption structures of selected XA extract constituents were achieved using the Forcite, and VAMP modules in the Material Studio 4.0 software (Accelrys, Inc.) as previously described [12,13,25].

3.0 Results and Discussion

3.1 Gravimetric studies

The values of inhibition efficiency as a function of concentration are shown in Figure 1. The results show that as the inhibitor concentration increases, the inhibition efficiency increases. The maximum inhibition efficiency values obtained at 0.5 g/L inhibitor concentration were: 66.6 (root extract) and 91.6 % (root bark extract) in H_2SO_4; and 86.9 (root extract) and 98.9 % (root bar extract) in HCl respectively.

Table 1 presents the effects of three factors, namely: (i) type of acid, (ii) extract type, and (iii) inhibitor concentration on inhibition efficiency. Values of F-statistic that are less than 0.05 imply significant contribution/ effect. Results presented in table 1 show that the following has significant effect on inhibition efficiency: acid type (AT), extract type (ET), inhibitor concentration (IC), inhibitor concentration/acid type interaction (IC*AT), and acid type/extract type interaction (AT*ET). Only less than 0.9 % variability cannot be accounted for as Table 1 reveals.

To understand the direction of these effects, regression analysis was performed. Equation 5 presents regression results on/for corrosion inhibition efficiency:

$$IE = -66.590 + 103.890IC + 20.190ET + 45.622AT \qquad 5$$

where IE is inhibition efficiency, IC is inhibitor concentration, ET stands for extract type and AT stands for acid type. Equation 5 shows that: increasing the inhibitor concentration by 0.1g/L would cause a 103.890 % increase in inhibition efficiency; using the root bark extract over the root extract, increased inhibition efficiency by 20.190 %; using the hydrochloric acid solution as corrodent over the sulphuric acid solution, increased inhibition efficiency by 45.666 %. These results suggest that *xylopia aethiopica* is a good corrosion inhibitor for mild steel corrosion in H_2SO_4 and HCl such that its performance: is better in the presence of low hydrogen ion concentration (HCl), improves by using the root bark extract, and increases with increase in concentration.

3.2 Adsorption isotherm studies

It is generally believed that inhibitors act through adsorption on metal surface and providing coverage. This shields the metal surface from the attacks of the corrodent thereby reducing the rate by which the metal corrodes in the corrosive media.

Figure 2 presents selected compounds extracted from XE root bark which possess structural features that are rich in electron densities: unsaturated π bonds (A and B) and electron lone pairs on oxygen atom (C) which could possibly serve as active sites for the adsorption processes.

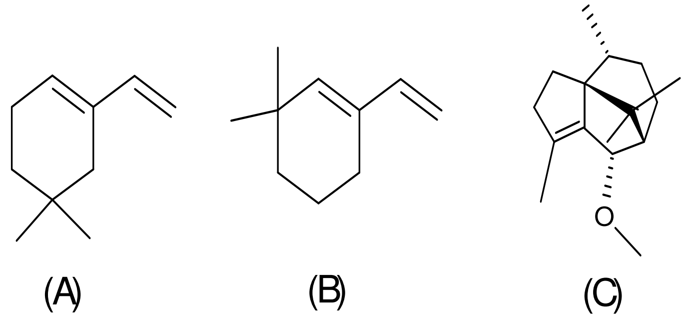

Figure 1: Isolated compounds from X. aethiopica root bark extract [Yapi et al, 2012]: (A) 4,4-dimethyl-2-vinylcyclohexene (xylopia A), (B) 3,3-dimethyl-1-vinylcyclohexene (xylopia B), and (C) endo-5-methoxy-3-patchoulene (xylopia C).

In order to confirm the adsorption of XE on mild steel surface, adsorption isotherms were studied. Adsorption isotherms help to describe the adsorption mechanism of an inhibitor, that is, they provide vital clues to the nature of the metal-inhibitor interaction(s). Therefore, the degree of surface coverage values (*θ*), at different inhibitor concentrations in 0.1 M HCl and H_2SO_4 were evaluated from weight loss measurements (equation 3) at 30 °C and fitted into suitable adsorption isotherms. The commonly used linearised adsorption isotherms are [10-12]: Langmuir model (equation 11); Fruendlich model (equation 12); Temkin model (equation 13); and El-Awady model (equation 14). Respectively they are represented thus:

$$C/\theta = 1/K_L + C \qquad 6$$

$$Ln\theta = LnK_F + \frac{1}{n}LnC \qquad 7$$

$$\theta = \frac{1}{f}\left(LnK_T + LnC\right) \qquad 8$$

$$Ln\left(\frac{\theta}{1-\theta}\right) = LnK_{EL} + YLnC \qquad 9$$

where K_L, K_f, K_T and K_{EL} are adsorption capacity values obtained from Langmuir, Fruendlich, Temkin and El-

Awady isotherm models respectively. Also, $\frac{1}{n}$ is Fruendlich constant, 'f' is the Frumkin lateral interaction factor related to Temkin heterogeneity 'a' (f = -2a) and Y is the El-Awady constant which is characteristic of the number of active sites on the aluminium surface.

Here, the simple linear regression was used to fit surface coverage (θ_{cal}) values into adsorption isotherms represented by equations 6-9. The linear equation 10 was taken to represent regression models:

$$Y = a + bX \qquad 10$$

where Y represents theoretical/calculated surface coverage values, X stands for the experimental surface coverage values, 'a' is the regression constant and 'b' is the regression coefficient.

Two 'normal' equations were generated and solved simultaneously to determine the regression constant and regression coefficient values. These 'normal' equations generated are represented thus

$$aN + b\sum X = \sum Y \qquad 11$$

$$a\sum X + b\sum X^2 = \sum XY \qquad 12$$

where N represents the number of $\theta_{\exp}$ values and Σ represents summation.

Furthermore, to account for how much of the $\theta_{\exp}$ values fitted into the adsorption isotherms, the coefficient of determination (R^2) was calculated using equation 13 [12].

$$R^2 = 1 - \frac{\sum\left(Y - \hat{Y}\right)^2}{\sum\left(Y - \bar{Y}\right)^2} \qquad 13$$

where $\bar{Y}$ is the mean value of the experimental surface coverage values. Values of the regression constant, the regression coefficient and coefficient of determination are presented in table 2.

Using adsorption capacity values obtained from the regression equations, free energy of adsorption was calculated by substituting into the following relationship

$$K_{ads} = \frac{1}{55.5}\ell^{-\frac{\Delta G_{ads}}{RT}} \qquad 14$$

where K_{ads} is any of the adsorption capacity values from equations 6-9. Calculated adsorption capacity values and values of free energy of adsorption are presented in Table 2.

Table 2 presents results which suggest that: in H_2SO_4, the Freundlich adsorption isotherm gave the best fit for the adsorption of root and root bark extracts; and in HCl, the El-Awady and Freundlich adsorption isotherms gave the best fits for the adsorption of root and root bark extracts respectively.

For the adsorption of XE root extract on mild steel in H_2SO_4, the coefficient of determination value of 0.9893 was highest with a corresponding χ^2 value of 0.0113. An adsorption capacity (K_F) value of 3.3706 was obtained which on substitution into equation 14 gave a free energy value of -13.179 kJmol^{-1}. This value is less than -40 kmol^{-1}, therefore, suggests physisorption mechanism.

The adsorption of XE root bark extract on mild steel in H_2SO_4 gave the coefficient of determination value of 0.9224 and a corresponding χ^2 value of 0.0367. An adsorption capacity (K_F) value of 1.3738 was obtained which on substitution into equation 14 gave a free energy value of -10.918 kJmol^{-1}. This value is less than -40 kmol^{-1}, therefore, suggests physisorption mechanism.

For the adsorption of XE root extract on mild steel in HCl, the coefficient of determination value of 0.9615 was highest with a corresponding χ^2 value of 0.0018. An adsorption capacity (K_{El}) value of 10.9726 was obtained which on substitution into equation 14 gave a free energy value of -16.512 kJmol^{-1}. This value is less than -40 kmol^{-1}, therefore, suggests physisorption mechanism.

The adsorption of XE root bark extract on mild steel in HCl gave the coefficient of determination value of 0.9895 and a corresponding χ^2 value of 0.0001. An adsorption capacity (K_F) value of 1.0525 was obtained which on substitution into equation 14 gave a free energy value of -10.247 kJmol^{-1}. This value is less than -40 kmol^{-1}, therefore, suggests physisorption mechanism.

3.3 Quantum chemical calculations

Frontier orbital theory holds that reactivity of molecules often occurs on the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). Higher E_{HOMO} values indicate a tendency of XE molecules to donate electrons to appropriate acceptor molecules with low energy or empty orbitals of Fe to form coordinate bond. Lower E_{LUMO} values suggest stronger electron accepting abilities of XE molecules and ensure electron back-donation bonding with its anti-bonding orbitals. Comparing values obtained elsewhere for other inhibitors [17], Table 3 presents high E_{HOMO} and low E_{LUMO} values for Xylopia A, B and C, suggesting that the adsorption of XE onto Fe explains their effectiveness as corrosion inhibitors in HCl and H_2SO_4 solutions.

Values of ΔN can be used to show that inhibition effect resulted from electrons donation. As posited by Lukovits [53], if $\Delta N < 3.6$, then inhibition efficiency most likely increased with increasing electron donating ability at the metal surface. This study therefore, as ΔN *values presented in table 3 shows, suggests that XE extracts were* donating electrons and the mild steel surface was the acceptor. This result supports the fact that the adsorption of inhibitor on the metal surface most likely occurred on the bases of donor- acceptor interactions between the π electrons of XE extract components and the vacant d-orbitals of the metal surface [54].

4. Conclusions

Extracts of XE (root and root bark) are effective corrosion inhibitors for mild steel in 0.1 M HCl and H_2SO_4. Weight loss technique gave inhibition efficiency values for XE root and root bark extracts at 0.5 g/L to be greater than 65 % in 0.1 M HCl and H_2SO_4 solutions at 30 ^oC. Inhibition efficiency values for root bark extract were higher. Adsorption of root and root bark extracts (in 0.1 M H_2SO_4 solution) on metal followed Freundlich adsorption isotherm while El-Awady and Frendlich adsorption isotherms were respectively obeyed by root and root bark XE extracts in 0.1 M HCl. Physisorption mechanisms have been proposed by the extracts in studied acidic media. Quantum chemical studies indicate that the O atom (xylopia C) and unsaturated C=C sites were the main adsorption centres for the corrosion inhibition action of XE.

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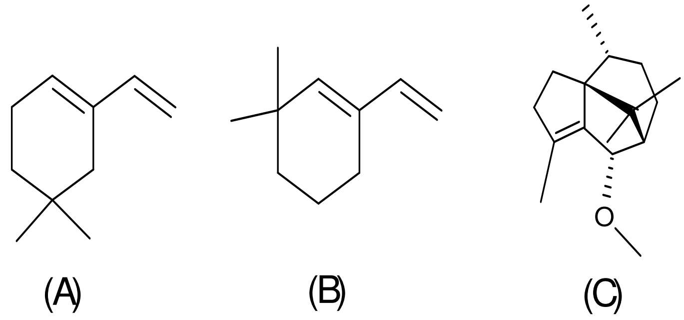
Figure 1: Isolated compounds from X. aethiopica root bark extract .



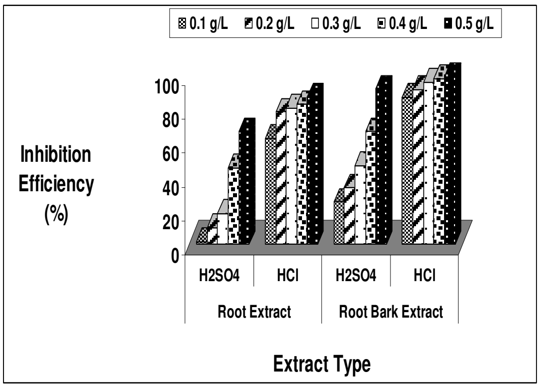


Figure 2: Inhibition efficiency of the extract (Root and Root bark) in different acidic media

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Table 1: ANOVA results on *Xylopia aethiopica* inhibition efficiency

Source	Sum of Squares	Degree of Freedom	Mean square	F-ratio	Sig
Corrected Model	18727.712[a]	15	1248.514	139.479	0.000
Intercept	80125.140	1	80125.140	8951.259	0.000
IC	4379.036	4	1094.759	122.302	0.000
ET	2038.180	1	2038.180	227.697	0.000
AT	10406.834	1	10406.834	1162.610	0.000
IC*ET	27.084	4	6.771	0.756	0.603
AT*ET	86.611	1	86.611	9.676	0.036
IC*AT	1789.966	4	447.491	49.992	0.001
Error	35.805	4	8.951		
Total	98888.657	20			
Corrected Total	18763.517	19			

a. R Squared = 0.998 (Adjusted R Squared = 0.991)
IC stands for inhibitor concentration; ET stands for extract type; and AT stands for acid type.

Table 2: Adsorption isotherm results

	Root Extract	Root Bark Extract
H_2SO_4		
Langmuir	$Y = 5.8170 - 11.0856X$ R^2 = -0.7871 K_L = 0.1719 $\chi^2 = 7.1691$	$Y = 0.4707 + 02901X$ R^2 = 02495 K_L = 2.1245 $\chi^2 = 0.4584$
Frendlich	$Y = 1.2151 + 2.2886X$ R^2 = 0.9893 K_F = 3.3706 $\chi^2 = 0.0113$	$Y = 0.3176 + 0.7922X$ R^2 = 0.9224 K_F = 1.3738 $\chi^2 = 0.0367$
Temkin	$Y = 0.7917 + 0.3781X$ R^2 = 0.7987 K_T = 8.1165 $\chi^2 = 0.2503$	$Y = 1.0442 + 0.3848X$ R^2 = 0.8271 K_T = 15.0835 $\chi^2 = 0.1216$
El-Awady	$Y = 2.4149 + 2.8805X$ R^2 = 0.9664 K_{El} = 11.1887 $\chi^2 = 7.1691$	$Y = 0.1951 - 0.0272X$ R^2 = -0.0468 K_{El} = 0.1719 $\chi^2 = 0.5416$
HCl		
Langmir	$Y = 0.0521 + 1.0588X$ R^2 = 0.7624 K_L = 19.1871 $\chi^2 = 0.01$	$Y = 0.3124 + 0.9706X$ R^2 = -119.9091 K_L = 3.201 $\chi^2 = 3.2995$
Freundlich	$Y = 0.0075 + 0.1941X$ R^2 = 0.1941 K_F = 1.0075 $\chi^2 = 0.0034$	$Y = 0.0512 + 0.0839X$ R^2 = 0.9895 K_F = 1.0525 $\chi^2 = 0.0001$
Temkin	$Y = 0.9729 + 0.1427X$ R^2 = 0.9349 K_T = 91.8807 $\chi^2 = 0.0031$	$Y = 1.0459 + 0.0778X$ R^2 = 0.9891 K_T = 6.893×10^5 $\chi^2 = 0.0001$
El-Awady	$Y = 2.3954 + 0.7929X$ R^2 = 0.9615 K_{El} = 10.9726 $\chi^2 = 0.0018$	$Y = 5.2628 + 1.5873X$ R^2 = 0.7980 K_{El} = 193.0212 $\chi^2 = 0.0023$

Table 3: Quantum chemical parameters for selected compounds of XE root bark extracts

Parameter	Value for selected compound (eV)		
	Xylopia A	Xylopia B	Xylopia C
$E_{HOMO} = -I$	-5.221	-5.239	-5.152
$E_{LUMO} = -A$	-1.379	-1.382	-0.470
$\chi_{inh} = \frac{I+A}{2}$	3.300	3.311	2.811
$\eta_{inh} = \frac{I-A}{2}$	1.921	1929	2341
$\delta = \frac{1}{\eta_{inh}}$	0.521	0.518	0.427
$\Delta N = \frac{\chi_{\mathrm{Fe}} - \chi_{inh}}{2(\eta_{\mathrm{Fe}} + \eta_{inh})}$	2.681	2.673	2.095
$\Delta E = E_{HOMO} - E_{LUMO}$	3.842	3.857	4.769

I stands for ionization potential, A means electron a**ffinity,** $\chi_{\mathrm{Fe}} = 7.0eV$ and χ_{inh} stand for absolute electronegativities of Fe and inhibitor molecule respectively, $\eta_{\mathrm{Fe}} = 0.0eV$ and η_{inh} stand for absolute hardness of Fe and inhibitor molecule respectively, δ stands for and ΔN stands for fraction of electron transferred.