Corrosion Inhibition and Adsorption Behavior of Extract of *Funtumia elastica* on Mild Steel in Acidic Solution

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Abstract. The corrosion and adsorption behavior of leaf extract of *Funtumia elastica* (FE) on mild steel corrosion was studied in 1 M HCl using gravimetric, electrochemical impedance spectroscopy, potentiodynamic polarization and Fourier transformed infrared spectroscopy methods. Quantum chemical calculations were performed to theoretically correlate the inhibition performance of the inhibitor with its electronic structural parameters. The gravimetric experiment revealed that the extract effectively inhibited the corrosion of mild steel even at a prolonged exposure time. The impedance and polarization results revealed that the extract inhibited both the cathodic and anodic partial reactions via the adsorption of the inhibitor on the metal/solution interface. The FTIR results revealed FE as an adsorption inhibitor. The calculated quantum chemical parameters associated with the molecular structure of FE confirmed its inhibiting efficacy.

INTRODUCTION

Mild steel has found applications in many industries, but excessive corrosion attack is known to affect this industrial raw material. The corrosion attack can be reduced to a very reasonable state by the use of corrosion inhibitors [1]. The high cost of most commercial corrosion inhibitors coupled with the recent environmental awareness has necessitated the motivation into the use of natural materials as corrosion inhibitors [2-10]. These materials have proven to be less toxic, cheap, environmental friendly and readily available and yet as effective as most commercial inhibitors such as chromate compounds [11-15]. It has been reported severally that most materials of plant origin which are used as corrosion inhibitors are rich in heteroatoms containing oxygen, nitrogen and/or sulphur in a conjugated system [16-20]. These materials function by adsorption of the material on the surface of the metal creating a barrier between the metal and the aggressive corrodent [21].

Again it has been reported that these natural materials contain a number of phytochemicals (tannins, alkaloids carbohydrates steroids e.t.c) which have electronic and molecular structures closely related to conventional corrosion inhibitors and which have been found to inhibit metal corrosion [22]. Oguzie et al [23] reported that acid extract of *Piper guineense* effectively reduced the corrosion of mild steel in both hydrochloric and tetraoxosulphate (VI) acid media. Also Patel and co-workers [24] have investigated the corrosion inhibition of mild steel by leave extracts of *Wrightia tinctoria*, *Clerodendrum phlomis* and *Ipomoea triloba* and the study revealed that the plants inhibited the corrosion of mild steel in 0.5 M H₂SO₄.

With regard to our continuous interest in the use of raw materials of plant origin as corrosion inhibitors, we here in report the corrosion inhibition of mild steel in 1 M HCl by ethanol extract of the leaves of *Funtumia elastica* using both gravimetric and electrochemical methods. FTIR was used to ascertain the adsorption behavior and density functional theory (DFT) was used to determine the individual contribution of the extract constituents to the total adsorption process.

DETAILS OF EXPERIMENTAL PROCEDURE

Material preparations: Tests were performed on mild steel with the following weight percentage composition: C- 0.05; Mn – 0.6; P - 0.36; Si – 0.3 and the balance Fe. The aggressive solution used was 1 M HCl prepared from analytical grade reagents. Stock solutions were prepared from the plant extract by refluxing weighed amount of the dried and ground plant material for 3 h in absolute ethanol. The resulting solution was cooled and triple filtered. The amount of plant material that was extracted into the absolute ethanol was quantified by comparing the weight of the dried residue with the weight of the dried material before extraction. Test solutions of concentration (50, 200, 400, 600, 800, 1000 and 1500 mg/L) were prepared from the stock solution by dilution.

Gravimetric experiments: The mild steel coupons used for the gravimetric experiment have the following dimension 3cm x 3 cm x 0.14 cm. The coupons were obtained from a commercial source and cut into the desired dimension. The coupons were wet polished with silicon carbide abrasive paper of grade 400# to #1000, rinsed in distilled water, dried in acetone and warm air, weighed and stored in moisture free desiccators for use when desired. Tests were performed on the prepared coupons by total immersion into the test solutions. The coupons were suspended in beakers containing 300ml of the solutions using hooks and rods. To determine the weight loss, the coupons were retrieved after 24 h intervals progressively for 120 h, and left for another 216 h un-retrieved making a total of 336 h. When retrieved the coupons were immersed in 20% NaOH solution containing 200 g/L of zinc dust, scrubbed with bristle brush, washed dried, reweighed and re-immersed into the test solutions. The weight loss was determined as a difference between the weight of the coupon at a given time and the initial weight of the coupon. All tests were performed in quadruplicate and the data gave good reproducibility. Average values were obtained and used for subsequent calculations.

Electrochemical experiments: The electrochemical experiments were performed on mild steel coupons with the following dimension 1 x 1 cm². And was fixed in polytetrafluoroethylene (PTFE) rods by epoxy resin in such a way that only one surface of area 1 cm² was exposed. The uncovered area was cleaned as described earlier in the gravimetric section. Electrochemical tests were conducted in a conventional three electrode glass cell of capacity 400 ml using a VERSASTAT 400 complete DC Voltammetry and corrosion system with a V3 software. The counter electrode was a graphite rod while the reference electrode was a saturated calomel electrode. The reference electrode was connected via luggin's capillary. The test solution was left for 1 h in an aerated and unstirred condition at 30°C. Impedance experiments were made at corrosion potentials (E_{corr}) over a frequency range of 100 kHz – 10 MHz using a signal amplitude perturbation of 5 mV. Potentiodynamic polarization experiments were performed in the potential range of ± 250 mV versus corrosion potential at 0.333 mV/s scan rate. Each experiment was performed in triplicate to ensure that the obtained results are reproducible.

Transformed Infrared Spectroscopy experiments: Fourier transformed infrared spectroscopy (KBr pellet) was recorded using a Nicolet Magma-IR 560 FTIR spectrophotometer. The spectra for FE powder before and after extraction were recorded. Also recorded was the spectra of the protective fumes scraped from the surface of the mild steel coupon after immersion in a solution containing 1500 mg/L FE extract by carefully removing the fumes, mixing it with KBr, and making the pellet.

Computational consideration: All computational calculations were done using the DFT electronic structure analysis programs VAMP and DMol³ as explained in the Material studio modeling 4.0 software (accelrys. Inc.).

RESULTS AND DISCUSSION

Gravimetric results: Gravimetric experiments were undertaken to study the effect of time on the inhibitive effect of the ethanol extract of FE on mild steel corrosion. The results presented are means of quadruplicate determinations. Figure 1 shows the variation of weight loss with time in the uninhibited and inhibited 1 M HCl. The result shows that FE extract effectively inhibited mild steel corrosion at all the concentrations studied. Figure 2 (a) shows the variation of inhibition efficiency with time for mild steel corrosion in the presence of different concentrations of FE and Figure 2 (b) shows the variation of inhibition efficiency with FE concentrations after 24 h of immersion. The result in Figure 2 (a) shows that efficiency

Table 1. Inhibition efficiency of FE extract on mild steel corrosion in 1 M HCl

System (mg/L) FE	24 h IE _W %	48 h IE _W %	72 h IE _W %	96 h IE _W %	120 h IE _W %	336 h IE _W %
50	74.3	73.5	72.2	71.2	65.5	55.2
200	78.3	76.1	75.8	73.3	72.5	60.5
400	83.5	79.9	78.6	76.7	76.4	71.9
600	85.2	83.5	81.7	79.9	78.5	72.5
800	86.2	84.3	82.5	81.5	79.2	74.2
1000	87.7	85.2	83.5	82.3	80.1	75.8
1500	90.1	88.3	86.5	85.2	80.5	79.5

Reduced with increase in exposure time and that FE extract maintained good inhibition efficiency even at 336 h. The least inhibition efficiency observed was 55.2% at a concentration of 50 mg/L at 336 h. The result in 2 (b) shows that inhibition efficiency increased with FE concentration. Table 1 presents the calculated inhibition efficiencies as a function of both FE concentration and immersion time. The result shows that inhibition efficiency increased with increase in FE concentration and reduced with increase in exposure time. It can also be observed from the result that FE extract is an efficient corrosion inhibitor for mild steel in 1 M HCl even after 336 h of immersion. Inhibition efficiency from the gravimetric experiment was estimated as follows;

$$IE_W\% = \left(1 - \frac{\Delta W_{inh}}{\Delta W_{blank}}\right) \times 100. \quad (1)$$

Where ΔW_{blank} and ΔW_{inh} are the weight loss of mild steel in the absence and presence of inhibitor, respectively. Figure 3 shows the variation of weight loss with concentration, the result shows that the FE extracts diminished the corrosion rate of mild steel in 1 M HCl.

Figure 1. Variation of weight loss with time for mild steel corrosion in 1 M HCl solution in the absence and presence of ethanol extract of FE.

Figure 2. Variation of inhibition efficiency with (a) time for mild steel corrosion in 1 M HCl solution in the presence of ethanol extract of FE (b) FE concentration for mild steel corrosion in 1 M HCl after 24 h.

Figure 3. Variation of weight loss with concentration for mild steel corrosion in 1 M HCl solution in the absence and presence of ethanol extract of FE.

Electrochemical Results:

Electrochemical impedance results: Electrochemical experiments were undertaken to study the inhibitive effects of FE extract on mild steel corrosion from an electrochemical point of view. The chosen concentrations for the electrochemical experiments are (50mg/L, 600mg/L and 1500 mg/L, these concentrations were chosen to cover the concentration range used for the gravimetric experiment. Nyquist plot for mild steel corrosion in 1 M HCl in the absence and presence of 50mg/L, 600mg/L and 1500 mg/L FE extracts are shown in figure 4. The Nyquist plot show single semicircles for all systems over the frequency range studied. The high frequency intercept with the real axis in the Nyquist plots assigned to the solution resistance (R_s) and the low frequency intercept with the real axis ascribed to the charge transfer resistance (R_{ct}). Figure 4 shows gradual increase in the size of the semicircle with increase in FE concentration. the impedance spectra were analyzed by fitting to the equivalent circuit models $R_s (Q_{dl}R_{ct})$ which has been used previously to model impedance spectra [25,26]. Table 2 embodies various impedance parameters such as charge transfer resistance (R_{ct}), double layer capacitance (Q_{dl}) and inhibition efficiency $IE_I\%$. A gradual decrease in the values of (Q_{dl}) with increase in the concentration of FE extracts was observed. This considerable decrease in the size of (Q_{dl}) has confirmed that FE molecules were adsorbed on the mild steel surface and has decreased the roughness of the metal surface created due to corrosion by 1 HCl solution. The values of the inhibition efficiency were calculated from the impedance data as follows:

$$IE_I\% = \left(\frac{R_{ct,inh} - R_{ct,bl}}{R_{ct,inh}} \right) \times 100. \quad (2)$$

Where $R_{ct,bl}$ and $R_{ct,inh}$ are the charge transfer resistance values in the absence and presence of the inhibitor respectively.

Figure 4. Nyquist plot for mild steel corrosion in 1 M HCl without and with FE extracts.

To calculate the values of Qdl, the frequency (f_{max}) at which the imaginary component of the impedance is maximum $-Z_{im(max)}$ was found and Qdl was obtained from the equation below:

$$Qdl = \frac{1}{2\pi f_{max} R_{ct}} \quad (3)$$

Table 2. Impedance Results for mild steel Corrosion in 1 M HCl without and with FE extracts.

System (mg/L)	$R_{ct} (\Omega cm^2)$	$Q_{dl} (\mu\Omega^{-1} S^n cm^{-2}) \times 10^{-4}$	n	IE _I %
HCl blank	46.1	1.38	0.9116	
FE 50 mg/L	155.4	0.53	0.9292	70.4
FE 600 mg/L	169.5	0.47	0.9012	72.8
FE 1500 mg/L	261.4	0.31	0.8078	82.4

Potentiodynamic polarization results: Potentiodynamic polarization experiments were undertaken to identify the effect of FE extract on the anodic dissolution of mild steel and the cathodic reduction of hydrogen ion. Typical potentiodynamic polarization curves for mild steel corrosion in 1 M HCl in the absence and presence of 50, 600 and 1500 mg/L of FE extracts are given in figure 5 while the electrochemical parameters derived from the polarization curves is given in table 3. From the results it can be seen that the addition of the FE extracts affected the anodic as well as the cathodic half reactions, shifting the corrosion potential (E_{corr}) slightly towards more negative (cathodic) values and reducing the anodic and cathodic current densities and also the reaction corrosion current density (i_{corr}). From the results obtained it can be said the FE extracts functioned as mixed type corrosion inhibitor for mild steel in 1 M HCl. The value of the inhibition efficiency was calculated from the polarization parameters using the equation below:

$$IEp\% = \left(\frac{I_{corr(bl)} - I_{corr(inh)}}{I_{corr(bl)}} \right) \times 100 \quad (4)$$

Where $I_{corr(bl)}$ and $I_{corr(inh)}$ represents the corrosion current density in the absence and presence of the inhibitor, respectively

Figure 5. Potentiodynamic polarization curves of mild steel corrosion in 1 M HCl solution without and with FE extracts.

Table 3. Potentiodynamic polarization parameters for mild steel corrosion in 1 M HCl with and without FE extracts

System (mg/L)	E (mV vs SCE)	i_{corr} ($\mu\text{A}/\text{cm}^2$)	IE _P %
1 M HCl (blank)	-488.3	49.28	
50 mg/L	-484.7	3.23	93.5
600 mg/L	-481.8	2.85	94.2
1500 mg/L	-480.2	1.06	97.9

From table 3, It is observed that the i_{corr} values gradually decreased with gradual increase in the concentration of FE up to 1500 mg/L from $3.23(\mu\text{A}/\text{cm}^2)$ in 50 mg/L to $1.06(\mu\text{A}/\text{cm}^2)$ in 1500 mg/L leading to increase in inhibition efficiency from 93.5% to 97.9% .The obtained values from table 3 can be seen to follow the same trend as the gravimetric and impedance data therefore highlighting the corrosion inhibiting efficacy of FE extracts.

Adsorption consideration: The inhibitive action of organic components present in the FE extracts is attributed to the adsorption of the FE extracts on the mild steel surface as already observed in the electrochemical impedance spectroscopy experiment. The adsorbed layer acts as a barrier preventing both mass and charge transfer leading to a reduction in the rate of mild steel corrosion. Further characterization of adsorption involved fitting the experimental data in frequently used adsorption isotherms. The fraction of the surface covered by adsorbed molecule (surface coverage) represented by θ is an indication of the effectiveness of the adsorbed specie and is directly proportional to the inhibition efficiency (IE). θ can be calculated from the inhibition efficiency from the equation below: [27]

$$\theta = \text{IE}/100. \quad (5)$$

Different adsorption isotherms were tried but it was observed that the best fit isotherm for this experiment is the Langmuir adsorption isotherm as determined from the gravimetric measurement after 24 h of immersion.

According to the Langmuir adsorption isotherm,

$$C/\theta = 1/b + C \quad (6)$$

Where C is the inhibitor concentration, b is the equilibrium constant and θ is the degree of surface coverage

The plot of C/θ versus C is shown in figure 6 to be linear for FE extract in 1 M HCl solution: with slope 1.097 and R^2 value of 0.99894 suggesting that the experimental data follows the Langmuir adsorption isotherm.

Figure 6. Langmuir adsorption isotherm for FE extracts on mild steel in 1 M HCl.

Fourier Transformed Infrared Spectroscopy Analysis:

The FTIR spectra of FE powder before and after extraction as well as that of the scrapings from the inhibitor films formed on the surface of mild steel after 3h immersion in 1 M HCl solution containing 1500 mg/L of FE extract is presented in figure 7.

Figure 7. FTIR spectra of FE powder before and after extraction in ethanol and the surface film on mild steel specimens immersed in 1 M HCl solution containing FE powder.

Examination of the plot in Figure 6a reveals the presence of some peaks; which is attributed to the existence of functional groups. Most of the peaks in FE powder before and after extraction are also observed for the film adsorbed on the mild steel surface, confirming the existence of these

functional groups in the inhibitor film adsorbed on the steel surface. Some of the peaks deviated, while some vanished. We observed a shift from 1648 to 1604 cm^{-1} due to the C=O stretching, the bands related to O-H/N-H at 3209 shifts to 3320 cm^{-1} , those associated with C-N at 1002 vanished. The shift of C=C and C-O stretching frequencies from 1650 to 1636 cm^{-1} and from 1250 to 1083 cm^{-1} , respectively, suggests the adsorption of FE molecules on the corroding metal surface. The shift due to O-H/N-H and C=O stretching frequencies from 3209 to 3386 cm^{-1} and from 1723 to 1703 cm^{-1} also confirm the adsorption of the inhibitor species on the metal surface.

Theoretical considerations

Our experimental results have shown that the Corrosion inhibition of mild steel by the ethanol extract of FE occurred through the adsorption of the inhibitor organic matter on the metal surface. The contributions of the individual molecules to the overall adsorption process could not be achieved experimentally. We therefore rely on performing theoretical computations in the framework of the density functional theory (DFT) and molecular dynamic simulation to theoretically overcome this problem. Density functional theory (DFT) has been used to calculate information relating molecular geometries and electron distributions, which influence corrosion inhibition performance [28, 29]. The structures of some major constituents of FE were modeled using a combination of DFT- based quantum chemical calculations and molecular dynamics simulations to theoretically evaluate the inhibiting potential based on structure-activity relationship to determine basic molecular descriptors. Three major constituents of FE modeled are Ascorbic acid, Methyl ursolate and N,N-Dimethylcon-5-enin-3-amine. The simulations were performed by means of density functional theory (DFT) electronic structure program DMol³ using a Mulliken population analysis [30,31]. Electronic parameters for the simulation include restricted spin polarization using the DND basis set and the Perdew–Wang (PW) local-correlation-density functional. The molecular structures were first subjected to geometry optimization using a COMPASS force field and the Smart minimization method by high-convergence criteria, more geometrical optimization of the molecules were carried out using neglect of diatomic differential overlap (NDDO) with AM1 Hamiltonian in the semi empirical molecular orbital package VAMP (MS Studio 4.0). The electronic structures of the molecules, including the distribution of frontier molecular orbital and Fukui indices were then determined.

Figure 8. Electronic properties of ascorbic acid (a) HOMO orbital (b) LUMO orbital (c) total electron density (d) F^+ (e) F^- . Atom legend: white = H; gray = C; red = O; blue = N. The blue and yellow isosurfaces depict the electron density difference: the blue regions show electron accumulation while the yellow regions show electron loss.

Figure 9. Electronic properties of Methyl ursolate (a) HOMO orbital (b) LUMO orbital (c) electron density (d) F^+ (e) F^- . Atom legend: white = H; gray = C; red = O; blue = N. The blue and yellow isosurfaces depict the electron density difference: the blue regions show electron accumulation while the yellow regions show electron loss.

Figure 10. Electronic properties of N,N-Dimethylcon-5-enin-3-amine ursolate (a) HOMO orbital (b) LUMO orbital (c) electronic structure (d) F^+ (e) F^- . Atom legend: white = H; gray = C; red = O; blue = N. The blue and yellow isosurfaces depict the electron density difference: the blue regions show electron accumulation while the yellow regions show electron loss.

Figure 11. Top view of the representative snapshots from molecular dynamics models of: (a) ascorbic acid, (b) methyl ursolate and (c) N,N-Dimethylcon-5-enin-3-amine

Figure 12. Side view of the representative snapshots from molecular dynamics models of: (a) ascorbic acid, (b) N,N-Dimethylcon-5-enin-3-amine

Figure 8 (a-e), shows the highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), the total electron density, center for electrophilic behavior (F^-) and center for nucleophilic behavior (F^+) of ascorbic acid, whereas figures 9 and 10 show similar properties for methyl ursolate and N,N-Dimethylcon-5-enin-3-amine respectively. The electron density can be seen to saturate all around each molecule: Which facilitate flat lying adsorption orientations. The regions of highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbitals also called the frontier orbitals determine the way the molecule interact with other species. The HOMO is the orbital that acts as an electron donor since it is the outermost orbital containing electron. The LUMO is the orbital that acts as an electron acceptor, since it is the innermost orbital that could act as electron acceptor. According to the frontier molecular orbital, the formation of the transition state is due to the interaction between the frontier orbitals of reaction [32]. A large HOMO-LUMO gap implies high stability for the molecule in chemical reactions.

The eigenvalues of the HOMO (E_{HOMO}), LUMO (E_{LUMO}) and the energy gap $\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}}$ are presented in table 4, as well as other quantum chemical parameters related to the molecular electronic structure of the most stable conformation of the molecules. High values of E_{HOMO} indicate the ability of the molecule to donate electrons to an appropriate acceptor, also low value of

ΔE will favor good inhibition efficiency since the energy needed to remove an electron from the last occupied orbital will be reduced [33,34]

I and A are related to E_{HOMO} and E_{LUMO} according to the equation:

$$I = -E_{\text{HOMO}}, A = -E_{\text{LUMO}}. \quad (7)$$

The absolute electronegativity (χ), absolute hardness (η) and softness (σ) of the molecules were calculated using the equation:

$$X = \frac{I+A}{2} \quad (8)$$

$$\eta = \frac{I-A}{2} \quad (9)$$

$$\sigma = \frac{1}{\eta} \quad (10)$$

Electron charge transfer, (ΔN) from Lewis base (the inhibitor) to Lewis acid (the metal surface) was quantified using the equation below

$$\Delta N = \frac{X_m - X_i}{2(\eta_m + \eta_i)} \quad (11)$$

Where X_m and X_i are the absolute electronegativity of the metal and inhibitor molecule, respectively, η_m and η_i are the absolute hardness of the metal and inhibitor molecule respectively. The ΔN values presented in table 4 were calculated using theoretical values of 7 eV/mol and 0 eV/mol for X_m and η_m respectively [35]. ΔN values has been reported to increase with increase in inhibition efficiency[36].

Table 4. Calculated quantum chemical properties for the most stable configuration of ascorbic acid, methyl ursolate and N,N-Dimethylcon-5-enin-3-amine.

Property	Ascorbic acid	Methyl ursolate	N,N-Dimethylcon-5-enin-3-amine.
E_{HOMO} (Ev)	-6.031	-4.966	-1.439
E_{LUMO} (Ev)	-2.294	-0.746	-1.433
$E_{\text{LUMO-HOMO}}$	3.737	4.220	0.006
Σ	0.535	0.473	333.3
X	4.163	2.856	1.436
η	1.869	2.110	0.003
ΔN	0.759	0.982	927.3
Adsorption energy (Kcal/mol)	-30.3	- 160.5	-231.0

The results show that N,N-Dimethylcon-5-enin-3-amine has the highest value of E_{HOMO} and the lowest value of ΔE therefore it may be said to be more stable than the other molecules.

Molecular dynamics simulation was used to sample different low energy adsorption configurations of the molecules on the Fe surface using Force quench molecular dynamics to sample many different low energy configurations and identify the low-energy minima. The Fe slab was cleaved along the (110) plane. The calculations were performed in a 12 x 10 supercell using a Compass force field and the Smart algorithm with NVE (microcanonical) ensemble, a time step of 1

fs and simulation time of 5ps. system was quenched automatically at intervals of 250 steps while maintaining the temperature at 303K.

Figure11(a-c) shows top view of the representative snapshots of the lowest energy adsorption configurations for single molecules of ascorbic acid, methyl ursolate and N,N-Dimethylcon-5-enin-3-amine respectively on the Fe (110) surface from our simulations. Figure12 show the side view positions for ascorbic acid and N, N-Dimethylcon-5-enin-3-amine. Each molecule is seen to maintain flat lying adsorption orientation on the Fe surface as expected from the delocalization of the electrons on the molecules. This adsorption position maximizes contact between the molecule and the Fe surface and then improves surface coverage.

In order to quantify the interaction between the molecules under study and the Fe surface, the binding energy (E_{bind}) of each system was calculated using the equation:

$$E_{\text{bind}} = E_{\text{total}} - (E_{\text{inh}} + E_{\text{Fe}}). \quad (12)$$

Where E_{inh} , E_{Fe} and E_{total} denotes the total energy of the single molecule, the Fe slab without adsorption and the total energy of the system containing the molecule/Fe surface, respectively. The total energies were obtained by averaging the energies of the five most stable adsorption configurations. the obtained values of E_{ads} values are -30 for ascorbic acid, -160.5 for methyl ursolate and -231.0 for N,N-Dimethylcon-5-enin-3-amine all the adsorption energies are all negative indicating stable adsorption structures. The trend in adsorption energy correspond to the trend in molecular size obtained earlier (N, N-Dimethylcon-5-enin-3-amine > methyl ursolate > ascorbic acid) showing that the larger molecules adsorb better than smaller ones.

The calculated values are presented in Table 3. Good linear correlation has been found to exist between inhibition efficiency and binding energy, wherein efficiency increased with binding energy [37].

Conclusion

From the result of this research, it has been established the ethanol extract of *Funtumia elastic* (FE) is an adsorption inhibitor mild steel in 1 M HCl solution. The gravimetric results showed that inhibition efficiency decreased with increase in exposure time but maintained high inhibition efficiency even at long exposure time (336 h). Polarization study revealed that the inhibitor is a mixed type corrosion inhibitor for mild steel in 1 M HCl solution. The FTIR results indicate that FE extract functioned by the adsorption of the organic matter on the corroding mild steel surface. Quantum chemical calculations performed on some active components of FE confirmed their strong contribution the overall inhibiting process.

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