

Corrosion Inhibition Studies on Low Carbon Steel in Hydrochloric Acid Medium Using o-Vanillin-Glutamine Schiff Base

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The o-Vanillin - Glutamine Schiff base [2-Hydroxy-3-Methoxy BenzylideneCarbonyl) -2-Butanoic Acid] was examined for low carbon steel corrosion inhibition in acid media. Weight loss studies were carried out at three different temperatures to determine the inhibition efficiency (IE). Electrochemical impedance spectroscopy revealed that the charge transfer resistance controlled the corrosion reaction and Tafel polarization indicated that the Schiff base acts as mixed mode of inhibitor. SEM images were recorded for the surface morphology of the low carbon steel surface. DFT studies revealed corrosion control mechanisms using quantum chemical parameters such as E_{HOMO} , E_{LUMO} , energy gap (ΔE), chemical Hardness (η), chemical Softness (σ), Electronegativity (χ), and the fraction of electron transferred (ΔN), which is calculated using Gaussian software 09. The gas-phase geometry was fully optimized in the Density Functional Theory (DFT/B3LYP-6-31G (d)). The DFT results are in good agreement with the experimental results. All the results proved that the Schiff Base (2-Hydroxy-3-Methoxy BenzylideneCarbonyl) -2-Butanoic is a suitable alternative for corrosion inhibition of low carbon steel in acid media.

Keywords: DFT, Electrochemical studies, Schiff base, SEM, Weight loss

1. Introduction

Metal corrosion is one of the major issues being encountered in various industrial fields, leading to enormous economic losses [1]. The use of corrosion inhibitors is one of the most effective measures for protecting metal surfaces against corrosion in acidic environments [2]. It is already proved that Schiff bases are effective inhibitors for the corrosion of steel in acidic media. Schiff bases are organic compounds with the general formula $R-C=N-R$, where R and R- are aryl, alkyl, or heterocyclic groups formed by the condensation of a primary amine and a carbonyl group, which are responsible for potential inhibition [3].

The greatest advantage of Schiff bases is that they could be conveniently and easily synthesized from relatively cheap starting materials. Schiff bases are effective inhibitors for the corrosion of steel in acidic media due to the presence of imine groups ($-C=N-$) and electronegative nitrogen, sulfur, and/or oxygen atoms present in the molecule [4,5]. In general, the tendency to form stronger

coordination bonds and, as a result, inhibitory efficiency increases in the following trends: $O < N < S < P$ [6].

The present study aims at to examine the corrosion inhibition effects of the Schiff base o-Vanillin-glutamine on low carbon steel in acid media by analyzing the efficiency of inhibition both from experimental and theoretical viewpoints. However, no work has been reported on the corrosion inhibition studies of the analyzed Schiff base, namely [2-Hydroxy-3-Methoxy Benzylidene-Carbonyl) -2-Butanoic Acid] to the best of our knowledge. Hence, in the present study, we have synthesized the Schiff base ligand derived from 2-hydroxy 3-methoxy- benzaldehyde and L- Glutamine. The effects of the Schiff base on the corrosion behavior of low carbon in a 5% HCl solution were analyzed by the weight loss method. Further, the inhibition efficiency of the synthesized Schiff base was evaluated using electrochemical studies and SEM studies. To explain the mechanism of inhibiting effect of heterocyclic organic compounds theoretically, the Density Functional Theory (DFT) method [7,8] was used. Quantum Chemical methods are proved very useful in determining molecular structures and explaining electronic structures and reactivity. They have been proved to be a very powerful

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tool for studying corrosion inhibition mechanisms [9]. Quantum chemical parameters can provide insight into the inhibitor-surface interaction. The relation between the corrosion inhibition efficiency with molecular orbital (MO) energy levels for many organic compounds has been successfully performed [10].

2. Materials and Methods

2.1 Preparation of the specimen and corrosive environment

Low carbon steel sheet of chemical composition C = 0.02%, Mn = 0.06%, P = 0.05%, S = 0.05%, and Fe = 99.26% were used for the study throughout. Low carbon steel sheets, previously degreased with trichloroethylene and polished using sand emery papers of various grades were cut into plates of size $4.0 \times 2.0 \times 0.19$ cm for weight loss studies. For electrochemical studies and scanning electron microscopic studies (SEM), low carbon steel specimens with a 1 cm^2 open area were used. The HCl solution of 5% (V / V), prepared by using pure HCl and double distilled water were used as a corrosive environment.

2.2 Synthesis of Schiff Base Ligand (SB)

A mixture of alcoholic o-Vanillin (0.5 N, 20 mL) and an aqueous solution of L-Glutamine (0.5 N, 20 mL) were refluxed for 5-6 hours at 60-65°C. The solution was concentrated till its volume reduces to one-fourth of its initial volume. Upon allowing this to stand overnight, a yellow precipitate of Schiff base was obtained. The obtained precipitate was filtered, washed repeatedly with diethyl ether, and dried to get pure Schiff base which was used for further analysis.

2.3 Weight Loss study

Previously polished and degreased low carbon steel specimens of size $4.0 \times 2.0 \times 0.19$ cm were used for weight loss studies. Low carbon steel plates of known weight were separately immersed in 100 mL of the corrosive environment and 100 mL each of the test solutions with 0.1, 0.2, 0.3, 0.4, 0.5 g of the Schiff base for one hour. After an hour, low carbon steel specimens were washed immediately with double distilled water, dried, and weighed again. The same experiment was carried out at three different temperatures of 305, 310, and 315K respectively. From the measured weight loss data, the

inhibition efficiency (IE) was calculated using the formula

$$IE\% = (W_0 - W_i) / W_0 \quad (1)$$

Where W_i & W_0 are the weight loss values in the presence and absence of the inhibitor [11]. All these data were tabulated

2.4 Electrochemical studies

Electrochemical parameters such as linear polarization resistance (LPR), Corrosion Potential (E_{corr}), Corrosion current (I_{corr}), Anodic Tafel Slope (B_a), Cathodic Tafel Slope (B_c), Charge Transfer Resistance (R_{ct}), Double Layer Capacitance (C_{dl}), Corrosion level and IE were obtained from electrochemical measurements [12]. Tafel polarization plot was recorded potentiodynamic using platinum electrodes, calomel electrodes, and low carbon steel specimens each as auxiliary, standard, and working electrodes.

Polarization studies were carried out at CHI 608 D model electrochemical analyzer using the working electrode (low carbon steel) is approximately 1 cm^2 , standard calomel electrode, a platinum electrode with 100 mL test solution at -0.250 and -0.750 V with the scan rate of 0.01 Vs^{-1} . Potential (E) versus the log current (log I) plots were then recorded. From the polarization studies, we can calculate the parameters like Anodic Tafel Slope (b_a), Cathodic Tafel Slope (b_c), and linear polarization resistance (LPR). By applying these parameters to the Stern –Geary equation we have calculated the Corrosion current (I_{corr}). The Stern –Geary equation is:

$$I_{\text{corr}} = \frac{b_a b_c}{2.303(b_a + b_c)R_p} \quad (2)$$

b_a = Anodic Tafel current

b_c = Cathodic Tafel current

R_p = Polarization Resistance

Electrochemical impedance was conducted in the frequency range of 10 kHz to 1 kHz at an open circuit potential by applying the alternating current signal of 0.005 V peak to peak. The Impedance parameters like Charge transfer resistance (R_{ct}) and Double-layer capacitance (C_{dl}) were obtained from the impedance study.

2.5 Scanning electron microscopy (SEM) studies

Surface morphology was evaluated using SEM photographs recorded for polished low carbon steel surfaces, specimens exposed to 5% HCl (V / V), and specimens exposed to a 0.5% test solution. Low carbon steel specimens with a 1cm² open area were used for SEM studies. SEM photos were recorded using Sigma HV - Carl Zeiss with Bruker Quantax 200 - Z10 Eds Detector Model scanning electron microscope structure which were as small as 1 nanometer (= billion millimeters) for the study of morphological, chemical, and analytical material.

2.6 Density functional theory (DFT)

2.6.1 Quantum Chemical Calculations

The density Functional Theory method (DFT / B3LYP-6-31G (d)) was used to calculate quantum chemical parameters. Parameters such as highest occupied molecular orbitals (E_{HOMO}) and lowest unoccupied molecular orbitals (E_{LUMO}), energy differences (ΔE) between E_{HOMO} and E_{LUMO} , dipole moment (μ), electronegativity (χ), the electrophilicity index (ω), electron affinity (A), global hardness (η), global softness (σ), ionization potential (I) and the electron fraction transferred (ΔN). Ionization potential (I) and electron affinity (A) related to E_{HOMO} and E_{LUMO} were calculated from the optimized structure obtained as follows [13]

$$I = -E_{\text{HOMO}} \quad (3)$$

$$A = -E_{\text{LUMO}} \quad (4)$$

$$\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}} \quad (5)$$

The quantities absolute electronegativity (χ) and global hardness (η) are related to electron affinity (A) and ionization energy (I) as follows [14]

$$\chi = \frac{I + A}{2} \quad (6)$$

$$\eta = \frac{I - A}{2} \quad (7)$$

Global chemical softness (σ), which describes the capacity of an atom or group of atoms to receive electrons [15] was estimated by using the equation:

$$\sigma = \frac{1}{\eta} = \frac{2}{E_{\text{HOMO}} - E_{\text{LUMO}}} \quad (8)$$

According to Pearson, the number of electrons transferred (ΔN) from the inhibitor molecule to the metal surface was calculated [16] as

$$\Delta N = \frac{\chi_{\text{Fe}} - \chi_{\text{Inh}}}{[2(\eta_{\text{Fe}} - \eta_{\text{Inh}})]} \quad (9)$$

Where χ_{Fe} and χ_{inh} denote the absolute electronegativity of iron and inhibitor molecule, η_{Fe} and η_{inh} denote the absolute hardness of iron and the inhibitor molecule respectively. In this study, we have used the theoretical value of $\chi_{\text{Fe}} = 7.0$ eV and $\chi_{\text{inh}} = 0$, for calculating the number of electrons transferred. The chemical reactivity parameter known as electrophilicity index (ω) is defined as [17]

$$\omega = \frac{\mu^2}{2\eta} \quad (10)$$

According to this definition, this index measures the tendency of chemical species to receive electrons. Good nucleophile, more reactive, marked with a low-value μ , ω , and vice versa electrophiles are well marked with high-value μ , ω . This new reactivity index measures stabilization in energy when the system acquires additional electronic charge ΔN from the environment.

3. Results and Discussion

3.1 Weight Loss Studies of o-Vanillin –Glutamine Schiff base

Weight loss studies were carried out at three different temperatures. Using the weight loss data, the percentage inhibition efficiencies were calculated and the results are

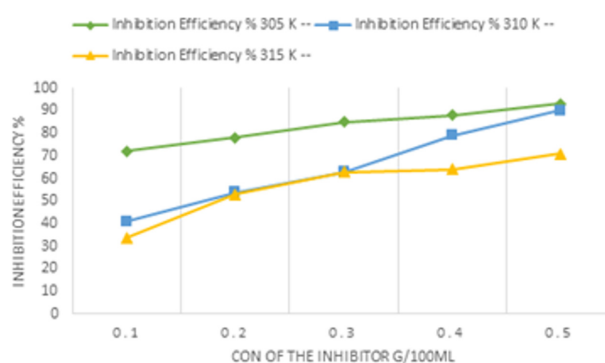


Fig. 1. Plot between IE % against the concentration of Schiff base inhibitor

Table 1. Weight loss data

Conc. of the inhibitor g/100mL	Weight loss g			Inhibition Efficiency %		
	305 K	310 K	315 K	305 K	310 K	315 K
0	0.11	0.182	0.374	--	--	--
0.1	0.03	0.107	0.246	72	41	34
0.2	0.024	0.082	0.174	78	54	53
0.3	0.016	0.066	0.135	85	63	63
0.4	0.013	0.038	0.134	88	79	64
0.5	0.007	0.018	0.105	93	90	71

shown in Table 1. The data obtained clearly show that the Inhibition efficiency depends on the concentration of inhibitors. Also, it was found that IE increased with an increase in the concentration of inhibitors which is evident from Fig. 1. It was also noted that at the highest concentrations, inhibition efficiency reduces with an increase in temperature as shown in Fig. 1.

3.2 Electrochemical studies

3.2.1 Electrochemical impedance spectroscopy

Electrochemical impedance Nyquist plot obtained for low carbon steel corrosion in the absence and the presence of the Schiff base o-Vanillin-Glutamine is shown in Fig. 3. Electrochemical impedance parameters Charge transfer resistance (R_{ct}), Double-layer capacitance (C_{dl}), and Inhibition efficiency (IE) were tabulated in Table 2. The diameter of the semi-circles of the Nyquist plot obtained in the presence and absence of the Schiff base was found to increase with an increase in the concentration of Schiff base [18]. Nyquist plots were often assigned to surface irregularities and solid surface heterogeneity due to the adsorption of inhibitors on metal surfaces.

The C_{dl} values and inhibitor concentration are inversely

related. A decrease in the C_{dl} value shows an increase in electric double layers on the metal solution interface and slowly replacing the corrosive environment with the

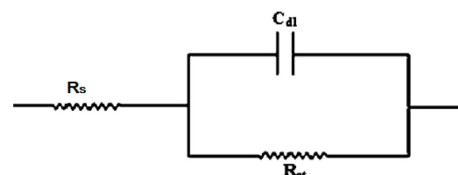


Fig. 2. The equivalent circuit for impedance studies

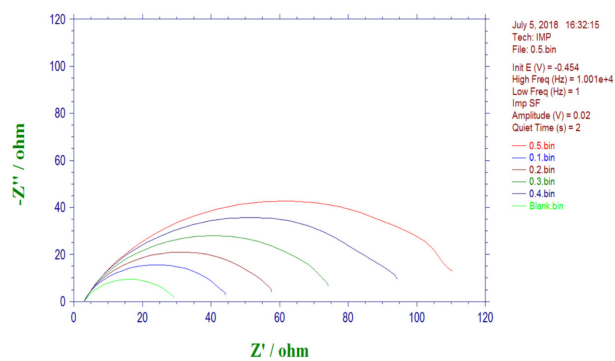


Fig. 3. Impedance spectra of low carbon steel in HCl in the absence and Presence of different concentrations of Schiff base

Table 2. Electro-Chemical Impedance and Polarization data

con of inhibitor g/100mL	C_{dl} F/cm ²	R_{ct} Ωcm ²	R_s Ωcm ²	b_c V/dec	b_a V/dec	I_{corr} A/cm ²	LPR Ωcm ²	E_{corr} V/SCE	% IE
Blank	0.003319	38.76	1.857	8.725	7.441	7.231	37	-0.4599	
0.1	0.003166	69.87	1.502	8.452	7.909	5.550	48	-0.4621	44
0.2	0.002926	101.3	1.466	8.201	7.884	4.863	56	-0.6315	61
0.3	0.002688	147.7	1.373	8.248	7.560	3.863	71	-0.4613	73
0.4	0.002443	209.2	1.217	8.381	7.374	2.959	93	-0.4613	81
0.5	0.00223	271.5	1.091	10.820	7.693	2.051	115	-0.4621	85

adsorption of organic molecules on the metal surface. The charge transfer resistance increases with an increase in the concentration of inhibitors, which illustrates that the charge transfer process highly controls corrosion of low carbon steel corrosion.

3.2.2 Tafel polarization

Tafel polarization curve for *o*-Vanillin -Glutamine Schiff Base for 5% HCl on low carbon steel is shown in Fig. 4. Tafel parameters such as corrosion potential (E_{corr}), corrosion flow (I_{corr}), Anodic Tafel Plot (b_a), Cathodic Tafel Plot (b_c), linear polarization resistance (LPR), and inhibitory efficiency (IE) are tabulated in Table 2. A shift in the cathodic and anodic curves at lower current densities in the presence of inhibitors is attributed to a decrease in corrosion reactions. A stable decrease in the I_{corr} value also predicts a decrease in corrosion reaction. The value of (E_{corr}), which does not increase or decrease regularly from the blank reveals that inhibitors act through mixed-mode [19]. The LPR value (linear polarization resistance) increases with an increase in the concentration of inhibitors which also proves a decrease in corrosion reaction. Changes in the b_a and b_c values in the presence of inhibitors reveal the reduced dissolution of anodic metal and the backward reaction of cathodic hydrogen evolution. This indicates that the inhibitor acts as a mixed-mode of inhibition but predominantly retards the cathodic reaction.

3.3 SEM studies

SEM photos of polished low carbon steel surfaces are given in Fig. 5a, which are found to be free of corrosion

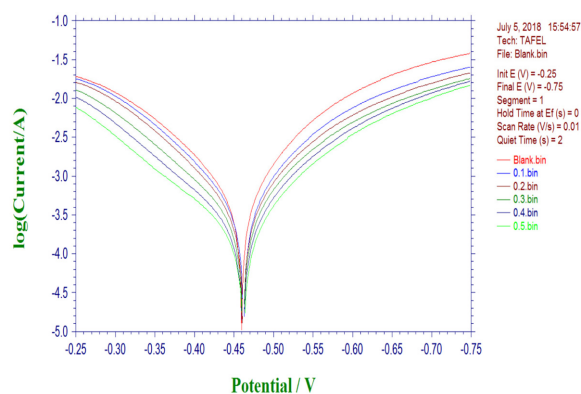
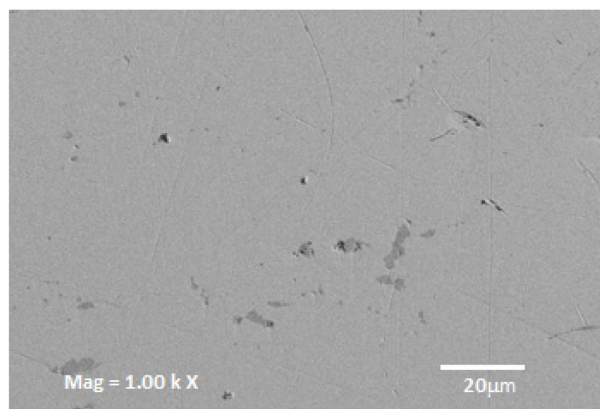
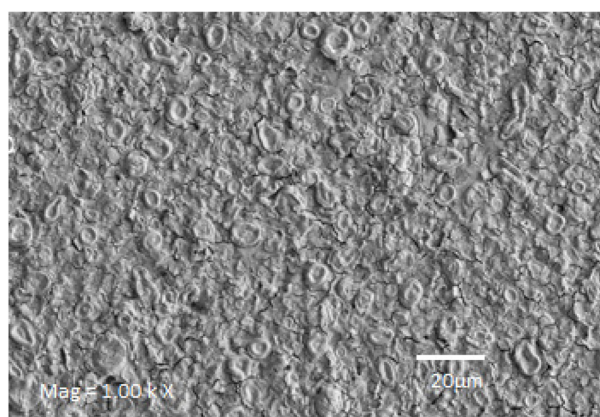


Fig. 4. Tafel Curve

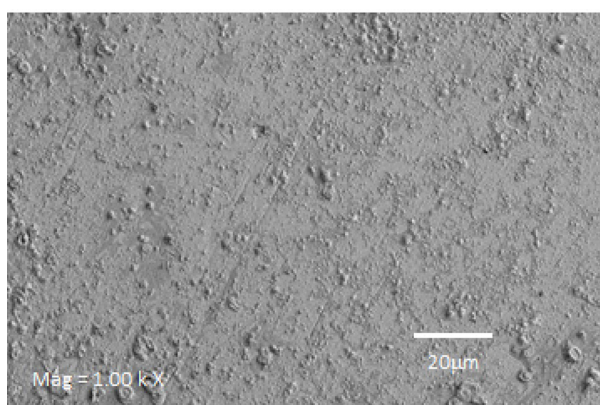
products. SEM images of low carbon steel exposed to 5% (V / V) HCl are given in Fig. 5b. The surface is severely attacked by the acid and hence has pits and cracks throughout the surface. SEM images from low carbon steel exposed to 0.5 g inhibitors with 100 mL acid solution



(a)



(b)



(c)

Fig. 5. (a) SEM image of polished low carbon steel surface, (b) SEM image of low carbon steel exposed to 5% HCl, (c) SEM image of low carbon steel exposed to 5% HCl having 0.5 g Schiff base

are given in Fig. 5c. It is observed that there is a remarkable decrease in cracks, pits, and corrosion products on the low carbon steel surface in the presence of inhibitors (Fig. 5c) when compared to Fig. 5b. The inhibitor is found to protect the exposed surface of low carbon steel from corrosion in the HCl medium through the formation of a protective layer by the adsorption of the Schiff base component of the inhibitor [20].

3.4 Density Functional Theory (DFT)

3.4.1 Quantum chemical simulations

The optimized structure, HOMO, and LUMO of the o-Vanillin–Glutamine Schiff base are shown in Fig. 6, 7, 8. The transfer of electrons and chemical reactivity of reacting species are due to the interaction between the

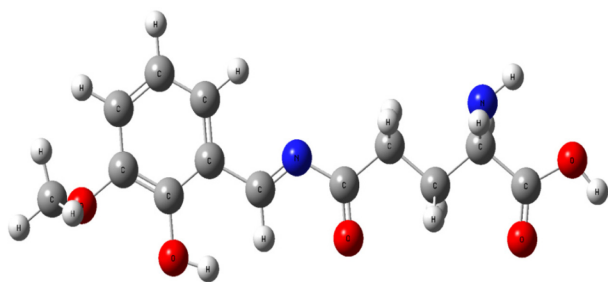


Fig. 6. Optimized structure of Schiff base

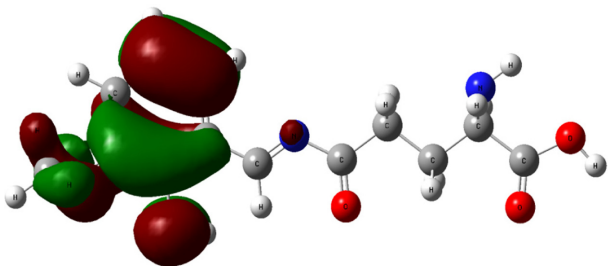


Fig. 7. HOMO of Schiff base

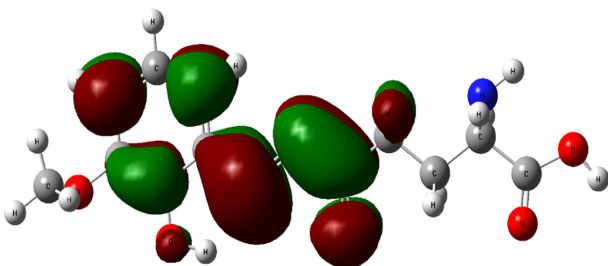


Fig. 8. LUMO of Schiff base

HOMO (Highest occupied molecular orbitals) and the LUMO (Lowest unoccupied molecular orbitals) [21].

E_{HOMO} is the ability of molecules that contribute electrons. The high E_{HOMO} value indicates that molecules tend to contribute electrons to acceptor molecules that are under low energy empty molecular orbitals [22]. E_{LUMO} shows the ability of molecules to receive electrons. The lower E_{LUMO} values endorse that the molecule would accept more electrons.

Energy gap between E_{HOMO} and E_{LUMO} molecular energy levels as a function of reactivity of molecular inhibitors towards adsorption on metal surfaces. Because ΔE reduces, increased molecular reactivity causing an increase in the percentage of IE of the molecule. The lower value of the difference in energy improves inhibition efficiency. This is due to the energy required to remove electrons from the last occupied orbital will be low [23].

The unequal sharing of charges on various atoms in the molecule results from the dipole moment (μ). A high dipole moment is required to confirm better molecular

Table 3. Quantum Chemical Parameters

Quantum parameters	(2-hydroxy-3-methoxybenzylidene carbonyl)-2-aminobutanoic acid
E_{HOMO} (eV)	-9.1042
E_{LUMO} (eV)	-3.3951
ΔE gap (eV)	5.7091
μ (debye)	3.5756
$I = -E_{\text{HOMO}}$	9.1042
$A = -E_{\text{LUMO}}$	3.3951
$\chi = \frac{I + A}{2}$	6.2497
$\eta = \frac{I - A}{2}$	2.8545
$\sigma = \frac{1}{\eta}$	0.3503
$\Delta N = \frac{\chi_{\text{Fe}} - \chi_{\text{Inh}}}{[2(\eta_{\text{Fe}} - \eta_{\text{Inh}})]}$	0.1314
$\omega = \frac{\mu^2}{2\eta}$	6.8414
E_{total}	-990.85

adsorption on metal surfaces [24].

Molecular stability and reactivity are measured using properties such as absolute hardness and softness. It was clear that chemical hardness shows resistance to deformation or polarizing clouds of atomic electrons, ions, or molecules in small disorders of chemical reactions. Hard molecules have large energy gaps and soft molecules have small energy gaps [25]. Usually, inhibitors with the highest value of global hardness are most expected to have the highest inhibitory efficiency [26].

The tendency of chemical species to accept electrons is measured in terms of electrophilicity index (ω) [17]. The electrophilicity index value is high and acts as a good electrophile while a small value of electrophilicity act as a good nucleophile. In this study we get the high value ($\omega = 6.8414\text{eV}$) that reveals the electrophilic nature of the studied molecule showing the possible transfer of electrons from the metal to the inhibitor.

ΔN , the fraction of electrons transferred for (2-hydroxy-3-methoxybenzylidene carbonyl)-2-aminobutanoic acid, was carried out using equation (9) using theoretical χ value of 7 eV/mol and η value of 0 eV/mol for iron. The ΔN values showed an inhibition effect resulting from electrons donation. It is evident that if the $\Delta N < 3.6$, the inhibition efficiency will increase [16] (R.G.Pearson et al). The obtained ΔN value of 0.1314 proves that the inhibition efficiency increases with the increasing electron-donating ability of the inhibitor to donate electrons to the metal surface [27].

4. Conclusion

The corrosion inhibition effect of Schiff base inhibitor on corrosion of Low carbon steel in HCl acid medium increases on increasing the concentration of Schiff base and decreases with rising in temperature. Weight loss study, revealed a maximum inhibition efficiency of 93%, is obtained with a 0.5 g Schiff base in 100 ml of 5% HCl acid.

The electrochemical impedance spectroscopy indicates that the charge transfer resistance is increasing with an increase in the concentration of inhibitors, which illustrate that the inhibitor controls the corrosion of low carbon steel in acid media.

The results of Tafel polarization reveals that Schiff's

base inhibitor acts as a mixed-mode of inhibitor but mainly retards the cathodic reaction.

SEM photographs obtained indicate that the inhibitor is found to protect low carbon steel surfaces that are open for corrosion on the HCl medium through layer formation by the adsorption of Schiff base inhibitor.

The results obtained from quantum chemical parameters (DFT) are under the trial data. The ΔN value of 0.1314 confirms that the inhibitory efficiency increased with an increase in the ability to donate electrons from the metal surface.

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