Experimental and Theoretical Study for Corrosion Inhibition in 1M HCl Solution by New 5-Chloroisatin Derivative

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Abstract

The theoretical study of the 5-chloro-1-(2-(dimethylamino) ethyl) indoline-2,3-dione (I1) by applying quantum chemical calculations based on DFT methods at the B3LYP / 6-31G level using the Gaussian 03 code. The objective of this work was to try to find relationships between the intrinsic electronic properties and efficient inhibition of the I1 inhibitor, which was previously studied as a corrosion inhibitor of mild steel in experimentally 1M HCl acid medium. The effectiveness of corrosion inhibitors and chemical reactivity depend on certain parameters, such as the highest occupied molecular orbital energy (EHOMO), the lowest unoccupied molecular orbital energy (ELUMO) energy gap (AE), dipole moment (μ), electronegativity (χ), electron affinity (A), total hardness (η), Softness (σ), the ionization potential (I), Fukui functions and softness indices which were calculated.

Keywords: Hydrochloric Acid, Corrosion, Adsorption, DFT Calculations

I. INTRODUCTION

Corrosion is the degradation of material properties, because of the physicochemical interactions with elements returning to their environment, which cause common problems in industry and high raw material costs [1, 2].

With the intent to prevent damage caused by corrosion in acidic medium, using organic inhibitors as an effective and practical method [3-5]

The mechanism of inhibition is generally explained by the formation of a film physically and / or chemically adsorbed on the metal surface [6].

The reaction of organic inhibitors on the metal surface provides vacuum electron or partially filled d orbital of the metal, so that these compounds depend on the functional groups present in their molecular structures, such as heteroatom, aromatic rings double or triple conjugated bonds [7].

Therefore, the effectiveness of corrosion inhibitors is strongly related to their structural and electronic properties.

Further theoretical study was used to correlate the electronic descriptors with the effectiveness of the corrosion inhibition and also to explain the experimental results, as well as to elucidate the mechanism of corrosion inhibition processes [8].

The ultimate goal of this present study is the prediction of the inhibitory efficacy of corrosion compound 5-chloro-1-(2-(dimethylamino) ethyl) indoline-2,3-dione (I1), using approaches to quantum chemical calculations appointed density functional theory (DFT) [9].

Inhibitors of the activity properties represent the geometry of the inhibitor in its ground state, so that the nature of their molecular orbital, the highest occupied molecular orbital (HOMO) and lowest vacant molecular orbital (LUMO) and other parameters.

The inhibitory effect of an organic compound has often been correlated with the energy of the HOMO, LUMO and HOMO-LUMO gap. The efficacy of inhibiting corrosion of the I1 inhibitor has been previously studied [10].

II. EXPERIMENTAL DETAILS

A. Inhibitor

The derivative 5-chloro-1-(2-(dimethylamino) ethyl) indoline-2,3-dione (Figure 1) was synthesized from 5-chloroisatin by the alkylation method under the conditions of phase transfer catalysis , in the following tested compound was characterized by the technique of nuclear magnetic resonance ^{1}H-NMR and ^{13}C-NMR and infrared spectroscopy, all the methods have been described in detail by Tribak et al [11].

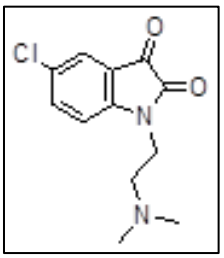


Fig. 1: Chemical structure of the inhibitor 5-chloro-1-(2-(dimethylamino) ethyl) indoline-2,3-dione (I1)

B. Weight Loss Measurements

The plates of mild steel were cut (1.5 cm x 1.5 cm x 0.3 cm) dimensions in a 1M HCl solution the exposed area of the plates was mechanically abraded with (120, 600 and 1200) categories of papers of emery, with the following composition 0.370% C, 0.230% Mn 0.680% Si, 0.016% S, 0.077% Cr, 0.011% Ti, 0.059% Ni, 0.009% Co, 0.160% of Cu and the balance Being iron (Fe) used for weight loss measures. The samples were washed with bidistilled water and dried degreased with acetone and weighed thereafter. Gravimetric and thermodynamic measurements are made with and without the addition of different concentrations of the I1 inhibitor. The immersion time for weight loss is 6 pm at (30 ± 1°C). In order to obtain good reproducibility, the experiments were performed in triplicate for each case.

C. Quantum Chemical Calculations

The majority of quantum chemical study was done using the functional theory of density (*DFT*) with *B3LYP* hybrid functional, with the exchange of the three parameters of functional Beck and the Lee-Yang correlation -Parr nonlocal functional (*B3LYP*) with 6-31G basis set is implemented in the package Gaussian 03 program [12]. This approach is made to determine favorable geometries for a wide variety of systems.

Good theoretical parameters were investigated to correlate with the inhibiting performance of derivative of 5-chloro-1*H*-indole-2,3-dione studied, using quantum chemical investigations. For this, some of the molecular properties describing the overall responsiveness were calculated from the optimized structure obtained such that: the energy of the orbital highest occupied molecular (E_{HOMO}), the energy of the Lowest Unoccupied Molecular orbital (E_{LUMO}), energy gap ($AE = E_{LUMO}$-E_{HOMO}) the dipole moment (μ), the ionization potential (*IP*), electron affinity (*EA*), electronegativity (χ), global hardness (η) and Fukui functions and softness indices were calculated. Other parameters describing the local selectivity of the studied molecules such as local land races and Fukui functions were also discussed.

In order to identify some of the previous descriptor, the theorem of Koopmans was used [13] to connect the HOMO and LUMO energies at the IP and EA respectively:

$$IP = -E_{HOMO} \quad (1)$$

$$EA = -E_{LUMO} \quad (2)$$

Furthermore, a linear combination between the *IP* and *EA* were calculated to determine the values of the electronegativity and the global hardness [14].

$$\chi = \frac{IP+EA}{2} \quad (3)$$

$$\eta = \frac{IP-EA}{2} \quad (4)$$

And the softness is the inverse of the hardness: $\sigma = \frac{1}{\eta}$ (5)

III. RESULTS AND DISCUSSION

D. Weight Loss Measurements

The simple application and reliability of the weight loss method of inhibition efficiency and monitoring, makes it a very useful technique in the field of corrosion [15]. The reproducibility of the results for the values of weight loss effectiveness and the percent inhibition for the determination of triplicate was very accurate.

Table.1 shows the values of the corrosion rate of mild steel in 1M HCl at 30°C in the absence and presence of various concentrations of the I1 inhibitor.

It is very clear that corrosion rate decreases after the addition of 5-chloro-1- (2-(dimethylamino) ethyl) selected indoline-2,3-dione, due to the fact that the adsorption of coverage increases, which protects the surface of the mild steel effectively in hydrochloric medium. While the efficiency of the augment inhibition with the addition of inhibitor concentration to reach 91% at 10^{-3}M.

Table - 1

The variation in the inhibition efficiency and the corrosion rate with and without the addition of I1 at different concentrations in 1M HCl

Concentration (M)	*C_R (mg.cm^{-2}.h^{-1})*	*H (%)*	*θ*
HCl 1M	*0.451*	--	--
10^{-3}	*0.038*	*91.57*	*0.915*
5.10^{-4}	*0.067*	*85.14*	*0.851*
10^{-4}	*0.075*	*83.37*	*0.833*
5.10^{-5}	*0.144*	*68.07*	*0.680*
10^{-5}	*0.218*	*51.66*	*0.516*
10^{-6}	*0.242*	*46.34*	*0.463*

E. Adsorption isotherm and standard adsorption free energy

There are several types' adsorption isotherms such as Frumkin, Langmuir, Temkin, which were used to fit the experimental data. In the presence study was found that the adsorption of the I1 inhibitor studied on the steel surface follows the adsorption equation the Langmuir isotherm [16-17].

$$\frac{C}{\theta} = \frac{1}{K} + C \qquad (6)$$

Where C is the concentration of the inhibitor, the constant K adsorption equilibrium, and θ is the surface coverage

The figure shows plots of C/θ with respect to inhibitor concentration, while and the corresponding linear regression parameters chosen isotherm are shown in Table 2.

The regression coefficients (R^2) and the slope is close to 1, indicating the adsorption of the I1 inhibitor on the steel surface obeys Langmuir adsorption isotherm.

In addition, K value means a better performance of inhibition of I1 given. This is in good agreement with the values of the inhibition efficiency obtained in the table.1.

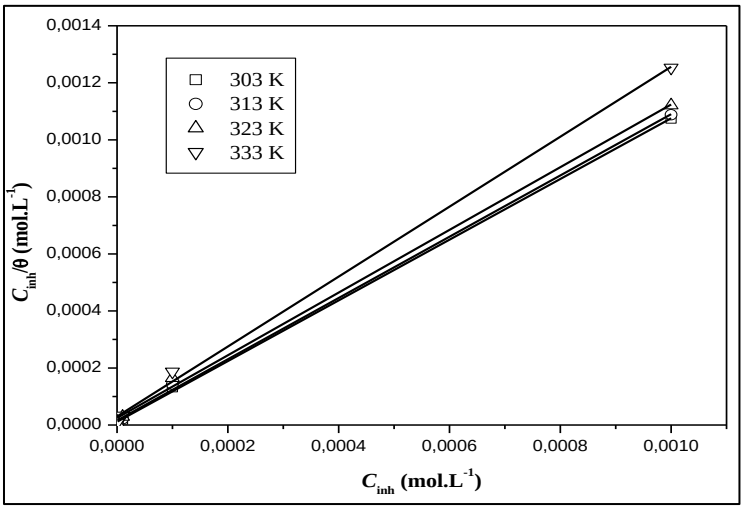


Fig. 2: Langmuir adsorption isotherm of the I1 inhibitor on mild steel in 1M HCl at 30°C

Table - 2

The inhibitor I1 adsorption parameters at different temperatures in 1M HCl obtained from the adsorption isotherm Langmuir

T (K)	*R^2*	*Slope*
303	*0.9996*	*1.0641*
313	*0.9992*	*1.0743*
323	*0.9983*	*1.0991*
333	*0.9983*	*1.2266*

Equation (7) represents the relationship between the adsorption equilibrium constant (K) and standard free energy adsorption (ΔG°) [18].

$$K_{ads} = \frac{1}{C_{H_2O}} \, exp\left(\frac{-\Delta G^{\circ}_{ads}}{RT}\right) \qquad (7)$$

Where R is the gas constant T the absolute temperature (K), and C_{H_2O} is the concentration of water in the solution.

Table - 3
Thermodynamic adsorption parameters of I1 determined at different temperatures in 1M HCl in mild steel

T (K)	*K_{ads} (mol/L)*	*R^2*	*$\Delta G°_{ads}$ (kJ.mol^{-1})*
303	*169546.2*	*0.9839*	*-40.45*
313	*90986.64*	*0.9754*	*-40.17*
323	*38008.58*	*0.9743*	*-39.11*
333	*15279.43*	*0.9966*	*-37.79*

Negative values (ΔG^0_{ads}) imply that the I1 inhibitor was spontaneously adsorbed onto the electrolyte mild steel interface. It has been reported that the values of (ΔG^0_{ads}) to -20 kJ / mol are in accordance with the physisorption; those around -40 kJ / mol or more are compatible with chemisorptions [19].

Note in case the (ΔG^0_{ads}) value were found in the range of -37.79 to -40.45 kJ mol-1 at different temperatures (303-333 K), probably means that adsorption of the I1 inhibitor on parts of the surface of the mild steel corresponds to a chemical adsorption.

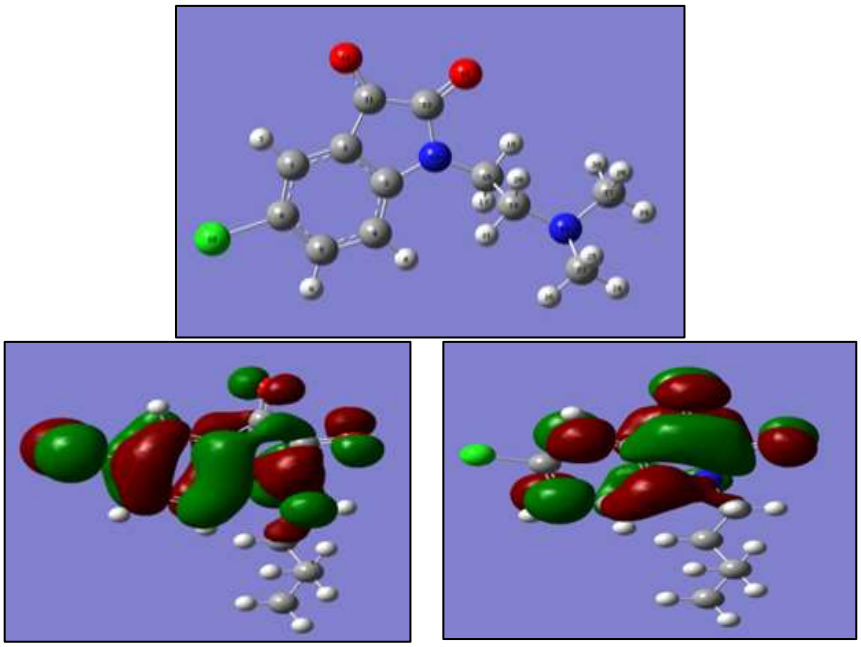
F. Global Molecular Reactivity

All chemical parameters obtained from quantum calculations DFT / B3LYP / 6-31G affect the efficiency of inhibition, for example molecular orbital (E_{HOMO}) held the highest energy more lowest unoccupied molecular orbital (E_{LUMO}), energy gap (ΔE), dipole moment (μ) and total energy (*TE*), electronegativity (χ), electron affinity (*A*) the global hardness (η), softness (σ), the ionization potential (*IP*) are summarized in table 4.

Table - 4
The calculated quantum chemical parameters of the studied I1 inhibitor

Parameters	*Inhibitor*
$-E_{HOMO}$ (ev)	*-0.23590*
$-E_{LUMO}$ (ev)	*-0.11859*
ΔE gap (ev)	*0.11731*
μ(debye)	*5.6982*
E_w (%)	*91%*
IP= $-E_{HOMO}$	*0.23590*
EA= $-E_{LUMO}$	*0.11859*
$\chi = \frac{IP + EA}{2}$	*0.177245*
$\eta = \frac{IP - EA}{2}$	*0.058655*
$\sigma = \frac{1}{\eta}$	*17.048844*

According to the molecular frontier orbital theory (*FMO*) in chemical reactivity, a transition of electrons is due to the interaction between the highest occupied molecular orbital (*HOMO*), and lowest unoccupied molecular orbital (*LUMO*) of the species reactive [13].



HOMO LUMO

Fig. 3: The obtained molecular structures and HOMO and LUMO orbitals of the inhibitor 5-chloro-1-(2-(dimethylamino) ethyl) indoline-2,3-dione (I1) by DFT/B3LYP/6-31G.

The energy of HOMO is a quantum chemical parameter that is often related to the ability of the electron donor molecule. The great value of E_{HOMO} is likely a tendency of the molecule to donate electrons to an acceptor molecule suitable low molecular weight empty orbital energy. [20] While the energy of LUMO indicates the ability of the molecule to accept electrons .Thus, the greater value of E_{LUMO}, more likely the molecule accepts electrons.

From the obtained values of the energy gap of which is an important parameter as a function of the reactivity of the inhibitor molecule to adsorption on the metal surface, means that the I1 inhibitor has a small. This parameter provides a measure of the stability of the complex formed on the metal surface.

The dipole moment of the molecule is the most widely used to describe the amount polarity [21] It is defined as the product of the load on the atoms and the distance between the two bonded atoms. The dipole moment (μ in Debye) is another important electronic parameter resulting from the non-uniform load distribution on the various carbon atoms in the molecule. The high value of the dipole moment probably increases the adsorption between the chemical product and metal surface.

Our theoretical results indicate that the I1 inhibitor has a small hardness (η) and softness (σ) [22].

Table - 5

Calculated Mulliken atomic charges, Fukui functions and softness indices for the atoms of I1 using DFT B3LYP/6-31G method

Atoms	q_N	q_{N+1}	q_{N-1}	f_k^+	f_k^-	S_k^+	S_k^-
1 C	*0,120968*	*0,16953*	*0,011893*	*0,048562*	*0,109075*	*0,413963*	*0,92980138*
2 C	*0,006813*	*0,008544*	*-0,004961*	*0,001731*	*0,011774*	*0,01475578*	*0,10036655*
3 C	*0,326785*	*0,339649*	*0,319447*	*0,012864*	*0,007338*	*0,10965817*	*0,06255221*
4 C	*0,064925*	*0,094115*	*-0,017182*	*0,02919*	*0,082107*	*0,24882789*	*0,69991476*
5 C	*0,065646*	*0,110527*	*-0,037959*	*0,044881*	*0,103605*	*0,3825846*	*0,88317279*
6 C	*-0,255488*	*-0,269229*	*-0,219463*	*-0,013741*	*-0,036025*	*-0,11713409*	*-0,30709232*
10 Cl	*0,085605*	*0,192354*	*-0,062824*	*0,106749*	*0,148429*	*0,90997357*	*1,2652715*
11 C	*0,228076*	*0,257375*	*0,164478*	*0,029299*	*0,063598*	*0,24975705*	*0,54213622*
12 C	*0,497428*	*0,502755*	*0,442868*	*0,005327*	*0,05456*	*0,0454096*	*0,46509249*
13 N	*-0,710139*	*-0,691661*	*-0,728294*	*0,018478*	*0,018155*	*0,15751428*	*0,15476089*
14 O	*-0,348505*	*-0,296005*	*-0,526974*	*0,0525*	*0,178469*	*0,44753218*	*1,52134515*
15 O	*-0,393821*	*-0,358272*	*-0,531041*	*0,035549*	*0,13722*	*0,30303469*	*1,16972125*
16 C	*0,261045*	*0,310273*	*0,214943*	*0,049228*	*0,046102*	*0,41964027*	*0,39299292*
19 C	*0,178813*	*0,287882*	*0,164944*	*0,109069*	*0,013869*	*0,92975023*	*0,11822522*
22 N	*-0,450813*	*-0,373956*	*-0,446049*	*0,076857*	*-0,004764*	*0,65516154*	*-0,04061035*
23 C	*0,15873*	*0,351958*	*0,121121*	*0,193228*	*0,037609*	*1,64715711*	*0,320595*
27 C	*0,16393*	*0,364163*	*0,135052*	*0,200233*	*0,028878*	*1,70687068*	*0,24616827*

The calculated Fukui indices are presented in Table 5. The parameters were calculated for C, N, O and Cl atoms. It has been reported that as the Mulliken charges of the adsorbed centre become more negative, more easily the atom donate its electrons to the unoccupied orbital of the metal [23].

From the Table 5, it is clear that carbon, nitrogen and oxygen and chlorine atoms have high charge densities. The regions of high charge densities are generally the sites to which electrophiles can attach [24]. Therefore C, N, O and Cl atoms are the active centers, which have the strongest ability to bond the metal surface.

The local reactivity of the I1 inhibitor can be analysed by condensed Fukui functions.

The condensed Fukui functions and condensed softness indices help to distinguish each part of the molecule based on its distinct chemical behavior due to the different functional groups. Thus, the site for nucleophilic attack will be more is more where f_k^+ value is high. In turn, the electrophilic attack is controlled by f_k^- .

The most reactive sites for nucleophilic attack for I1 are C23, C27 and N22.

The most reactive sites for electrophilic attack for I1 are O14, C 10.

Table 5 shows these results. The condensed local softness indices S_k^+ and S_k^- are related to the condensed Fukui functions. The local softness follows the same trend of Fukui functions.

IV. CONCLUSION

The correlation between the effectiveness of the inhibition of 5-chloro-1- (2- (dimethylamino) ethyl) indoline-2,3-dione (I1) and quantum chemical parameters was studied using DFT / B3LYP /6-31G calculation.

The effectiveness of inhibition of the I1 inhibitor is squarely related to quantum chemistry parameters, such as molecular orbital (E_{HOMO}) of longest high energy of the lowest unoccupied molecular orbital (E_{LUMO}), energy gap (ΔE), softness (σ), global hardness (η), and the values of the Fukui functions.

This is in a good agreement with the experimental observations suggesting that the I1 inhibitor has the highest inhibition efficiency.

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