

A Corrosion Inhibition Study of Some Organic Substances Using DFT Calculations

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Department of chemistry, college of science of women, University of Baghdad,
Baghdad, Iraq

Corresponding author email: manalohamzah@gmail.com

Abstract

The density functional theory DFT at B3LYP hybrid and 6-311++G basis set have been implemented to investigate the corrosion inhibition of mild steel Fe and copper Cu using some organic compounds that have amid group. The surface energies and electronegativity equations of Pauling and Mullikan were used to calculate the quantum scales factors of inhibition (electronegativity, hardness, softness, and the fraction and energy of charge transfer) of these compounds. For mild steel metal, the results showed that some compounds have high tendency to donate electrons to the metal, Fe since these have low electronegativity scales. Conversely, the others tend to accept electrons and forming the feedback bond of inhibition. But for copper, it is found that all compounds have tendency to accept the charge from the metal since its electronegativity lower than that of inhibitors. Thus it is expected that some compounds have high efficiency of inhibition towards Fe. The other substances have lower inhibition efficiency. But for copper, the corrosion inhibition using these compounds is less efficient.

Keywords: corrosion inhibition, DFT, electronegativity, organic, mild steel.

1. Introduction

In industry, the organic substances are used widely for applications of a corrosion inhibition. Corrosion is defined as the act of loss of metal when expose to corrosive agents such as acids solutions. And it has bad impacts on economic and environment (Pathak & Mishra 2016),(Onwumelu et al. 2018). Non-metallic materials such as plastics, ceramic, concrete and rubber also found affected by the corrosive agents (Grilli et al. 2018). The manufactured substances that have hetero atoms such as (O, N, P and S) and π -bond were used as corrosion inhibitors since it have the ability to adsorbed on the metal surface (Uwiringiyimana et al. 2016), (Bakri et al. 2017). The process of inhibition is happened by form a protective layer of inhibitor on the surface of metal substances prevents the diffusion of oxygen and water throughout the metal. And it is driven by the difference of potential energies of the metal

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and the corrosion product (Murthy & Vijayaragavan 2014). Sometimes these inhibitors are added to the paints to help protection (Grilli et al. 2018). Corrosion inhibition was studied experimentally and theoretically. Experimental studies involved using the weight-loss and electrochemical techniques. The corroded metals that studied commonly were the carbon steel (Chen et al. 2019),(Fouda et al. 2017),(Idouhli et al. 2018), mild steel (Onwumelu et al. 2018),(Gupta et al. 2017),(Hazani et al. 2019),(Guo et al. 2017), copper (Tasić et al. 2019), Zinc (Sachin et al. 2019), and aluminum (Uwiringiyimana et al. 2016). Using drugs as corrosion inhibitors consider a new route of research. This method as so-called green corrosion inhibition is an alternative of using organic substances to avoid the poisonousness of these substances. This safely protection is related in some drugs to a heterocyclic group that is eco-friendly to the environment. Besides, drugs are available and do not cost much money (R. S. Abdel Hameed 2013),(Gupta et al. 2017),(Rani & Basu 2012). Experiments showed that the high concentrations of organic substance decreased the corrosion (Uwiringiyimana et al. 2016). Rani and Basu (Rani & Basu 2012) also stated that the high basicity and electron density behind the good ability of organic substances as corrosion inhibitors in addition to their chemical structures and physicochemical properties. Some theoretical models are built to discuss this effect. The frontier molecular orbital theory through the quantum mechanics calculations was also used to study the effect of some drugs as anti-corrosion of carbon steel and mild steel in acidic solutions (Bakri et al. 2017),(Gupta et al. 2017),(Tasić et al. 2019),(Rani & Basu 2012),(Lgaz et al. 2016),(Sinph et al. 2019).

In the present study, the density functional theory calculations DFT were carried out to study the corrosion inhibition of mild steel and copper using some organic compounds. The obtained surface energies, the highest occupied molecular orbital HOMO and the lowest unoccupied molecular orbital LUMO which are relatively linked to the inhibitors were used to calculate the electronegativity, hardness, softness, and the fraction and energy of the charge transfer, the corrosion parameters that help to discuss the mechanism and magnitude of corrosion inhibition on these metals. The physical and chemical properties of inhibitors also calculated.

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2. The Method of calculations

The set of compounds under study consist of 10 dimers of acids and esters, Table 1. These organic compounds contain amid group which they used finally as inhibitors of corrosion of mild steel Fe and copper Cu. The models of inhibitors are built and their physical and chemical properties are analyzed, Table 2. The Density functional theory with B3LYP hybrid and 6-311++G basis set was applied to optimize energy of compounds at their equilibrium geometries. The scale factors of corrosion inhibition (electronegativity χ , hardness η , softness S , the fraction of electron transfer ΔN and the energy of charge transfer $E_{transfer}$) were then calculated using the follow equations (Pearson 1985),

$$\chi = 1 / 2 (EA + EI) \quad \dots\dots\dots (1)$$

$$\eta = 1 / 2 (EI - EA) \quad \dots\dots\dots (2)$$

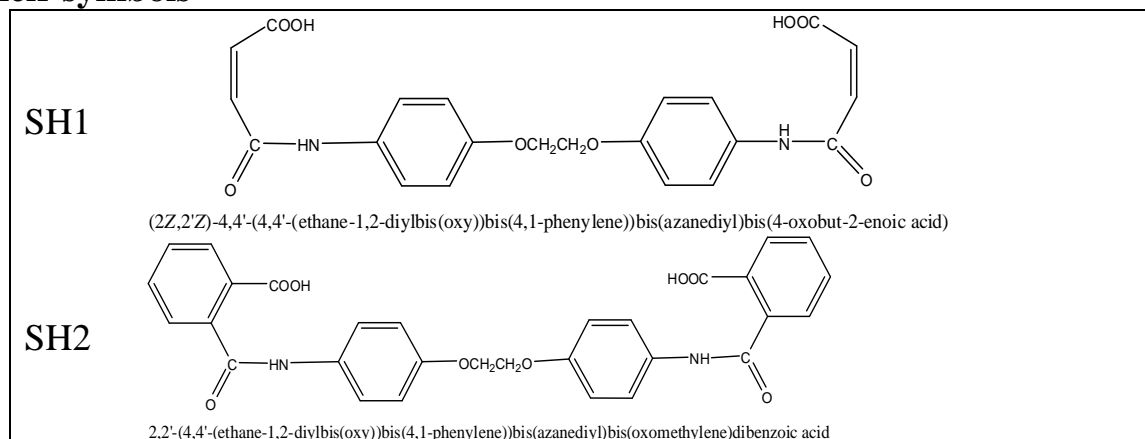
$$S = 1 / \eta \quad \dots\dots\dots (3)$$

$$\Delta N = \frac{[\chi_A - \chi_D]}{2[\eta_A + \eta_D]} \quad \dots\dots\dots (4)$$

$$E_{transfer} = \frac{[\chi_A - \chi_D]^2}{4[\eta_A + \eta_D]} \quad \dots\dots\dots (5)$$

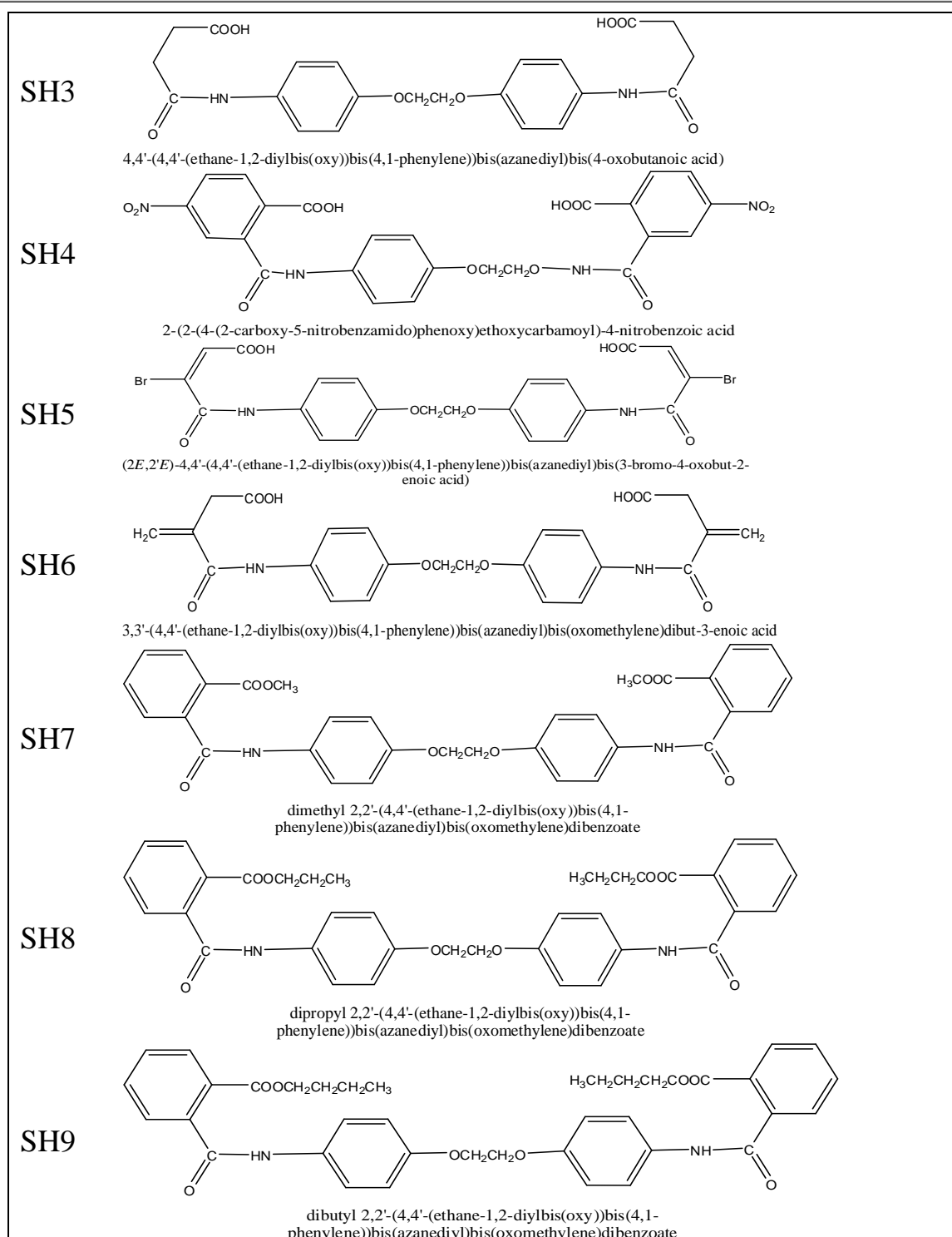
where, EI is the ionization energy, EA is the electronic affinity towards adsorption, the electronegativity of the metal (acceptor of electrons) χ_A was appointed as (7) for Fe and (4.48) for Cu and their hardness η_A as (0), χ_D is the calculated electronegativity of the inhibitor (donor) and η_D is its calculated hardness factor.

Table 1: The geometrical structures of organic compounds and their symbols



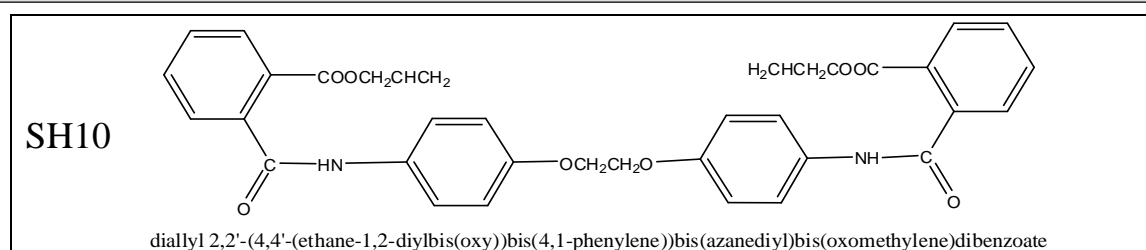
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3. The Results and discussion

3.1. The physical and chemical properties

As shown in Table 2 which includes the calculated physical and chemical properties of inhibitors, the heat of formation ΔH_f of all models (SH1-SH10) obtained using PM3 calculations at their minima energies are with (-) sign. This sign indicates an exothermic process of compounds formation in addition to big stability. In comparison, SH3 has the smallest value of formation enthalpy (-272.129) Kcal/mol, the smallest value of boiling point (1351.96) K and the smallest value of Gibbs energy (-676.06) KJ/mol. Thus, thermodynamically SH3 considers the most stable than others. The value of Gibbs energy was found allow strong and spontaneous adsorption of the compound on the metal surface when they are in contact (Tasić et al. 2019).

Table 2: The physical and chemical properties of organic compounds (inhibitors)

| Comp. | Chemical Formula | Molecular Weight | Heat of Formation [Kcal/mol] | Boiling Point [K] | Melting Point [K] | Gibbs Energy [KJ/mol] |
|-------|---|------------------|------------------------------|-------------------|-------------------|-----------------------|
| SH1 | C ₂₂ H ₂₀ N ₂ O ₈ | 440.12 | -210.843 | 1360.28 | 1103 | -515.62 |
| SH2 | C ₃₀ H ₂₄ N ₂ O ₈ | 540.52 | -198.280 | 1598.32 | 1281.2 | -403.14 |
| SH3 | C ₂₂ H ₂₄ N ₂ O ₈ | 444.43 | -272.129 | 1351.96 | 1113.16 | -676.06 |
| SH4 | C ₃₀ H ₂₂ N ₄ O ₁₂ | 630.52 | / | / | / | / |
| SH5 | C ₂₂ H ₁₈ Br ₂ N ₂ O ₈ | 598.19 | -204.763 | 1492.36 | 1194.68 | -504.08 |
| SH6 | C ₂₄ H ₂₄ N ₂ O ₈ | 468.46 | -235.084 | 1390.84 | 1104.26 | -500.64 |
| SH7 | C ₃₂ H ₂₈ N ₂ O ₈ | 568.57 | -184.855 | 1469.5 | 1067.2 | -319.22 |
| SH8 | C ₃₆ H ₃₆ N ₂ O ₈ | 624.68 | -199.984 | 1561.02 | 1112.28 | -285.54 |
| SH9 | C ₃₈ H ₄₀ N ₂ O ₈ | 652.73 | -209.322 | 1606.78 | 1134.82 | -268.7 |
| SH10 | C ₃₆ H ₃₂ N ₂ O ₈ | 620.65 | -106.888 | 1554.38 | 1108.78 | -109.86 |

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3.2. The parameters of corrosion inhibition

The calculated parameters of corrosion inhibition using DFT calculations are listed in Table 3. As illustrated in (Idouhli et al. 2018) and (Gupta et al. 2017), the HOMO energy correlate to the ionization energy EI (the energy absorbed when an atom donates the electron). On the other side, the LUMO energy link to the electron affinity EA (the energy released when atoms accepting electrons). The inhibitor expects to react with the metal to form a complex by sharing the electron pairs rather than oxygen. In consequences, the formation of the corrosion production is inhibited. The stability of the formed complex depends on the interaction between the metal as the acceptor of electrons and the inhibitor as the donor through a charge transfer. As shown in Table 3, SH4 has the highest value of HOMO (-8.118) eV. For this reason it has the highest tendency of electrons donation when it absorbed on the metal surface. In contrast, SH8 has the lowest value of HOMO (-10.998) eV. Thus it has the lowest tendency to donate electrons. Conversely, SH3 has the highest value of LUMO (-1.617) eV thus it has the lowest ability to accept electrons whereas SH4 has the lowest energy of LUMO (-7.212) eV subsequently it has the highest tendency of electrons acceptance. As stated by Idouhli et al. when the HOMO energy of the compound is high, it tends to donate electrons. Subsequently, the inhibition efficiency expects to increase. And when the LUMO energy is low, the compound tends to accept electrons and the inhibition efficiency expected to decrease (Idouhli et al. 2018). The difference between HOMO and LUMO (E_{gab}) describes the reactivity of a molecule towards adsorption inhibition. SH4 has the smallest E_{gab} (0.906) eV, whereas SH8 the highest E_{gab} and it is equal to (9.293) eV. The other compounds have moderate values of E_{gab} . Their sequences are found as (SH1 < SH2 < SH6 < SH5 < SH3 < SH7 < SH10 < SH9). The molecule with low E_{gab} has better reactivity towards adsorption on the metal surface. Hence the inhibition efficiency of corrosion has the opposite sequence.

Electronegativity χ , the tendency of the atom to attract the electron pairs towards itself or the accumulation of charges on the atom, is another important factor affects the corrosion inhibition of metal by organic substances. The results showed that SH1 has the highest scale of electronegativity and it is equal to (8.287). This factor is lowered by (0.706) in SH2, the acid that substituted with phenyl group. And it decreased to the lowest value in SH3 ($\chi= 5.457$). Since SH1 is alkene and SH3 is alkane,

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hence the π -bond of alkene in addition to presence the phenyl ring caused the increasing of electronegativity to the highest. Conversely, the sigma bond of SH3 caused the decreasing of electronegativity to the least. SH4 has the next highest value of this factor ($\chi= 7.665$) whereas SH5 has just (6.917). It is expected that the NO_2^- group as donating group of electron caused this increasing in this factor more than Br^- group in SH5. That scale factor of SH6 is equal to (7.056). Significantly, for the esters (SH7-SH9), the χ of these compounds decreased in sequences as the length of alkyl substitution increased as SH7 with methyl group is (6.492), SH8 with propyl group is (6.351) and SH9 with butyl group is (6.331). The allyl group of SH10 also lowered the electronegativity to the least ($\chi= 6.111$). It noticed that the π -bond and NO_2^- cause increasing the electronegativity whereas sigma bond, alkyl and allyl groups cause decreasing this factor. But the substitution with Br^- still has moderate effect on this factor despite the presence of π -bond. The general correlation of this factor for all compounds under study is (SH1 > SH4 > SH2 > SH6 > SH5 > SH7 > SH8 > SH9 > SH10 > SH3). The charge is moving from a species with low electronegativity to that with high electronegativity (Pearson 1985). Therefore this correlation is the opposite of tendency to donate electrons to the metal. And it expected it is the opposite of the efficiency of corrosion inhibition. Also, for the corrosion inhibition of mild steel it is expected that some compounds (SH3, SH5, SH7-SH10) tend to donate electrons to the metals since their electronegativity lower than that of mild steel (Fe). The other molecules (SH1, SH2, SH4 and SH6) tend to accept the charges from the metal and form the feedback-bond because their high electronegativity. The significant result is that all compounds under study expected to accept electrons from the metal (Cu) during the adsorption since their electronegativity higher than that of the metal, copper. This could decrease their efficiency of inhibition (Tasić et al. 2019). This result improved by the charge transfer fractions of inhibitors with Cu since these values are found below the zero (0).

In coordination chemistry, the hardness is a non-polarization property and the softness is a polarization property (Pearson 1963). These factors consider good indicators of reactivity towards adsorption inhibition (Tasić et al. 2019),(Gupta et al. 2017). Table 3 shows that SH4 has the lowest value of hardness ($\eta= 0.453$). Thus it has the lowest anti-polarization ability. Whereas SH8 has the highest value of anti-polarization ability and it is equal to (4.646). As the softness is the inverse of hardness, Equation 2, SH4 has the highest significant value of softness ($S= 2.207$) but SH8 has the lowest value

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of softness ($S= 0.215$). As shown in Table 4, the charges in SH4 focused highly on the NO_2^- since this group has high ability of charge polarization. In contrast, the alkyl group showed high ability to withdraw the charges towards other atoms. Hence its ability of polarization decreased to the least. Thus SH4 consider the softest base and SH8 the hardest base. The overall correlation of softness is (SH4 > SH1 > SH2 > SH6 > SH5 > SH3 > SH7 > SH10 > SH9 > SH8). As noticed it is the same relation as that of reactivity E_{gab} . It is mentioned that the more softness of molecule causes the higher tendency of adsorption on the metal surface. accordingly, the efficiency of corrosion inhibition has the same correlation (Lgaz et al. 2016).

The other factor that affect the inhibition is the fraction of electron transfer ΔN . As shown in Table 3, SH4 has the highest value of ΔN (0.733). And SH6 has the lowest ΔN (0.008). In accordance, the efficiency of charge transfer of SH4 is high and that of SH6 is low. For the esters (SH7-SH9), this factor increased as the length of alkyl substitution increased. The SH10 found has the highest value of ΔN among the other esters and it is equal to (0.103). It is expected this increasing due to the allyl group. The general sequence of charge transfer is (SH4 > SH1 > SH3 > SH10 > SH2 > SH9 > SH8 > SH7 > SH5 > SH6). This correlation indicates the amount of charge transferring during the adsorption of compounds on the metal surface. Regarding the energy of charge transfer E_{transfer} , it is shown, for the acids group (SH1-SH6), the highest energy required for charge transfer from inhibitor to the metal is related to SH4 and it is equal (0.2440). And the lowest energy is associated with SH6 ($E_{\text{transfer}}= 0.00024$). The E_{transfer} of esters group (SH7-SH10) also increased as the length of substitutions increased. The sequence of charge transfer energy is (SH4 > SH1 > SH3 > SH10 > SH9 > SH8 > SH2 > SH7 > SH5 > SH6).

The inhibition sites of the organic compounds

Table 4 shows the figures of inhibitors (SH1-SH10) with their atom labels and serial number on the left side and their surface molecular orbitals, HOMO and LUMO on the right side. These surfaces as labeled with red (HOMO) and blue (LUMO) colors show clearly the charge distribution or the active sites of adsorption since these orbitals correlate to ionization energy and electron affinity, respectively. As shown, for (SH1-SH3) and (SH6-SH10), the active sites are (C2-C7, C9-C10), (O8, O11) and N1. For these compounds, the oxygen atom (O8) with high electronegativity has the highest ability to attract the charges. And N and the other C atoms come next. The

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alkyl groups of (SH7-SH10) have high ability of anti-polarization (withdrawing electrons). Thus, these groups offer the electrons and enable these compounds to act as donors. These positive charge species are exposed to attack by the molecules with the negative charges (nucleophilic attack). For the other compounds, the active sites of SH4 are (C12-C17), N21, and (O22 and O23). And those sites for SH5 are (C12-C17), N21, and Br17. In these two compounds, NO₂ and Br groups have higher ability to attract the charges than the other atoms (electrophilic attack). Thus these compounds expected to act as charge acceptors. But it is found that the polarization of NO₂ is much more than that of Br. This difference is shown clearly through the value of softness, a scale factor of polarization, Table 3. Accordingly, SH5 tends to act as a donor because it's electronegativity also lower than that of Fe. All these sites expected to receive the charges from the copper Cu since its electronegativity χ smaller (4.48) than that of inhibitors.

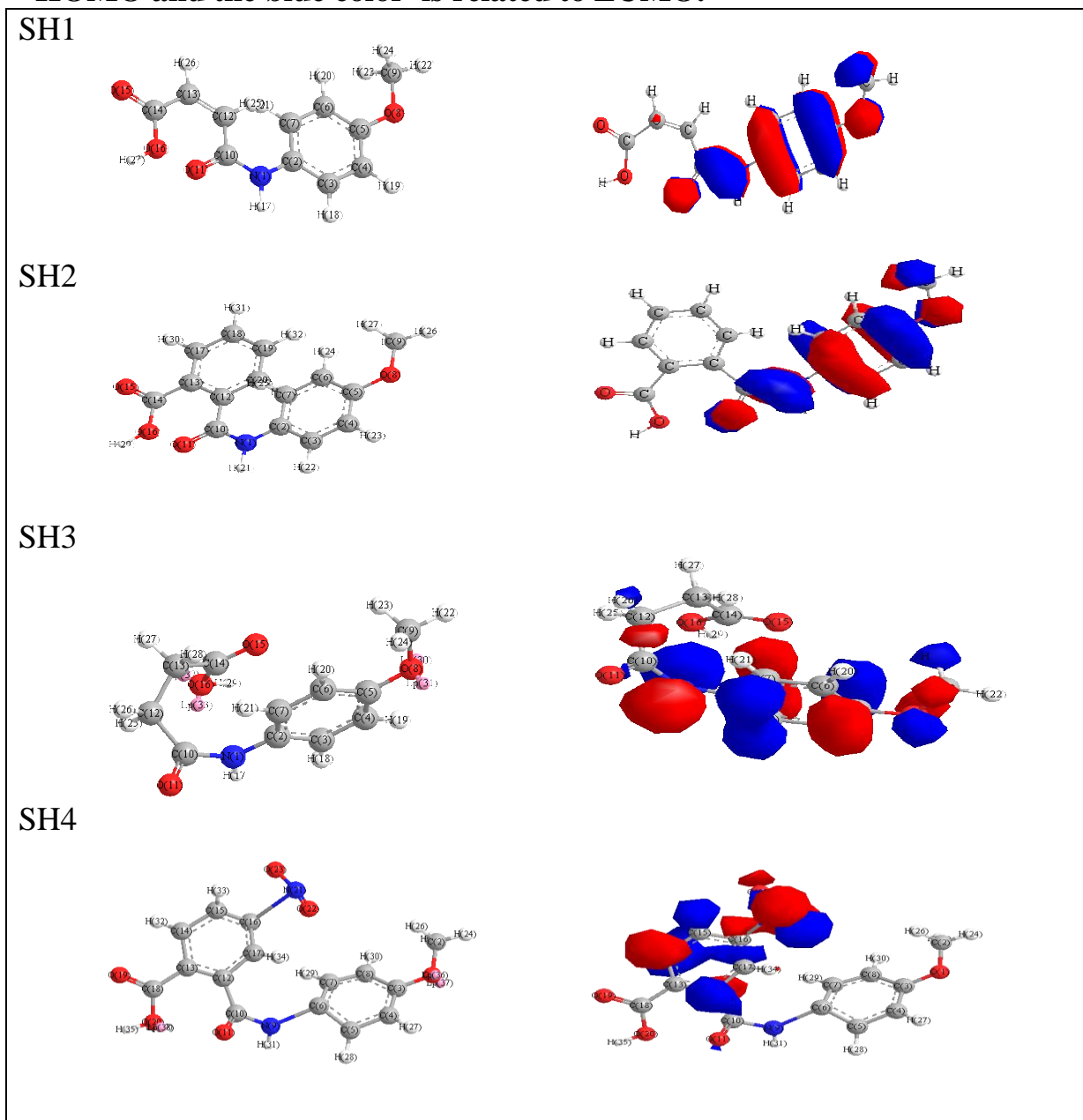
Table 3: The parameters of corrosion inhibition of inhibitors calculated using DFT calculations

| Comp | HOMO | LUMO | E _{gab} | χ | η | S | ΔN_{Fe} | $\Delta E_{trans.}$ | ΔN_{Cu} |
|------|---------|--------|------------------|--------|--------|-------|-----------------|---------------------|-----------------|
| SH1 | -10.801 | -5.773 | 5.028 | 8.287 | 2.514 | 0.397 | 0.255 | 0.1647 | -0.757 |
| SH2 | -10.638 | -4.365 | 6.273 | 7.501 | 3.136 | 0.318 | 0.080 | 0.0203 | -0.285 |
| SH3 | -9.297 | -1.617 | 7.680 | 5.457 | 3.840 | 0.260 | 0.200 | 0.1550 | -0.127 |
| SH4 | -8.118 | -7.212 | 0.906 | 7.665 | 0.453 | 2.207 | 0.733 | 0.2440 | -3.515 |
| SH5 | -10.655 | -3.179 | 7.476 | 6.917 | 3.738 | 0.267 | 0.011 | 0.0004 | -0.325 |
| SH6 | -10.195 | -3.917 | 6.278 | 7.056 | 3.139 | 0.318 | 0.008 | 0.0002 | -0.410 |
| SH7 | -10.793 | -2.192 | 8.601 | 6.492 | 4.300 | 0.232 | 0.059 | 0.015 | -0.468 |
| SH8 | -10.998 | -1.705 | 9.293 | 6.351 | 4.646 | 0.215 | 0.069 | 0.022 | -0.402 |
| SH9 | -10.904 | -1.758 | 9.146 | 6.331 | 4.573 | 0.218 | 0.073 | 0.024 | -0.404 |
| SH10 | -10.427 | -1.796 | 8.631 | 6.111 | 4.315 | 0.231 | 0.103 | 0.045 | -0.377 |

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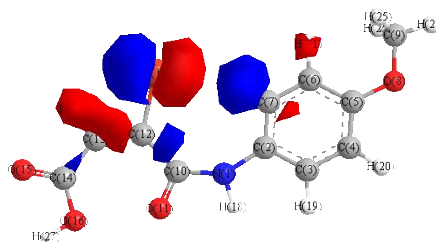
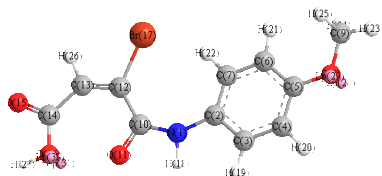
Table 4: The left side is the 3D structures and the right side is the HOMO and LUMO molecular orbitals of inhibitors as calculated using DFT/B3LYP and 6-311++ G calculations where the red color is related to HOMO and the blue color is related to LUMO.



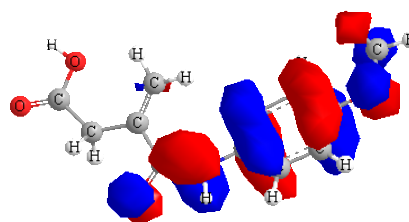
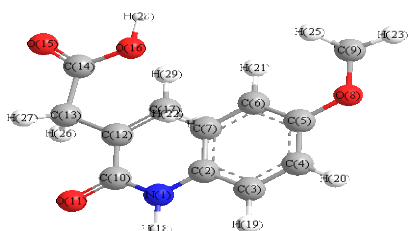
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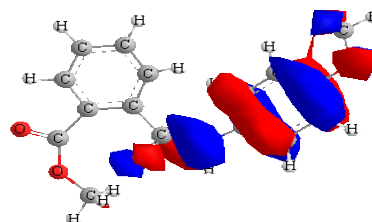
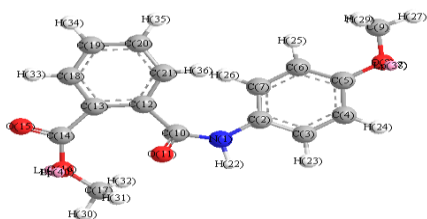
SH5



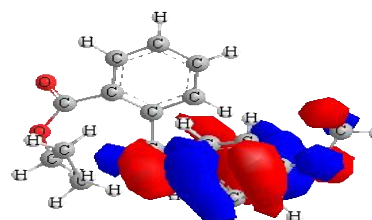
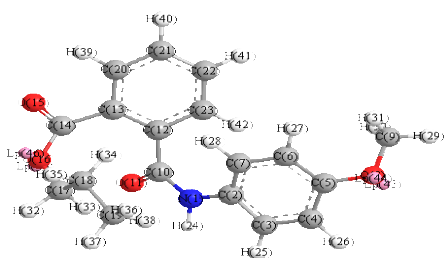
SH6



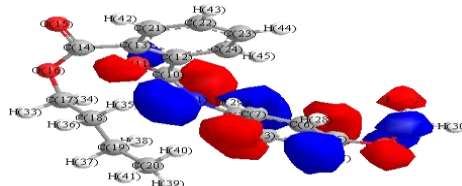
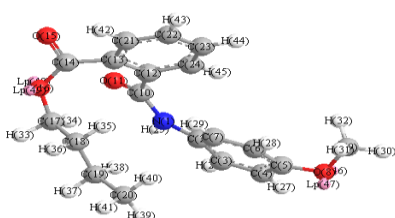
SH7



SH8

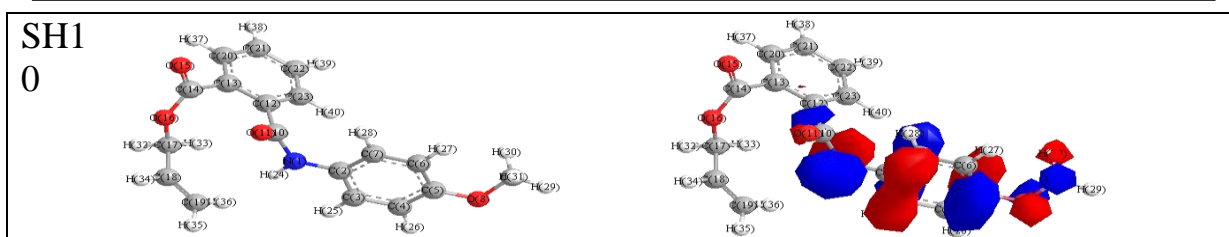


SH9



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Conclusions

The frontier molecular orbital theory offers a good insight of corrosion inhibition. The calculated scale factors help to understand and discuss the direction and the scale of corrosion inhibition. The results revealed that all the organic compound under study have the ability to adsorbed and inhibit the corrosion of mild steel in different values throughout their active site. The esters (SH7-SH10) in addition to two of the acids (SH3 and SH5) have the ability to offer electrons to the unoccupied orbital of the metal, d-orbital. The other acids (SH1, SH2, SH4 and SH6) have the ability to accept electrons from the metal and forming feedback bond as a result of this acceptance. The interaction between these compounds and the metal assist to inhibit the corrosion. For the copper, its electronegativity lower than that of inhibitors hence it is expected the inhibition is not efficient. It tends to donate the charge rather than accept it. This result is confirmed by the negative values of ΔN .

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