



Theoretical Determination of Corrosion Inhibitor Activities of Naphthalene and Tetralin

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Highlights

- Inhibitor derivatives can be effective anti-corrosion agents.
- Organic corrosion inhibitor has a relationship with the quantum chemical parameters.
- The naphthalene molecule has the most beneficial corrosion inhibition impact compared to tetralin.

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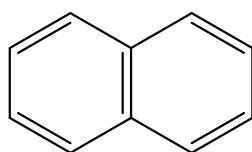
Inhibitor activity

Abstract

Quantum mechanical methods were used to investigate the corrosion inhibitor activities of tetraline and naphthalene compounds. In this study, some parameters were estimated, including, the energy of the highest occupied molecular orbital (E_{HOMO}), the energy of the lowest occupied molecular orbital (E_{LUMO}), the energy bandgap ($\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}}$), and the dipole moment (μ). The aforementioned parameters give information about the corrosion efficiency of organic compounds. Furthermore, the density functional theory (DFT) was handled to determine the geometry of the molecules and electronic characteristics of the compounds. B3LYP/6-31G (d, p) was utilized to determine physical parameters such as hardness (η), softness (σ), and electronegativity (χ). We also evaluated quantum chemistry characteristics including the fraction of electrons transported (ΔN) between the iron surface and our title compounds. This study also discusses which parameters have a significant linear relationship with inhibitory performance. The findings suggest that the behavior of organic-based corrosion inhibitors is correlated with the effectiveness of good corrosion inhibitors and the quantum chemical parameters measured from this process. As a result, the behavior of corrosion inhibitors can be determined without the need for an experiment.

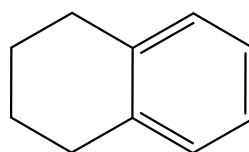
1. INTRODUCTION

Naphthalene is made of two benzene rings bonded in ortho positions (Figure 1A). Naphthalene is colorless and possesses the odor of mothball and at room temperature, it can form a shiny flaked crystalline structure. At room temperature, it slowly sublimates and melted at 82.2 °C. Naphthalene is hydrophobic, while it can dissolve in alcohol and highly soluble in ether and benzene. It is very volatile and burns with a smoky flame [1]. There are some drugs containing naphthalene, such as nafcillin, naftifine, tolinaftate, and terbinafine [2], which play a crucial role in the management of microbial infections. Naphthalene mono hydroxide derivatives are called naphthol [3, 4].



naphthalene

A



1,2,3,4-tetrahydronaphthalene

B

Figure 1. Chemical structure for A) naphthalene B) tetralin

Tetralin (1,2,3,4-tetrahydronaphthalene), on the other hand, is made up of two moiety: aromatic and alicyclic (Figure 1B). The chemical can be found in coal tar and petroleum, moreover, it can be made from naphthalene using catalytic hydrogenation or anthracene through cracking for industrial use. Tetralin compound is commonly used in the petrochemical industry as a solvent, where it is especially used in conjunction with liquefaction coal. It can be also used as an alternative for turpentine in each of paints and waxes [5]. Tetralin was increasingly degraded by mixed microorganism cultures [6] or by the presence of substrate [7].

Corrosion-preventive (inhibitor) characteristics are found in many organic compounds, and they have major economic implications [8]. Corrosion of metals, such as mild steel, causes many problems for various sectors. This condition can occur in several stages, especially during stages such as steel pickling, acid washing, and etching [9, 10]. The corrosion inhibitors are a tiny number of chemical substances that prevent metal from corroding in harsh settings. These inhibitors are extensively employed in production industry for chemical cleaning solutions, industrial water, and petrochemical engineering because they are a cost-effective and efficient way to prevent metal and alloy corrosion [11]. It can be stated that inhibitors act by altering the kinetics of electrochemical processes including the corrosion mechanism.

According to the available evidence, nearly all organic inhibitors function through adsorption on the metal surface. It is reported that the organic inhibitor molecules may usually adsorb onto metal and change physical or chemical properties [12]. Calculations based on quantum chemistry have shown to be a reliable tool for investigating corrosion inhibition mechanism [13] because significant associations were observed between the efficiencies of most compounds and various semi-empirical corrosion inhibition characteristics. The quantum chemical theory is a valuable method for predicting the inhibition capacity that are structurally related organic compounds [14-16].

The purpose of this research was to see how effective naphthalene and tetralin were at inhibitor activity. B3LYP/6-31G (d,p) was utilized to estimate structure of the molecules attributes of the aforementioned compounds. Molecular orbital computations are commonly utilized to satisfy good theoretical parameters to identify inhibitors in order to understand the corrosion inhibition process and then to imitates the inhibitor adsorption method on the metal surface.

2. CALCULATION METHODS

GaussView5.0, a molecular imaging tool, was used to map the three-dimensional form of the molecular compounds in the gas phase and the base case [17, 18]. The GaussView 5.0 packet program was used to establish the starting geometries of the molecules, and the Gaussian09W software was used to perform the calculations [19, 20]. Because the electron density is taken into consideration in the DFT approach, it can produce the needed data for a more accurate measurement of the electronic characteristics of compound structures [21, 22]. DFT was also one of the first techniques to show a significant advantage against Hartree-Fock [23]. For various reasons, B3LYP is commonly used [24], which is faster than most techniques used for Post Hartree-Fock and usually yields comparable performance [21]. For a DFT process, it's also pretty robust. In addition, in the Gaussian09W program, the hybrid feature B3LYP is suited for the number of workstations and 6-31G G capacity (d, p) as the basis set [25]. From geometry-optimized structures, identifiers of electronic structures were found, and E_{HOMO} , E_{LUMO} , ΔE , σ , χ , nucleophilicity (ϵ) index, electrophilicity (ω) index, chemical potential (μ), μ and ΔN linked to corrosion inhibitory action were estimated. Also, the identifier's electronic structure was investigated.

3. RESULTS AND DISCUSSION

3.1. Geometry Optimization

Table 1 lists the electronic structures and geometric properties, including the lengths of the bonds, bond angles, and dihedral angles of the naphthalene and tetralin inhibitors obtained in a gaseous phase. Figure 2 shows the molecular structures after optimization with calculated ground energies. B3LYP/6-31G(d,p) base sets were used to obtain sophisticated geometry improvements.

Table 1. Some essential parameters, including bond length, Bond angle, and dihedral angle for both naphthalene and tetralin molecule

Naphthalene		Tetralin	
Symbol	Bond Length	Symbol	Bond Length
C1-C2	1.376307	C2-C1	1.5267557
C3-C2	1.4210268	C3-C2	1.5008836
C4-C3	1.433655	C4-C3	1.4105343
C5-C4	1.4210387	C5-C4	1.5008836
C6-C5	1.3763042	C6-C1	1.4476828
H7-C3	2.1645062	H7-C3	2.158854
H8-C1	1.0860828	H8-C1	1.0813542
H9-C2	1.087031	H9-C2	1.0849676
C10-C3	1.4210414	C10-C3	1.3829612
C11-C4	1.421033	C11-C4	1.3829612
H12-C5	1.0870321	H12-C5	1.0849676
H13-C6	1.0860824	H13-C6	1.0813542
C14-C11	1.3763034	C14-C11	1.4076745
C15-C10	1.3763032	C15-C14	1.392677
H16-C11	1.0870301	H16-C11	1.0867578
H17-C14	1.0860836	H17-C14	1.0862293
H18-C15	1.0860825	H18-C15	1.0862293
Symbol	Bond angle	Symbol	Bond angle
C3-C2	120.8679712	C3-C2-C1	108.7644895
C4-C3-C2	118.8476397	C4-C3-C2	104.6849883
C5-C4-C3	118.8454393	C5-C4-C3	104.6849883
C6-C5-C4	120.8684748	C6-C1-C5	61.7057142
H7-C3-C2	96.1731527	H7-C3-C2	108.8794089
H8-C1-C2	120.1002612	H8-C1-C6	135.2665001
H9-C2-C1	120.4211545	H9-C2-C1	120.2338254
C10-C3-C2	122.3068893	C10-C3-C2	134.320234
C11-C4-C3	118.8480087	C11-C4-C3	120.9947768
H12-C5-C4	118.7104922	H12-C5-C4	123.68896
H13-C6-C5	120.1004651	H13-C6-C1	135.2665001
C14-C11-C4	120.8673684	C14-C11-C4	118.1906017
C15-C10-C3	120.8679366	C15-C14-C11	120.8146207
H16-C11-C4	118.7105053	H16-C11-C4	121.4207727
H17-C14-C11	120.1010219	H17-C14-C11	119.49422
H18-C15-C10	120.1003839	H18-C15-C14	119.6911593
Symbol	dihedral angle	Symbol	dihedral angle
C4-C3-C2-C1	-0.0003329	C4-C3-C2-C1	30.0525829
C5-C4-C3-C2	0	C5-C4-C3-C2	-0.0056504
C6-C5-C4-C3	0.0002866	C6-C1-C5-C4	100.5365783
H7-C3-C2-C1	180	H7-C3-C2-C1	-149.9635128
H8-C1-C2-C3	-179.9996731	H8-C1-C6-C2	126.094165
H9-C2-C1-C6	180	H9-C2-C1-C6	108.2771407
C10-C3-C2-C1	180	C10-C3-C2-C1	-149.9586165

C11-C4-C3-C2	-180	C11-C4-C3-C2	-179.9963031
H12-C5-C4-C3	180	H12-C5-C4-C3	-179.9947554
H13-C6-C5-C4	179.9997201	H13-C6-C1-C5	126.094165
C14-C11-C4-C3	0	C14-C11-C4-C3	-0.0069456
C15-C10-C3-C2	-180	C15-C14-C11-C4	-0.0047713
H16-C11-C4-C3	180	H16-C11-C4-C3	179.9765771
H17-C14-C11-C4	-180	H17-C14-C11-C4	179.9930536
H18-C15-C10-C3	-180	H18-C15-C14-C11	-179.9870416

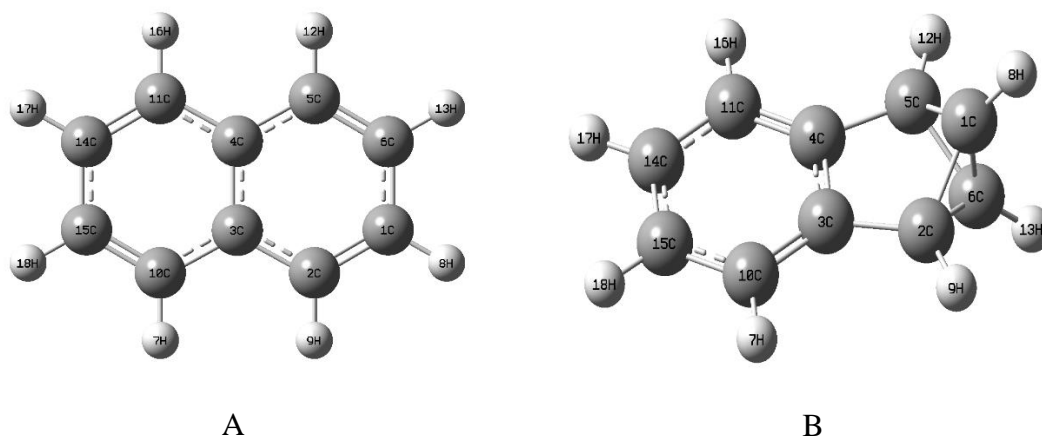


Figure 2. The inhibitor compounds' was optimized; A) naphthalene; B) tetralin

3.2. Inhibitor Parameters Activity

The molecular electronic structure indicates the bond structure of the molecules and identifiers of the electronic structure. The corresponding electronic structural parameters, including E_{HOMO} , E_{LUMO} , ΔE_{gap} , σ , χ , ρ , σ , χ , ε , μ , HOMO, and LUMO were derived from the Gaussian output of the molecular profile. The energy level of the highest occupied and lowest unoccupied are defined as E_{HOMO} and E_{LUMO} , respectively, whereby their values determine the reactivity or passivity of a material. The following equations show the electron affinity (A) and the ionization potential (I) of the compounds:

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

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

Calculate other identifies using equations was existed in the literature. Table 2 shows that there is a big difference between A and I value, moreover, the corresponding value of naphthalene are slightly more than tetralin. Additionally, ionization energy levels are linked to E_{HOMO} and E_{LUMO} values of any chemical type and electron affinity values, which were estimated according to Koopmans' theorem. Koopmans' theorem indicates that the negative energy of the HOMO equals the first ionization energy of a molecule [26, 27]. Normally inhibitors have a higher energy bandgap ($E_{\text{LUMO}} - E_{\text{HOMO}}$) compared to metallic materials. The energy bandgap (ΔE) of both inhibitors were calculated by the following equation:

$$\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}} \quad (3)$$

Atomic band structure achieves different properties when they bonded to other elements to make a compound. In this case, instead of atomic energy levels, we should deal with molecular orbitals, which are quite different from the components. The energy bandgap of naphthalene and tetralin are 4.823 and 5.579 eV, which extremely higher than metallic materials, and they are listed in the insulator materials. The hardness (η) and (χ) inhibitor are theoretically determined through the equation:

$$\eta = (I - A) / 2 \quad (4)$$

and

$$\chi = (I + A) / 2. \quad (5)$$

While Pearson experimentally calculates the χ and η for the single atoms. The electron affinity (A) and ionization potential (I) of a single metal are supposed to be equal ($I = A$), according to Pearson, the η metal value for a single metal is assumed to be zero. In this study, we are used iron single metal χ equal to 7 and η zero.

The softness (σ) and (Pi) were respectively calculated by using the following equations [28-30]:

$$\sigma = 1/\eta \quad (6)$$

$$Pi = -\chi. \quad (7)$$

The electrophilicity (ω) and nucleophilicity (ϵ) indexes are also related to the value of Pi and η :

$$\omega = Pi^2/2\eta \quad (8)$$

$$\epsilon = Pi \cdot \eta. \quad (9)$$

The electrophilicity index is the energy loss resulting from the entire electron flow between the transmitter and the receiver [31], whereas the new molecular structure identifier is the nucleophilicity index [23]. The following equation measures the ΔN by using the theoretical values of χ and η , it is show the the electrons transferred between the inhibitor and the metal [8]:

$$\Delta N = \frac{(\chi_{\text{metal}} - \chi_{\text{inhibitor}})}{2(\eta_{\text{metal}} - \eta_{\text{inhibitor}})} \quad (10)$$

Table 2. Identifiers electron structure calculated using B3LYP/6-31G(d, p) basis set

Parameters	Molecule Name	
	Naphthalene	Tetralin
Total Energy (a.u)	-385.905	-385.8
μ (D)	0	1.5713
E_{HOMO} (eV)	-5.802601584	-5.788995784
E_{LUMO} (eV)	-0.979345484	-0.209257204
ΔE (eV)	$\Delta E = E_{\text{HOMO}} - E_{\text{LUMO}}$	-4.8232561
I (eV)	$I = -E_{\text{HOMO}}$	5.802601584
A (eV)	$A = -E_{\text{LUMO}}$	0.979345484
χ (eV)	$\chi = (I + A) / 2$	3.390973534
η (eV)	$\eta = (I - A) / 2$	2.41162805
σ (eV)	$\sigma = 1/\eta$	0.414657642
Pi (eV)	$Pi = -\chi$	-3.390973534
ω (eV)	$\omega = Pi^2/\eta^2$	1.977097775
ϵ (eV)	$\epsilon = Pi \cdot \eta$	-8.177766891
ΔN	ΔN	0.717036013

Table 2 lists the electron structural descriptors for the compounds investigated. The energy values of HOMO and LUMO indicated that there is a general trend between the constructions studied. Since HOMO is connected to electron donating capacity, so it is critical in corrosion investigation. The HOMO of the

naphthalene is greater than the tetralin. The inhibitory action of inhibitor compounds becomes stronger as HOMO values rise [32], therefore, the naphthalene shows a better inhibitor feature compared to tetralin. This characteristic enables inhibitory chemicals to work on the charge transfer process throughout the surface of the metal while also allowing them to withstand the adsorption process. Based on the high E_{HOMO} value, the naphthalene molecule has the most potent inhibitor and the tetralin molecule possesses the lowest inhibitory activity (Figure 3).

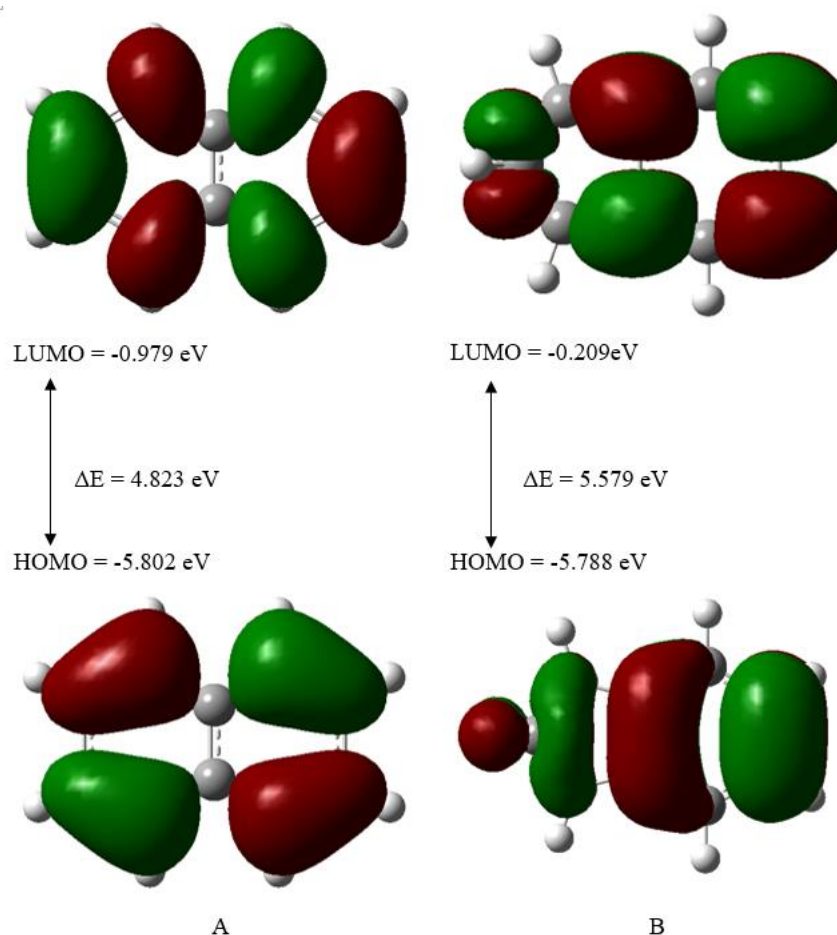


Figure 3. HOMO-LUMO and Energy bandgap of A) naphthalene B) tetralin

Because E_{LUMO} has a low value, the inhibitor might charge the metal surface with a further negative charge. Tetralin LUMO energy possesses the lowest energy, whereas naphthalene has the highest value of LUMO energy. For this reason, the naphthalene molecule inhibitor was found to be reactive by acting as a donor. As a result, its inhibitory activity was high. The undermost values of E_{LUMO} and E_{HOMO} are seen in the tetralin molecule inhibitor. Despite the fact that low- E_{HOMO} inhibitors diminish reactivity to metal inhibitors, the metal acts as a donor to the inhibitor. The inhibitor's action is reduced, while the metal's reactivity is boosted. The naphthalene molecule has the most powerful inhibition of corrosion based on energy band gaps (HOMO-LUMO).

For studying the inhibitor proficiency, it is necessary to compare the ΔE . The energy difference between E_{HOMO} and E_{LUMO} has a lot of preliminary relevance and clarification when it comes to determining theoretical inhibitory effectiveness and static molecular reactivity. The energy bandgap for naphthalene is smaller than tetralin. The lower value of the energy bandgap, the greater the inhibition efficacy. The energy bandgap's value is determined by E_{HOMO} instead of E_{LUMO} . With a high HOMO energy and low ΔE , inhibitor derivatives can be utilized as effective anti-corrosion agents [32]. According to the highest value of HOMO energy and the lowest value of ΔE , naphthalene will provide effective inhibitory action. Table 3 reveals that the charge distribution on the naphthalene and tetralin molecules. Mulliken population analysis (charge

Distribution) is a commonly utilized technique for estimating inhibitor adsorption [32]. Many researchers have reported that the existence of negatively charged heteroatoms enhances the ability of donor-acceptor mechanisms to adsorb on the metal surface [33]. With this fact, naphthalene has an important inhibitory effect owing to a higher negative charge at the center of the molecule. Molecular electrostatic potential map (MEP) Figure 4 shows the charge distribution on the molecule by color. It is seen the center of the naphthalene molecule has denser red color than the tetralin molecular center, the is indicated that naphthalene more absorb on the surface of the metal.

Table 3. Charge distribution on the atoms for both naphthalene and tetralin

Naphthalene		Tetralin	
Atoms	Charge distribution	Atoms	Charge distribution
C1	-0.092621	C1	-0.0872
C2	-0.128589	C2	-0.21306
C3	0.101945	C3	0.104271
C4	0.102287	C4	0.104271
C5	-0.128295	C5	-0.21306
C6	-0.09298	C6	-0.0872
H7	0.084669	H7	0.088095
H8	0.085517	H8	0.108209
H9	0.084611	H9	0.138355
C10	-0.128213	C10	-0.12439
C11	-0.128707	C11	-0.12439
H12	0.084744	H12	0.138355
H13	0.085556	H13	0.108209
C14	-0.092621	C14	-0.0942
C15	-0.092937	C15	-0.0942
H16	0.084528	H16	0.088095
H17	0.085522	H17	0.079917
H18	0.085582	H18	0.079917

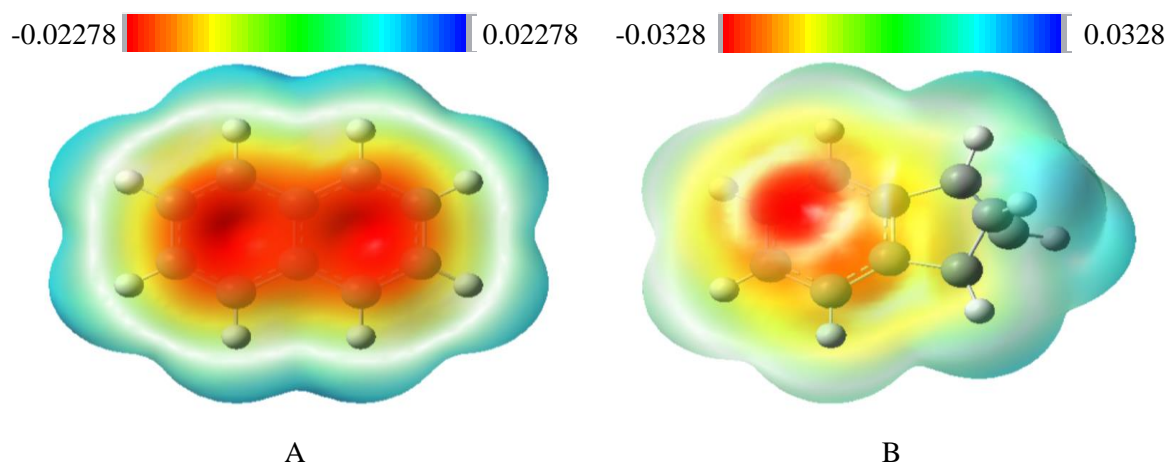


Figure 4. Molecular electrostatic potential map A) naphthalene B) tetralin

Other significant parameters that provide information on the stability, reactivity, and inhibitor activity of the inhibitor molecules are hardness and softness. The hardness (η) of naphthalene is less than tetralin, while the softness (σ) of tetralin is lower than naphthalene. Because the organic inhibitor chosen is Lewis-based, and soft inhibitors are more reactive than hard inhibitors, they act as more effective corrosion inhibitors [34-36]. Therefore, for this situation, the naphthalene inhibitor with high EHOMO and low ΔE was shown to have high softness and low hardness scores.

Additionally, χ and π are two important parameters, which were calculated to determine and compare the inhibitor activity of the compounds. The calculated values of the χ provide details about how the coordinated covalent bond happens between the metal and the inhibitor. In the current investigation, iron metal was used to examine our molecular inhibitor activity. It is found that the χ values of the inhibitors (Table 2) are smaller compared to the corresponding reported value for the iron metal. The iron metal takes electrons from the inhibitor compound to form bonds. Also, naphthalene was shown higher inhibitor reactivity with a lower χ value. The ΔN values for iron and metal inhibitors were obtained (Table 2) show that the naphthalene molecule can transfer more electrons to the iron metal that makes it a more powerful inhibitor.

Although there are no studies mentioned the direct correlation between dipole moment (μ) and the activity of inhibition, in some studies, the behavior of molecules with a higher μ have been determined as a good inhibition, whereas in other studies, the inhibition activity increases with a decrease in μ value. There is a low dipole moment in the naphthalene inhibitor, which is in line with other parameters. This can be translated at low μ values as a stronger coating of the metal surface.

The ω and ϵ indices are major features employed in the operations of inhibitors. Additionally, the ω index shows the inhibitor molecules' ability to admit electrons, whereas the ϵ index indicates the inhibitors' capacity to donate electrons [23, 31]. The activity of inhibition rises as the ϵ value decreases or the ω value increases. Naphthalene molecule has a lower value for ϵ and a higher value for ω which is opposite to tetralin molecule. It is noted that, according to ω and ϵ features, the naphthalene inhibitor possesses the highest powerful inhibitory effect.

4. CONCLUSION

In this study, the inhibitory of naphthalene and tetralin compounds were studied theoretically using the Gaussian package program. According to the results, the E_{HOMO} and E_{LUMO} of the inhibitor molecules have a higher value, also it is found that naphthalene inhibitor was more reactive compared to tetralin by taking on the role of a donor. With high E_{HOMO} and low ΔE , inhibitor derivatives can be utilized as good anti-corrosion agents. Based on the obtained results of E_{HOMO} and ΔE , naphthalene has the greatest value of E_{HOMO} , there is a substantial inhibitory activity. The Mulliken atomic charges of naphthalene showed that the inhibitory action is influenced significantly by electronegativity of atoms. It is possible to connect the negatively charged atoms at the centers of the naphthalene molecule to the metal surface. When compared to tetralin, the determined η , σ , χ , π , ω , and ϵ parameters support the naphthalene molecule having the maximum effective corrosion inhibition impact. The higher χ value of the inhibitor the more likely the iron metal forms a bond by stealing electrons from the inhibitor's molecule, and so ΔN can have the maximum value. Consequently, there is a near connection between the organic corrosion inhibitory with the quantum chemical parameters obtained for the compounds.

CONFLICTS OF INTEREST

No conflict of interest was declared by the authors.

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