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STUDYING α-TERPINENE, β-CARYOPHILLENE, α-ELEMENT AND α-HUMULENE COMPOUNDS AS CORROSION INHIBITORS USING THE DENSITY FUNCTIONAL THEORY (DFT) METHOD

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Corrosion Inhibitor
α-Terpinene
β-Caryophillene
α-Element and α-Humulene
DFT

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ABSTRACT

*The compounds α-Terpinene, β-Caryophillene, α-Element and α-Humulene are the main components of Toona sinensis leaf essential oil and have the highest % area from the research results of Toona sinensis leaf essential oil components. This research uses the Gaussian 16W program package with the Density Functional Theory (DFT) calculation method and the B3LYP/6-31G database which produces the optimal structure of the inhibitor molecule, the Highest Occupied Molecular Orbital (HOMO) contour, the Lowest Unoccupied Molecular Orbital (LUMO) contour, EHOMO, ELUMO and mulliken charge density. The inhibitor molecules analyzed were the compounds α-Terpinene, β-Charyophillene, α-Element and α-Humulene. Analysis of the reactivity of inhibitor molecules was carried out in the gas phase and with water as a solvent medium. Calculation of quantum chemical parameter values in the form of bandgap (ΔE), electronegativity (χ), ionization potential (I), hardness (η), softness (σ), electrophilicity (ω), nucleophilicity (ε), charge transfer (ΔN), interaction energy (Δψ), back donation energy (ΔEb-d). Based on the parameter results obtained, the best compound with potential as a corrosion inhibitor is α-Terpinen. Data on bond energy, Gibbs free energy (ΔG) and entropy (ΔS), bond length and bond angle were used to determine the interaction of α-Terpinene with Fe. The interaction that occurs is a chemical interaction because the ΔG value obtained is small from -40 kJ/mol,*namely -201,142 kJ/mol.

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INTRODUCTION

Corrosion is a decrease in the quality of metal due to electrochemical reactions with its environment. Many factors can cause corrosion of a material, one of which is the influence of the concentration of corrosion inhibitors. According to the basic ingredients they are made from, corrosion inhibitors can be divided into two types, namely inhibitors made from inorganic and organic materials. Organic inhibitors are a type of inhibitor that are non-toxic, cheap, readily available in nature, easily renewable and do not damage the environment. These organic inhibitors are obtained by extracting several materials found in nature (Sastri et al, 2011).

Most of the inhibitors that are often used are organic inhibitors because these inhibitors tend to be more environmentally friendly. Organic inhibitors derived from natural extracts that can be used effectively are compounds containing N, O, P. S atoms and atoms that have lone pairs of electrons. Natural extracts have been widely used as corrosion inhibitor compounds such as melinjo bark extract (Gnetum gnemon. L) (Emriadi et al., 2018), cocoa leaf extract (Theobroma cacao) (Yetri et al., 2017), cassava leaf extract (Manihot esculenta) (Gusti et al., 2016) and red suren (Toona sinensis) leaf extract (Emriadi et al., 2016)

The method for determining whether a compound can be said to be a corrosion inhibitor is divided into two, namely computational methods and experimental methods. With the development of technology, many researchers have conducted research using computational methods. One computational method is density functional theory (DFT). DFT is one of several popular approaches for calculating the electronic structure of many particles using quantum mechanics for molecular systems and dense materials.

Research by Adlis Santoni et al (2015) regarding the essential oil of Toona sinensis and the insecticidal activity test where the results of this research show that the compounds α-Terpinen, β-Caryophilen, α-Element and α-Humulen contained in the essential oil components of Toona sinensis leaves are the main components and have % area The highest results from research on the essential oil components of Toona sinensis leaves. (Santoni, A., Nurdin, H., Manjang, Y., & Achmad, SA, 2015). The compounds α-Terpinen, β-Caryophilen, α-Element and α-Humulene have potential as iron corrosion inhibitors because they have double bonds in their structural framework.

Therefore, based on this description, research was carried out to study the compounds α-terpinene, β-caryophilen, α-element and α-humulene as corrosion inhibitors using the density functional theory (DFT) method.

RESEARCH METHODS

In this research, computer equipment was used with an Intel® Core™ Intel Core i7-4650U CPU @ 1.70 GHz, 16 GB memory (RAM). The software used to process data obtained from literature is the Windows™ 2010, Gausian™ 09 operating system to optimize the geometry of α-Terpinen, β- Caryophilen, α-Element and α-Humulen Compounds.

Method 1

The α-Terpinene, β-Caryophilene, α-Element and α-Humulene molecules in the gas phase and H_2O solvent medium were optimized with optimization settings plus frequency using the Gaussian 16 W program package. The output data used was the optimal geometric

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structure, EHOMO, ELUMO, Contour HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital), total energy, dipole moment and mulliken charge density using calculation methods.

DFT and B3LYP/6-31G basis set. The more detailed procedure is as follows:

1. Molecules or atoms are depicted in Gauss view 6.0 by selecting element fragment, ring fragment or R-group fragment.
2. In the optimization process, click on the calculation setup option, then in the job type section select opt+freq. In the method section, ground state is selected for structure optimization in the ground state, then DFT, Default spin and B3LYP/6-31G basis set are selected.
3. Select solvation, SDM model, solvent water (specifically for using solvents)
4. Submit is clicked.
5. Save is clicked, the optimization process takes place at Gaussian 16W and is immediately saved in three folders, namely chk (output), gfj (input) and notepad.

Then determine the bandgap (ΔE), ionization potential (I), electron affinity (A), electronegativity (χ), hardness (η), softness (σ), electrophilicity (ω), nucleophilicity (ε), ΔN (transfer charge), ΔEBack Donation, interaction energy (□□) and dipole moment (MD). These values are obtained based on the following equation: Based on these parameters, the stability of the inhibitor is then analyzed.

Method 2

Freq+opt was carried out using the Gaussian 16 W program package with the DFT calculation method and the B3LYP/6-31G basis set on one of the best molecules that binds to the Fe atom. The optimization results are in the form of optimal geometric structure, enthalpy, Gibbs free energy and entropy. After that, the adsorption energy and binding energy values are determined using the following equation:

$$E_{ads} = E_{complex} - (E_{Fe} + E_{inh})$$
$$E_{binding} = -E_{ads}$$

Based on the parameters mentioned above, then analyzed:

1. Mechanism of interaction between molecules and Fe atoms
2. Molecular inhibition efficiency against iron corrosion
3. Efficient molecular structure as a corrosion inhibitor.

RESULTS AND DISCUSSION

Figure 1. Geometric Structure of α-Terpinene, β- Caryophilen, α-Element and α-Humulene Compounds without solvent

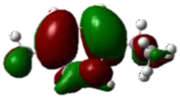
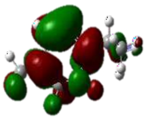
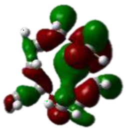
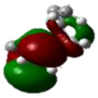
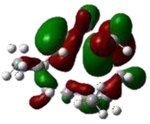
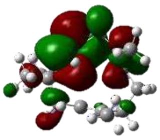
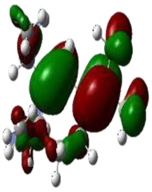
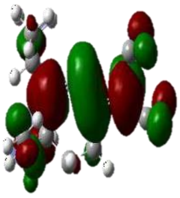
Test Compound	Geometric Structure	HOMO Contour	LUMO Contours
α-Terpinene			
B-Caryophyllene			
α-Humulene			
α-Element			

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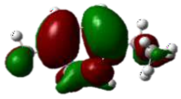
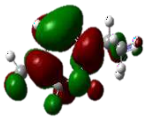
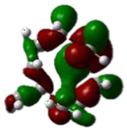
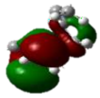
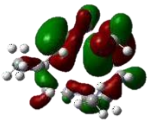
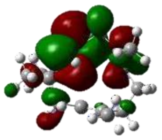
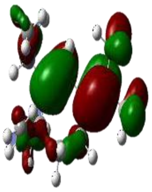
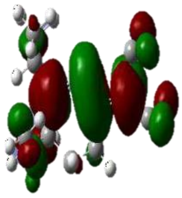
Figure 2. Geometric Structure of α-Terpinene, β-Caryophilen, α-Element and α-Humulene Compounds using H2O as a solvent

Test Compound	Geometric Structure	HOMO Contour	LUMO Contours
α-Terpinene			
B-Caryophyllene			
α-Humulene			
α-Element			

Based on the HOMO and LUMO contours of the α-Terpinene, β- Caryophilene, α-Element and α- Humulene compounds, it can be explained that in the α-Terpinene compound there is a conjugated -C=C- bond and a CH3 group which acts as an electron donor which shows the occurrence of π electron resonance in the aromatic ring towards the CH3 group attached to the C4 atom. The presence of two CH3 groups attached to the C1 atom has an electron-pushing effect as shown in Figure 2 where electron resonance begins with the 2 CH3 groups and also resonates on the benzene ring and ends with one CH3 group attached to C4 which causes the CH3 group to become electron-attracting.

Table 1. Reactivity parameters of inhibitor compounds in the DFT-B3LYP/6-31G method without water as a solvent

Molecule	**EHOMO (eV)**	**ELUMO (eV)**	**ΔE (eV)**
α-Terpinene	**-0.19244**	**-0.00974**	**0.1827**
β-Caryophilene	-0.21882	0.01875	0.23757
α-Elements	-0.21367	0.02225	0.23592
α-Humulene	-0.19337	-0.00859	0.18478

Table 2. Reactivity parameters of inhibitor compounds in the DFT-B3LYP/6-31G method with water as a solvent medium

Molecule	**EHOMO (eV)**	**ELUMO (eV)**	**ΔE (eV)**
α-Terpinene	-0.19233	**-0.00918**	**0.18315**
β-Caryophilene	-0.21349	0.02319	0.23668
α-Elements	**-0.19196**	-0.0065	0.18546
α-Humulene	-0.21543	0.0198	0.23523

Table 1. and Table 2. show the chemical reactivity parameters of the compounds α-Terpinen, β- Caryophilen, α-Element and α-Humulene. E_{HOMO} states the ability of a compound to donate electrons to a metal surface. High E_{HOMO} values tend to donate electrons to the metal surface. The E_{HOMO} value of the α-Terpinen compound (-0.19244 eV) has the greatest value compared to other compounds, so the α-Terpinen compound is more dominant in donating electrons to empty d orbitals in metals. Meanwhile, in table 2. the compounds that have this value E_{HOMO} is highest when the solvent medium is water, namely α-Element.

Value E_{LUMO} indicates the ability of a molecule to accept electrons from a metal surface. A high E_{LUMO} value has a tendency to accept electrons from the metal surface, so it will cause the molecule to accept electrons from the metal surface to a greater extent. The E_{LUMO} value of the α-Terpinene compound (-0.00974 eV) has the smallest E_{LUMO} value when compared to other compounds, so the α-Terpinene compound is dominant in accepting electrons from the metal surface. Meanwhile, in table 2. the compound that has the lowest E_{LUMO} value when using water as a solvent is α-Terpinene. When compared with other compounds, the α-Terpinene compound is dominant in accepting electrons from the metal surface.

Gap energy (ΔE) is an indicator of the reactivity and stability of a compound. Compounds that have a low gap energy are generally associated with high chemical reactivity and low molecular stability. The lower gap energy value is the α-Terpinene compound (0.1827 eV) compared to other compounds. This indicates that the reactivity of

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the molecules increases, causing the adsorption strength to increase. Meanwhile, in table 2, the compound that has the smallest ΔE value when used as a water solvent is α-Terpinene when compared to other compounds.

Table 3. Quantum chemical parameter values of inhibitor compounds without solvent

Parameter	α-Terpinene	β-Caryophilene	α-Element	α-Humulene
I (eV)	**0.19244**	0.21882	0.21367	0.19337
A (eV)	**0.00974**	-0.01875	-0.02225	0.00859
X (eV)	-0.09135	0.100035	0.009571	**0.10098**
η (eV)	**0.09135**	0.18785	0.11796	0.09239
σ (eV-1)	**10.9469075**	8.41857137	8.47744998	10.8236822
ω (eV)	0.045675	0.04212232	**0.00388284**	0.05518433
ε(eV-1)	21.893815	23.7403828	**254.543448**	18.1210862
ΔN	**0.97536643**	0.19910298	0.48839855	0.2355158
μ(D)	0.515822	0.353698	**0.338498**	0.352324
ΔEbd (eV)	**0.0228375**	0.02969625	0.02949	0.0230975

Table 4. Quantum chemical parameter values of inhibitor compounds with water as a solvent medium

Parameter	α-Terpinene	β-Caryophilene	α-Element	α-Humulene
I (eV)	0.19233	0.21349	**0.19196**	0.21543
A (eV)	**0.00918**	-0.02319	0.0065	-0.0198
X (eV)	0.100755	**0.09515**	0.09923	0.097815
η (eV)	**0.091575**	0.11834	0.09273	0.117615
σ (eV-1)	**10.92001092**	8.450228	10.783996	8.502317
ω (eV)	0.000465	0.0005357	**0.00045654**	0.00056266
ε(eV-1)	2151.3935	1866.7272	**2190.40163**	1777.2821
ΔN	0.002964	**0.0041377**	0.0030737	0.0039512
μ(D)	**1.042977**	0.379697	0.58742	0.692672
ΔEbd (eV)	-0.02289375	**-0.029585**	-0.0231825	-0.02940375

In addition to the value parameter E_{HOMO}, E_{LUMO} and ΔE can also be seen from the quantum chemical parameters which can be seen in Table 3 and Table 4. According to the optimization results that have been carried out, the lowest ionization potential (I) value is obtained for the α-Terpinen compound (0.19244 eV) compared to other compounds, while the compound that has the lowest ionization potential value when used as a water solvent is α-Element. The low ionization potential indicates that the molecule can more easily release electron pairs which causes the compound to become reactive, but if the value

A large ionization potential means that a large amount of energy is needed to remove electrons so that the compound becomes less reactive.

The largest electron affinity (A) value is the α-Terpinene compound (0.00974 eV) when compared to other compounds, while the compound that has the largest electron affinity value when used as a water solvent is α-Terpinene. A high electron affinity value indicates that the compound is easy to capture electrons so that the compound will bond easily, whereas a low electron affinity value makes it more difficult for molecules to capture electrons so that the molecules have difficulty bonding.

The lowest hardness value (η) compared to other compounds is the compound α-Terpinen (0.09135 eV), while the compound that has the lowest hardness value when using water is α-Terpinene. A low hardness value will make it easier for the compound to react with the metal surface.

The softness value (σ) is inversely proportional to the hardness value, it does not show any resistance to the polarization of the electron cloud so the compound is easy to react. The highest softness value compared to other compounds is the compound α-Terpinen (10.9469075 eV-1), while the compound that has the highest softness value when using water as a solvent is α-Terpinen. The greater the softness value, the easier it is for the compound to react with the metal surface.

The largest electronegativity (χ) value compared to other compounds is the compound α-Humulene (0.10098 eV), while the compound that has the lowest hardness value when used as a water solvent is β-Caryophilene. A large electronegativity value indicates that the molecule has more electronegative properties. The greater the electronegativity value makes it easier for the molecule to reach electronic equilibrium so that the molecule becomes more reactive, while a low electronegativity value indicates the opposite. This shows that the α-Humulene compound will more easily gain electron balance so that the compound becomes more reactive than other compounds.

A high electrophilicity value (ω) indicates that it is difficult for molecules to react with metal surfaces, while a low electrophilicity value indicates that molecules more easily bind to metal surfaces that are more electropositive. The low electrophilicity value compared to other compounds is the α-element compound (0.00388284 eV). This indicates that α-Element compounds react more easily with metal surfaces than other compounds because α-Element can bond with more electropositive metal surfaces better than other compounds.

A high nucleophilicity (ε) value indicates that the molecule reacts more easily with the metal surface, while a low nucleophilicity value indicates that the molecule has difficulty reacting with the more electropositive metal surface. The largest nucleophilicity value compared to other compounds is the α-Element compound (254.543448 eV-1), while the compound that has the largest nucleophilicity value when using water as a solvent is α-Element.

The dipole moment value (μ) is a quantity that is often used to describe the polarity of molecules in polar covalent bonds. The lowest dipole moment value compared to other compounds is the α-Element compound (0.338498 D), while the compound that has the lowest dipole moment value when used as a water solvent is α-Terpinen. A lower dipole moment value indicates that it is easier for the molecule to polarize.

Back-donation energy value (EA low bd) indicates the metal's ability to donate electrons back to the inhibitor. The smaller the back-donation energy, the fewer electrons are transferred from the iron to the inhibitor. The lowest back-donation energy value compared to other compounds is the compound α-Terpinene (0.0228375 eV), while the compound that has the lowest back-donation energy value when using water as a solvent is β-Caryophilen.

Electron transfer (ΔN) is the transfer of electrons from molecules that have low electronegativity values (organic inhibitors) to molecules that have large electronegativity values (metal surfaces) so that the potential values become the same. The greater the electron transfer value indicates the greater the number of electrons transferred by the inhibitor. The largest electron transfer value compared to other compounds is the compound α-Terpinen (0.97536643), while the compound that has the largest electron transfer energy value when using water as a solvent is β-Caryophilen.

Based on the calculation results, it is known that the α-Terpinen compound is the best corrosion inhibitor compared to other compounds, both in the gas phase and in the water solvent medium. Therefore, the α-Terpinen compound will increase the efficiency of corrosion inhibition on metal surfaces. This is because the α-Terpinen compound has 2 CH3 groups and one CH3 group below it and the -C=C- bond which acts as an electron donor and facilitates the conjugation of electrons on the metal surface, which is most important as a good inhibitor compared to other compounds. other. It can be concluded that the α-Terpinen compound is the best corrosion inhibitor compound in this research.

Muliken Charge Density of α-Terpinene, β-Caryophilen, α-Element and α-Humulene Compounds

Mulliken charge analysis states that heteroatoms with negative charges are binding areas between the inhibitor and the metal surface. Centers with a higher negative charge donate more electrons to the empty d-orbitals of the metal. Muliken charge analysis of the inhibitor compound has a negative charge on the C atom. It can be predicted that the O atom has the greatest ability to bond with the metal surface. In Figure 3, it can be seen that inhibitor compounds on average have C atoms with their respective values. Because the α-Terpinen compound is a compound that has good quantum chemical parameters for anti-corrosion, it can be seen from the muliken charge of the α-Terpinen compound in Figure 3. It has an active center at the C atom which consists of C1 (0.135), C2 (-0.131) atoms. , C3 (-0.111), C4 (0.113), C5 (-0.231) and C6 (-0.235).

The C6 atom has the most negative atomic charge. Therefore, it can be concluded that the C6 atom has the largest active center and has the ability to bond strongly to metal surfaces. Through this atom, the inhibitor compound can receive free electron pairs from the metal surface, so that the compound can function as a corrosion inhibitor compound. A good corrosion inhibitor compound is not only a good electron donor on the metal surface, but also an electron acceptor on the metal surface.

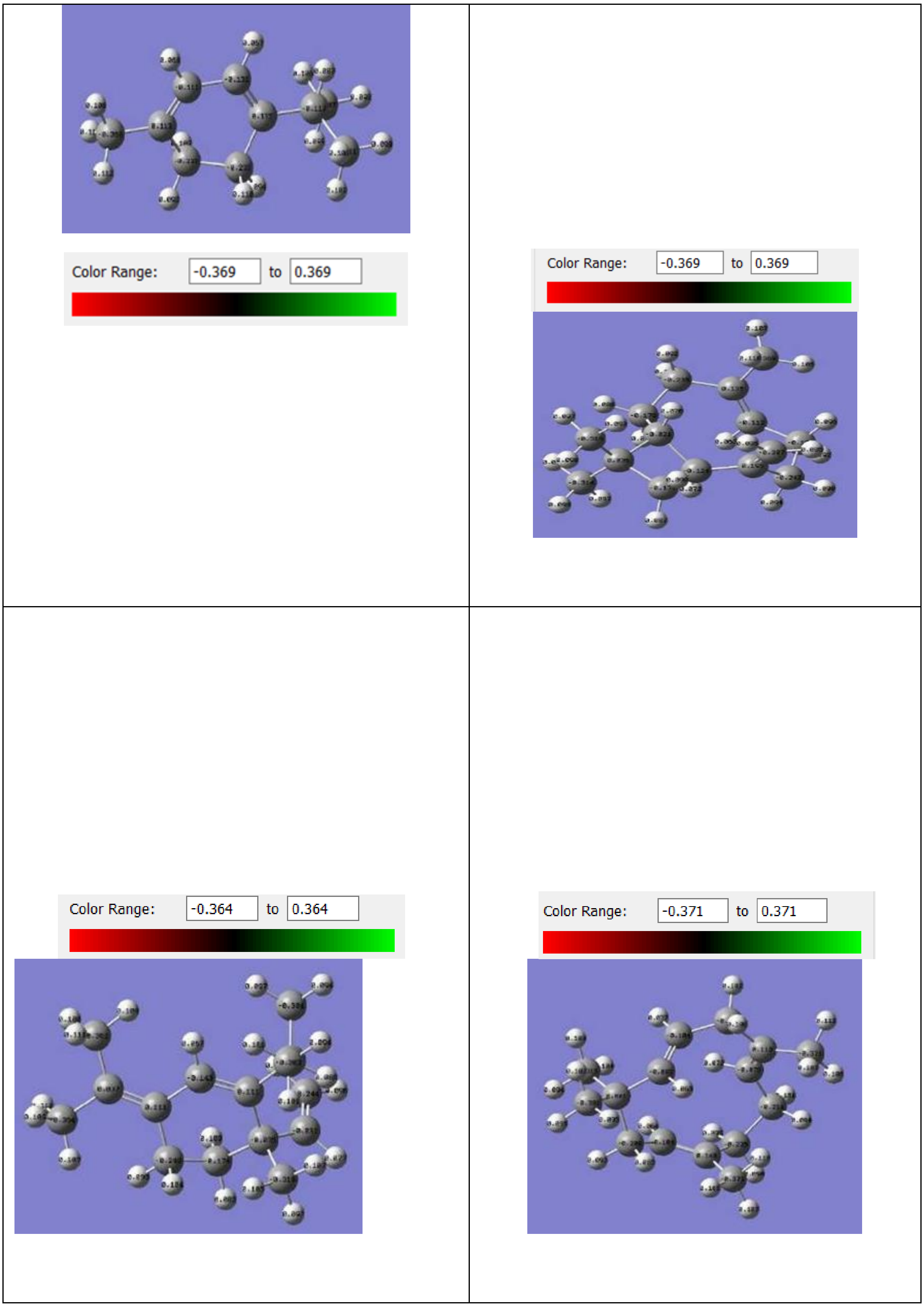


Figure 3. Mulliken charge density of inhibitor compounds

Electron Resonance Mechanism in α-Terpinene, β-Caryophilen, α-Element and α-Humulen Compounds. Figure 4 displays the reaction mechanisms that might occur with each inhibitor compound. In Figure 4, you can see that each inhibitor has a methoxy group (-CH3) as an electron pushing group, so that the inhibitor is substituted by a CH3 group which results in electrons from CH3 being pushed towards the benzene ring and resonating at the -C=C- bond and continuing to resonate again towards the direction of the CH3 group attached to the C4 atom. In the α-Terpinene compound, it has a substituent hydrogen atom that bonds to the C2 atom and functions as an electron booster which causes the electrons to be concentrated in the benzene ring. The hydrogen atom substituent in the α-Terpinen compound has greater reactivity compared to other compounds because only the α-Terpinen compound has the hydrogen atom substituent and the -C=C- bond conjugation. If a compound has a very high level of reactivity then that compound has the potential to be an excellent corrosion inhibitor compound.

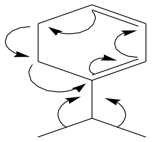
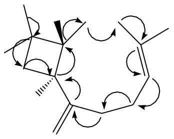
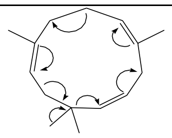
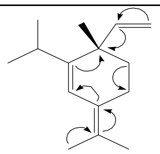
	
α-Terpinene	**β-Caryophilene**
	
α-Humulene	**α-Elements**

Figure 4. Electron resonance mechanism of corrosion inhibitor compounds

Adsorption of α-Terpinene, β-Caryophilen, α-Element and α-Humulene Compounds on Metal Surfaces. The aim of optimization with iron surfaces is to see the position of a stable interaction between iron and the inhibitor, which is characterized by a low interaction energy value. When optimizing using iron atoms, which serves to simplify calculations, the inhibitor is seen to bind to the hydroxy group which has the most negative mulliken charge. As previously discussed, the adsorption process between the inhibitor and the iron surface occurs in two stages, namely chemical adsorption and physical adsorption.

This research focuses on chemical adsorption because inhibitor compounds form coordinating covalent bonds with metal surfaces. The process of corrosion can be minimized by adding inhibitors, but not all inhibitors can cover the metal surface. Inhibitors that have large active centers have an important role in covering metal surfaces so that the rate of corrosion that occurs can be minimized. Inhibitor Interaction with Fe Atoms

The interaction between α-Terpinen and the Fe atom can be seen in Figure 5. The strength of the inhibitor interaction that binds to the Fe atom can be expressed by the values of adsorption energy (Eads), bond energy (Ebinding), Gibbs free energy (ΔG) and entropy (ΔS).) are stated in Table 3.

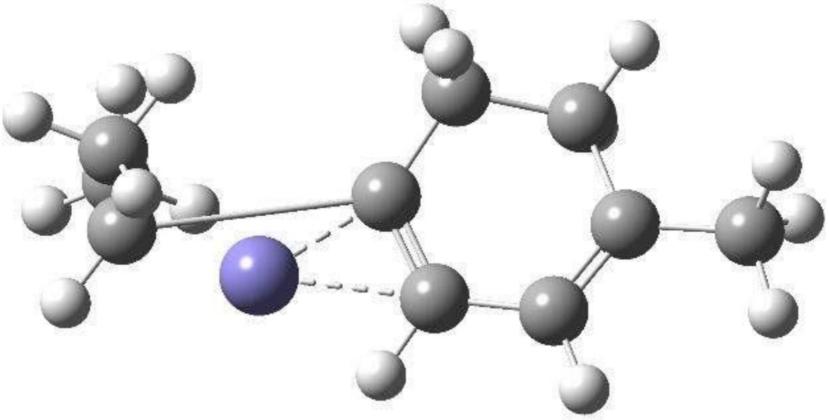


Figure 5. Interaction of α-Terpinene with Fe atoms

Table 5. E value$_{ads}$, Ebinding, ΔG, ΔS, α-Terpinene bond length with Fe atoms (r) and molecular bond angle with Fe atoms

System	Eads	Ebond	ΔG	ΔS	Bond length (r)	Bond angle
α-Terpinene with Fe atoms	-227,861	227,861	-201,142	-0.104	1.44243	54,414

The adsorption strength of the inhibitor on the Fe surface can be determined through the binding energy, bond length and thermodynamic parameters which can indicate the performance of the inhibitor. Inhibitors adsorbed on more than one adsorption center are characterized by their large bond energy values. Based on table 5, it can be seen that the adsorption energy has a negative sign (-) which indicates that the reaction that occurs is an exothermic reaction. The adsorption energy and bond energy for α-Terpinene with Fe atoms are -227.861 kJ/mol and 227.861 kJ/mol.

Gibbs free energy (ΔG) is a parameter used to express the spontaneity of a reaction between an inhibitor and a metal. Thermodynamically, the more negative the Gibbs free energy, the more spontaneous the reaction will be. Based on table 3, the Gibbs free energy value of α-Terpinen with Fe atoms is -201.142 kJ/mol. A ΔG value that is large than -20 kJ/mol indicates that the interaction that occurs between the inhibitor and the Fe atom is a physical interaction, whereas if it is small than -40 kJ/mol, it indicates that there is a chemical interaction. Based on table 5, the type of interaction between α-Terpinen and the Fe atom is chemical interaction because the ΔG value obtained is small at -40 kJ/mol.

Entropy energy is energy that expresses the degree of disorder of the system, where the formation of inhibitory complexes with Fe is directly proportional to the entropy value.

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Based on table 5, the entropy energy value for the α-Terpinen compound with Fe atoms is -0.104 kJ/mol.

The bond length between the inhibitor and Fe can also determine the reactivity of a molecule as an inhibitor, where the smaller the bond length, the stronger the bond between the inhibitor and the Fe atom. The bond length of the α-Terpinene compound with the Fe atom is 1.44243.

The structural form of an inhibitor also influences the reactivity of the molecule as an inhibitor, where the more planar a molecule is, the easier it is for the inhibitor to transfer electrons to the Fe atom. The planarity of a compound can be seen when the angle approaches 0o and 180o. Based on table 5, the bond angle for α-Terpinene with the Fe atom is 54.414˚.

Conclusion

The corrosion inhibition ability of α-Terpinene, β-Caryophilene, α-Element and α-Humulene compounds can be determined using the DFT method as proven by the presence of images of the optimal structure of the inhibitor molecule, the Highest Occupied Molecular Orbital (HOMO) contour, the Lowest Unoccupied Molecular Orbital (LUMO) contour, E_{HOMO}, E_{LUMO} and mulliken charge density. Based on the results of quantum chemical calculations, the compound that has the most potential as a corrosion inhibitor both without solvent and with water as a solvent is α-Terpinene. The inhibitor interaction that occurs with the Fe atom is a chemical interaction because the ΔG value obtained is small from -40 kJ/mol, namely -201.142 kJ/mol.

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