Scientific Analysis of Rose Essential Oils: Viewed from Various Perspectives

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ABSTRACT

The use of essential oils in the world each year has increased with the increasing development of modern industries such as the perfume industry, cosmetics, food, aroma therapy and medicine. Essential oils or also known as etheric oils are a large group of vegetable oils in the form of viscous liquids at room temperature but volatile so that they give a distinctive aroma. Some components of essential oils are hydrocarbon compounds (hydrogen-carbon) and oxygen. One source of essential oils can be obtained from rose extract. This study aims to analyze the physical, chemical, and beneficial properties of several components of the rose essential oil. This research approach uses a qualitative approach with a literature study method, then the data were analyzed using descriptive analysis. The results obtained conclude that the essential oil content in roses with the highest percentage is n-nonadekane, -phenylethylacetate, phenylethylalcohol, and 2-Isopropyl-5-methyl-9-methylene-bicyclo-1-decene, -Fernesene, and -cadinene. From these structures there are 2 types of hybrid orbitals, namely sp^3 and sp^2, when viewed from the type of bond π and σ; whereas if viewed from the isomerism, these structures have skeletal, functional groups, and optical isomers. Some of the constituents in the volatile oil components can be reacted (nucleophilic addition with HCl and electrophilic with bromine). The existence of these differences causes the chemical and physical properties of the structure of the essential oil content to vary according to their usefulness.

Keywords : Rose flower, Essential oil, Hybridization, Stereochemistry, Reaction Mechanism

INTRODUCTION

With the growth of modern industry like the fragrance industry, cosmetics industry, food industry, aroma therapy industry, and medical industry, the use of oils has increased globally each year. A vast class of vegetable oils in the form of viscous liquids at room temperature but volatile so that they give off a distinct aroma are known as essential oils, also known as etheric oils, and essential oils. Hydrocarbon molecules (hydrogen-carbon compounds) and oxygen are some of the constituents of essential oils.

Essential oils are formed due to the reaction between various chemical compounds in the presence of water. The oil is synthesized in glandular cells in plant tissues or some is formed in resin vessels. Based on their location in plants, external glands are in the epidermal cells and their modifications (for example, in the soft hairs on the leaf surface) and internal glands are between plant tissue cells[1]. According to Gunther (1990)[2]Essential oils are odorous substances contained in plants. This oil is also called volatile oil, etheric oil, essential oil because at room temperature it easily evaporates. The term essential itself is used because essential oils have the smell of the original plant. In its fresh and pure state, essential oils are generally colorless. However, on long storage, the essential oils can be oxidized. To prevent this, essential oils should be stored in dark glass vessels, fully filled, tightly closed, and stored in a dry and cool place.

At present, essential oils have been developed and become Indonesian export commodities, one of which is roses. The part of the rose plant

that produces essential oils is in the flower. Essential oils can be obtained apart from flowers, namely in the leaves, stems and roots[3]. Based on research Sukardi et al (2018)found that the chemical composition of rose oil contains 9 constituent components, and the highest 3 components, respectively, are eicosane compounds of 38.79%; phenyl ethyl alcohol by 31.58%, and tetradecane by 8.55%[4], while according to research Malasari et al (2019) found that the main chemical component of rose essential oil detected by KGSM was phenyl ethyl alcohol as high as 6.53%[5]. Seeing the many components or content of essential oils in roses can be used in many ways, both in basic scientific fields such as studying compound hybridization, compound isomers, structures, and reactions of their compounds as well as applied science such as the application of components or content in useful or selling products.

Research by Shohayeb (2014) reported that rose essential oil contains high levels of phenolic so that it can act as antibacterial, antioxidant, and anti-inflammatory[6]. This causes rose flower extract to be widely used as a source of medicine as reported in the results of the activity test of rose essential oil as an anti-bacterial. The essential oil extract has antibacterial properties that are effective against gram-positive and gram-negative pathogenic bacteria. With Gram-positive bacteria, the most sensitive bacteria are Staphylococcus aureus, Bacillus subtilis and Streptococcus. And the most sensitive gram-negative bacteria is Klebsriella pneumonia[7]. The presence of phenolic compounds in roses causes roses to have very strong antioxidant activity[7],[8]. In addition, roses are also proven to have anti-inflammatory properties. Where this important effect of rose extract significantly reduces edema which may act by inhibiting mediators of acute inflammation[7].

Based on the background that has been described, by looking at the urgency and trends in the development of rose essential oil science from various points of view, the researchers conducted a review of research articles on the analysis of rose essential oil from various points of view. The questions underlying this article are:

1. What are essential oils and the source for obtaining them?
2. What are the benefits of essential oils?
3. What is the activity of essential oils?
4. What are the components, structure, hybridization, isomerism of essential oils in roses?
5. How is the synthesis of compounds from components of rose essential oil?
6. What is the mechanism of the addition reaction to the components of rose essential oil?
7. What is the stereochemistry of the reactants and products of rose essential oil?
8. What are the compounds of rose essential oil that have more potential use value?

MATERIALS AND METHODS

This type of research is descriptive qualitative. Qualitative research is a search to find and understand a symptom or phenomenon[9][10]. The subject of this research is in the form of findings on the essential oil in roses. The data collection in this study used several literatures and was associated with actual conditions[11]. The data analysis technique uses the Miles and Hubermen model, namely data reduction, data presentation, and drawing conclusions[12]. Analyzing the data in this study is when collecting data. So that the data can be reduced, data reduction is an attempt to conclude the data, then sort the data into certain categories. The results of the data reduction are processed in such a way that the points are seen more fully in accordance with the existing conditions**.**

RESULT AND DISCUSSION

Definition, sources and benefits of Essentials Oils

Essential oils, also known as essential oils, are oils that are often used as aromatherapy. Essential oils are consist of a mixture of liquid compounds obtained from distillation of various plant parts, such as bark, leaves, roots, stems, fruits, seeds and flowers. These oils are also referred to as etheric oils and essential oils

because they are volatile at room temperature. The term essential is used because the essential oil represents the smell of the original plant[4], [13], [14].

Essential oils are produced from metabolic processes in plants because of the reaction of several chemical compounds and water [1]. This oil has the property of having a bitter taste or pungent taste, fragrant according to the origin of the plant. In addition, essential oils are also easily soluble in organic solvents, such as alcohol, ether, petroleum, benzene, and insoluble in water.

Essential oils have characteristics, namely (1) having a low vapor point so that it evaporates easily; (2) contains strong components that affect the sense of smell; (3) difficult to dissolve in water and other polar solvents; and (4) the preparation is made from a mixture of various compounds that produce a distinctive odor or aroma according to the source.

Essential oils can be obtained from the distillation process, there are several types of plants and their parts, such as leaves, flowers, fruit, seeds, stems or bark and roots. Several types of plants have the potential that can be cultivated to meet the needs of essential trade. In Indonesia, there are about 40 types of essential oil-producing plants, although only some of them are being used, including: (a)root, as in vetiver, yellow; (b)leaves, like patchouli leaves, cloves, lemongrass, lemongrass, betel, mentha, eucalyptus, gandapura, kaffir lime, karmiem, krangean, yellow, kenikir, turmeric,basil, basil; (c)seeds, such as nutmeg, pepper, celery, avocado, cardamom, klausena, kasturi, kosambi;(d)fruits such as fennel, citrus, cumin, cubeb, anise, coriander; (e) flowers, such as clove flowers, remembrance, ylang-ylang, jasmine, tuberose, yellow cempaka, thousand leaves, gandasuli kuning, Srikanta, Angsana, Srigading; (f) bark, such as cinnamon, acacia, mace, sandalwood, masoi, selasihan, sintok; (g)branches, like twigsfirdreadlocks and fan; (h) rhizomes, such as ginger, turmeric, bangel, baboan, jeringau, kencur, galangal, lempuyang sari, black meeting, temulawak, princess meeting; (i) all parts, in the form of cat roots, bandaton, inggu, salasih, sudamala, trawas [2].

Essential oils are generally used as binders to make perfumes, fragrances, fragrances in cosmetics, pharmaceuticals, flavoring agents for food and beverages. In addition, essential oils also have many health benefits, including the following:

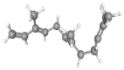
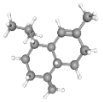
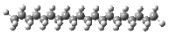
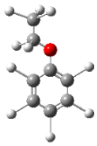
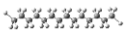
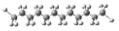
1. Helping Heart Disease Patients
   Essential oils are often used as aromatherapy. A study conducted by the British Association of Critical Care Nurses in 2015 used lavender oil as aromatherapy for 60 heart disease patients who couldn't sleep well. The results showed that lavender oil can improve sleep quality and reduce anxiety in patients suffering from heart disease, especially coronary heart diseases [2].
2. Sleep Disorders or Insomnia
   Insomnia or difficulty sleeping is a symptom experienced by a person and can result in disruption of physical, mental and emotional health. A 2014 study examined 15 types of essential oils used to improve sleep quality. The method used to detect it is by inhaling the aroma of essential oils, especially lavender oil. Inhaling aromatherapy from lavender oil is an alternative way to using drugs. The result is known that lavender oil can improve the quality of one's sleep [2]
3. Improve Memory
   Inhaled essential oils can stimulate a system in the part of the brain that functions in regulating emotions, behavior, sense of smell and long-term memory. The system has an important role in the formation of memory. This is in accordance with studies which state that smells can trigger an increase in memory and emotions. The limbic system is a part of the brain that plays a role in controlling subconscious physiological systems, such as breathing, heart rate and blood pressure. Some therapists use and claim that essential oils have a good impact on the body [2].

4. Reduce Stress and Depression
   The use of essential oils as aromatherapy can also be used to reduce stress and depression. Research conducted by Molecules in 2015 explained that 43% of people with stress and depression used essential oils as treatment ingredients and showed good effects. Generally, therapists use essential oils to massage patients who are depressed and stressed [2].
5. Overcoming Headaches and Migraines
   Since the 90s, the use of aromatherapy from a mixture of peppermint and ethanol applied to the forehead and temples can relieve headaches. Recent research, states that essential oils mixed with peppermint and lavender oil can relieve headaches. In addition, using another mixture of essential oils, cammomile and sesame oil, can treat headaches and migraines [2]
6. Reduce Inflammation
   Heat, infection, chemical exposure, and infection with organisms such viruses, bacteria, and fungi can all cause inflammation in the body. Essential oils are known to have substances that contain antibiotics and anti-microbial agents that prevent bacterial infections. Based on the content of these substances, a study was conducted using a mixture of thyme and oregano oil which was tested on a rat. As a result, it can be seen that a mixture of thyme and oregano oil can relieve colitis remission (inflammation of the large intestine). Another study was also conducted to examine the effects of using cumin and rosemary oil which were tested on rats. The test results obtained the same benefits.

Components and compound structure of Rose Essential Oil

The part of the rose that is used as the main raw material for extracting essential oils, namely flower crowns because it is considered to have a more fragrant aroma compared to other parts of the flower. During the extraction process, swelling of plant cells occurs which causes rupture of the gland so that the essential oil can be removed from the plant matrix in the vapor phase. Evaporation is regulated at a moderate temperature which aims to prevent degradation of the essential oil components. After that, a cooling process is carried out to condense the distillation results so that the desired rose flower liquid extract can be obtained. Based on the results of studies from several articles, it is known that the components of essential oils with the highest percentages are phenylethyl alcohol, nonadekane, -phenylethyl acetate, and 2-Isopropyl-5-methyl-9-methylene-bicyclo-1-decene.

Tabel 1. Compound Components in Rose Essential Oil Extract.

Component	Compound Structure	Rate (%)	Method	Source
Nonadecane		17.61	SFME	[15]
β-Phenylethyl acetate		17.26		
2-Isopropyl-5-methyl-9-methylene-bicyclo-1-decene		13.67		
α-Fernesene		8.75		
γ-cadinene		8.32		
Eicosane		38.79	Solvent evaporates	[4]
Phenyl ethyl alcohol		31.58		
Tetradecane		8.55		
n-Dodecane		2.85		

Hybridization of Rose Essential Oil Components

Organic compounds in nature are very abundant. One of the reasons is the ability of carbon atoms in organic compounds to bond with other compounds to produce various structures. Variations in the structure can not be separated from the concept of hybridization on carbon atoms. One example is that the

component content in rose essential oil has many components as shown in Table 1.

Hybridization is the joining of two or more atomic orbitals to form hybrid orbitals in the same number and have the same shape and energy level. In this section, the hybridization of essential oil components will be explained, namely nonadecane, phenylethyl alcohol, -phenylethyl acetate, and 2-Isopropyl-5-methyl-9-methylene-bicyclo-1-decene.

On nonadecane molecules all of the orbitals are hybridized to form sp3 hydride orbitals. The molecular structure of nonadecane can be seen in Figure 1.

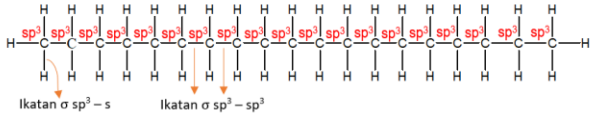


Figure 1. Nonadecane Hybrid Molecular Structure and Orbitals

In Figure 1 above, it can be seen that the nonadecane molecule ($C_{19}H_{40}$) contains 19 carbon atoms that form sp^3 hybrid orbitals. In the hybridization process, the 2s and 2p orbitals of carbon form four sp^3 orbitals which have the same energy level, where the angle of each orbital is 109.5^0. The sp^3 orbitals overlap each other to form a C-C sigma bond. Furthermore, each carbon atom has a residual sp^3 orbital, and each of these overlaps the 1s orbital of the hydrogen atom to form a C – H sigma bond. This causes each carbon atom in nonadekane to have a tetrahedral molecular geometry. So it can be concluded that at nonadecane molecules all of the orbitals are hybridized to form sp^3 hydrid orbitals. This is in accordance with Fessenden (1986) that in every molecule, every carbon atom bonded to four other atoms is in a sp^3 hybrid state, and the four bonds of the carbo are sigma bonds. When carbon is bonded to four other atoms, sp^3 hybridization overlaps maximally. So the sp3 orbitals repel each other as far as possible so that they form an angle of 109.5^o; however, other factors such as dipole-dipole repulsion or the geometry of the cyclic compound can cause deviations from the ideal bond angle.

On the phenylethyl acetate molecule hybridizes to form sp^3 and sp^2 hydride orbitals. The molecular structure of -phenylethyl acetate can be seen in Figure 2.

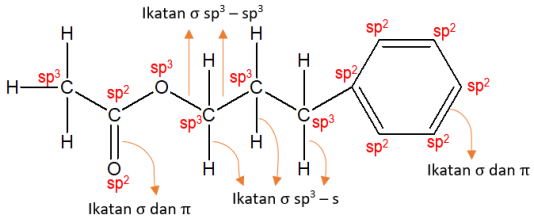


Figure 2. Hybrid Molecular Structure and Orbitals-*phenylethyl acetate*

In Figure 2 above, it can be seen that the double bond in the carbon atoms in the benzene structure) have sp^2 hybridization where one 2s orbital and two 2p orbitals form three sp^2 orbitals, while the remaining 2p orbitals are not hybridized. The three sp^2 orbitals around the carbon nucleus repel each other as far as possible so that they lie in a 120^o angle plane and form a trigonal planar molecular geometry. The unhybridized 2p orbitals will form a pi (π) bond, while the hybridized orbital will form a sigma (σ) bond. This is in accordance with Fessenden (1986) that benzene is a cyclic compound with six carbon atoms joined in a ring. Each carbon atom is sp^2 hybridized and the ring is planar. Each carbon atom has one hydrogen atom bonded to it. Each carbon atom also has an unhybridized p orbital perpendicular to the sigma bond plane of the ring. Each of these six p orbitals can donate one electron to the pi bond. With six p electrons, benzene can contain three pi bonds.

On the carbon atom number one (far left) it can be seen that the carbon atom has four groups around the carbon atom, so there are four orbitals used so that there are four types of hybrid orbitals, one 2s orbital and three 2p orbitals, so the type of hybrid orbital is sp^3. The sp^3 orbitals overlap each other to form a C-C sigma bond. Furthermore, each carbon atom

has a residual sp^3 orbital, and each of these overlaps the 1s orbital of the hydrogen atom to form a C – H sigma bond. A carbon atom having sp^3 hybridization will have a tetrahedral shape.

On the oxygen atom bonded to the number two carbon atom (CO bond) it can be seen that the oxygen atom has three groups (one carbon group and two lone pairs of electrons), then the orbitals used are three so that there are three types of hybrid orbitals, one 2s orbital and two 2p orbitals, so the type of hybrid orbital is sp^2. Furthermore, on the oxygen atom bonded between carbon atoms number two and three, it can be seen that the oxygen atom has four groups (two carbon groups and two lone pairs of electrons), then the orbitals used are four so that there are four types of hybrid orbitals, namely one 2s orbital. and three 2p orbitals, so the hybrid orbital type is sp^3.

In the phenylethyl alcohol molecule. The molecular structure of phenylethyl alcohol can be seen in Figure 3.

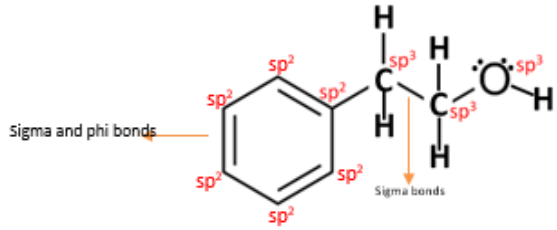


Figure 3. Phenyl-ethyl Alcohol Hybrid Molecular Structure and Orbitals

In Figure 3 above, it can be seen that the phenyl-ethyl alcohol molecule has 2 carbon atoms, each of which binds one phenyl group and one OH group respectively. In the phenyl group, all the carbon atoms have sp2 hybridization because one 2s orbital and two 2p orbitals are used. This is because one electron in the p orbital is donated to form a double bond. Therefore, all the carbon atoms in phenyl form a cyclic ring consisting of carbon atoms in a trigonal planar shape. At the C atom number 2 binds a phenyl group, one C atom and two H atoms so that the orbitals used are two 2s orbitals and two 2p orbitals and form sp3 hybridization. At the C atom number 3 binds one C atom, two H atoms, and one O atom, so that the orbitals used are one 2s orbital and three 2p orbitals to form sp^3 hybridization. Atom C in this number 2 and 3 has a tetrahedral shape and each bond has a bond. The O atom located on the far-right binds one C atom and one H atom and has two lone pairs of electrons. So it is known that the orbitals used are one 2s orbital and three 2p orbitals which form sp3 hybridization and are tetrahedral in shape.

On the molecule 2-Isopropyl-5-methyl-9-methylene-bicyclo-1-decene. The molecular structure of 2-Isopropyl-5-methyl-9-methylene-bicyclo-1-decene can be seen in Figure 3.

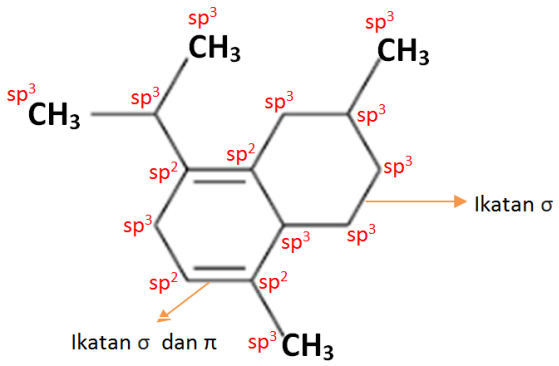


Figure 4. Molecular Structure and Orbital Hybrid 2-Isopropyl-5-methyl-9-methylene-bicyclo-1-decene

In Figure 4 above, it can be seen that the 2-Isopropyl-5-methyl-9-methylene-bicyclo-1-decene molecule has two types of hybridization, namely sp^2 and sp^3. Sp^2 hybridization is formed because one electron in the 2p orbital is donated to form a double bond and so that only one 2s orbital and two 2p orbitals are used to form sp2 hybridization. While the other carbon atoms form sp^3 hybridization because the bonds formed are only single bonds and used two 2s orbitals and three 2p orbitals.

Isomers of Rose Essential Oil Components

The essential oil components can change shape but do not change the general formula. This change in shape is called an isomerism[16]. Isomers are divided into two parts, namely

constitutional isomers and stereoisomers[17]. The constitutional isomers have different physical properties. The difference may not always be large, but constitutional isomers are always found to have different melting points, boiling points, densities, refractive indices, and so on. Part of the constitutional isomers include skeletal isomers, position isomers, and functional group isomers. While the stereoisomer, has the same qualitative, quantitative and functional structure but has a different spatial orientation of the molecule or its parts. Parts of stereoisomers are configurational, geometric, optical, and conformational isomers[17], [18]. In this section, several isomers of the essential oil components have been described which have been in sub-components and hybridization, namely nonadecane, phenylethyl alcohol, -phenylethyl acetate, and 2-Isopropyl-5-methyl-9-methylene-bicyclo-1-decene.

In nonadekane compounds, there are only constitutional isomers, namely in the structural or skeletal isomers which amount to 148,284. Nonadekane only have structural or skeletal isomers because they belong to the homologs of alkanes. One of the isomers of nonadecane is 2-methyloctadecane, 3-methyloctadecane, and 2,2-dimethylheptadekane.

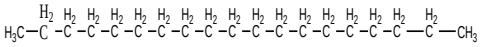


Figure 5. Nonadecane structure

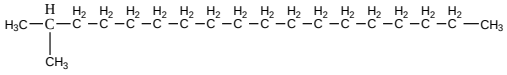


Figure 6. 2-methyloctadecane structure

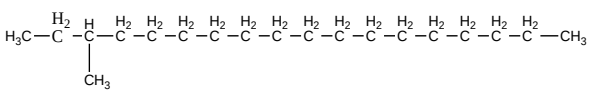


Figure 7. 3-methyloctadecane structure

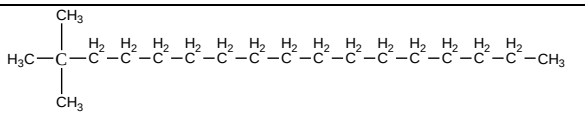


Figure 8. 2,2-dimethylheptadecane structure

The nonadecane ($C_{19}H_{40}$) isomer, although it has the same molecular formula but has a different geometric shape. The difference in the geometry of the compound is caused by the size of the energy generated by each of these molecules. The large difference in energy greatly affects the stability of the structure of a compound. The greater the energy, the more unstable the compound, on the contrary, the smaller the energy produced, the more stable the geometric structure of the compound. Geometric differences include differences in bond lengths possessed by each element forming a compound, as well as differences in bond angles in these compounds. The geometric characteristics of the $C_{19}H_{40}$ isomer are large differences in angles, on the carbon element which has branches, the bond angle is smaller than that of a straight chain and the length of the bond in the branches is also farther than that of a straight chain. This is caused by the energy produced by the larger branched chains due to the electron repulsion of the elements that make up the compound. Geometric structure also affects the boiling and melting points of each compound. The greater the bond length or the smaller the bond angle in a compound, the easier it is to break the bonds (higher boiling and melting points).

The compound -phenylethyl acetate is an alkyl alkanoate (ester). So it has a functional group isomer, namely alkanoic acid (acid-5-phenylpentanoic) with the following structure:

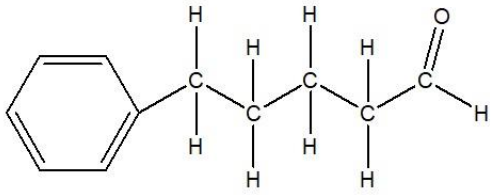


Figure 9. Structure of 5-phenylpentanoic acid

In addition to having functional group isomers, -phenylethyl acetate compounds also have skeletal isomers. According to Fessenden (1986), skeletal isomers are isomers that have different frameworks but have the same molecular formula. One of the skeletal isomers in question is 2-phenylethylacetate.

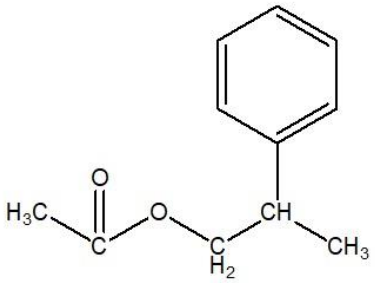


Figure 10. Structure of 2-phenylethylacetate

In compound phenyl-ethyl alcohol has three types of isomers, namely functional isomers, skeletal isomers, and optical isomers. This compound has alcohol functional group, so that the functional isomer with ether (methoxyphenylmethane) with the following structure:

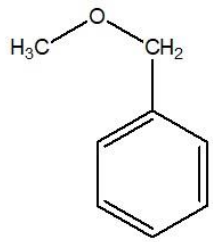


Figure 11. Methoxyphenylmethane structure

In addition, the compound has a skeletal isomer with the name 1-phenylethanol. The structure of 1-phenylethanol can be seen in Figure 12.

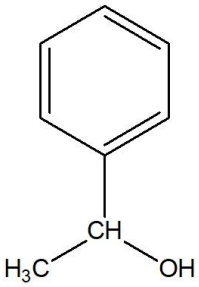


Figure 12. Structure of 1-phenylethanol

The phenylethyl alcohol compound has a chiral C atom, so it can be optically isomerized. Based on Fessenden (1986), the characteristics of the chiral C atom are that it has sp3 hybridization, binds four different atomic groups and when reflected is not close together. In a chiral compound it has pairs or mirror images called enantiomers. Enantiomer pairs in phenylethylalcohol compounds can be seen in Figure 13.

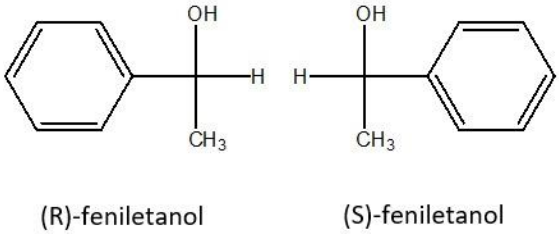
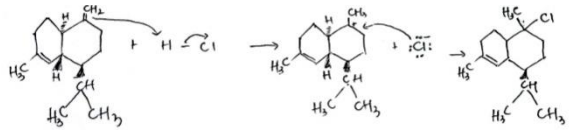


Figure 13. Structure of (R)-phenylethanol (left) and (S)-phenylethanol (right)

Addition Reaction Mechanism

Several components of the compound in the essential oil in roses can be added by using hydrochloric acid (HCl) and bromine water (Br_2). The components of volatile oil compounds that can be added include -cadinene and -Fernesene. This compound can be added because it has 2 double bonds. The reaction mechanism for the addition of -cadinene by HCl can be seen in Figure 14.

First addition mechanism



Second addition mechanism

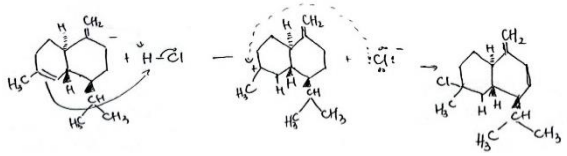


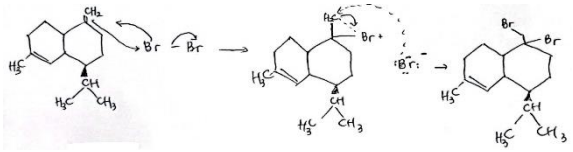
Figure 14. Mechanism of Addition of -cadinene by HCl

HCl can add -cadinene compounds on both sides of the double bond. The first addition

occurs at the double bond between the CH_2 group and the cycle group. Electrophilic addition occurs when -cadinene is added to HCl. The H^+ ion from HCl which is an electrophile opens the double bond and is bound by one of the open double bonds. Then, the next carbon atom forms a carbocation. The carbocation then binds to a Cl- ion which is a nucleophile. The second addition occurs at the double bond in the cycle group. Electrophilic addition occurs when -cadinene is added to HCl. The H^+ ion from HCl which is an electrophile opens the double bond and is bound by a carbon atom that does not bind to CH_3. Then, the carbon atom that binds to CH_3 forms a carbocation. The carbocation then binds to a Cl- ion which is a nucleophile.

The reaction mechanism for the addition of -cadinene by Br_2 can be seen in Figure 5.

First addition mechanism



Second addition mechanism

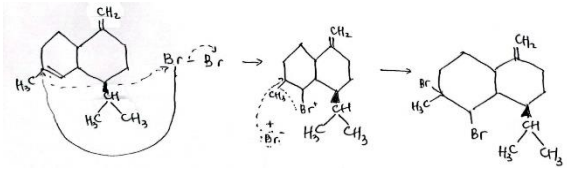


Figure 15. Mechanism of Addition of -cadinene by Br_2

Bromine water (Br_2) can add -cadinene compounds on both sides of the double bond. The first addition occurs at the double bond between the CH_2 group and the cycle group. Electrophilic addition occurs when -cadinene is added to Br_2. The Br atom which has a positive charge (electrophile) attacks the double bond and then bonds to the C atom in the open double bond on the side of the cycle group. Then, the next carbon atom that binds CH_2 forms a carbocation. The carbocation then binds to the negatively charged Br atom (the nucleophile). The second addition occurs at the double bond in the cycle group. Electrophilic addition occurs when -cadinene is added to Br_2. The positively charged Br atom (electrophile) attacks the double bond and then bonds to the C atom in the open double bond. Then, the next carbon atom that binds to CH3 forms a carbocation. The carbocation then binds to the negatively charged Br atom (the nucleophile).

The reaction mechanism for the addition of -Fernesene by HCl can be seen in Figure 16.

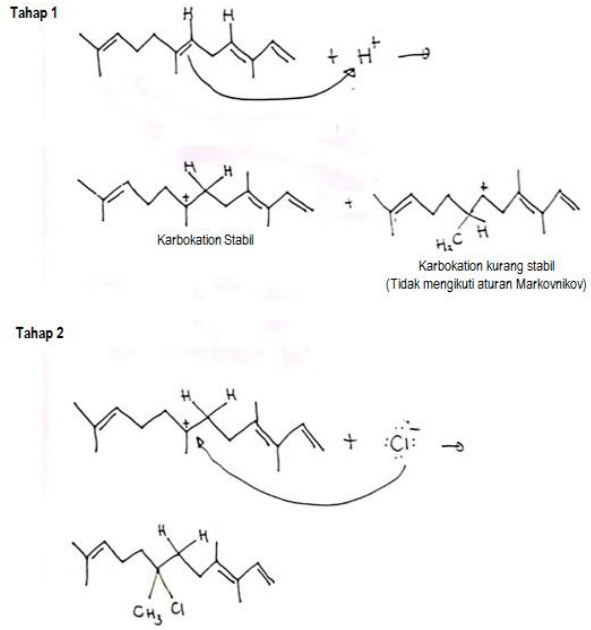


Figure 16.Mechanism of Addition of -Fernesene Compound by HCl

HCl can add -Fernesene compounds. In the first step there is an electrophilic addition of -Fernesene compound by HCl. The H^+ ion from HCl which is an electrophile attacks the double bond and then binds to the secondary C atom because fewer alkyl groups are attached. Carbocations are formed on tertiary atoms. This carbocation is more stable and conforms to Markovnikov's rule. Markovnikov's rule states that by adding a protic acid HX to an asymmetrical alkene, the acidic hydrogen (H) will attach to the carbon with fewer alkyl substituents, and the halide group (X) will attach to the carbon with more alkyl substituents (Fessenden, 1999). Furthermore, the carbocation binds to the Cl^- ion which is a nucleophile.

The reaction mechanism for the addition of -Fernesene by Br_2 can be seen in Figure 17.

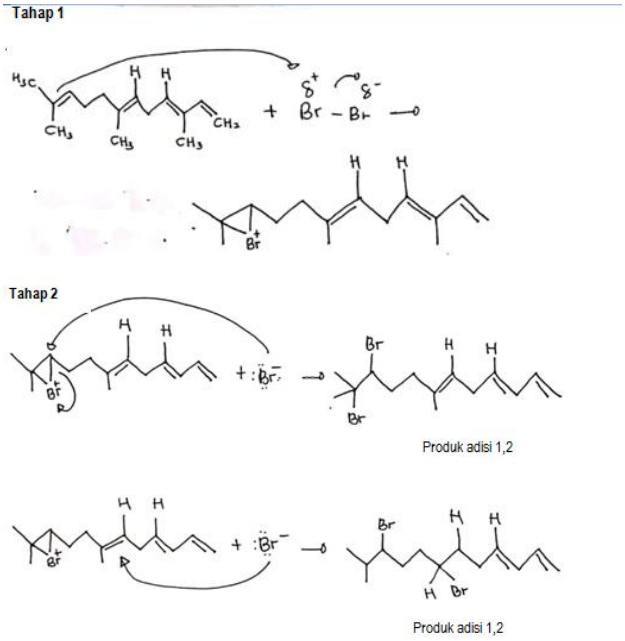


Figure 17. Mechanism of Addition of α -Fernesene Compound by Br_2

Bromine water (Br_2) can add -Fernesene compounds. In the first step, the double bond in the α-Fernesene compound is attacked by a positively charged (electrophilic) Br atom. Then a carbocation is formed which then binds to a negatively charged Br atom (nucleophile). The addition product by Br_2 forms 2 products namely the addition product 1,2 and the addition product 1,4 as shown in Figure 17.

Essential Oil Components That Have More Value Prospects

Based on the analysis of several articles regarding the components of essential oils in roses, it was found that several components have more prospect or usefulness values. These compounds, among others, can be seen in Table 2 below.

Table 2. Benefits of Rose Flower Essential Oil Components.

Component	Function	Source
Nonadecane	Used as an antibacterial agent	[19]
β-Phenylethyl acetate	Perfume raw material	[5], [20], [21]
α-Fernesene	raw material in diesel and jet fuel as well as pheromone alarms to eradicate fleas	[22]
γ-cadinene	Antioxidant	[23]
Eicosane	used as a substance,antibacterial , antifungal, and cytotoxic effects on HeLa and MCF-7 . cancer cells	[19]
Phenyl ethyl alcohol	Perfume raw material	[5], [13]
Tetradecane	antiviral, anti-microbial and anti-inflammatory	[24]
n-Dodecane	Used as an antibacterial agent	[19]

These compounds are very useful for human life. These compounds are very useful in the fields of health, industry, energy, and even beauty.

CONCLUSION

Based on the results of the article analysis, it can be concluded that the volatile oil content in roses with the highest percentage is n-nonadekane, -phenylethylacetate, phenylethylalcohol, and 2-Isopropyl-5-methyl-9-methylene-bicyclo-1-decene, -Fernesene, and -cadinene. Based on the type of bond, specially and, these structures have 2 types of hybrid orbitals, namely sp3 and sp2, whereas when viewed from the isomerism, these structure have skeletal, molecular orbitals, and optic isomers. Some of the volatile oil's ingredients can react with one another (nucleophilic addition with HCl and electrophilic with bromine). According to these variations, the chemical and physical characteristics of the structure of the essential

oil content change depending on how useful they are.

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