Evaluation of the Essential Oils Constituents from the Leaves, Seed Buds and Fruits of *Eucalyptus torelliana* F. Muel Plant by Gas Chromatography-Mass Spectral Analysis

Dashak, D. A.¹, Daben, J. M.², Olaoye, F.M.¹, Agunbiade¹, A.T, Ogbole, E.³

¹Department of Chemistry, ²Department of Science Laboratory Technology, Faculty of Natural Sciences, University of Jos, Jos, Plateau State, Nigeria.

³Biochemistry and Biotherapy Division, Nigerian Institute for Trypanosomiasis Research, Vom, Plateau State, Nigeria

Abstract: Essential oils obtained from the leaves, seed buds and fruits of Eucalyptus torelliana F. Muel plant by hydro-distillation technique were evaluated using Gas Chromatography-Mass Spectrometry method. The major components of all the essential oils from the Gas Chromatography-Mass Spectral analysis are: 4-hexen-2-one, phenol, 7-Azabicyclo[4.1.0] heptane, 2-isopropyl phenol, 2,5-dimethyl-3-methylene-1,5-Hexadiene, 1,8-nonadiyn, 1-phenylmethanol, n-Hexanol, 2-phenylethanol, Methyl propanoate and haptanitrile. The presences of these compounds suggest potentials of the leaves, seed buds and fruits of Eucalyptus torelliana plant for possible uses as antiseptics, disinfectants and food additives.

Keywords: Eucalyptus torelliana, fruits, gas chromatography-mass spectroscopy, hydro-distillation, leaves, mass spectral, n-hexane extracts and seed buds.

I. Introduction

Eucalyptus species belong to the family Myrtaceae. It is a large genus of aromatic trees far known to be indigenous to Australia, Tasmania and the neighbouring islands but today can be found growing in subtropical regions of the world [1]. This genus, which includes over 800 species, [2], [3] is the second most widely planted multipurpose woody tree species in the world, they occur under a wide range of environmental conditions. The remarkable adaptability of eucalypts coupled with their fast growth and superior wood properties has driven their rapid adoption for plantation forestry in more than 100 countries [3].

There are several *Eucalyptus* tree improvement programs, but *Eucalyptus* domestication can still be considered as being at an early stage. Their general importances are described as short rotation hardwoods for a variety of products and ornamentals with specific emphasis on existing and emerging markets as energy products [4]. The oils of the *Eucalyptus* plant are frequently used as a remedy for cold and cough. They are used in pharmaceuticals such as cough syrups, lozenges, nasal drops and mouthwash [1]. Eucalypts constituents, is an ingredient in over-the-counter pharmaceuticals as temporary relief of minor aches and pains of muscles. *Eucalyptus* essential oils have long history of safe use in food preservation, pharmaceuticals, physiotherapies, pesticides [5].

Researches from Nigeria, Mali, Australia and Congo-Brazzavilla have reported that *E. torelliana* essential oils are rich in hydrocarbon monoterpenol, spatulenol, α and β -pinenes, ocimene, aromadendrene and caryophyllene oxide as its characteristic constituents [6].

Essential oils from leaves and seed of the plant were reported to have possessed antibacterial activities against enteric pathogens [7], antiviral, anti-inflammatory, anti-oxidant antifungal antimicrobial antibiotic and anti-carcinogenic properties. Analyses of the seed essential oils extracts resulted in the identification of 70 compounds representing 98% of the oil [5].

In Nigeria, *E. torelliana* is used to treat gastrointestinal disorders; decoction of the leaves is used for sore throat remedy and other bacterial infections of respiratory and urinary tract. The poultice of the leaves is applied over wounds and ulcers. It decreases gastric acid production and used for the treatment of gastric and duodenal ulcers, cough associated with most pulmonary diseases. The essential oil of the leaves have been used in treatment of lung diseases, and were stated to have anti-inflammatory and remedies cancer-related symptoms, and intestinal disorders [6], [8], [9].

Eucalyptus seed essential oil contain eucalyptol which is the principal component of the seed essential oil, it is an oxygenated monoterpenoid which can readily penetrates tissues, due to its efficacy, it is used in various decognestants, pain relief products, anti-catarrh hale, anti microbial, antiviral properties [10], [11], [12].

This work evaluates the essential oils constituents, showing the fragmentation patterns and mechanisms of formation of ions obtained from GC-MS analysis of the leaves, the seed buds and fruits of E. torelliana in Ishong Agwon, Jos, Plateau- Nigeria.

2.1 Preparation of Samples

II. Materials and Methods

The leaves, seed buds and fruits of *Eucalyptus torelliana* were collected separately from Ishong Agwon community of Jos North Local Government Area of Plateau State, Nigeria. Samples were cleaned free of debris, air dried, milled and stored in an airtight container for analysis.

2.2 Extraction of Essential Oils.

Fifty grams (50g) each, of the powdered samples was subjected to hydro-distillation for 7hours using Clevenger-type apparatus. N-hexane was used to separate the essential oil from the aqueous layer. The two layers were dried by anhydrous Na₂SO₄ and stored in vial at low temperature.

2.3 Gas Chromatography and Mass-Spectrophotometer Analysis.

Analysis of the essential oils of the leaves, seed buds and fruits of E. torelliana using Gas Chromatography and Mass-Spectrophotometer (Shimadzuma Japan QP2010 PLUS); under the following conditions: AOC-20i auto-injection, column flow rate 1.58ML/ min, injection volume of 1μ L at 250°C with initial temperature of column at 80°C, pressure of 108pKa, total flow of 6.2mL/min and total run time-28mins. Carrier gas Helium at a constant flow rate of 0.99ml/min.

2.4 Identification of GC-MS Chromatograms

Identification of essential oils chromatograms were compared with published Electron Impact-Mass Spectral (EI-MS) in the NIST (National Institute of Standards of Technology), Shimadzu's Flavours and Fragrance of Natural Synthetic Compounds (FFNSC), and published spectral data. The retention indices were determined based on a homologous series of n-alkanes internal standard analyzed under the same operating conditions. Calibration based on the Automatic Adjustment of Compound Retention Time (AACRT) function of the GC-MS. Relative concentration of the essential oil component were calculated based on GC peak area with computer matching using NIST libraries provided with computer controlling the GC-MS System. The spectrum of unknown component was compared with the spectrums of known components stored in the libraries. The name, molecular weight and structure of the components of the test materials ascertained. [13], [14].

III. Results 3.1 Gas Chromatography-Mass Spectral (GC-MS) Analysis



Figure 1: GC-MS chromatograms of n-hexane fraction of the leaves oil

3.1.1 Molecular Structure, Mass Spectrum and Fragmentation Pattern of 4-hexen-2-one (C₆H₉O).

$$CH_3$$
-CH=CH-CH₂-C-CH₂ 4-hexen-2-one

ion

Retention Time (RT) 21.092minutes



The fragmentation patterns of 97, 79, 68, 44 and 42 in figure 2 has its most stable molecular mass ion and major ion in the fragments is 79. The mass of fragments lost between these fragmentations are $18(H_2O)$, $11(-CH_2, +3H)$, 24(-HC=CH, +2H) and 2(-2H), therefore the compound is 4-hexen-2-one with molecular weight of 97.

The ions to be accounted for are 97, 79, 68, 44 and 42 as shown in the spectrum.

There is a loss of water molecule to give an ion with m/z of 79 which is hexyne-4-ene ion as shown below.

$$CH_3-CH=CH-CH_2-C-C+CH_2-C=\dot{C}$$

Now there is a formation of an ion with m/z of 68 (2-pentene ion) from the ion with m/z of 79. Where there is a loss of a methylene group and an addition of 3H as given below.

$$CH_3-CH=CH-CH_2$$
 CH_2 $CH_3-CH=CH-CH_2-\dot{C}H$

Furthermore, where there is a loss of ethylene group and an addition of 2H, an ion with m/z of 44 (propane) will be form.

$$CH_{3}$$
 $CH=CH-CH_{2}$ $-\dot{C}H \rightarrow CH_{3}$ $-\dot{C}H=CH$ $+2H$ CH_{3} $-CH_{2}$ $-\dot{C}H$

There is finally a loss of 2H to give an ion with m/z of 42 which is 2-propene



3.1.2 Molecular structure, Mass Spectrum and Fragmentation pattern of phenol (C₆H₇O)





The fragmentation patterns of 95, 70, 68, 45 and 41 in figure 3 has its most stable molecular mass ion and major ion of the fragments is 45. The mass of fragments loss between these fragmentations are 25(-

CH=CH, +H), 2(-2H), $23(-C \equiv C, +H)$ and 4(-4H), therefore the compound is phenol with molecular weight of 95 as shown in the mass spectrum is shown below.

The structure and bond cleavage of phenol with molecular weight of 95 (2, 4-hexadienol ion) shown in the mass spectrum is given below.



The formation of an ion with m/z of 70 (2-butenol ion) from m/z of 95 comes from the loss of a methylene group and an addition of H.

There is a loss of 2H to gain an ion with m/z of 68 which is 2- butyneol ion

HO-
$$\dot{C}H$$
- $C=C$ - CH_2 $\xrightarrow{-2H}$ HO- $\dot{C}H$ - $C=C$ - $\dot{C}H_2$

There is a loss of ethyne group and a gain of H to form an ion with m/z of 45which is ethanolic ion

HO-CH_TC=C-CH
$$\xrightarrow{-C=C}$$
 HO-CH-CH

4H

There is a loss of 4H to give an ion with m/z of 41. This ion may be a transient ion.

O=C=





3.1.3 Molecular structure, Mass Spectrum and Fragmentation pattern of 7-Azabicyclo [4.1.0] heptanes or 2, 3-Tetramethylene aziridine ($C_6H_{10}NH$)



The fragmentation patterns of 96, 81,68, 54, 43 and 40 in figure 5 has its most stable molecular mass ion and major ion of the fragments is 68. The mass of fragment lost between these fragmentations are $16(-CH_{2,-}2H)$, $13(-CH_{2,+}H)$, $25(+3H, -CH_{2}CH_{3,+}H)$ and 3(-3H) therefore the compound is 7-Azabicyclo [4.1.0] heptanes with molecular weight of 97.

The ions to be accounted for are 96,81,68,54, 43 and 40 as shown in the spectrum.

The structure and ring opening of the compound is shown below.



The formation of an ion with m/z of 81 (an imine, an intermediate compound 3-Penten-imine ion) from an ion with m/z of 97 comes from the loss of methylene group and 2H.

$$\vec{\ddot{C}}H - CH - CH - CH - CH_2 - CH = NH \xrightarrow{-\dot{C}H_2} \vec{\ddot{C}}H - CH = CH - CH_2 - CH = NH$$

From the ion with molecular weight of 81, there is a loss of methylene group and an addition of H at the terminal carbon to give an ion with m/z of 68 (2-Buten-imine ion)

$$\dot{C}H-CH=CH-\dot{C}H_{27}CH=NH \xrightarrow{-\dot{C}H_2} \dot{C}H-CH=CH-CH=NH$$

There is also a gain of 3H at C_2 , C_3 and C_4 , then a loss of terminal ethyl follow by a gain of H at C_2 to give an ion with m/z of 43 (Ethane-imine)

$$CH_2-CH=CH-CH=NH \xrightarrow{+3H} CH_3-CH=NH$$

Finally there is a loss of 3H to give an ion with m/z of 40 which is acetonitrile ion



3.1.4 Molecular structure, Mass Spectrum and Fragmentation pattern of 2-isopropyl phenol (C₉H₁₂O)



The fragmentation patterns of 136, 121, 111, 95, 83, 67, 43, 41 and 40 in figure 6 has its most stable molecular mass ion and major ion of the fragments is 43. The mass of fragment lost between these fragmentations are 15(-OH, +2H), 10(-CH₂, +4H), 16(-CH₃, -H), 12(-CH₂, +2H), 16(-CH₃, -H), 24(-CH=CH, +2H), 2(-2H) and 1(-H) therefore the compound is 2-isopropylphenol with molecular weight of 136.

The ions to be accounted for are 136, 121, 111, 95, 83, 67, 43, 41 and 40 as shown in the spectrum.

The structure and cleavage of bond at the 6th position will give 2-isopropyl-2,4-hexedienol ion as given below.



From the ion with molecular weight of 136, there could be a loss of -OH and an addition of 2H at the 1st and 6th position to give an ion with m/z of 121 which is 2-isopropyl-2, 4-hexendiene ion



When a terminal group of methylene is lost and 4H is added at the 1^{st} , 2^{nd} and 3^{rd} position it will give an ion with m/z of 111which is 2-isopropyl-4-hexene ion



Further loss of methyl group at the isopropyl group and a loss of H at C_1 will give an ion with m/z of 95 (4-methylene hexene ion) from the 111 molecular weight compound.



There is a loss of another methylene group and an addition of 2H to gain an ion with m/z of 67 which is hexene ion.



There is a loss of methyl group to form an ion with m/z of 67 (Pentene ion).

$$\dot{C}H=CH-CH_2-CH_2-CH_2-CH_3$$
 $\xrightarrow{CH_3}$ $\dot{C}H=CH-CH_2-CH_2-\dot{C}H_3$

There is a loss of terminal ethylene group to form an ion with m/z of 43 (Propane).

$$\dot{C}H = CH_2 - CH_2 -$$

There is a loss of 2H from an ion with m/z of 43 to give an ion with m/z of 41(Propene ion)

$$\begin{array}{c} \begin{array}{c} -2H' \\ \hline \\ H \\ H \\ \end{array} \begin{array}{c} -2H' \\ \hline \\ CH_2-CH_2-\ddot{CH} \\ \hline \\ H \\ \end{array}$$

Finally there is a loss of H to give an ion with m/z of 40 (1, 2-propene ion).

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3.1.5 Molecular structure, Mass Spectrum and Fragmentation pattern of 2, 5-dimethyl-3-mthylene-1, 5-hexadiene (C₉H₁₃).

$$CH_2 = C - C - CH_2 - C = \dot{C} - H$$

$$I \qquad I \qquad I$$

$$CH_3 \quad CH_2 \quad CH_3 \qquad 2, 5 - dimethyl-3 - mthylene-1, 5 - hexadiene ion$$



The fragmentation patterns of 121, 105, 91, 77, 65, 51, and 41 in figure 7 has its most stable molecular mass ion and major ion of the fragments is 41. The mass of fragments lost between these fragmentations are $16(-CH_3, -H)$, $14(-CH_3, +H)$, $14(-CH_2)$, $12(-CH_2, +2H)$, $14(-CH_2)$, and $10(+4H, CH_2)$ therefore the compound is 2, 5-dimethyl-3-mthylene-1, 5-hexadiene with molecular weight of 121.

The ions to be accounted for are 121, 105, 93, 77, 65, 51, and 41 as shown in the spectrum.

There is a loss of methyl group and H as shown below to give the ion with m/z of 105 (5-methyl-3-mthylene-1,5-hexadiene ion)

There is a further loss of methyl group and addition of H at C_2 to give an ion with m/z of 91which is 3-mthylene-1, 5-hexadiene ion

There could also be formation of an ion with m/z of 77 (3-mthylene-1, 4-pentadiene ion) from the ion with molecular weight of 91 when there is a loss of methylene group.

$$CH_2 = \dot{C} - C_1 - C_1 - C_2 + \dot{C}_1 - C_2 - \dot{C}_1 - C_1 - \dot{C}_2 - \dot{C}_1 - \dot{C}_1 - \dot{C}_2 - \dot{C}_1 - \dot{$$

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Where there is a loss of another methylene group and addition of 2H at C_3 and C_4 , an ion with m/z of 65 (1,4-pentadiene ion) obtain.

$$CH_2 = \dot{C} - CH = \dot{C} \qquad \xrightarrow{-CH_2} \qquad CH_2 = C - \dot{C} - CH = \ddot{C} \qquad \xrightarrow{+2H} \qquad CH_2 = C - \dot{C} - CH = \ddot{C} \qquad \xrightarrow{+2H} \qquad H \qquad H$$

Further loss of methylene group from an ion with m/z of 65 will give an ion with m/z of 51 (1, 3-butadiene ion).

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There is a gain of 4H at C_{1-4} and a loss of terminal methylene group to give an ion with m/z of 41(Propene ion) as the most thermodynamically stable fragment ion.

$$\dot{C}H=CH-CH=\dot{C} \xrightarrow{+4H'} \dot{C}H_2-CH=CH_2$$

3.1.6 Molecular structure, Mass Spectrum and Fragmentation pattern of 1, 8-nonadiyne (C₉H₁₁).

$$CH \equiv C-CH_2-CH_2-CH_2-CH_2-C = \overset{\bullet}{C}_{1, 8-\text{nonadiyne ion}}$$



The fragmentation patterns of 119, 105, 91, 79, 65, 53, 43 and 40 in figure 8 has its most stable molecular mass ion and major ion of the fragments is (41). The mass of fragments lost between these fragmentations are $14(-CH_2)$, $14(-CH_2)$, $12(-CH_2, +2H)$, $14(-CH_2)$, $12(-CH_2, +2H)$, $12(-CH_2, +2H)$, $12(-CH_2, +2H)$, and 1(-H) therefore the compound is 1,8-nonadiyne with molecular weight of 119.

The ions to be accounted for are 119, 105, 91, 79, 65, 53, 43 and 40 as shown in the spectrum.

There is a loss of methylene group from an ion with m/z of 119 to give an ion with m/z of 105 which is 1,7-octadiyne ion

There is also a loss of another methylene group to give an ion with m/z of 91(1,6-Heptadiyne ion)

A loss of methylene and addition of 2H at C_5 and C_6 will give an ion with m/z of 79 (5-Hexenyne ion).

$$CH \equiv C-CH_2-CH_2 \xrightarrow{-CH_2} C \stackrel{-CH_2}{\longrightarrow} CH \equiv C-CH_2-CH_2-C=C$$

There is now a loss of methylene group to give an ion with m/z of 65which is 4-Petenyne ion

$$CH \equiv C-CH_2 \xrightarrow{-CH_{27}} CH = CH \xrightarrow{-CH_2} CH \equiv C-CH_2-CH = CH$$

The loss of methylene continue and an addition of 2H at C_1 and C_2 to give an ion with m/z of 65 (1, 3-Butadiene ion)

$$CH \equiv C \stackrel{-CH_2}{\xrightarrow{}} CH = CH \xrightarrow{-CH_2} CH = C - CH = \stackrel{-CH_2}{\xrightarrow{}} H \stackrel{-CH_2}{\xrightarrow{} H \stackrel{-CH_2}{\xrightarrow{}} H \stackrel{-CH_2}{\xrightarrow{}} H \stackrel{-CH_2}{\xrightarrow{} H \stackrel{-CH_2}{\xrightarrow{}} H \stackrel{-CH_2}{\xrightarrow{} H \stackrel{-CH_2}{\xrightarrow{}} H \stackrel{-CH_2}{\xrightarrow{} H \stackrel{-CH_2}{\xrightarrow{} H \stackrel{-CH_2}{\xrightarrow{}} H \stackrel{-CH_2}{\xrightarrow{} H \stackrel{-C$$

A loss of methylene and addition of 2H at C_2 and C_4 give an ion with m/z of 53 (Propene ion).

There is a loss of H at C_2 to give an ion with m/z of 40 (Propene ion).



3.1.7 Molecular structure, Mass Spectrum fragmentation pattern of 1-phenylmethanol (C7H9O)





The fragmentation patterns of 109, 95, 81, 65, 41 and 40 in figure 9 has its most stable molecular mass ion and major ion of the fragments is 41. The mass of fragments lost between these fragmentations are 14(-CH₂), 14(-H₂O, +4H), 16(-CH₃, -H), 24(-CH=CH, +2H), and 1(-H) therefore the compound is 1-phenylmethanol with molecular weight of 109.

The ions to be accounted for are 109, 95, 81, 65, 41 and 40 as shown in the spectrum.

The structure and cleavage of bond will give 2, 4-Heptadienol ion as given below.



There is a loss methylene group to form an ion with m/z of 95 which is 2, 4-hexadienol.

There is a loss of water molecule and addition of 4H at C_1 and C_6 to obtain an ion with m/z of 81 (2, 4-Hexadiene ion).



The formation of an ion with m/z of 65 (1, 3-Pentadiene ion) is brought about by a loss of methyl group and a loss of H at C_1

There is a loss of ethylene group and a gain of 2H will give an ion with m/z of 41(Propene ion).

$$\dot{C}H=CH=CH=CH-\ddot{C}H=CH$$
 $\xrightarrow{-\dot{C}H=CH}$ $CH_2=CH-\dot{C}H_2$

There could be a loss of H to obtain an ion with m/z of 40 is which1,2-Propandiene ion

$$CH_2=CH-\dot{C}H_2 \xrightarrow{-H} CH_2=C=CH_2$$

3.1.8 Molecular structure, Mass Spectrum and fragmentation pattern of n- hexanol $(C_6H_{13}O)$.

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The fragmentation patterns of 101, 87, 74, 57, 43, 41 and 40 in figure 10 has its most stable molecular mass ion and major ion of the fragments is 74. The mass of fragments lost between these fragmentations are 14(-CH₂), 13(-CH₂, +H), 17(-HO,), 14(-CH₂), 2(-2H) and 1(-H) therefore the compound is hexanol with molecular weight of 101.

The ions to be accounted for are 101, 87, 74, 57, 43, 41 and 40 as shown in the spectrum. A loss of methylene brings about the formation an ion with m/z of 87 (Pentanol ion) from an ion with m/z of 101.

The loss of methylene and a gain of H at C_5 bring about the formation an ion with m/z of 74 from an ion with m/z of 87 (Butanol).

$$: CH_2 - CH_2 - CH_2 - CH_2 - CH_2 - OH \xrightarrow{-CH_2} CH_2 - CH_2 -$$

There is a loss of hydroxyl group to give an ion with m/z of 57 which is Butane ion

There is now a loss of methylene group to give an ion with m/z of 43 (Propane ion).

$$CH_3-CH_2-CH_2-CH_2 \longrightarrow CH_3-CH_2-CH_2$$

There is a formation of unsaturated ion with m/z of 41(Propene ion) by the loss of 2H at C₁ and C₂.

$$\begin{array}{c} \begin{array}{c} -2H' \\ CH_2-CH-CH_2 \\ H \\ H \\ \end{array} \end{array} \xrightarrow{-2H'} CH_2=CH-\dot{C}H_2$$

Finally there is a loss of H to give an ion with m/z of 40 (Propene ion).



3.1.9 Molecular structure, Mass Spectrum and fragmentation pattern of 2-phenyl ethanol ($C_8H_{11}O$).





The fragmentation patterns of 123, 98, 87, 74, 69, 55, 41 and 40 in figure 11 has its most stable molecular mass ion and major ion of the fragments is 55. The mass of fragments lost between these fragmentations are $25(+4H,-CH_2CH_3)$, $11(-CH_2, +3H)$, $13(-CH_2, +H)$, 5(-5H), $14(-CH_2)$, $14(-CH_2)$, and 1(-H) therefore the compound is 2-phenyl ethanol with molecular weight of 123.

The ions to be accounted for are 123, 98, 87, 74, 69 and 55 as shown in the spectrum. Opening the ring structure of 2-phenyl ethanol could be rewritten as given below.



When 4H is added at C_6 , C_7 and C_8 , and a loss of the terminal ethyl will give an ion with m/z of 98 (4-Hexenol ion)

$$H\ddot{C}$$
- CH = CH - CH = CH - CH - CH_2 - CH_2 - CH_2 - OH
- CH_2CH_3 $\dot{C}H_2$ - CH = CH - CH - CH - CH_2 - CH_2 - OH

Here there is a loss of terminal methylene group and addition of 3H at C_{3} , C_{4} and C_{5} to give an ion with m/z of 87which is Pentanol ion

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$$\dot{C}H_2$$
- $\dot{C}H$ =CH-CH-CH₂-CH₂-OH $\xrightarrow{-C}H_2$ $\dot{C}H$ -CH-CH-CH-CH₂-CH₂-OH $+3H$ \dot{H} \dot{H} \dot{H} \dot{H}

The loss of terminal methylene group continued and addition of H to give an ion with m/z of 74 Butanol.

$$\begin{array}{c} \overbrace{CH_2} \xrightarrow{CH_2-CH_2-CH_2-CH_2-OH} & \xrightarrow{-CH_2} & \xrightarrow{CH_2-CH_2-CH_2-CH_2-OH} \\ & \xrightarrow{H} & \xrightarrow{H} \end{array}$$

Where there is a loss of 5H the formation of an ion with m/z of 69 is possible.

To obtain the molecular mass of the thermodynamically stable ion of the compound, there will be a loss of terminal methylene group to attain the stability m.wt of 55 (2-Propenal ion)



Figure 12: GC-MS chromatogram of n-hexane fraction of the fruits oil

3.1.10 Molecular structure, Mass Spectrum and fragmentation pattern of methyl propanoate $(C_4H_7O_2)$ H₃C-CH₂-C-O-CH₂

Methyl propanoate ion



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The fragmentation patterns of 87, 74, 57, and 41 in figure 13 has its most stable molecular mass ion and major ion of the fragments is 74. The mass of fragments lost between these fragmentations are $13(-CH_2, +H)$, 17(-OH), and $16(-CH_3, -H)$, therefore the compound is methyl propanoate with molecular weight of 87.

The ions to be accounted for are 87, 74, 57, and 41 as shown in the spectrum. There is a loss of methylene group attached to the oxygen and then H is attached to oxygen to give the ion with m/z of 74 which is propanoic acid.

The hydroxyl group from the acid could be loss in order to gain an ion with m/z of 57 (Propanone ion).

$$H_3C-CH_2-C$$
 $\rightarrow OH$ $-OH$ $CH_3-CH_2-\dot{C}=O$

There is a further loss of methyl and H to form an ion with m/z of 41 (Ethenone ion)

$$\underbrace{CH_{37}CH_{2}}_{-H^{-}}CH_{2}-\dot{C}=O \xrightarrow{-CH_{3}}_{-H^{-}}CH_{2}=C=O$$

3.1.11 Molecular structure, Mass Spectrum and fragmentation pattern of heptantrile (C₇H₁₃N). CH₃-CH₂-CH₂-CH₂-CH₂-CH₂-C ≡ N



The fragmentation patterns of 111, 84,74, 69, 55, 41 and 40 in figure 14 has its most stable molecular mass ion and major ion of the fragments is 41. The mass of fragments lost between these fragmentations are 27($-C \equiv N, +H$), 10 +5(CH₃), 14(-CH₂), 14(-CH₂), and 1(-H) therefore the compound is heptantrile with molecular weight of 111.

The ions to be accounted for are 111, 84, 74, 69, 55, 41 and 40 as shown in the spectrum.

For the formation of an ion with m/z of 84which is hexane to occur, there is a loss of nitrile group and gain of H from an ion with m/z 111.

The concurrent formation of ions with m/z of 74 and 69 (pentane ion) is possible when a methyl group is loss from the ion with m/z of 84.

$$CH_3$$
- CH_2 - CH_2 - CH_2 - CH_2 - CH_3 \rightarrow CH_2 - CH_3 - CH_2 - CH_2 - CH_2 - CH_3 - CH_2 - CH_2 - CH_3 - CH_3 - CH_2 - CH_3 - $CH_$

There is now a loss of methylene group to give an ion with m/z of 55 which is Butane ion.

$$CH_2$$
 CH_2 CH_2

Where there is another loss of methylene group an ion with m/z of 41(Propane ion) is form.

$$CH_2$$
-CH₂-CH₂-CH₂-CH₃ $-CH_2$ -CH₂-CH

There is a loss of H to give an ion with m/z of 40 which is Propene ion

$$: CH_2 - CH_2 - CH_2 \longrightarrow : CH_2 - CH_2 = CH_2$$

IV. Discussion

The GC-MS spectral analysis of the n-hexane fraction of the leaves extract showed the presence of 4-hexen-2-one and phenol, has high medicinal application particularly the disinfectant and antiseptics uses as earlier reported [15]. Similarly, the discovery of phenol in the leaves of *E. torelliana*, which have been found to be non toxic but have antiviral properties and therapeutic value in the treatment of tuberculosis, thus, have been used in composing cough syrup, aspirin and chewable medicinal tablets as contributed by Adeniyi & Ayepola, and Coffi and colleagues [1], [16], places high potential for medicinal value.

Meanwhile, GC-MS analysis of the essential oil obtained from the seed buds were found to contain 7-Azabicyclo[4.1.0] heptane, 2-isopropyl phenol, 2,5-dimethyl-3-methylene-1,5-Heptadiene, 1,8-nonadiyn, 1phenylmethanol, n-Hexanol, 2-phenylethanol. Some of the essential oils constituents' 2-isopropyl phenol has the ability to degrade bacteria strains of *pseudomonas* species, as reported byToyama and others [17]. Further, presence of 1-phenylmethanol, 2-phenylethanol and n-hexanol, places it as possible constituents of flavor in food industries, and applications like serving as solvents in the paint and varnishes industries, which is in consonants with earlier works of Falbe and colleagues [18]. However, the GC- MS analysis of the essential oil extracted from the fruits (*E. torelliana*), revealed the presence of methyl propanoate and heptanitrile, which could serve as source of fragrance used in the manufacturing industries. This is also similar to the works of Tranzeat and others [19], hence, can improve the economic base of the locals where the plant is cultivated on a large scale.

V. Conclusion

The results of this work have shown the presence of essential oils of the leaves, seed buds and fruits of *Eucalyptus torelliana*. Some of these components have medicinal and pharmacological properties. They also have applications in the food and manufacturing industries, especially in the wake of advocate for agriculture by the present government. Therefore, high potential for revenue generation whether at the local, state or federal level.

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