Cathkin High School
CfE Higher Chemistry

Nature's Chemistry
Fragrances and Skin Care

No.	Learning Outcome	Understanding?
1	Essential oils are concentrated extracts of the volatile, non-water soluble aroma compounds from plants.	☺ 😐 ☹
2	Essential oils are widely used in perfumes, cosmetic products, cleaning products and as flavourings in food.	☺ 😐 ☹
3	Essential oils are mixtures of organic compounds.	☺ 😐 ☹
4	Terpenes are key components in most essential oils.	☺ 😐 ☹
5	Terpenes are unsaturated compounds formed by joining together isoprene (2-methybuta-1, 3-diene) units.	☺ 😐 ☹
6	Terpenes are components in a wide variety of fruit and floral flavours and aromas.	☺ 😐 ☹
7	Terpenes can be oxidised within plants to produce some of the compounds responsible for the distinctive aroma of spices.	☺ 😐 ☹
8	Ultraviolet radiation (UV) is a high-energy form of light present in sunlight.	☺ 😐 ☹

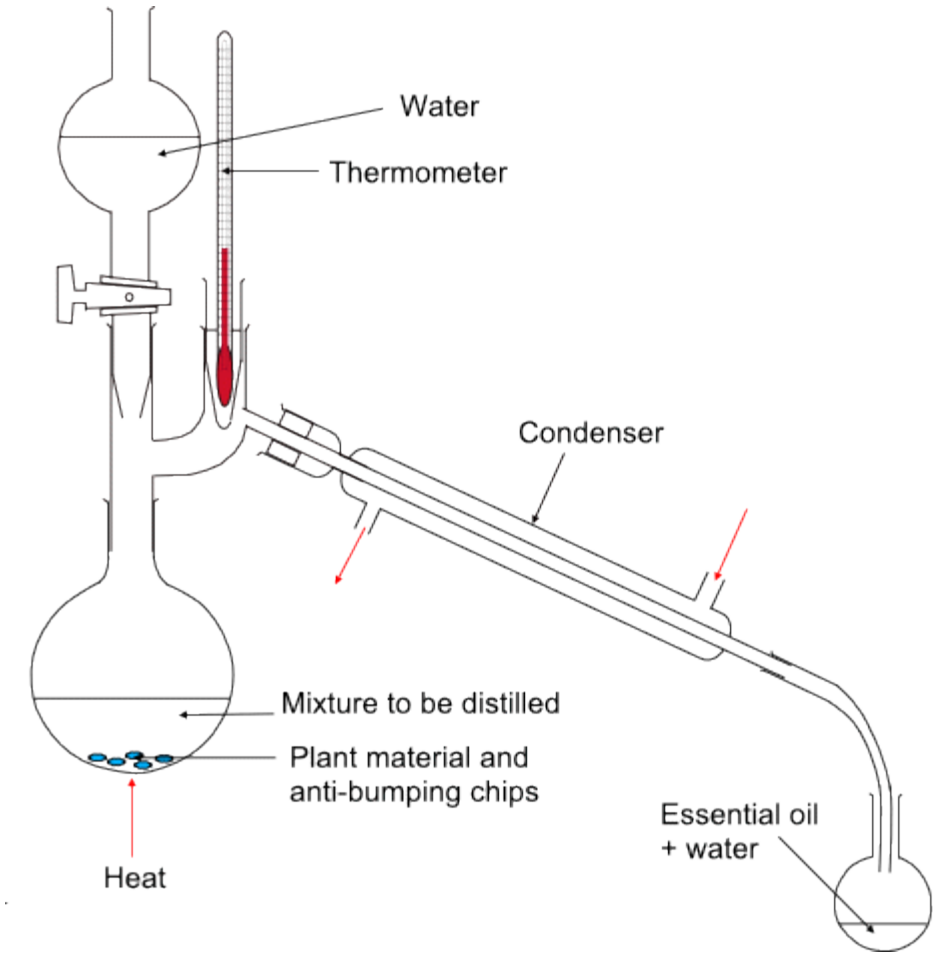
9	Exposure to UV light can result in molecules gaining sufficient energy for bonds to be broken. This process is responsible for sunburn and contributes to aging of the skin.	☺ 😐 ☹
10	Sun-block products prevent UV light reaching the skin.	☺ 😐 ☹
11	When UV light breaks bonds, free radicals are formed.	☺ 😐 ☹
12	Free radicals have unpaired electrons and, as a result, are highly reactive.	☺ 😐 ☹
13	Free radical chain reactions include the following steps: • Initiation • Propagation • Termination	☺ 😐 ☹
14	Many cosmetic products contain free radical scavengers; molecules which can react with free radicals to form stable molecules and prevent chain reactions.	☺ 😐 ☹
15	Free radical scavengers are also added to food products and to plastics.	☺ 😐 ☹

Essential Oils

Essential oils are concentrated extracts of the volatile, non-water soluble (hydrophobic) aroma compounds from plants. The oils have the aroma of the plant from which they are extracted. They include lavender, peppermint, orange, lemon, and eucalyptus oils.

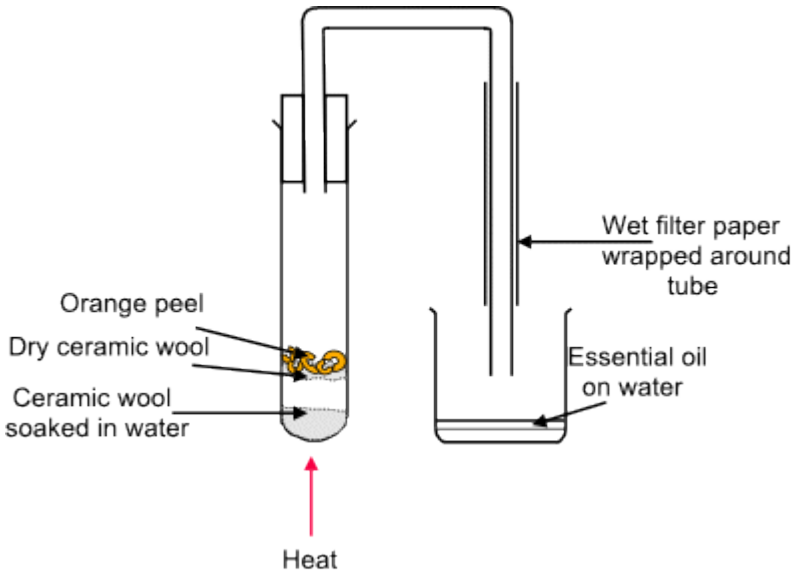
Unlike essential amino acids (which are essential as some living things cannot make them) essential oils simply mean oils related to the essence of the plant (so are described as essential).

They are extracted from plant sources by a process called steam distillation.



In this process the volatily of the oil is important so that it is carried by the steam. More water can be added from the funnel.

The essential oil collects as a mixture of oil and water, but as the two do not mix, they are easily separated.



A simpler laboratory extraction can be achieved with the apparatus shown.

This simple steam distillation process will produce a scented product in the beaker within about 5 minutes. Various plant materials can be tried.

Essential oils are widely used in perfumes, cosmetic products, cleaning products and as flavourings in foods. They are mixtures of organic compounds rather than just one pure compound.

An important component in essential oils is known as a terpene.

Terpenes

Terpenes are key components in most essential oils. They are components in a wide variety of fruit and floral flavours and aromas.

Terpenes are responsible for the distinctive flavours of spices such as cloves, cinnamon and ginger. Terpenes can be extracted from many materials in the laboratory such as the extraction of limonene from citrus fruits.

Limonene can be extracted from oranges using ethyl ethanoate as a solvent in a process called *solvent extraction*. You may have the opportunity to extract terpenes from plant material.

Solvent extraction is often used in organic chemistry to remove one substance from a mixture of substances, particularly where one substance is soluble in aqueous solvents and the other is more soluble in organic solvents. This can be used to purify the substance.

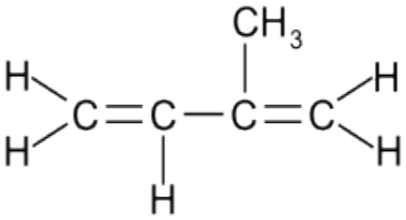
For example terpenes may dissolve well in ethyl ethanoate where they are soluble and very poorly in water. If an impure terpene in an aqueous extract is shaken with ethyl ethanoate, most of the terpene will dissolve in the ethyl ethanoate and very little will remain in the lower aqueous layer. Impurities which are more soluble in water will move into the water layer. Using a separating funnel the water layer can be removed and further treated with ethyl ethanoate to remove more of the terpene. Impurities which are more soluble in water are then removed from the terpene.

The ethyl ethanoate portions can be combined and the ethyl ethanoate removed by flash distillation to leave the purified terpene.

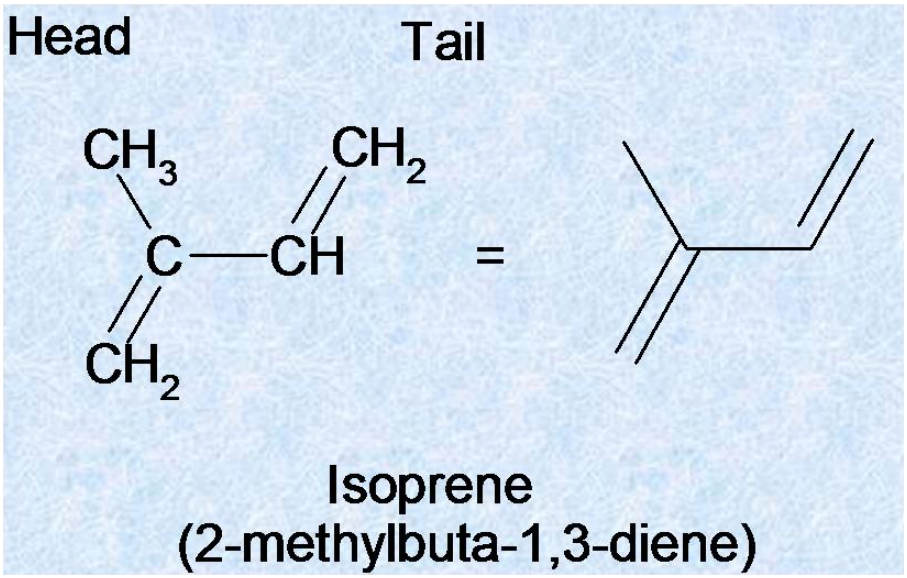
Terpenes can be oxidised within plants producing some of the compounds responsible for the distinctive aroma of spices.

Structures of Terpenes

Terpenes are *unsaturated* compounds formed by joining together isoprene (2-methylbuta-1, 3-diene) units.

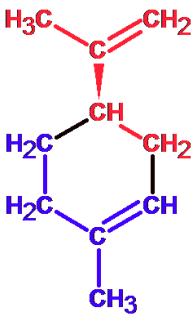


2-methylbuta-1,3-diene



Isoprene units can be linked head to tail to form linear terpenes or in rings to form cyclic terpenes.

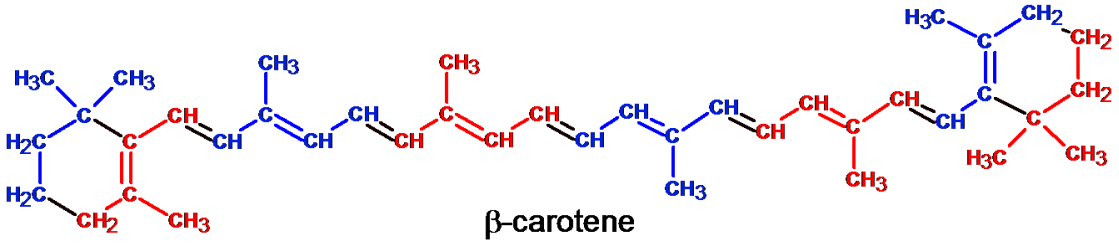
Limonene is a cyclic terpene found in citrus fruits. It is made of two isoprene units linked in a ring.



Limonene

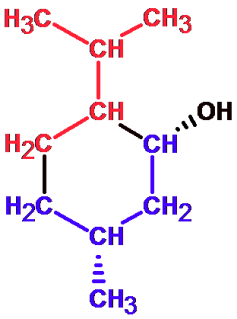
(skin of citrus fruits)

B-carotene is a linear terpene found in carrots. It is made from 8 isoprene units linked head to tail.



β-carotene

Menthol is a cyclic terpenoid – a terpene which has been oxidised. It is found in peppermint and has a distinctive aroma.



Menthol

(peppermint)

Skin Care Products

Effect of Ultraviolet Light

Ultraviolet radiation (UV) is a high-energy form of light, present in sunlight. The energy of light is inversely proportional to the wavelength of the light, so that shorter wavelength light is of higher energy and causes more damage. UV light is divided into UVA, UVB and UVC light. UVA is the highest energy UV light and causes most damage. UVC light does not penetrate the atmosphere and so causes no problems.

UVA and UVB cause wrinkles by breaking down collagen, create substances called free radicals, and inhibit the natural the repair of the skin. **Exposure to UV light can result in molecules gaining sufficient energy for bonds to be broken. This is the process responsible for sunburn and also contributes to aging of the skin. Sun-block products prevent UV light reaching the skin.** UVB light, but not UVA light is stopped by glass. You may notice labels on sunglasses to indicate their effectiveness.

UV Photography reveals the effects of "photo-aging", or aging of skin caused by light. Photo-aging refers to the damage that is done to the skin from prolonged exposure to UV radiation, over a person's lifetime. Most of the skin changes that occur as we get older are accelerated by sun exposure. Examples of skin changes from photo-aging include dark spots, wrinkles, leathery skin and skin cancer (malignant melanoma).

UV sensitive polymer beads are now available from many educational suppliers. These beads change colour when exposed to UV light. They can provide a fun and cheap way of allowing students to experiment with the effectiveness of different sun-block molecules.

Free Radical Reactions

When UV light breaks bonds *free radicals* are formed. Free radicals have unpaired electrons and, as a result, are highly reactive.

Free radical chain reactions include the following steps: *initiation*, *propagation* and *termination*.

Hydrogen reacts with explosively with chlorine in the presence of U.V. light. The reaction can be shown as follows:

$$H_2(g) + Cl_2(g) \longrightarrow 2HCl(g)$$

The presence of acid HCl in the product can be shown with moist pH paper.

The reaction follows a free radical chain reaction, initiated by U.V. light (hv). For convenience, the reaction can be split into three stages.

- Initiation

  U.V. light provides the energy for the homolytic fission of halogen into reactive halogen atoms or free radicals (atoms with an unpaired electron).

$$Cl_2(g) \longrightarrow Cl^{\cdot}(g) + {}^{\cdot}Cl(g)$$

- Propagation

  In this stage, free radicals collide with other species but the number of free radicals is maintained (hence the term propagation).

$$H_2(g) + {}^{\cdot}Cl \longrightarrow H^{\cdot}(g) + HCl(g)$$

The product of this reaction is known as a hydrogen radical.

$$H^{\cdot}(g) + Cl_2(g) \longrightarrow HCl(g) + Cl^{\cdot}(g)$$

These reactions continue until reactants are used up, or until free radicals are used up by collision with each other.

- Termination

  In this stage, free radicals are used up by collision with each other.

$$H^{\cdot}(g) + {}^{\cdot}Cl(g) \longrightarrow HCl(g)$$
$$H^{\cdot}(g) + {}^{\cdot}H(g) \longrightarrow H_2(g)$$
$$Cl^{\cdot}(g) + {}^{\cdot}Cl(g) \longrightarrow Cl_2(g)$$

Another free radical reaction takes place when halogen is substituted into an alkane in the presence of UV light. This reaction is not explosive and results in the decolourisation of bromine.

Free radical substitution of halogen into alkanes

Alkanes react with chlorine and bromine in the presence of U.V. light, though the reaction with bromine is slow. The reaction can be shown as follows:

$$CH_4(g) + Cl_2(g) \rightleftharpoons CH_3Cl(g) + HCl(g)$$
$$CH_4(g) + Br_2(g) \rightleftharpoons CH_3Br(g) + HBr(g)$$

The presence of acid HCl or HBr in the product can be shown with moist pH paper.
However, the reaction does not end here and further *substitution* can occur with hydrogen atoms progressively replaced by halogen atoms.

The slow substitution reaction follows a free radical chain reaction, initiated by U.V. light (hv). For convenience, the reaction can be split into three stages.

- Initiation

  U.V. light provides the energy for the *homolytic fission* of halogen into reactive halogen atoms or free radicals (atoms or molecular fragments with an unpaired electron).

$$Br_2(g) \longrightarrow Br^{\cdot}(g) + {}^{\cdot}Br(g)$$

- Propagation

  In this stage, free radicals collide with other species but the number of free radicals is maintained (hence the term propagation).

$$CH_3\text{-}H(g) + {}^{\cdot}Br \longrightarrow CH_3^{\cdot}(g) + HBr(g)$$

  The organic product of this reaction is known as a methyl radical.

$$CH_3^{\cdot}(g) + Br_2(g) \longrightarrow CH_3 - Br(g) + Br^{\cdot}(g)$$

  These reactions continue until reactants are used up, or until free radicals are used up by collision with each other.

- Termination

  In this stage, free radicals are used up by collision with each other.

$$Br^{\cdot}(g) + {}^{\cdot}Br(g) \longrightarrow Br_2(g)$$
$$CH_3^{\cdot}(g) + {}^{\cdot}Br(g) \longrightarrow CH_3 - Br(g)$$
$$CH_3^{\cdot}(g) + {}^{\cdot}CH_3(g) \longrightarrow CH_3 - CH_3(g)$$

The product of the last equation is ethane. However, to minimise the range of possible products, an excess of the original alkane is used and the products separated from the excess alkane by distillation.

Evidence to Support this Mechanism

- The reaction is initiated by U.V. light and, once started, can continue in the dark.
- Other substitution products are made such as CH_2Br_2, $CHBr_3$, CBr_4 together with longer alkanes (and smaller amounts of substitution products of these alkanes.

However, these other substitution products can be minimised by using an excess of the original alkane to try to ensure collision of the relatively small number of free radicals produced by sunlight quickly uses up the bromine.

Free-radical Scavengers

Many cosmetic products contain *free radical scavengers*. These are molecules which can react with free radicals to form stable molecules and prevent chain reactions. As UV light can cause wrinkling of skin, some skin-care products claim to contain chemicals which prevent wrinkling. These are claimed to be anti-aging creams. Free radicals remove electrons from skin cells and damage them and wrinkles start to develop.

Melatonin and Vitamin E are examples of natural free radical scavengers.

Adverts for anti-aging products can be examined to identify the scientific basis of the claim. **Free radical scavengers are also added to food products and to plastics.**

Fragrances and Skincare - Glossary

Word	Meaning
Unsaturated	Compounds which have double (or triple) covalent bonds between carbon atoms e.g. alkenes such as ethane.
Solvent Extraction	A method to separate compounds based on their relative solubilities in two different immiscible liquids.
Free Radical	A reactive unit made when a covalent bond is broken and each fragment has an unpaired electron. Radicals can be atoms e.g. $H^{\cdot}$ or fragments of molecules such as a methyl radical, $CH_3^{\cdot}$
Initiation	The starting reaction of a chain reaction
Propagation	A stage in a chain reaction where the numbers of radicals is maintained.
Termination	The last stage in a chain reaction, where all of the remaining radicals are used up.
Homolytic Fission	Fission means 'splitting'. When a bond breaks and the bonding electrons are shared equally among the fragments, the fission is described as homolytic. $H\text{-}Cl(g) \longrightarrow H^{\cdot}(g) + {}^{\cdot}Cl(g)$ is homolytic but $H\text{-}Cl(g) \longrightarrow H^{+}(g) + Cl^{-}(g)$ is not homolytic.
Substitution	A reaction where one atom is replaced by another atom.
Free Radical Scavenger	A molecule that can react with and remove free radicals.