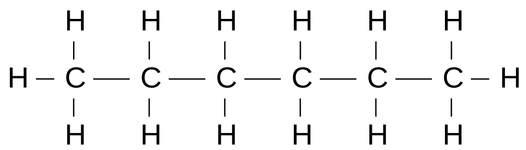
AS 90730 version 2
Describe selected organic compounds and their uses
Level 3 Credits 4

<u>Alkanes and alkenes</u> (limited to unbranched chains)

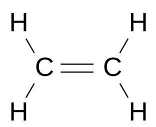
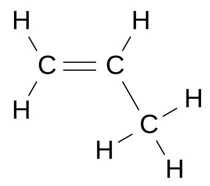
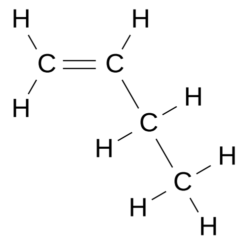
Alkanes, C_nH_{2n+2}
C1-10: methane, ethane, propane, butane, pentane, hexane, heptane, octane, nonane, decane
The alkanes are saturated; contain C-C single bonds. (All C atoms are bonded to 4 other atoms).

Example: hexane C_6H_{14}

$CH_3CH_2CH_2CH_2CH_2CH_3$ or



Alkenes, C_nH_{2n}
Example: ethene C_2H_4, propene, butene etc
Alkenes are unsaturated, containing a C=C double bond. (Not all C atoms are bonded to 4 other atoms).

Solubility
All hydrocarbons are non-polar; they will dissolve in each other as 'like compounds dissolve in like'. Hydrocarbons have C–H or C–C bonds, which are not polar, so cannot form hydrogen bonds with water; Hydrocarbons will not mix with or dissolve in polar water. Hydrocarbons will dissolve in soap or detergent solutions (see later).

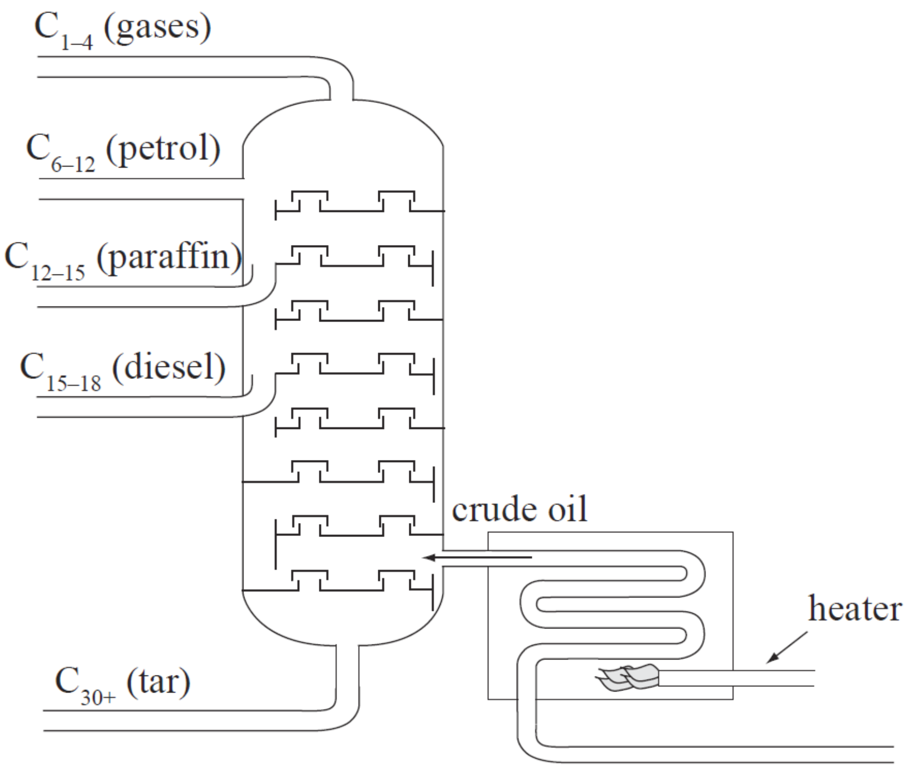
Melting and boiling points
With increasing carbon chain length, melting and boiling points increase. Weak forces (bonds) / intermolecular forces / van der Waal forces exist between the chains. The longer the chain, the greater the number of such forces, therefore the greater the strength of attraction between the molecules.

Fractional distillation uses the boiling point of the components (fractions) in crude oil to separate them. Crude oil will turn to gas when heated, but when cooled, the different fractions condense to a liquid when they reach their boiling points. Boiling point dependents on carbon chain length.

The fraction with a shorter C chain has a lower boiling point. Fractions with a longer C chain length have a higher boiling point due to the fact these have more intermolecular bonds between the chains.

Consider petrol and diesel. The molecular sizes (chain lengths) in petrol are smaller than those of diesel. Petrol forms less attractive forces (intermolecular forces) between the carbon chains than diesel as petrol has less surface area for intermolecular forces to form, than diesel. Petrol has a lower boiling point than diesel because of its shorter chain lengths, and condenses at a lower temperature than diesel.

As the fuels rise up the column, the diesel will condense first due to the longer chain lengths / greater number of attractive forces between chains, and higher boiling point, while the petrol with its shorter chain lengths / lesser number of attractive forces between chains, will condense further up the column due to its lower boiling point.



Reactions
Combustion of alkanes and alkenes – burning in oxygen.
Combustion may be complete or incomplete depending on the availability of oxygen.
Complete: hydrocarbon burns to form CO_2 and H_2O e.g. $C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$
Incomplete: hydrocarbon burns to form CO_2 CO, C and H_2O e.g. $C_3H_8 + 2O_2 \rightarrow 3C + 4H_2O$ or
$C_3H_8 + 3½\ O_2 \rightarrow 3CO + 4H_2O$ (what you will get will of course depend on the amount of O_2 available but you need to be able to write a "possible" balanced equation).

When alkanes (and alkenes) burn with reduced oxygen, they release CO, carbon monoxide, which is a colourless, odourless but very poisonous gas. A well ventilated room provides oxygen, which means that the hydrocarbon is completely combusted or burnt to carbon dioxide. Therefore carbon monoxide (or carbon) is not produced.

With complete combustion, a lot of energy is released as many bonds are formed, whereas there is less energy from incomplete combustion as there are fewer bonds formed. Differing amounts of oxygen, resulting in differing amounts of energy released because more bonds are formed during complete combustion.

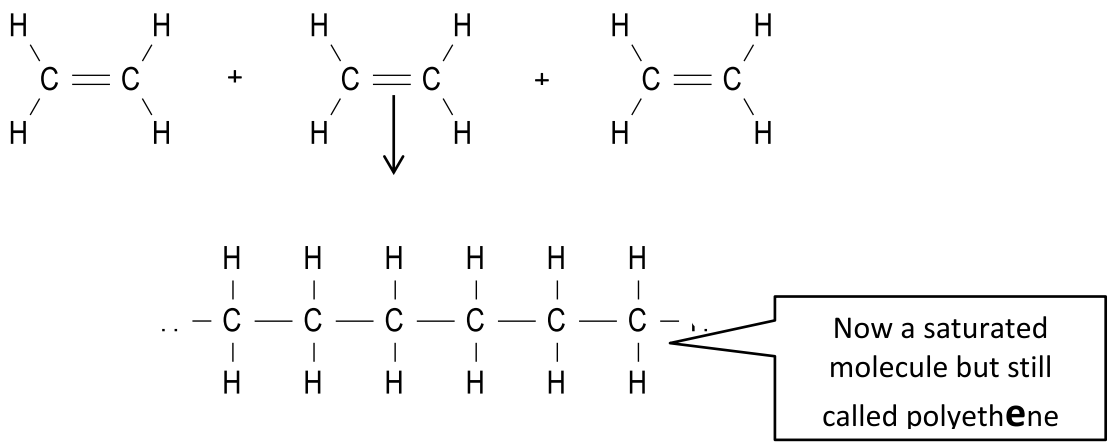
As the size of the alkane increases, the energy released also increases. As the number of carbons of the alkane chain increases, the energy released increases: energy is released each time a (C – C) bond is broken.

Addition reactions of alkenes
Addition reactions with hydrogen (hydrogenation)
E.g. $C_2H_4 + H_2 \rightarrow C_2H_6$

The addition polymerisation of ethene

The polymer polyethene is a long-chain (carbon compound) made up of many (ethene) units (called monomers) joined together.

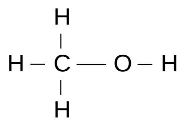
- Need high temperatures, pressure & catalyst
- Many momomer molecules → polymer molecule
- Addition reaction – called "addition polymerisation"
- E.g. ethene → polyethene, propene → polypropene etc
- Feature that allows this is the C=C double bond

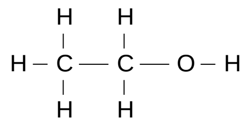


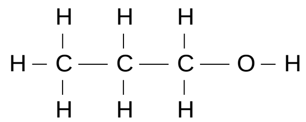
$$nC_2H_4 \rightarrow -[C_2H_4]-_n$$

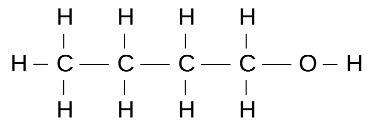
Uses
Alkanes – mainly as fuels
Alkenes – for polymer production

<u>Alcohols</u> (limited to unbranched, primary alcohols)
$C_nH_{2n+1}OH$

methanol


ethanol


propan-1-ol (1-propanol)


butan-2-ol (2-butanol)


Properties
Solubility

Alcohols and water are both polar; hydrogen bonds form between water and the polar -OH (hydroxyl) group of the alcohol. Smaller alcohols are able to dissolve in water because hydrogen bonds are easily made between them (the broken hydrogen bonds between water molecules and between alcohol molecules are compensated by the new hydrogen bonds formed when water bonds to the alcohol). Larger alcohols have a longer hydrocarbon chain (a non-polar region), which reduces the overall number and effectiveness of the hydrogen bonds (due to weaker van der Waals bonds forming) leading to a reduction in solubility.

Melting and boiling points

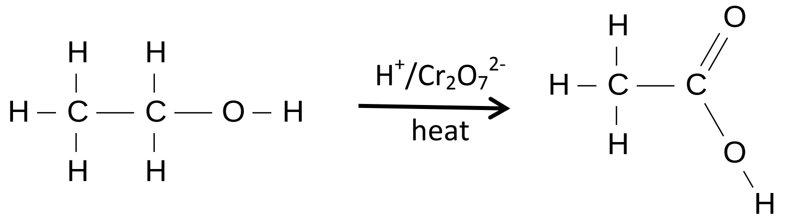
The boiling point of an alcohol is always much higher than that of the alkane with the same number of carbon atoms. This is due to hydrogen bonding between the alcohols because of the –OH group. The boiling points of the alcohols increase as the number of carbon atoms increases. The patterns in boiling point reflect the patterns in intermolecular attractions - weak forces (bonds) / intermolecular forces / van der Waal forces exist between the chains. The longer the chain, the greater the number of such forces, therefore the greater the strength of attraction between the molecules.

Reactions

Combustion. Alcohols can be used as fuels.

Complete oxidation of (primary) alcohols.

If a primary alcohol is warmed with acidified potassium dichromate it is oxidised to the carboxylic acid. The orange dichromate ion $Cr_2O_7^{2-}$ is reduced to the green chromium(III) ion, Cr^{3+}.

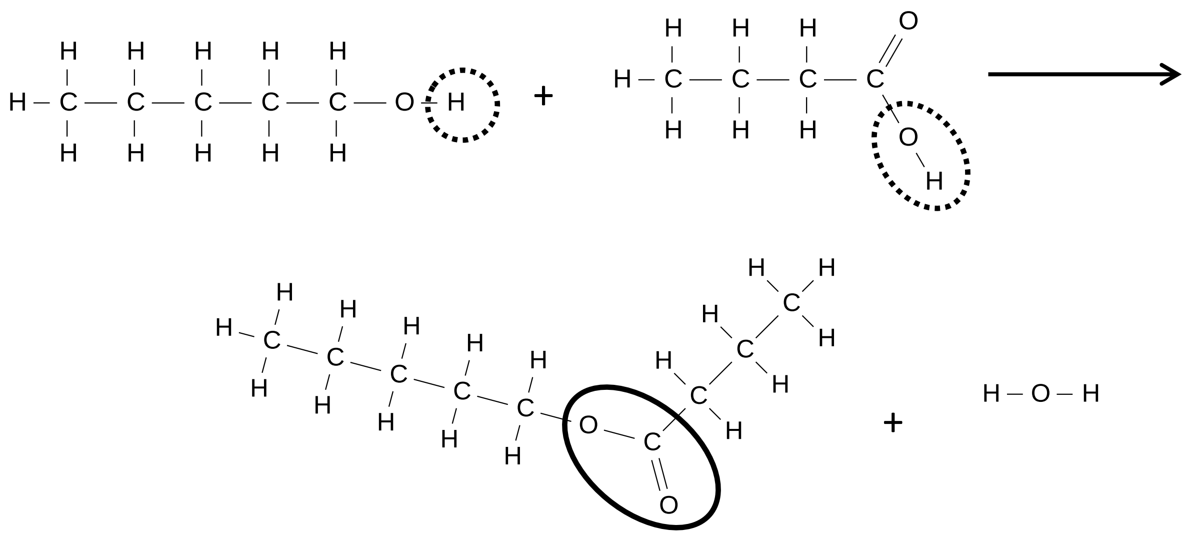


e.g.

ethanol (C_2H_5OH) ethanoic acid (CH_3COOH)

The carboxylic acids have sour, sharp and often disagreeable odours: ethanoic acid (vinegary), and butanoic acid (rancid butter smell). They are weak acids (pH 3-4). The smaller ones C1-3 are soluble in water; larger ones are not due to increased size of the non-polar hydrocarbon region).

Esterification. Esters have the ester functional group –COO- . Many have fragrant smells. The smell of apricot flavouring is due to the ester pentyl butanoate.



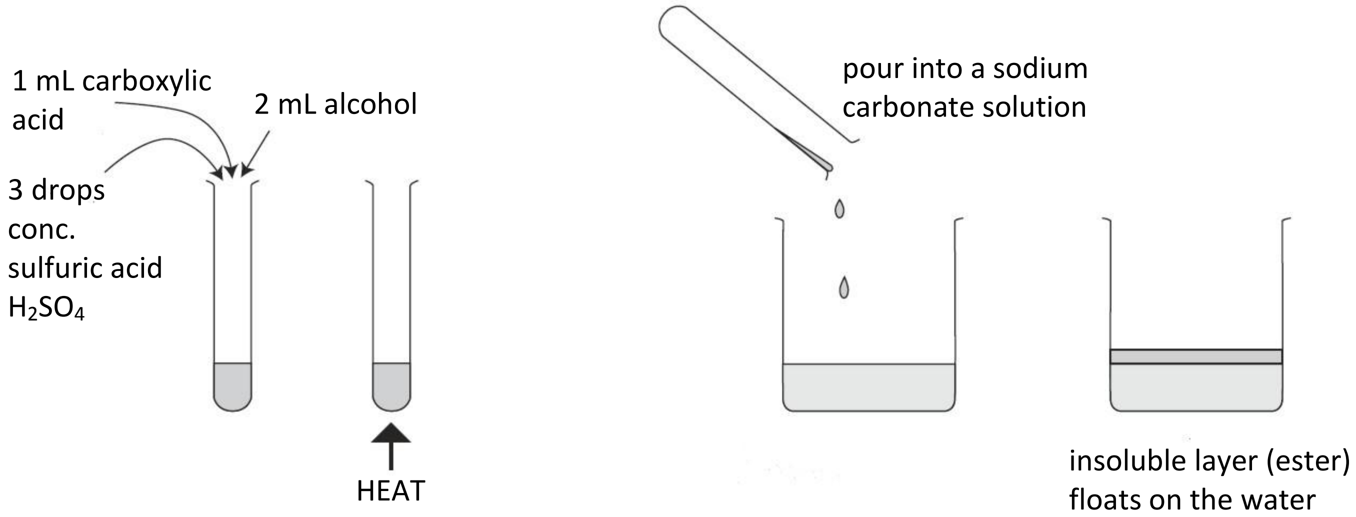
Water is also formed; the -H from the -OH of the alcohol. The -OH comes from the -OH of the -COOH.

Laboratory preparation – from the reaction of an alcohol and a carboxylic acid.

Heat (under reflux); reflux condenses vaporised reactants and products.
Addition of concentrated sulfuric acid, conc. H_2SO_4

- Acts as a catalyst to speed up the reaction.
- Acts as a dehydrating agent to remove the water produced in the equilibrium reaction to allow the reaction equilibrium to move towards making more product / therefore drives reaction to products

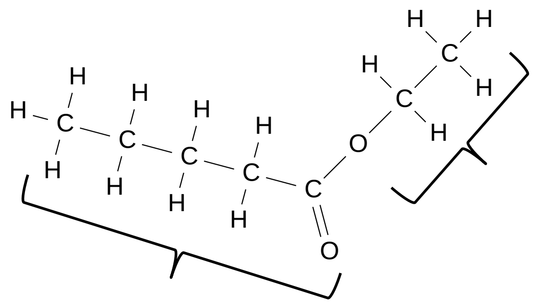
Pour into Na_2CO_3 added at end to remove excess H_2SO_4, and unreacted carboxylic acid (therefore removing sharp smell).



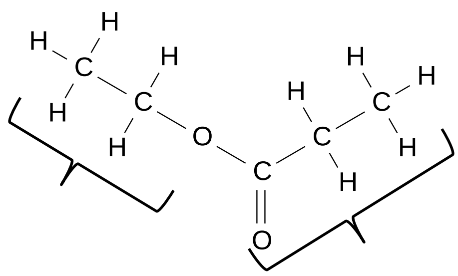
Naming esters: Esters have the names something-yl something-oate and are named depending upon the alcohol and carboxylic acid used.

e.g. methanol + ethanoic acid → methyl ethanoate + water
butanol + propanoic acid → butyl propanoate + water

Drawing esters – watch out for "which way round" they have been written / drawn
The –yl bit came from the alcohol, and the –oate part from the carboxylic acid with the C=O



ethyl pentanoate



ethyl propanoate

Alcohol is a solvent that can dissolve both polar and nonpolar chemicals. Ethanol contains the –OH hydroxyl group which makes the molecule polar. The polar hydroxyl portion will be attracted to the polar water molecules while the non-polar $-C_2H_5$ ethyl group will have an affinity to non-polar molecules. Esters are only slightly polar. The esters are attracted to the non-polar parts of the alcohol molecules & dissolve in the alcohol. Therefore alcohol is used as a solvent in perfumes and aftershaves. The alcohol evaporates on the skin to release the perfume / aftershave smell.

Low polarity of ester means weak attraction between molecules, therefore low boiling point and high volatility.

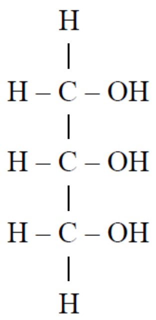
<u>Carboxylic acids</u> (limited to mono carboxylic acids)

- contain the –COOH functional group
- the -COOH group is very polar; C1-3 are soluble in water, C4 and above not (due to long hydrocarbon portion)
- higher m.pt. and b.pt. than alcohols of similar mass due to stronger intermolecular attractions
- odour (e.g. ethanoic acid "vinegary" and butanoic acid "sharp, rancid butter")
- long chain carboxylic acids are called fatty acids – are component part of triglycerides (fats/oils)
- are weak acids – only partly ionised when placed in water

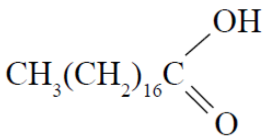
$$CH_3COOH + H_2O \rightleftharpoons CH_3COO^- + H_3O^+$$

<u>Fats and oils</u> (fats, oils and their constituent fatty acids)

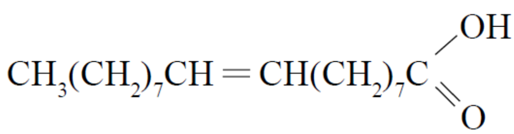
Structure of fats and oils; Fats and oils are esters of glycerol, the simplest triol (tri-alcohol), in which each of the three hydroxyl groups has been converted to an ester. The acid portion of the ester linkage usually contains an unbranched chain of twelve to twenty carbons atoms. These acids are called fatty acids. The glycerol (triol) forms a triester with 3 fatty acids *which can be the same as each other or different. Palmitic acid and stearic acids are saturated fatty acids, as both has only single bonds between the C atoms. Oleic acid is unsaturated as it has double bonds between the C atoms. Oleic acid is mono unsaturated.



glycerol

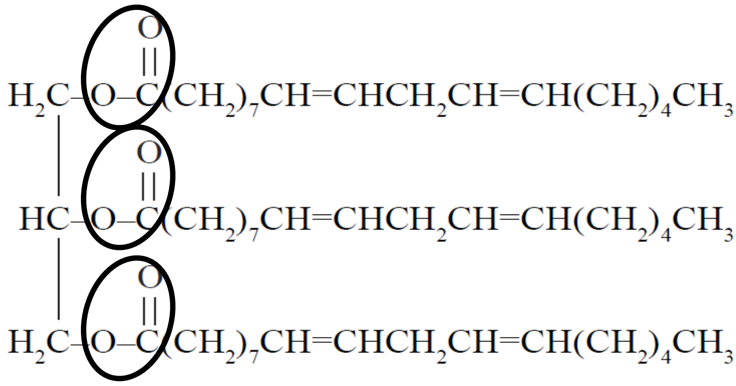


stearic acid



oleic acid

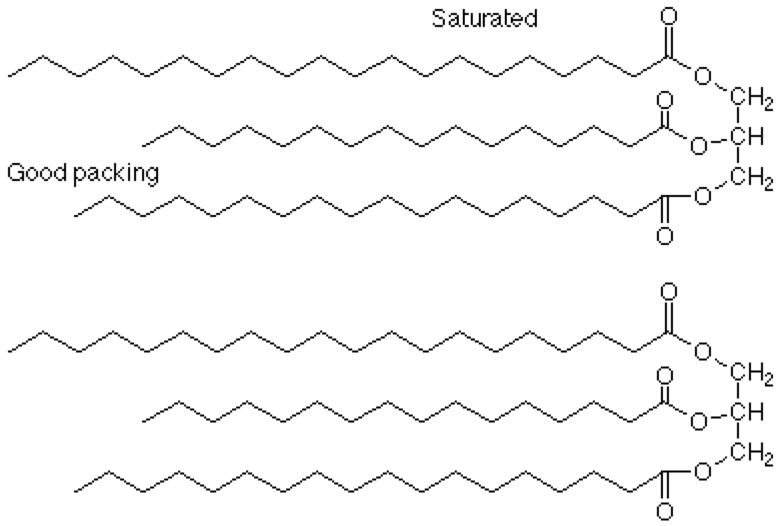
Triglycerides contain three ester groups – see opposite.



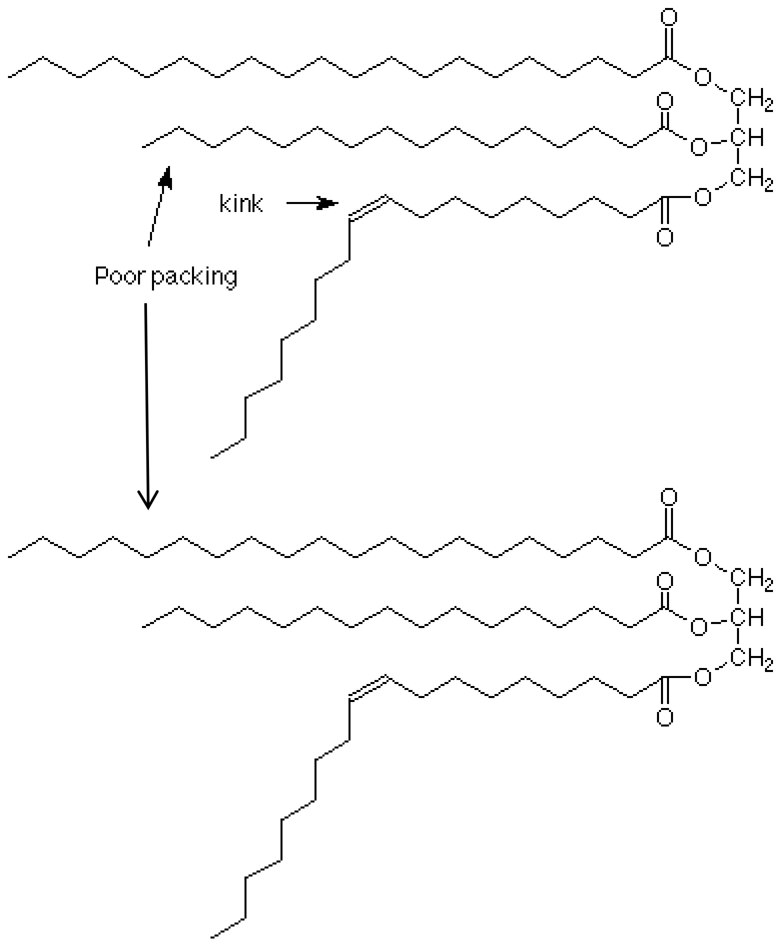
Fats tend to be saturated (and solid at room temperature), while oils are unsaturated (liquids at room temperature). Saturated means no C=C.

Melting point. This is affected by structure: Oil has C=C, which has a fixed C=C around which there is no rotation – this means molecules can't pack together well. This results in weaker intermolecular forces between fatty acid chains. (The more unsaturated, the lower the melting point.) The presence of several double carbon to carbon (C=C) bonds results in the compound having an irregular shape. (The irregular shape (kinks) lowers the melting point.) Due to the shape the compounds cannot fit together with it easily, thus lowering the melting point making the triglyceride a liquid at room temperature. Unsaturation refers to the amount of C=C. Unsaturated can be monounsaturated 1 × C=C or polyunsaturated 2 or more C=C).

The hydrocarbon chains of the fatty acids may be completely saturated or may be unsaturated (contain one or more double bonds).



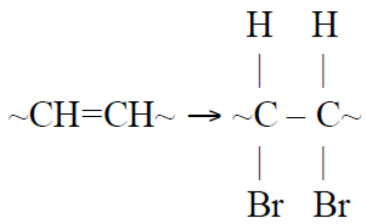
If a double bond is present, the configuration is normally cis. If a chain includes more than one double bond, the fat is called polyunsaturated.



Fatty acid notation e.g. 18:0 and 18:3. The first number refers to the number of C atoms; The second number of the notation represents the number of C=C bonds present in the fatty acid. As the number of C=C bonds increases, the melting point of the fatty acid decreases.

Fatty Acid	Notation	Melting Point (°C)
Stearic	18:0	71.5
Oleic	18:1	16
Linoleic	18:2	–5
Linolenic	18:3	–11

Bromine: Bromine can be used to test for unsaturation; Bromine solution is a brownish coloured liquid and will decolourise when added to an unsaturated fat / oil, showing the presence of carbon to carbon double bonds (C=C) / unsaturation.

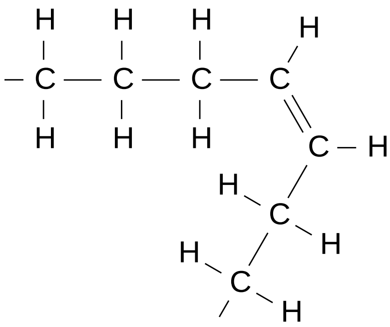


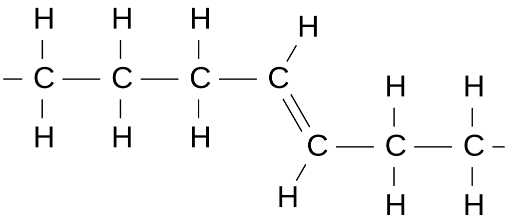
Iodine: Iodine will also react with C=C in a similar way to Br_2 (see above). The “iodine number” of a fat/oil (no. of g of I_2 that react with 100 g of fat/oil). The bigger the iodine number the more C=C bonds, the more unsaturated a triglyceride is.

FAT OR OIL	AVERAGE IODINE NUMBER
Butter fat	28
Beef fat	28
Cocoa butter	38
Olive oil	84
Cottonseed oil	107
Corn oil	120
Linseed oil	177

Fats/ Oils & Health

Good’ fatty acids contain more ‘cis’ fatty acids / fewer ‘trans’ fatty acids. ‘Cis’ fatty acids are healthier for the body. Trans are “not natural” and act like saturated fat due to packing and can actually increase bad cholesterol and decrease good cholesterol. Saturated fats are harder for the body to break down.
Mono unsaturated fatty acids contain higher levels of ‘cis’ fatty acids, which produce ‘kinks’ in the structure of the fatty acid chain. Unsaturated oils are easier to break down due to C=C.

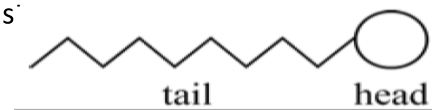




cis arrangement

trans arrangement

As triglycerides contain a lot of energy per gram excess triglycerides are stored as fat, which can lead to obesity. Excess fats / oils – can clog arteries. Saturated acids increase cholesterol which can lead to heart disease. Monounsaturated fatty acids reduce cholesterol levels in blood vessels. Monounsaturated fatty acids form fewer intermolecular bonds between chains resulting in a reduction of cholesterol / heart disease. Oils, such as soya bean oil, which are unsaturated, protect agains

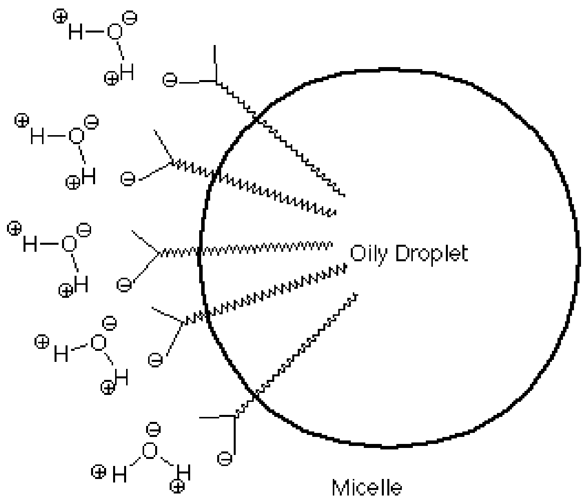


Soaps/detergents

Detergents are members of a class of compounds called surfactants or surface active agents. Surfactants are classified by their ionic (electrical charge) properties in water: anionic (negative charge), nonionic (no charge), cationic (positive charge) and amphoteric (either positive or negative charge depending upon the pH). Soap is an anionic surfactant. Other anionic as well as nonionic surfactants are the main ingredients in today's detergents.

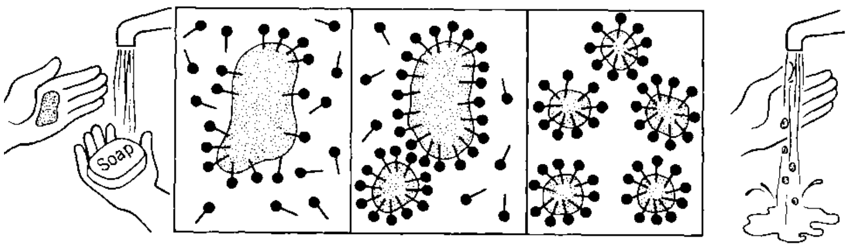
Soap and detergent molecules have a hydrophobic tail and hydrophilic head.

Grease is fat/oil is non-polar and water is polar, so won't dissolve. Hydrocarbons like alkanes are the same.



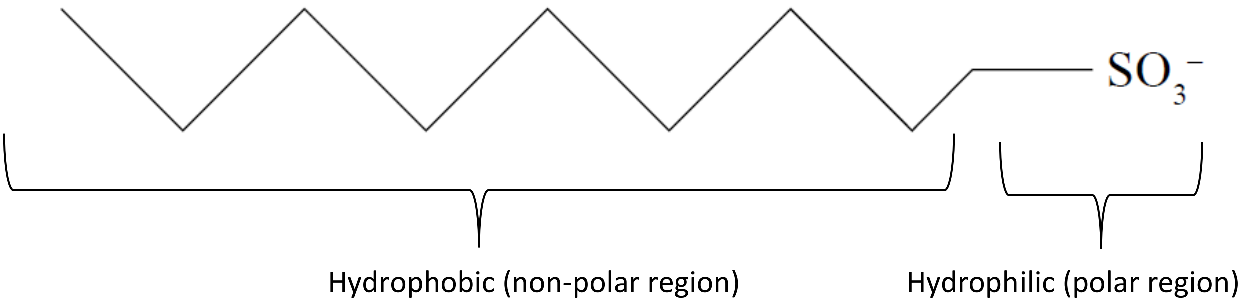
The hydrophobic (nonpolar) end of soap/detergent is attracted to fat or oil. The hydrophilic / polar end dissolves in the (polar) water. Micelles form (some grease molecules are surrounded by soap molecules with their tails in the grease and heads in the surrounding water) which interact to cause fats and oils to be removed.

Detergent molecules (micelles) emulsify the oil, dispersing it making it look as if it has disappeared.



Synthetic detergents serve the same function and have very similar structures. The major differences are that the hydrocarbon chains are derived from petroleum and that the ionic ends are salts of sulfonic acids ($-SO_3^-$ rather than carboxylic acids).

Anionic detergent (- charged)



Cationic detergent (+ charged)