3.7 Organic naming and Isomerism continued

See chapter 3.1 for basic naming of organic molecules. This chapter extends the naming for functional groups met in next few chapters

| | | prefix / suffix | | |
|----------------------|----------------------|------------------------------------|-------------------------------------|----------------------------------|
| homologous series | functional group | (* = usual use) | example | |
| aldehydes | о —с—н | suffix -al prefix formyl- | H O H C C H H H | ethanal |
| ketones | c | suffix* -one prefix oxo- | H O H H—C—C—C—H | Propanone |
| carboxylic acids | о сон | suffix -oic acid | H O H | Ethanoic acid |
| nitriles | —-C == N | suffix -nitrile prefix cyano- | H H | Propanenitrile |
| amines | ——C—NH ₂ | suffix* -amine prefix amino- | H H H | Propylamine Or propan-1-amine |
| esters | | -yl –oate | н о н | methylethanoate |
| Acyl chloride | o | -oyl chloride | CH ₃ ——C | ethanoylchloride |
| Amide | O NH ₂ | -amide | CH ₃ ——C NH ₂ | ethanamide |
| Acid Anhydrides | R——C | -oic anhydride | CH₃−C O CH₃−C | Ethanoic anhydride |

When compounds contain more than one functional group, the order of precedence determines which groups are named with prefix or suffix forms. The highest precedence group takes the suffix (and the lowest number on the carbon chain), with all others taking the prefix form. However, double and triple C-C bonds only take suffix form.

Order of priority highest first:

Carboxylic acids >carboxylic acid derivative>nitriles>aldehydes>ketones>alcohols>amines>alkenes>halogenoalkanes

Aldehydes

An aldehyde's name ends in -al It always has the C=O bond on the first carbon of the chain so it does not need an extra number. It is by default number one on the chain

Ethanal

If two aldehyde groups then **di** is put before **–al** and an **e** is added to the stem.

pentanedial

Carboxylic acids

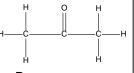
These have the ending oic acid but no number is
necessary for the acid
group as it must always be
at the end of the chain.
The numbering always
starts from the carboxylic
acid end

Propanoic acid

Ketones

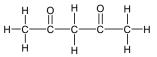
Ketones end in **-one**

When ketones have 5C's or more in a chain then it needs a number to show the position of the double bond. E.g. pentan-2-one



Propan**one**

If two ketone groups then **di** is put before **–one** and an **e** is added to the stem



Pentane-2,4-dione

The prefix oxo- should be used for compounds that contain a ketone group in addition to a carboxylic acid or aldehyde

2-oxopropanoic acid

If there are carboxylic acid groups on both ends of the chain then it is called a - dioic acid

Ethanedioic acid

Note the e in this name

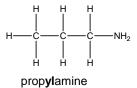
Amines

These end in -amine.

There is, however, rather confusingly two ways of using this suffix.

The exam board tend to use the common version where the name stem ends in **-yl** prop**yl**amine.

The IUPAC version of the same chemical is propan-1-amine. (This is used in the same way as naming alcohols)



Or propan-1-amine

If there is another priority functional group as well as the amine group then the prefix amino is used.

2-aminopropanoic acid.

If the amine is secondary and has two alkyl groups attached to the nitrogen, then each chain is named and the smaller alkyl group is preceded by an –N which plays the same role as a number in positioning a side alkyl chain

In the common naming version if the chain lengths are the same an –N is not used

If a tertiary amine similar rules apply, and each alkyl side group is given an N

CH₃CH₂CH₂NHCH₃ N-methylpropylamine (common name) N-methylpropan-1-amine (IUPAC name)

Diethylamine (common name- does not use N if chains are same length)

N-ethylethanamine (IUPAC name does still use N)

N,N-dimethylpropylamine (common name) N,N-dimethylpropan-1-amine (IUPAC name)

If there are two amine groups then name as following

It could also be named 1,6-diaminohexane

Nitriles

These end in **–nitrile**, but the C of the CN group counts as the first carbon of the chain. Note the stem of the name is different: butanenitrile and not butannitrile.

butanenitrile

2-hydroxy-2-methylpropanenitrile

Carboxylic acid derivatives

Esters

Esters have two parts to their names

The bit ending in **–yl** comes from the alcohol that has formed it and is next to the single bonded oxygen. The bit ending in **–anoate** comes from the carboxylic acid. (This is the chain including the C=O bond)

methylpropanoate

Acid Anhydrides

This is called **ethanoic anhydride.** It is ethanoic because it is two ethanoate groups joined together.

If the alkyl groups are of different lengths then each one is named e.g. ethanoic propanoic anhydride

Acyl Chlorides

add **-oyl chloride** to the stem name

ethanoyl chloride

2-methylpropanoyl chloride

$$CH_2$$

Pentanedioyl dichloride

Amides

Add **-amide** to the stem name

ethanamide

Secondary and tertiary amides are named differently to show the two (or three) carbon chains. The smaller alkyl group is preceded by an –N which plays the same role as a number in positioning a side alkyl chain

N, N-dimethylpropanamide

$$H_3C$$
— CH_2 — C — NH — CH_3

N-methylpropanamide

N,N,2-trimethylpropanamide

Isomers

Structural isomers: same molecular formula different structures (or structural formulae)

See 3.1 for more on structural isomerism

Structural isomerism can arise from

- Chain isomerism
- Position isomerism
- •Functional group isomerism

Functional group isomers: Compounds with the same molecular formula but with atoms arranges to give different functional groups

Aldehydes and ketones of the same chain length would be classed as functional group isomers- e.g. Propanal and propanone (both C₃H₆O)

Questions often involve functional group isomers of carboxylic acids: including esters etc

$$\begin{array}{ccc} \mathsf{OH} & \mathsf{OH} \\ \mathsf{H}_2\mathsf{C} -\! \mathsf{CH} \!=\! \mathsf{CH} \!-\! \mathsf{CH}_2 \end{array}$$

A carbon atom that has

attached is called a chiral

four different groups

(asymmetric) carbon

Stereoisomerism

Definition: Stereoisomers have the same structural formulae but have a different spatial arrangement of atoms

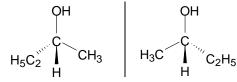
See 3.1 for EZ isomerism

There are two types of **stereoisomerism**: geometrical (E- Z isomerism) and optical isomerism

Optical Isomerism

Optical isomerism occurs in carbon compounds with 4 different groups of atoms attached to a carbon (called an asymmetric carbon).

These four groups are arranged tetrahedrally around the carbon.



Two compounds that are optical isomers of

mirror images

This causes two different isomers that are not superimposable to be formed. They are

A mixture containing a 50/50 mixture of the two isomers (enantiomers) is described as being a racemate or racemic mixture.

atom

Many naturally occurring molecules contain chiral C atoms, but are usually found in nature as a pure enantiomer

each other are called enantiomers.

Optical isomers have similar physical and chemical properties, but they rotate plane polarised light in different directions.

One enantiomer rotates it in one direction and the other enantiomer rotates it by the same amount in the opposite direction.

One optical isomer will rotate light clockwise (+)(called dextrorotatory). The other will rotate it anticlockwise(-)(called laevorotatory).

A racemic mixture (a mixture of equal amounts of the two optical isomers) will not rotate plane-polarised light.

Different systems of nomenclature are is existence for optical isomers. D/L or +/- are commonly used, but both have been superseded by the more useful and informative R/S system (this is not on the syllabus - for information only).



-ve enantiomer Anticlockwise rotation



+ve enantiomer clockwise rotation



no rotation

Chemical Reactions and Optical Isomers

Formation of a racemate

A racemate will be formed in a reaction mechanism when a reactant or intermediate has a **trigonal planar group** in the molecule is approached from both sides by an attacking species

Nucleophilic addition of HCN to aldehydes and ketones (unsymmetrical) when the **trigonal planar carbonyl group** is approached from both sides by the HCN attacking species: results in the formation of a racemate

A racemate can also be formed in the AS reaction of the electrophilic addition of HBr to an unsymmetrical alkene

Drug action and optical isomers

Drug action may be determined by the stereochemistry of the molecule. Different optical isomers may have very different effects

Thalidomide

One enantiomer of thalidomide causes birth defects in unborn children whilst the other had useful sedative problems. Unfortunately it was given in a racemic mixture when first used.

Ibuprofen