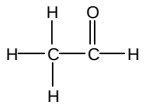
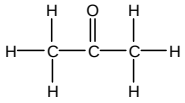
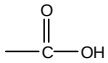
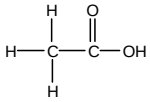
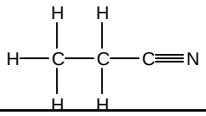
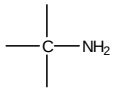
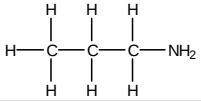
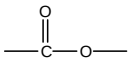
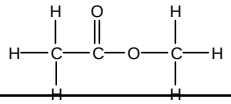
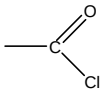
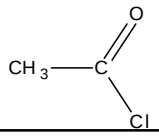
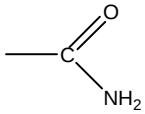
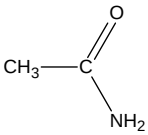
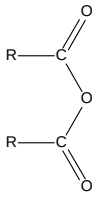
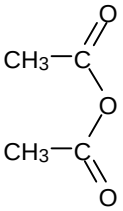
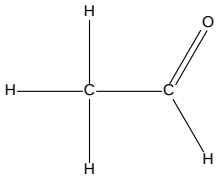
3.7 Organic naming and Isomerism continued

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

homologous series	functional group	prefix / suffix (* = usual use)	example
aldehydes		*suffix* **-al** *prefix* **formyl-**	 ethanal
ketones		*suffix** ***-one*** *prefix* **oxo-**	 Propanone
carboxylic acids		*suffix* **-oic acid**	 Ethanoic acid
nitriles		*suffix* **-nitrile** *prefix* **cyano-**	 Propanenitrile
amines		*suffix** **-amine** *prefix* **amino-**	 Propylamine Or propan-1-amine
esters		*-yl –oate*	 methylethanoate
acyl chloride		*-oyl chloride*	 ethanoylchloride
amide		*-amide*	 ethanamide
acid anhydrides		*-oic anhydride*	 Ethanoic anhydride

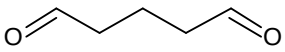
When compounds contain more than one functional group, the order of precedence determines which groups are named with prefix or suffix forms. The highest precedence group takes the suffix (and the lowest number on the carbon chain), with all others taking the prefix form. However, double and triple C-C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



ethan**al**

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

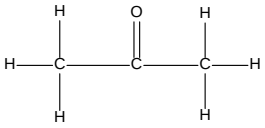


pentan**e**dial

Ketones

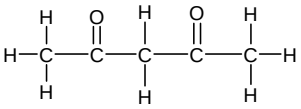
Ketones end in **-one**

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



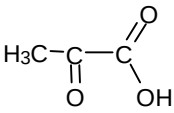
propan**one**

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



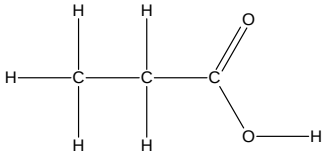
pentan**e**-2,4-dione

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



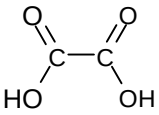
2-oxopropanoic acid

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



Propan**oic acid**

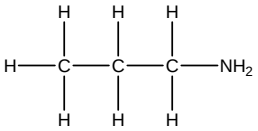
If there are carboxylic acid groups on both ends of the chain then it is called a - dioic acid



Ethan**edioic acid**

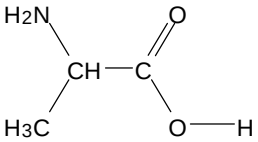
Note the **e** in this name

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



prop**yl**amine
Or propan-1-amine

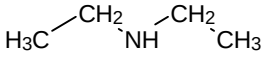
If there is another priority functional group as well as the amine group then the prefix amino is used.



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

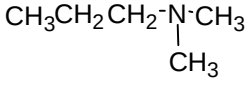
$CH_3CH_2CH_2NHCH_3$
N-methylpropylamine (common name)
N-methylpropan-1-amine (other name)



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

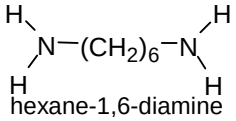
diethylamine (common name- does not use N if chains are same length)
N-ethylethanamine (other name does still use N)

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



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

If there are two amine groups then name as following

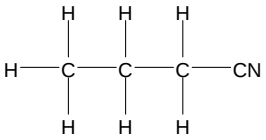


hexane-1,6-diamine

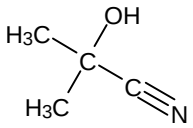
It could also be named 1,6-diaminohexane

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 : but**ane**nitrile and not butannitrile.



butanenitrile



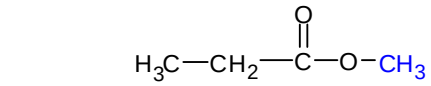
2-hydroxy-2-methylpropanenitrile

Carboxylic acid derivatives

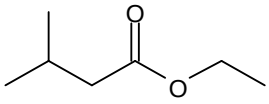
Esters

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)

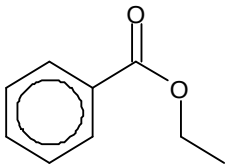


methylpropanoate



Ethyl 3-methylbutanoate

ethylbenzoate



Acid Anhydrides

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

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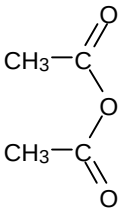
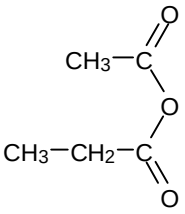
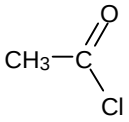


If the alkyl groups are of different lengths then each one is named e.g. ethanoic propanoic anhydride

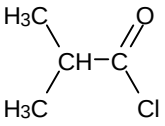


Acyl Chlorides

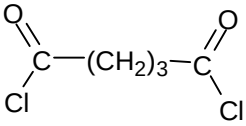
add **–oyl chloride** to the stem name



ethanoyl chloride



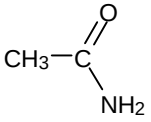
2-methylpropanoyl chloride



pentan**e**dioyl dichloride

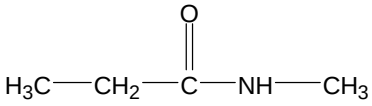
Amides

Add **–amide** to the stem name

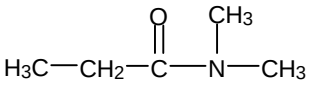


ethanamide

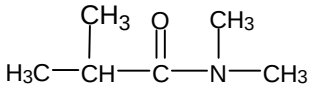
Secondary and tertiary amides are named differently to show the two (or three) carbon chains. The smaller alkyl group is preceded by an –N which plays the same role as a number in positioning a side alkyl chain



N-methylpropanamide



N,*N*-dimethylpropanamide



N,*N*,2-trimethylpropanamide

Isomers

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

See 3.1 for more on structural isomerism

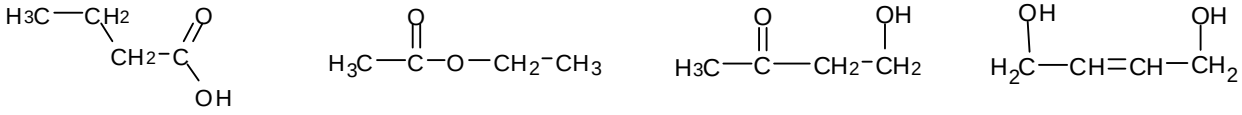
Structural isomerism can arise from

- 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 C_3H_6O)

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



Stereoisomerism

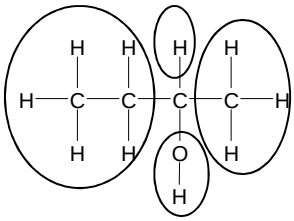
Definition: Stereoisomers have the same structural formulae but have a different spatial arrangement of atoms

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

See 3.1 for EZ isomerism

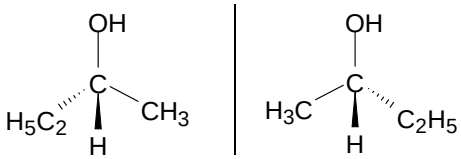
Optical Isomerism

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



A carbon atom that has four different groups attached is called a **chiral** (asymmetric) carbon atom

These four groups are arranged tetrahedrally around the carbon.



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

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

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

Two compounds that are optical isomers of each other are called **enantiomers**.

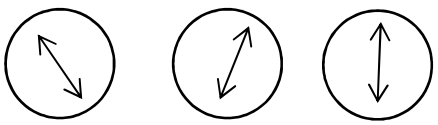
Optical isomers have similar physical and chemical properties, but they rotate plane polarised light in different directions.

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

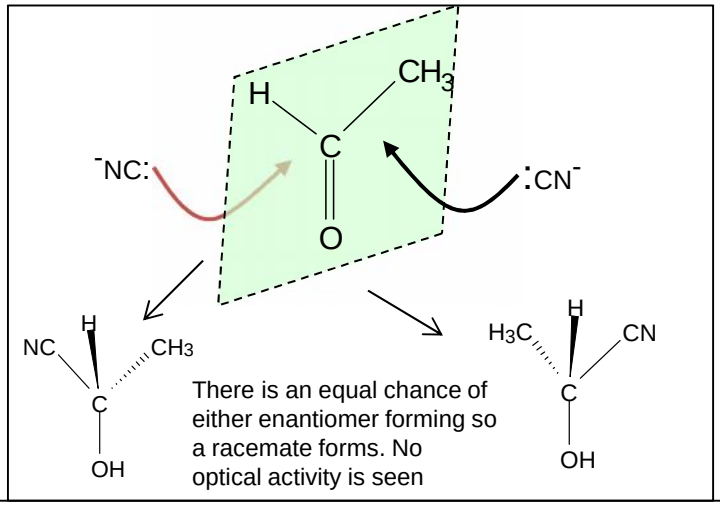
+ve enantiomer clockwise rotation

Racemate no rotation

Chemical Reactions and Optical Isomers

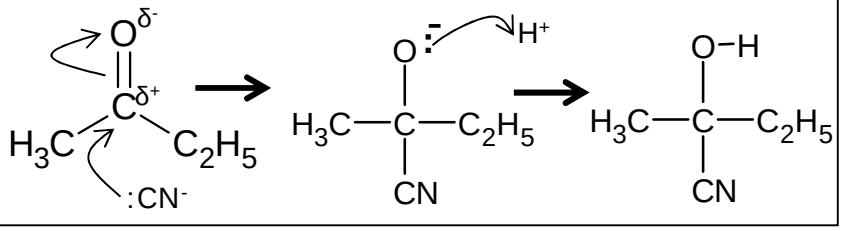
Formation of a racemate

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

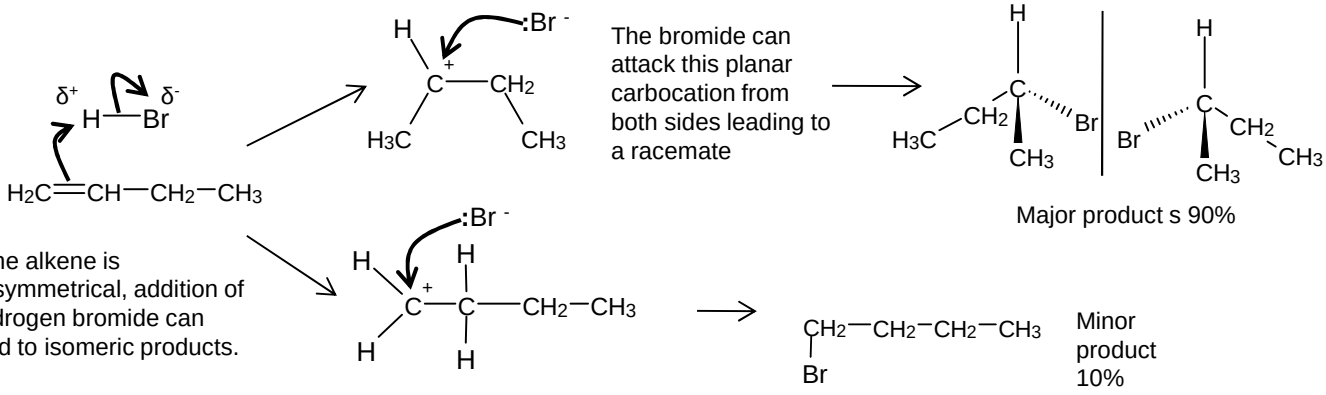


Nucleophilic addition of HCN to aldehydes and ketones (unsymmetrical) when the **trigonal planar carbonyl group** is approached from both sides by the HCN attacking species: results in the formation of a racemate

Mechanism for the reaction (drawn the same for both enantiomers)



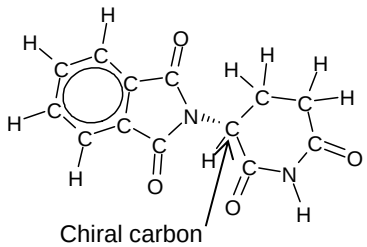
A racemate can also be formed in the AS reaction of the electrophilic addition of HBr to an unsymmetrical alkene



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