# 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     сн	suffix -al prefix formyl-	H 0 	ethanal
ketones	c	suffix* -one prefix <b>oxo</b> -	H O H        H—C—C—C—H 	Propanone
carboxylic acids	о <u>—</u> с—он	suffix -oic acid	н о      н—с—с—он   н	Ethanoic acid
nitriles	——C <b>≡</b> N	suffix -nitrile prefix cyano-	H H     H—C—C—C≡≡N 	Propanenitrile
amines	——C—NH <sub>2</sub>	suffix* -amine prefix amino-	H H H 	Propylamine Or propan-1-amine
esters	co	-yl –oate	н о н 	methylethanoate
acyl chloride	0	-oyl chloride	CH <sub>3</sub> ——C	ethanoylchloride
amide	NH <sub>2</sub>	-amide	CH <sub>3</sub> C NH <sub>2</sub>	ethanamide
acid anhydrides	R—————————————————————————————————————	-oic anhydride	CH <sub>3</sub> -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

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



propanone

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

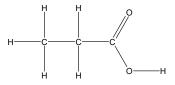
pentane-2,4-dione

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

2-oxopropanoic acid

## 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

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

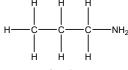
#### **Amines**

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.

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.

$$H_2N$$
  $O$   $CH-C$   $H_3C$   $O-H$ 

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

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>NHCH<sub>3</sub> N-methylpropylamine (common name) N-methylpropan-1-amine (other name)

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

N-ethylethanamine (other name does still use N)

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

If there are two amine groups then name as following

$$H$$
  $N-(CH_2)_6-N$   $H$   $H$  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: 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)

H<sub>3</sub>C—CH<sub>2</sub>—C—O-CH<sub>3</sub>

methylpropanoate

ethylbenzoate

## **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

$$CH_3 - C'$$
 $CH_3 - CH_2 - C$ 

## **Acyl Chlorides**

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

ethanoyl chloride

2-methylpropanoyl chloride

$$C - (CH_2)_3 - C$$

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

$$H_3$$
C— $CH_2$ — $C$ — $NH$ — $CH_3$ 

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  $C_3H_6O$ )

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

$$H_{3}C - C - O - CH_{2} - CH_{3}$$
  $H_{3}C - C - C$ 

$$\begin{array}{ccc} \text{OH} & \text{OH} \\ | & | \\ \text{H}_2\text{C}\text{---}\text{CH}\text{---}\text{CH}_2 \end{array}$$

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

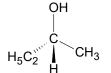
See 3.1 for EZ isomerism

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.



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

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

 $\begin{array}{c|c} & & & \\ & & & \\$ 

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

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 equally from both sides by the CN- attacking species: results in the formation of a racemate (equal amounts of both enantiomers)

A racemate can also be formed in the 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

$$\begin{array}{c} \text{CH}_3 \\ \text{H}_3\text{C-HC} \\ \text{CH}_2\text{-C} \\ \text{CH-CH} \\ \text{CH-CH} \\ \text{C=O} \\ \text{HO} \\ \end{array}$$