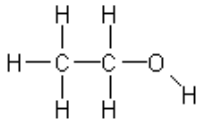
Topic 7 – Basic Concepts
Revision Notes

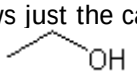
1) Formulae

Be able to recognise and use the different ways of showing organic compounds.

- **Molecular formula** is the actual number of atoms of each element in a molecule e.g. C_2H_6O for ethanol
- **Empirical formula** is the simplest whole number ratio of the atoms of each element in a molecule e.g. CH_2 for ethene (from molecular formula $C_2H_4 \div 2$)
- **General formula** is the simplest algebraic formula for a member of a homologous series e.g. C_nH_{2n+2} for alkanes
- **Structural formula** is the minimum detail that shows the arrangement of the atoms in a molecule e.g. CH_3CH_2OH for ethanol
- **Displayed formula** shows the relative positioning of atoms and the bonds between them e.g. for ethanol:



  All bonds should be shown. **Do not** put –OH for the alcohol group

- **Skeletal formula** shows just the carbon skeleton and functional groups e.g. for ethanol  (see also Appendix 1)

2) Functional groups and naming organic compounds

Be able to recognise and use the following terms.

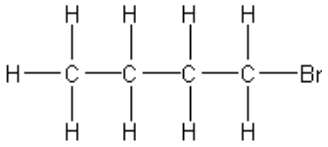
- **A homologous series** is a series of organic compounds having the same functional group with successive members differing by CH_2
- Alkanes, alkenes, alcohols and halogenoalkanes are all homologous series
- **A functional group** is a group of atoms responsible for the characteristic reactions of a compound e.g. C=C for alkenes and –OH for alcohols

The rules for naming organic compounds are as follows.

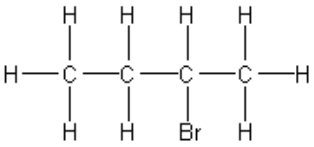
1) The functional group gives the ending of the name e.g. –ol for an alcohol
2) The number of carbons gives the first part of the name e.g. prop- or propan- for 3 carbons
3) Number the carbon chain to give the functional group carbon the lowest number
4) Any side chains (branches) or halogens go at the front of the name with commas between numbers and dashes between numbers and words e.g. 2,2-dimethylhexane
5) With more than 1 side chain or halogen, use alphabetical order e.g. 1-bromo-2-methylbutane

3) Structural isomers

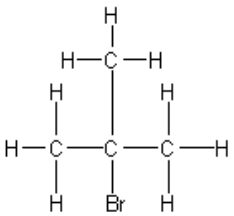
- Structural isomers have the same molecular formula but different structural formulae e.g. the molecular formula $C_4H_{19}Br$ can produce four different structures
- Differences between structural isomers arise from the position of the functional group and/or the arrangement of the carbon chain e.g. C_4H_9Br has four isomers



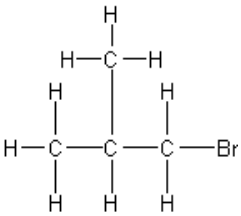
1-bromobutane



2-bromobutane



2-bromo-2-methylpropane



1-bromo-2-methylpropane

4) Cyclic Alkanes

- Carbon can form rings as well as chains
- Cyclic alkanes have general formula C_nH_{2n} (same as alkenes)
- Cyclopentane is 5 CH_2's in a ring with molecular formula C_5H_{10}. Skeletal formula is a pentagon
- Cyclohexane is 6 CH_2's in a ring. Skeletal formula is a hexagon

5) Percentage yield

- Most organic reactions do not give 100% conversion of reactant to product
- Reasons for this include the fact that most organic reactions are reversible, there may be side products and there will be loss of the desired product during purification

$$\% \text{ yield} = \frac{\text{Actual moles of product}}{\text{Possible moles of product}} \times 100\%$$

Example

In the following reaction, 2.18g of bromoethane produce 0.75g of ethanol. Calculate the percentage yield.

$$CH_3CH_2Br + NaOH \rightarrow CH_3CH_2OH + NaBr$$

Moles of reactant (bromoethane)	= mass/molar mass
	= 2.18/109
	= 0.020 mol
Possible moles of ethanol	= 0.020 mol (from equation)
Actual moles of ethanol	= 0.75/46.0
	= 0.0163 mol
Percentage yield	= 0.0163/0.020 x 100%
	= 82%

6) Atom economy

$$\textbf{Atom economy} = \frac{\textbf{Molecular mass of desired products}}{\textbf{Sum of molecular masses of all products}} \times 100\%$$

Example

In the above example

Molecular mass of desired product	= 46.0
Molecular masses of all products	= 46.0 + 102.9
	= 148.9
Atom economy	= 46.0/148.9 x 100%
	= 30.9%

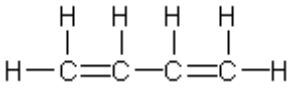
- Chemical processes with a high atom economy produce fewer waste materials
- Atom economy can be improved by developing a use for the by-product (unwanted product) or finding an alternative process with a higher atom economy

6) More on naming organic compounds

This section covers naming compounds with more than one alkene or alcohol functional group

a) Dienes

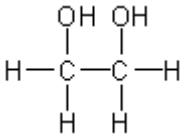
Compounds containing two alkene groups are called dienes e.g.



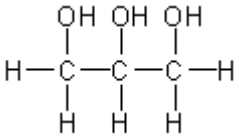
The name of this compound is buta-1,3-diene

b) Diols and triols

Compounds containing two alcohol groups are called diols while three –OH groups makes a triol e.g.



Ethane-1,2-diol



propane-1,2,3-triol (glycerol)

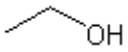
Appendix 1 - Skeletal Formulae

Skeletal formulae show carbon-carbon bonds and functional groups

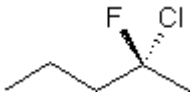
Alkane e.g. hexane

Alkene e.g. hex-3-ene

Alcohol e.g. ethanol

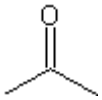


Halogenoalkane e.g. 2-chloro-2-fluoropentane

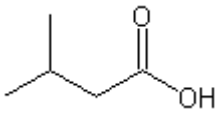


Aldehyde e.g. butanal

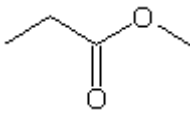
Ketone e.g. propanone



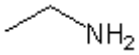
Carboxylic acid e.g. 3-methylbutanoic acid



Ester e.g. methyl propanoate



Amine e.g. ethylamine



Benzene