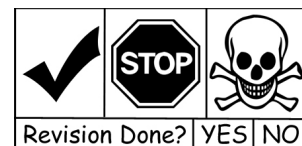


Unit 20 Organic Synthesis, NMR & Chromatography. (Paper 2 & 3)

20.1 Organic synthesis

The synthesis of an organic compound can involve several steps. **You should be able to:**

- explain why chemists aim to design processes that do not require a solvent and that use non-hazardous starting materials
- explain why chemists aim to design production methods with fewer steps that have a high percentage atom economy
- use reactions in this specification to devise a synthesis, with up to four steps, for an organic compound.



20.2 Nuclear magnetic resonance spectroscopy

Appreciation that scientists have developed a range of analytical techniques which together enable the structures of new compounds to be confirmed.

Nuclear magnetic resonance (NMR) gives information about the position of ^{13}C or ^1H atoms in a molecule.

^{13}C NMR gives simpler spectra than ^1H NMR.

The use of the δ scale for recording chemical shift.

Chemical shift depends on the molecular environment.

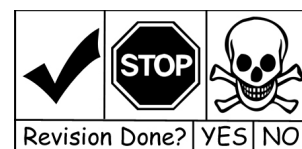
Integrated spectra indicate the relative numbers of ^1H atoms in different environments.

^1H NMR spectra are obtained using samples dissolved in deuterated solvents or CCl_4

The use of tetramethylsilane (TMS) as a standard.

You should be able to:

- explain why TMS is a suitable substance to use as a standard
- use ^1H NMR and ^{13}C NMR spectra and chemical shift data from the Chemistry Data Booklet to suggest possible structures or part structures for molecules
- use integration data from ^1H NMR spectra to determine the relative numbers of equivalent protons in the molecule
- use the $n+1$ rule to deduce the spin-spin splitting patterns of adjacent, non-equivalent protons, limited to doublet, triplet and quartet formation in aliphatic compounds.



20.3 Chromatography

Chromatography can be used to separate and identify the components in a mixture.

Types of chromatography include:

- thin-layer chromatography (TLC) – a plate is coated with a solid and a solvent moves up the plate
- column chromatography (CC) – a column is packed with a solid and a solvent moves down the column
- gas chromatography (GC) – a column is packed with a solid or with a solid coated by a liquid, and a gas is passed through the column under pressure at high temperature.

Separation depends on the balance between solubility in the moving phase and retention by the stationary phase.

Retention times and R_f values are used to identify different substances.

The use of mass spectrometry to analyse the components separated by GC.

You should be able to:

- calculate R_f values from a chromatogram
- compare retention times and R_f values with standards to identify different substances.

