

## Topic 11a – Halogenoalkanes

### Revision Notes

#### 1. General

- Functional group is a halogen i.e. F, Cl, Br or I
- General formula is  $C_nH_{2n+1}X$  where X is F, Cl, Br or I

#### 2. Substitution to form an alcohol

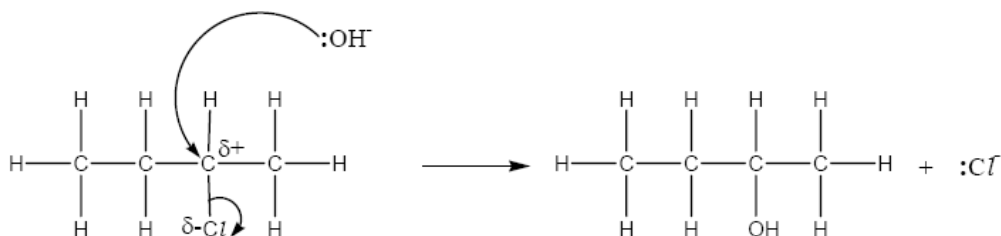
- Substitution = replacing one atom or group with another atom or group
- Reagents = the other chemicals needed
- Conditions = required temperature, pressure, catalyst etc

##### a) Equation

- Reaction is called hydrolysis
- **Example**  $C_4H_9Cl + NaOH \rightarrow C_4H_9OH + NaCl$
- Reagents Aqueous NaOH or KOH (dissolved in water)
- Conditions Heat to reflux

##### b) Mechanism

- Mechanism is called nucleophilic substitution
- Nucleophile = electron pair donor
- Mechanism includes curly arrows, lone pairs and dipoles



##### c) Rate of reaction

- Rate of hydrolysis  $C_4H_9I > C_4H_9Br > C_4H_9Cl > C_4H_9F$  *because*
- Order of bond strength  $C-F > C-Cl > C-Br > C-I$
- Shown by adding  $AgNO_3(aq)$  and timing how long silver halide precipitate takes to form

#### 3. Uses of halogenoalkanes

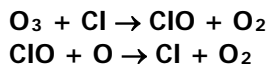
##### a) CFCs (chlorofluorocarbons) e.g. $CCl_3F$

- CFCs were used as refrigerants, propellants in aerosols and in air-conditioning. These uses were based on their properties. They are unreactive, non-toxic and highly volatile

- CFCs are no longer used as they deplete the ozone layer. In the upper atmosphere ultraviolet light breaks the C-Cl bond e.g.



- Ozone,  $\text{O}_3$ , is then broken down in a pair of propagation steps



- Green chemistry has minimised the damage to the environment caused by CFCs. Chemists have developed biodegradable alternatives to CFCs such as alkanes and HCFCs e.g.  $\text{CF}_3\text{CHCl}_2$ . In addition,  $\text{CO}_2$  has replaced CFCs as a blowing agent for expanded polymers

**b) To make plastics**

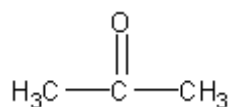
- Chloroethene ( $\text{CH}_2=\text{CHCl}$ ) is polymerised to make PVC
- Tetrafluoroethene ( $\text{CF}_2=\text{CF}_2$ ) is polymerised to make PTFE (Teflon)

## Topic 11b – Modern Analytical Techniques Revision Notes

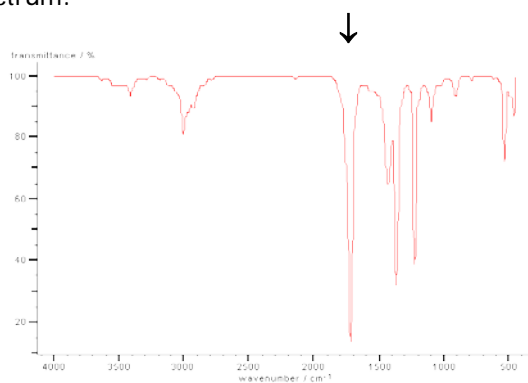
### 1) Infrared spectroscopy

- Absorption of infrared radiation causes covalent bonds to vibrate
- The frequencies that are absorbed can be used to identify the presence of certain bonds
- The absorptions you need to know are:
  - a) C=O 1680 - 1750  $\text{cm}^{-1}$
  - b) -OH in alcohols 3230 - 3550  $\text{cm}^{-1}$
  - c) -OH in carboxylic acids 2500 - 3300  $\text{cm}^{-1}$  (broad peak)
  - d) C-O 1000 - 1300  $\text{cm}^{-1}$

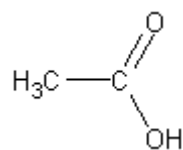
#### Example 1 – propanone



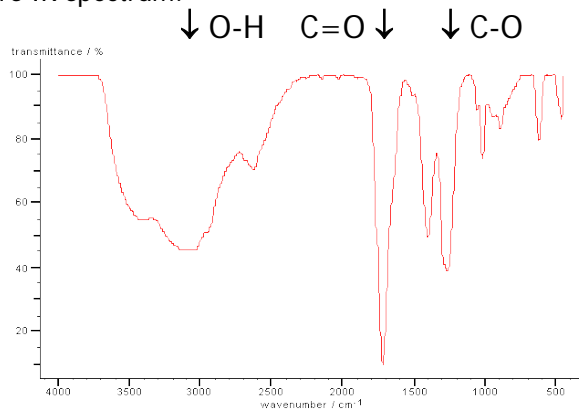
Of the absorptions mentioned above, only the C=O peak will be present in propanone's IR spectrum:



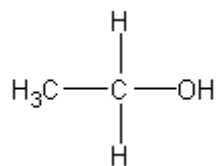
#### Example 2 – Ethanoic acid



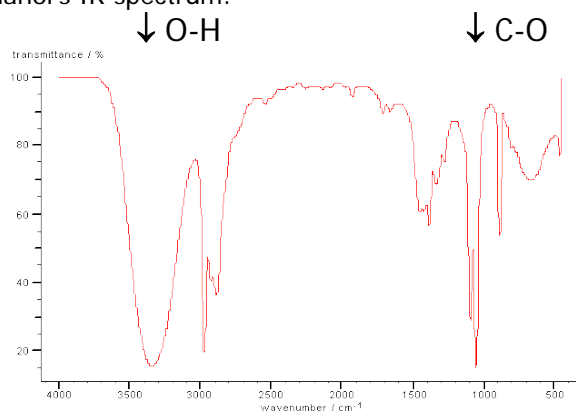
Of the peaks mentioned above, the -OH in acids, the C=O and the C-O peaks will be present in ethanoic acid's IR spectrum:



### Example 3 – ethanol



Of the absorptions mentioned above, the –OH in alcohols and the C-O peaks will be present in ethanol's IR spectrum:



- Modern breathalysers measure ethanol in the breath by analysis using infrared spectroscopy

## 2) Mass spectrometry

Mass spectrometry is a technique for measuring the masses of particles accurately

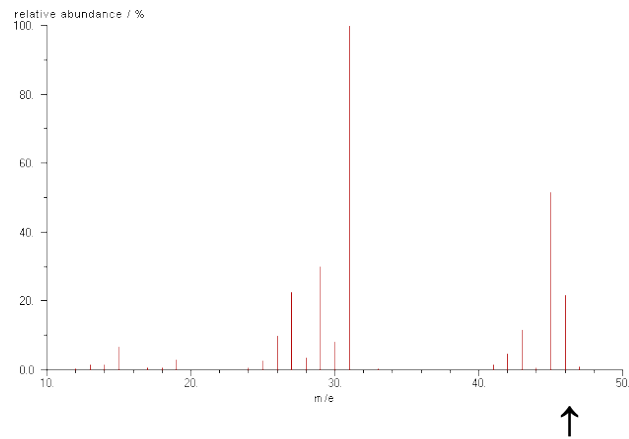
### a) Elements

- Most elements have more than one isotope
- The mass spectrum of an element gives accurate values for relative isotopic masses and says how much of each isotope there is (also called relative abundance)
- This information can be used to calculate relative atomic mass (mass number x abundance/100 + mass number x abundance/100 etc)
- Mass spectrometry can be used to identify the elements present in a sample e.g. in the Mars space probe and for monitoring levels of lead pollution in the environment

### b) Organic molecules

- In the mass spectrum for an organic molecule, the peak furthest to the right (or highest  $m/z$ ) is called the molecular ion peak and it gives the molar mass of the compound

### Example – ethanol



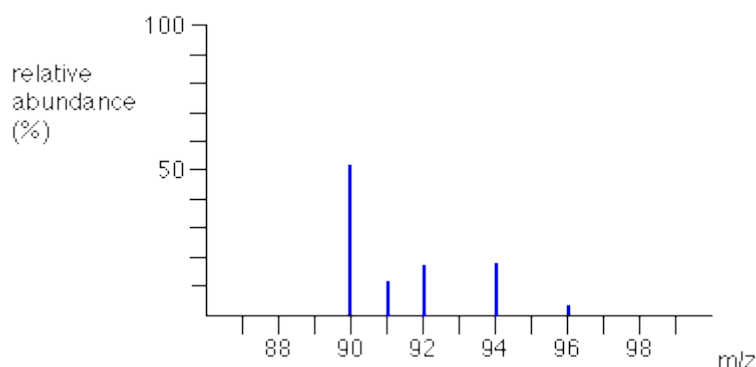
- The molar mass of ethanol is 46. The molecular ion peak is indicated by the arrow
- The molecular ion is unstable and fragments to give a characteristic spectrum
- Common fragments are  $\text{CH}_3^+$  at  $m/z$  15,  $\text{CH}_3\text{CH}_2^+$  at  $m/z$  29 and  $\text{CH}_2\text{OH}^+$  at  $m/z$  31
- A mass spectrum is essentially a fingerprint for the molecule that can be identified by computer using a database of spectra

## Appendix - Mass spectrometry for elements

The mass spectrum of an element gives the following information.

- Number of peaks = number of isotopes
- M/z of peak = mass number of isotope
- Size of peak = relative abundance (i.e. percentage)

### The mass spectrum for zirconium



#### *The number of isotopes*

The 5 peaks in the mass spectrum shows that there are 5 isotopes of zirconium - with relative isotopic masses of 90, 91, 92, 94 and 96 on the  $^{12}\text{C}$  scale.

#### *The abundance of the isotopes*

In this case, the 5 isotopes (with their relative percentage abundances) are:

zirconium-90	51.5
zirconium-91	11.2
zirconium-92	17.1
zirconium-94	17.4
zirconium-96	2.8

The relative atomic mass of Zr can be calculated from the well-known formula:

#### **Mass number x percentage/100 + Mass number x percentage/100 etc**

On another planet, such as Mars, the number of isotopes and their mass numbers will be the same as on Earth. However, the relative abundances may well be different so the relative atomic mass will be different as well.

The presence of lead in environment can be detected using mass spectrometry. There will be peaks for the four isotopes of lead at m/z 204, 206, 207 and 208 with relative abundances of 1.4%, 24.1%, 22.1% and 52.4% respectively.