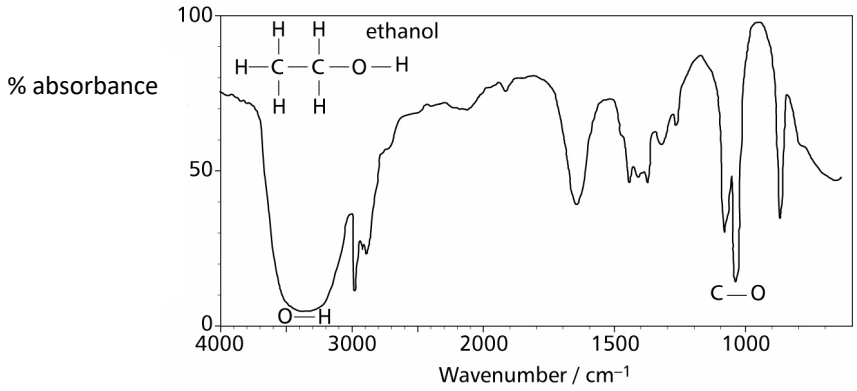
IR Spectroscopy and Mass Spectrometry

Infrared Spectroscopy

Absorption of infrared radiation causes covalent bonds to vibrate.
The infra-red spectrum can be used to identify the functional groups present in a molecule
The spectrum plots % absorbance against wavenumber (cm^{-1})



The groups which can be identified are

Functional group	Bonds		Absorption		
ALCOHOLS	O—H		1000-1300	3200-3600 broad	
ALDEHYDES/KETONES	C=O		1700-1750 sharp		
CARBOXYLIC ACIDS	C=O	O—H	1650-1720	2500-3200 broad	1000-1300

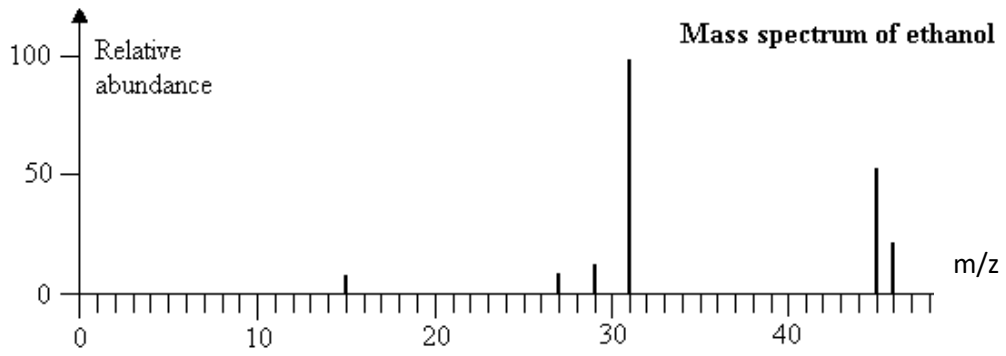
It is very important not to try to identify all of the peaks - look for particular wavenumbers only

Most organic compounds produce a peak at approximately 3000 cm^{-1} due to absorption by C–H bonds.

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

Mass Spectroscopy

Mass spectrum the molecular ion peak (usually the major peak with the largest m/z value) will give the relative molecular mass of the molecule



The molecular ion peak at 46 gives the molecule's molecular mass

Uses of mass spectrometry

1. **Determination of relative isotopic masses** The horizontal axis of a mass spectrum gives the mass to charge ratio. As the ions have a charge of one, this axis shows the relative isotopic mass.

2. **Identification of elements in a compound** e.g.

- Mass spectrometers on the Viking space probes found no traces of organic compounds in soil sampled on Mars
- Monitoring levels of environment pollution, such as lead.

Isotopic abundance The heights of the peaks, read off the vertical axis of a mass spectrum show the abundance of the isotopes which may be expressed as % composition of the sample.

Fragmentation patterns

The smaller mass peaks are the results of fragmentation; that is the parent ion falling apart under the extreme conditions present in the mass spectrometer. When suggesting the formula for the ions which cause these fragment peaks make sure they add up and the atoms are present in the original molecule.
The presence of certain fragments gives us clues as to the structure of the original molecule.

From the spectrum for ethanol:
Loss of the OH hydrogen atom (-1) produces $C_2H_5O^+$ at 45

Loss of a methyl group (-15) gives CH_2OH^+ at 31

$C_2H_5^+$ is seen at 29 (loss of OH, -17) and $C_2H_3^+$ at 27 (loss of a further H_2)

A small CH_3^+ peak is seen at 15

In the examination fragmentation patterns will be limited to alkanes, alkenes and alcohols.

A mass spectrum is essentially a fingerprint for the molecule that can be identified by computer using a spectral database.