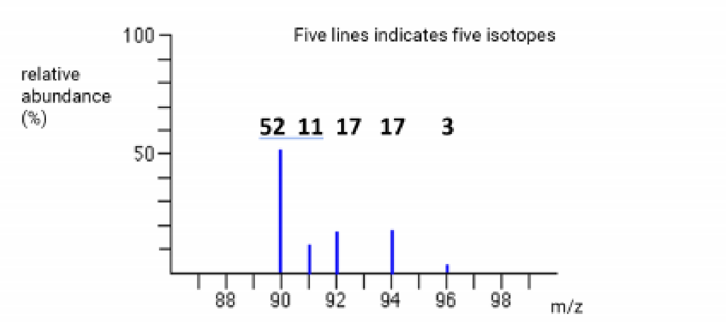
Atomic structure Knowledge organiser

Keywords

Mass Number:	Total number of protons and neutrons
Atomic number:	number of protons (smaller no.) also the
Isotope:	An atom that has the same number of pro-
Ionisation:	Removal of one or more electrons
First Ionisation Energy:	The energy needed to remove 1 electron from each atom in 1 mole of **gaseous** atoms.
Second ionisation energy:	The energy needed to remove 1 electron from each atom in 1 mole of **gaseous** +1 ions. M^{+} (g) à M^{2+} (g) + e^{-}
Successive ionisation energies:	Removing each electron in turn from a mole of gaseous atoms. Provides evidence of en-
Mass spectrometry	Technique used to calculate the mass of atoms and molecules

Determining relative atomic mass (A_r) of an element



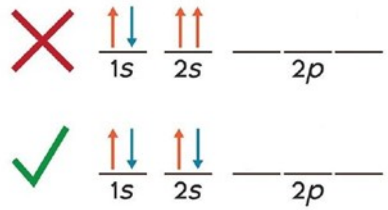
$$A_r = \frac{(52 \times 90) + (11 \times 91) + (17 \times 92) + (17 \times 94) + (3 \times 96)}{100} = 91.3$$

Rules for electron configuration

1	Aufbau "building up" principle	Electrons always fill the lowest energy level first
2	Hund's rule of maximum multiplicity (bus rule)	Electrons will fill the empty orbital of an energy level before pairing
3	Pauli's exclusion principle	When electrons pair in an orbital they have opposite spin

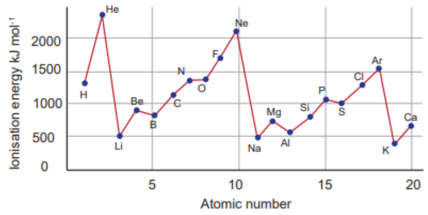
Energy levels

Energy level	Sub levels	Orbitals	Electrons
1	s	1	2
2	s,p	1,3	8
3	s,p,d	1,3,5	18
4	s,p,d	1,3,5	18



Drops in 1st ionisation energies across period 3

Ar	symbol	Electron config	Reason for drop?
13	Al	$3s^2\ 3p^1$	Electron is in p orbital further from nucleus to easier to remove
16	S	$3s^2\ 3p^4$	Electron is paired in 3p orbital so easier to remove



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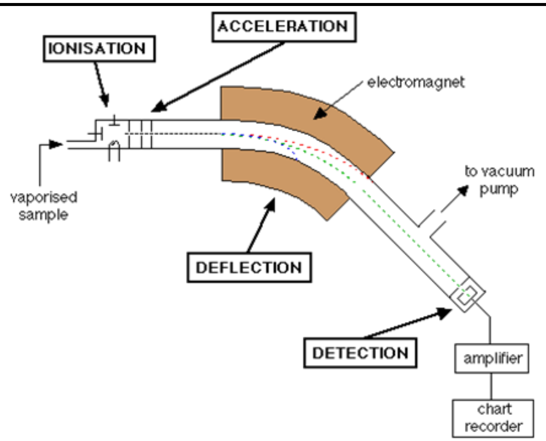
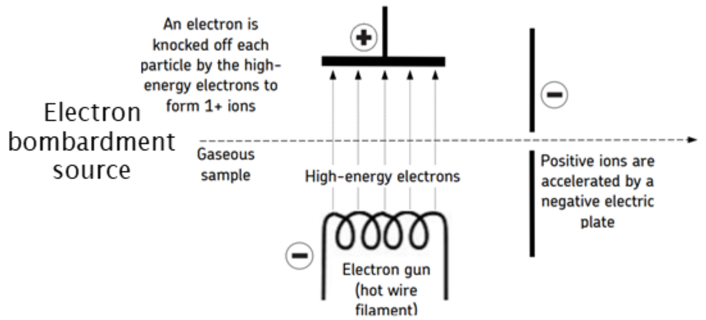
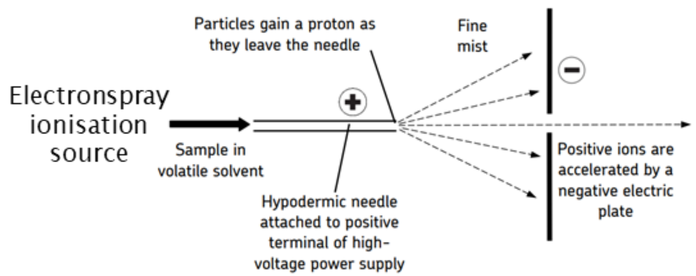
Fragmentation	In MS, the process in which a molecular ion breaks into smaller ions, radicals, and/or
m/z value	Mass/charge value used in MS to identify peaks.







Time of flight mass spectrometry

1	**Ionisation**	Sample dissolved and pushed through nozzle at high pressure and 4000v. As solvent evaporates particles gain a H^+ ion
2	**Acceleration**	+ ions accelerated by -5000v electric field. Have a fixed kinetic energy
3	**Ion drift**	Region of no electric field, so drift (lighter move faster, heavier ions slower.)
4	**Detection**	+ ions discharge creating a flow of electrons in the detector which registers the current and plots the mass spectrum.

Electrospray ionisation

- The sample X is dissolved in a volatile solvent and injected through a fine hypodermic needle to give a fine mist (aerosol).
- The tip of the needle is attached to the positive terminal of a high-voltage power supply.
- The particles are ionised by gaining a proton from the solvent as they leave the needle producing XH^+ ions (ions with a single positive charge and a mass of Mr + 1).
- The solvent evaporates away while the XH^+ ions are attracted towards a negative plate where they are accelerated. $C_2H_5OH (g) + H^+ \rightarrow C_2H_6OH^+ (g)$
- Fragmentation rarely takes place

Fragmentation

- If fragmentation occurs, the peak at the highest m/z on the mass spectrum is formed by the heaviest ion that passes through the spectrometer. Unless all molecules of the original substance break up, this corresponds to the molecular ion of the sample substance.
- Although the molecular ion peak for 2 isomers will be the same m/z value, fragmentation patterns will be different