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1.1 - Fundamental Particles

Developing ideas about the atom

- 1661 - Robert Boyle proposed there were some substances that can't be seperated - chemical elements
- 1803 - John Dalton suggested elements were made up of individual atoms - indivisible
- 1896 - Henri Beqwerel discovered radioactivity that showed particles could from inside an atom
- 1897 - JJ Thompson discovered electron (1st subatomic particle discovered) - negatively charged
  - suggested electrons located in circular arrays in a sphere of positive charge 'plum pudding model'
- 1911 - Ernest Rutherford and his team found that most of the mass and all of the positive charge of the atom was in a tiny central nucleus

Sub-atomic particles:

- three fundamental particles of an atom;
  - protons
  - neutrons
  - electrons
    - surround nucleus

protons + neutrons → make up the nucleus
- nucleons

→ properties of subatomic particles are given relative values to make it easier to use / remember

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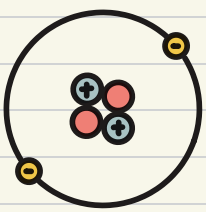
	Proton (p)	Neutron (n)	Electron (e)
Relative Mass	1	1	1/1840
Relative Charge	+1	0	-1

- atom has no overall charge because there are an equal number of protons as electrons and they have equal but opposite charges which cancel out

Arrangement of subatomic particles:



- protons and neutrons held together in the centre by strong nuclear force
  - much stronger than the electrostatic force of attraction that holds proton and electrons together in the atom
  - ∴ overcomes repulsion between protons in the nucleus but only acts over very short distances

- electrons surround nucleus and are found in a series of levels, orbits or shells - get further and further from the nucleus

1.2 - Mass Number, Atomic Number and Isotopes

Atomic number - proton number (Z)

- electron number = proton number
  - no. of electrons on outer shell determine the chemical properties / what sort of element it is

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∴ atomic number defines the chemical identity of an element

Atoms of the same element have the same atomic number and atoms of different elements have different atomic numbers

Mass number (A)

└ total number of nucleons - number of protons + neutrons

Isotopes

└ atoms of the same element with the same atomic number but different number of neutrons

- have the same electron configuration, so all isotopes of an element have identical chemical properties
- only the mass number changes

1.3 - The Arrangement of the electrons

The atom and electrons

- 1933 - Niels Bohr suggested that the atom consisted of a tiny positive nucleus orbited by negatively-charged electron, that orbit in fixed energy shells at set distances - movement of electrons from one shell to another explains how atoms absorbed and gave out

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light - beginning of quantum theory

- 1926 - Erwin Schrödinger - found equation that used the idea that electrons had properties of both waves as well as particles - this led to a theory called quantum mechanics (used to predict the behaviour of sub-atomic particles

- 1932 - James Chadwick discovered neutrons

American, Gilbert Lewis;

- inertness of noble gases was related to their having full outer shells of electrons
- ions were formed by atoms losing or gaining electrons to attain full outer shells
- atoms could also bond by sharing electrons to form full outer shells
  - form basis of modern ideas about chemical bonding

Evolving Ideas

- Dalton's model still used to explain the geometries of crystals
- Bohr's model used for a simple model of ionic and covalent bonding
- charge cloud idea used for a more sophisticated explanation of bonding and shapes of molecules
- simple model of electrons orbitting in shells is useful for many purposes, particularly working out bonding between atoms

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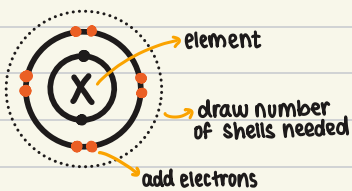
Electron Shells:

- first shell, which is closest to the nucleus, fills first then the second ...
- number of electrons in each shell = $2n^2$

Electron Diagrams

- can be written out by writing the number of electrons in each shell, starting with innermost shell and seperate by comma



→ written as; (2,8,...)

1.4 - The Mass Spectrometer

- most useful instrument for accurate determination of relative atomic mass (A_r) - based on a scale of ^{12}C as it is the only isotope with an exact, whole number A_r

$$\text{Relative atomic mass } (A_r) = \frac{\text{average mass of one atom of element}}{1/12 \text{ mass of one } C^{12} \text{ atom}}$$

$$\text{Relative molecular mass } (M_r) = \frac{\text{average mass of 1 molecule} \times 12}{\text{mass of one carbon}^{12} \text{ atom}}$$

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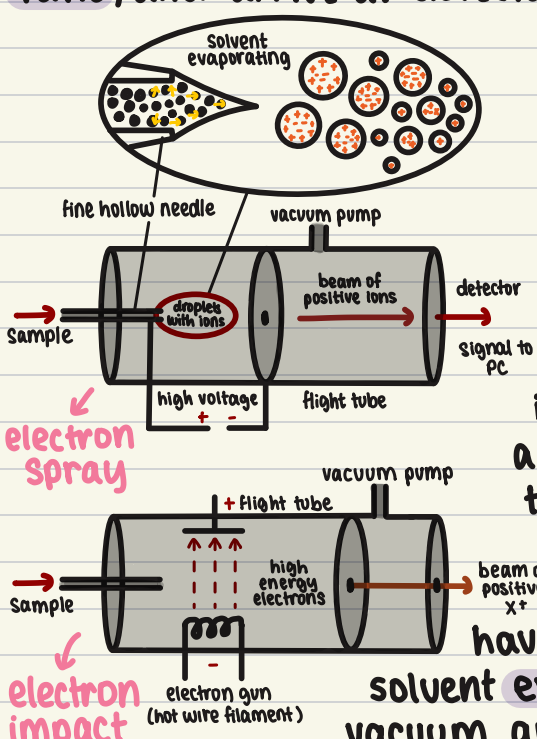
- **mass spectrometer** determines the **mass of seperate atoms / molecules**
  - different types of **mass spectrometer** but all follow the **principle of forming ions** from sample and seperating the ions **according to the ratio of their charge to their mass**

Time of Flight (TOF) Mass Spectrometer:

- **substances in the sample are converted into positive ions, accelerated to high speeds**, depending on **their mass to charge ratio**, and arrive at detector;



- **Vacuum** - whole apparatus is **kept under a high vacuum** to **prevent ions that are produced colliding with molecules from the air**
- **Ionisation** - two types of ionisation are described here. In **electrospray ionisation**, the sample is dissolved in **a volatile solvent** and forces into **a fine hollow needle** that is connected to the **positive terminal of a high voltage supply** - produces tiny **positively charged droplets** that **have gained a proton from the solvent** solvent **evaporates** from the droplets into the vacuum and the droplets get smaller and smaller until they may contain no more than a single positively charged ion - $X_{(g)} + H^+ \rightarrow XH^+_{(g)}$

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In electron impact, the sample is vaporised and high energy electrons are fired at it from an electron gun, which is a hot wire filament with a current running through it that emits beam of high energy electrons, usually knocking off one electron from each particle forming 1+ ion

$X_{(g)} + e^- \rightarrow X^+_{(g)} + 2e^-$

- Acceleration - positive ions are attracted towards a negatively charged plate and accelerated towards it, lighter ions and more highly charged ions achieve a higher speed
- Ion drift - ions pass through a hole in the negatively charged plate, forming a beam and travel along a tube, called the flight tube, to a detector
- Detection - ions with the same charge arrive at the detector, the lighter ones are first as they have higher velocities and the flight times are recorded. Positive ions pick up an electron from the detector, which causes current to flow
  - ions detected by gain of electrons + abundance relative to current
- Data analysis - signal from the detector is passed to a computer which generates a mass spectrum

Mass Spectra of elements

- mass spectrometer can be used to identify the different isotopes that make up an element
- detects individual ions, so different isotopes are detected seperately because they have different masses
- height of mass spectra shows relative abundance of each isotope
- horizontal scale gives the m/z (mass / charge ratio), for a singly charged ion is numerically the same as mass no. A

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- mass spectrometers can measure relative atomic masses to 5 d.p. of an atomic mass unit - high resolution mass spectrometry

Low resolution mass spectrometry
↳ done to 1 d.p.

M_r found using abundance of each isotope

$$\frac{(\text{Abundance} \times M_r) + (\text{Abundance} \times M_r)}{100} = \text{overall } M_r \text{ of element using its isotopes}$$

→ use mass spectrometers in space - on Mars Rover - identifies elements in rock samples

1.5 - More about Electron Arrangements in Atoms

Energy Levels

- electrons in different shells have differing amounts of energy
↳ can be represented on energy level diagrams
- shells are called main energy levels are labelled 1, 2, 3 ...
- each main energy shell can carry a max. number of electrons
↳ $2n^2$ (n = principal quantum number)
- except the first level, which only has an s-sub-level, these main energy levels are divided into sub-levels; s, p, d and f
↳ all have slightly different energies
- Level 2 → s and p sub level
- Level 3 → s, p and d sub level

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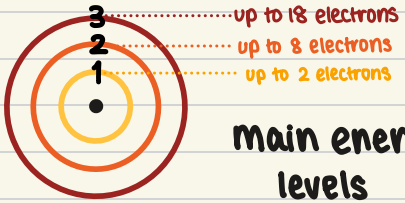
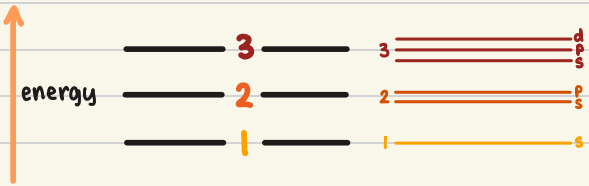


electron shells

main energy levels



main energy levels

sub-level

Quantum Mechanics

- developed in 1920s; gives a more complete description of electrons in atoms - uses maths to describe an atom as an equation (Schrödinger's equation)
- solutions give the probability of finding an electron in a given volume of space - atomic orbital

Atomic Orbitals

- electron is no longer considered to be a particle but a cloud of negative charge
- electron fills a volume of space called its atomic orbital
- concept of main/sub-levels;

- different atomic orbitals have different energies, each orbital has a number that tells us the main energy level it corresponds with
- atomic orbitals of each main level have different shapes, which in turn have slightly different energies - these are sub-levels
  - s, p, d and f

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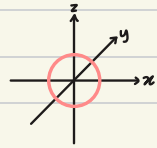
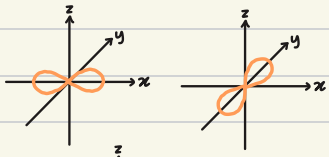
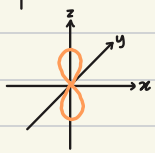
Shapes of the subdivisions of orbitals:

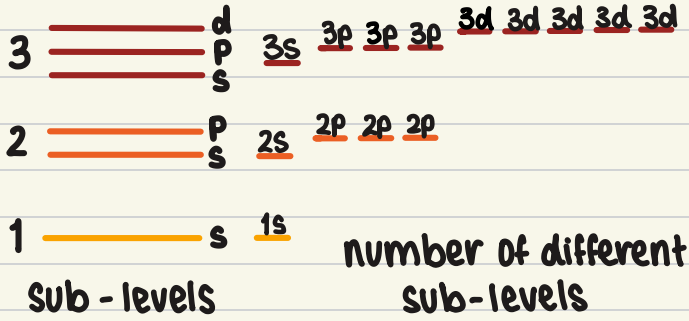


s-orbital





p-orbital



- these shapes represent a volume of space in which there is a 95% probability of finding an electron and they influence the shapes of molecules
- 1st main energy level consists of a single s-orbital, 2nd main level has a single s-orbital and three p-orbitals of slightly higher energy, 3rd main level has a single s-orbital, three p-orbitals of slightly higher energy, and five d-orbitals of slightly higher energy
- any single atomic orbital can hold a maximum of 2 electrons
  - s-orbitals can hold up to 2 electrons
  - p-orbitals can hold up to 2 electrons each; come in groups of 3 of same energy - give total of 6 electrons at p-sub-level
  - d-orbitals can hold up to 2 electrons each; come in groups of 5 of same energy - gives total of 10 electrons at d-sub-level

Main Energy Level (shell)	1	2		3			4			
Sub-levels	s	s	p	s	p	d	s	p	d	f
no. of orbitals in sub-level	1 (2e⁻)	1 (2e⁻)	3 (6e⁻)	1 (2e⁻)	3 (6e⁻)	5 (10e⁻)	1 (2e⁻)	3 (6e⁻)	5 (10e⁻)	7 (14e⁻)
total no. of electrons in main energy level	2	8		18			32			

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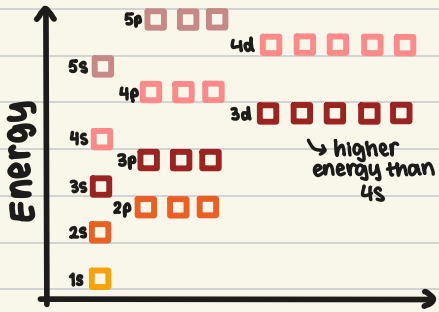

→ the energy level diagram shows the energies of the orbitals for the first few elements
└ each 'box' represents an orbital of the appropriate shape that can hold up to 2 electrons

Spin

└ electrons have a property called spin
- two electrons in the same orbital must have opposite spins
- the electrons are usually represented by arrows pointing up or down showing different directions of spin

Putting electrons into atomic orbitals

1. Atomic orbitals of lower energy are filled first + within this level, sub-levels of lower energy are filled first
2. Atomic orbitals of the same energy fill singly before pairing starts, because electrons repel each other
3. No atomic orbitals can hold more than 2 electrons

Writing electronic structures:

ORDER: $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2, 3d^6, 4p^6$...

[Kr] = $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2, 3d^6, 4p^6$...

[Ne] = $1s^2, 2s^2, 2p^6$

[Ar] = $1s^2, 2s^2, 2p^6, 3s^2, 3p^6$

→ can use noble gases for shorthand notation

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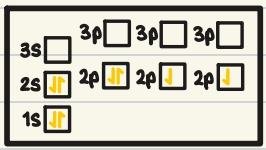
Example for oxygen:



$1s^2, 2s^2, 2p^4$ $[He]\,2s^2, 2p^4$

1.6 - Electron arrangements and ionisation energy

Ionisation energy (IE)

↳ energy required to remove a mole of electrons of atoms in the gaseous state and is measured in $KJmol^{-1}$

Removing electrons one by one

↳ can measure energy needed to remove each electron

- the first electron needs the least energy to remove it because it is being removed from a neutral atom → 1st IE
- second electron needs more energy than the first because it is being removed from a +1 ion → 2nd IE
- third electron needs even more energy to remove it because it is being removed from a +2 ion → 3rd IE

↳ successive ionisation energies

IE is not the energy change

$\therefore n^{th}\ IE = 1^{st}\ IE + 2^{nd}\ IE \ldots + n^{th}\ IE$

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- groups of similar ionisation energies indicate the number of electrons in each main level
- electron easiest to remove is on the furthest level away from positive nucleus
- most difficult to remove are closest to the positive nucleus

↳ found by jumps in successive ionisation energies

Trends in ionisation energies across a period in the Periodic table

- generally increase across a period, as the nuclear charge of the atom increases, making it more difficult to remove an electron

- some exceptions, e.g when orbital has a higher energy, it needs less energy to remove electron
  ↳ (e.g. aluminium has a lower 1st IE than magnesium)

- Paired electrons in an orbital are easier to seperate/remove due to their spin-pair repulsion, despite increase in nuclear charge (e.g. sulphur)

- Atoms with more electrons in the same main energy level are smaller in terms of atomic radius, due to unchanged amount of shielding but increased nuclear charge

Trends in ionisation energies down a group in the Periodic table

↳ general decrease in first ionisation energy going down groups

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- outer electron is in a main level that gets further from nucleus in each case

- nuclear charge increases but positive charge 'felt' by an electron in the outer shell is less than the full charge
  ↳ due to the effect of inner electrons shielding the nuclear charge