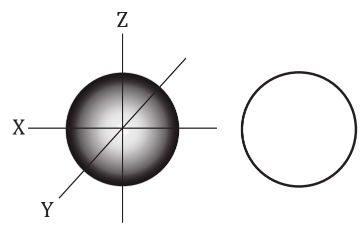
3. Electronic structure

- Electrons are involved in the changes that happen during chemical reactions.
- Electrons within atoms occupy fixed energy levels/shells which are numbered 1, 2, 3 etc (**principal quantum numbers**, n). The lower the value of n, the closer the shell is to the nucleus and the lower the energy level.
- In a shell there are areas of space (**atomic orbitals**) around the nucleus where there is a high probability of finding an electron of a given energy. Orbitals of the same type are grouped together in a subshell (s, p, d, f).
- Electrons have a property called 'spin'. For two electrons to exist in the same orbital they must have opposite spins (reduces the effect of repulsion).

Shapes of orbitals

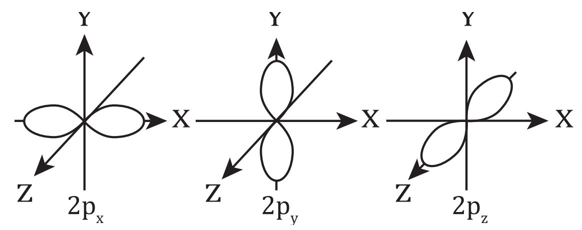
s orbital

- spherical
- can hold up to two electrons



p orbital

- dumb-bell shaped lobes at right angles (p_x, p_y, p_z)
- can hold up to six electrons in total (two in each orbital)



d orbital

- five different orbitals
- can hold up to 10 electrons in total (two in each orbital)

f orbital

- seven different orbitals (do not need to recognise/draw)
- can hold up to 14 electrons in total (two in each orbital)

Filling shells and orbitals

- Electrons fill orbitals from lower to higher energy.
- A maximum of two electrons can occupy any orbital, each having an opposite spin.
- If two or more orbitals of equal energy are available, electrons will occupy them singly at first with parallel spins before filling in pairs.

The way in which the electrons are arranged in an atom is called **electronic configuration** or **electronic structure**.

Order of filling electron shells and electronic structure

e.g. K atom, 19 electrons

$1s^22s^22p^63s^23p^64s^1$

(4s is filled before 3d as 3d is of a higher energy – also for calcium)

e.g. Cu atom, 29 electrons

$1s^22s^22p^63s^23p^63d^{10}4s^1$

(structure with a full 3d subshell is more stable than $3d^94s^2$ –

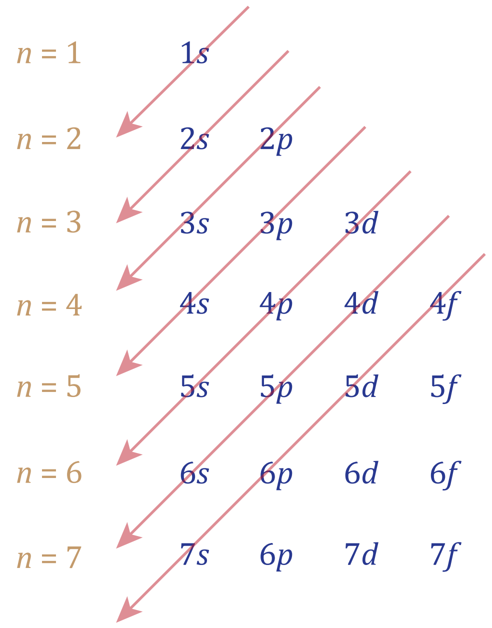
same for half-filled subshell in Cr)

e.g. Cu²⁺ ion, 27 electrons

$1s^22s^22p^63s^23p^63d^9$

(4s electrons are lost first when

d block elements form ions)



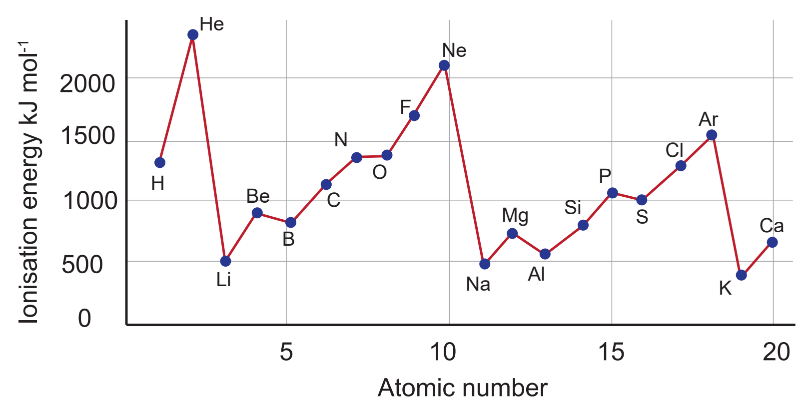
Ionisation energies

Ionisation is the process of removing electrons from an atom.

Successive ionisation energies always increase because:

- there is a greater 'effective' nuclear charge as the same number of protons are holding fewer and fewer electrons
- as each electron is removed, each shell will be drawn slightly closer to the nucleus
- as the distance of each electron from the nucleus decreases, the nuclear attraction increases.

Graph showing first ionisation energy against atomic number



The first ionisation energy of elements varies going across a period and down a group. The differences are linked to electronic structure. The attraction depends on three factors:

- the size of the positive **nuclear charge**
- the **distance** of the outer electron from the nucleus
- the **shielding** effect of electrons in fully occupied inner shells.

4. Emission and absorption spectra

Light is a form of electromagnetic radiation that travels as waves. The frequency (f), wavelength (λ) and speed of light (c) are related by the equation: $\mathbf{c = f\lambda}$

If atoms are given energy through heating or from an electrical field, electrons are pushed up from a lower energy level to a higher energy level (**promoted**). When the source of energy is removed, the electrons fall from their higher energy level (**excited state**) to a lower energy level and energy lost is released as a photon (**quantum of energy**).

The frequency (f) of electromagnetic radiation is related to its energy (E) by the equation: $\mathbf{E = hf}$ (h is a constant called Planck's constant (6.63×10^{-34} J s).

Frequency is proportional to energy and wavelength is inversely proportional to energy.

The whole range of frequencies of electromagnetic radiation is called the **electromagnetic spectrum**. Frequency and energy increase from infrared through visible light to the ultraviolet region.

Absorption spectra

The light of a frequency corresponding to the energy of the photon is **removed**. Black lines appear in the spectrum where the light of some wavelengths has been absorbed. The wavelengths of these lines correspond to the energy taken in by atoms to promote electrons to higher energy levels.

Emission spectra

When the source of energy is removed, electrons in the excited state fall to a lower energy level. Energy lost is released as a photon with a specific frequency. The spectrum consists of a number of coloured lines on a black background.

The hydrogen spectrum

The atomic spectrum of hydrogen consists of many separate series of lines. Transitions between different energy levels result in the emission of radiation of different frequencies and therefore produce different lines in the spectrum. As the **frequency increases**, the lines get **closer together** because the **energy difference** between the shells **decreases**.

Paschen series (infrared region) – each line is due to electrons returning to the **3rd shell, n = 3** energy level.

Balmer series (visible region) – each line is due to electrons returning to the **2nd shell, n = 2** energy level.

Lyman series (ultraviolet region) – each line is due to electrons returning to the **1st shell, n = 1** energy level.

The higher frequency spectral lines eventually become a continuous band of radiation and separate lines cannot be distinguished. This is the **convergence limit**. For the Lyman series, the convergence limit represents the ionisation of the hydrogen atom.