

# Topic 2: Atomic structure

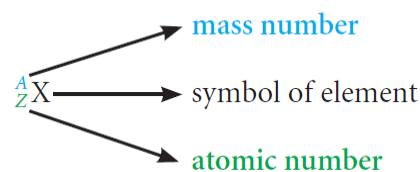
## 2.1 The nuclear atom

U1	Atoms contain a positively charged dense nucleus composed of protons and neutrons (nucleons).
U2	Negatively charged electrons occupy the space outside the nucleus.
U3	The mass spectrometer is used to determine the relative atomic mass of an element from its isotopic composition.
A1	Use of the nuclear symbol notation to deduce the number of protons, neutrons and electrons in atoms and ions.
A2	Calculations involving non-integer relative atomic masses and abundance of isotopes from given data, including mass spectra.

### Atomic structure

**Protons** and **neutrons** (**nucleons**) are found in the **nucleus**. **Electrons** are found in energy levels or 'shells' surrounding the nucleus.

particle	relative mass	relative charge
proton	1	+1
neutron	1	0
electron	$\frac{1}{1836}$	-1



### IB definitions

**Mass number (A)** – the mass number of an atom is the total number of protons plus neutrons in its nucleus.

**Atomic number (Z)** – the atomic number of an atom is the number of protons in its nucleus. It is also equal to the number of electrons it contains. The atomic number defines the element and its position in the Periodic Table.

**Isotopes** – atoms of the same element (and so have the same atomic number, Z) but have different numbers of neutrons (and so have different mass number, A).

### Calculations

- Number of protons = atomic number
- Number of electrons = atomic number – charge e.g.  $O^{2-} \rightarrow 8 - (-2) = 10$  electrons
- Number of neutrons = mass number – atomic number

### Properties of isotopes

Isotopes show the same chemical properties as neutrons do not participate in chemical reactions. A larger relative atomic mass means a **larger** density and a **slower** movement of atoms for a given temperature. These differences affect the melting and boiling points and can be used in separation of isotopes

### Uses of radioisotopes

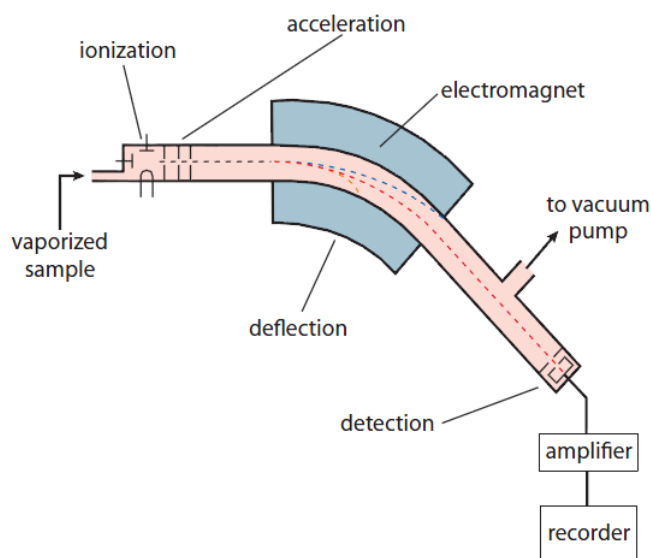
Uses of radioisotopes include: nuclear power generation, the sterilisation of surgical instruments in hospitals, crime detection, finding cracks and stresses in metals and the preservation of food, specifically:

- Carbon-14 is used in carbon-dating.
- Cobalt-60 is used in radiotherapy.(treat cancer)
- Iodine-131 is used as a tracer in medicine for treating and diagnosing illnesses
- Uranium-235 is used for nuclear fission in power plants.

## The mass spectrometer

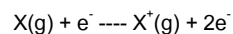
A **mass spectrometer** is used to determine relative atomic masses. (Work under a **vacuum**)

The stages of operation are:



**1. Vaporisation:** a vaporised sample is injected into the instrument; this allows individual atoms to be analysed

**2. Ionisation:** atoms are bombarded with a stream of high energy electrons, knocking off valence electrons, generating positively charged species



**3. Acceleration:** the positive ions are attracted by the negatively charged plates; they are accelerated (focused) by the **electric field**

**4. Deflection:** the ions are deflected by an external magnetic field placed at right angles to their path; the amount of deflection is proportional to the charge/mass ratio.

Lighter, highest charged atoms ----- deflected most

Heavier, smallest charged atoms ----- deflected least

**5. Detection:** ions of a **particular** mass/charge ratio are detected (other ions will hit the wall and get neutralised) and a signal is sent to a recorder; the strength of the signal is a measure of the number of ions

## Calculating the $A_r$

Using a mass spectrum, we can find out the relative atomic mass. The relative atomic mass is equal to the sum of the relative abundances multiplied by their respective masses divided by the sum of the relative abundances (which should be 100 if you're dealing with percentages):

$$A_r = \frac{\sum(\text{relative abundance} \times \text{mass})}{\sum \text{relative abundances}}$$

Problems on this subject are usually quite easy; however there is one case which is not immediately obvious: working out the abundances of isotopes given that there are only two and that you know the  $A_r$ . The trick is that if one isotope has an abundance  $x$ , then the other must have an abundance of  $100 - x$ , thus there is only one variable so the problem is capable of being solved.

### Problem solving

Chlorine has two isotopes –  $^{35}\text{Cl}$  and  $^{37}\text{Cl}$  and a relative atomic mass of 35.5. What are the abundances of the two isotopes?

Let  $x$  represent the abundance of  $^{35}\text{Cl}$ .

$$35.5 = \frac{x \times 35 + (100 - x) \times 37}{100}$$

$$35.5 \times 100 = 35x + 3700 - 37x$$

$$2x = 150$$

$$x = 75\%$$

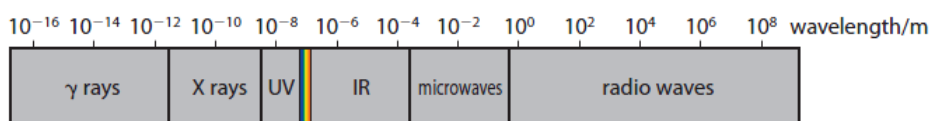
So the abundance of  $^{35}\text{Cl}$  is 75% and the latter is 25% abundant.

## 2.2 Electron configuration

- |    |   |
|----|---|
| U1 | Emission spectra are produced when photons are emitted from atoms as excited electrons return to a lower energy level.                                |
| U2 | The line emission spectrum of hydrogen provides evidence for the existence of electrons in discrete energy levels, which converge at higher energies. |
| U3 | The main energy level or shell is given an integer number, $n$ , and can hold a maximum number of electrons, $2n^2$                                   |
| U4 | A more detailed model of the atom describes the division of the main energy level into s, p, d and f sub-levels of successively higher energies.      |
| U5 | Sub-levels contain a fixed number of orbitals, regions of space where there is a high probability of finding an electron.                             |
| U6 | Each orbital has a defined energy state for a given electronic configuration and chemical environment and can hold two electrons of opposite spin.    |

A1	Description of the relationship between colour, wavelength, frequency and energy across the electromagnetic spectrum.
A2	Distinction between a continuous spectrum and a line spectrum.
A3	Description of the emission spectrum of the hydrogen atom, including the relationships between the lines and energy transitions to the first, second and third energy levels.
A4	Recognition of the shape of an s atomic orbital and the p <sub>x</sub> , p <sub>y</sub> and p <sub>z</sub> atomic orbitals.
A5	Application of the Aufbau principle, Hund's rule and the Pauli exclusion principle to write electron configurations for atoms and ions up to Z = 36.

Students should be able to identify the ultraviolet, visible and infrared and variation of wavelength and frequency across the spectrum:



A continuous spectrum shows an unbroken sequence of frequencies, such as the spectrum of visible light. A line spectrum is an emission spectrum that has only certain frequencies of light. It is produced by excited atoms and ions as they fall back to a lower energy level

## Continuous Spectrum



Energy of electromagnetic radiation is inversely proportional to wavelength and proportional to frequency of the radiation.

## Emission Lines

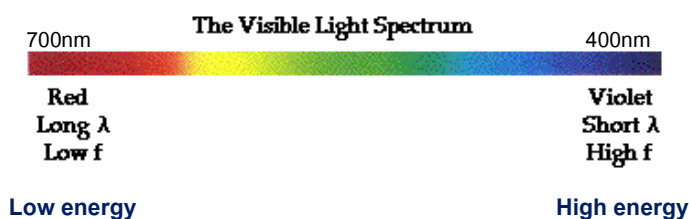


Planck's Equation:  $E = h \times f$  ( $h$  – Planck Constant =  $6.634 \times 10^{-34}$  Js)

## Absorption Lines



$$f = \frac{c}{\lambda} \quad (\lambda \text{—wavelength})$$



## The Bohr model

According to the **Bohr model**, an electron moves into a higher energy level when it absorbs energy, from the **ground state** to an **excited state**. This absorption produces the **absorption lines**. When the electrons fall back to the ground state they emit energy, producing the **emission lines**. The fact that only a few distinct colours can be observed shows there are only certain orbits in which an electron can be placed. (Deexcitation of electron releases energy and captured on the emission spectrum)

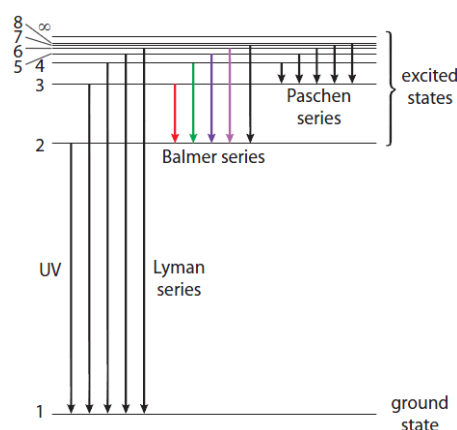
$$\Delta E_{\text{electron}} = E_{\text{photon}} = hf$$

## Energy of a particular energy level

$$E = -R_H \left( \frac{1}{n^2} \right)$$

$$\text{Energy of deexcitation of an electron } \Delta E = R_H \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right) = hv = \frac{hc}{\lambda}$$

## The emission spectrum of hydrogen



The observed emission spectrum show above results from the energy differences between energy levels that correspond to frequencies in the visible light region (the Balmer series). These are jumps from higher energy levels to the second energy levels. Jumps to the first energy level (the ground state) produce higher frequency emissions (ultraviolet) and jumps down to the third level produce lower frequency infrared radiation. The lines converge at higher energies because the energy levels inside the atoms become closer together.

Only electrons in Balmer series can be capture within the visible light range (Electrons coming back to  $n=2$  energy level)

## Relationships between lines in emission spectrum of hydrogen

As shown in the emission spectrum, lines towards violet colour are getting closer and closer. Also there are only certain distinct lines in the spectrum. So we can conclude that energy levels inside the atom are **discrete and certain**, and energy level are getting **closer** and closer to together as they become more energetic (e.g.  $n=4$  and  $n=3$  is closer than  $n=3$  and  $n=2$ )

## $2n^2$ Rule

Maximum number of electrons in a given energy level =  $2n^2$

(e.g.  $n=2$  maxi. 8 electrons;  $n=3$  maxi. 18 electrons)

## Four Quantum Numbers:

### #1 $n$ – principal quantum number

$n$ : Values of the energy level (1,2,3,4,5,.....  $\infty$ )

### #2 $l$ – angular momentum quantum number

$l$ : shape of the 3D space (sub-shell) where the electrons may be found (0,1,2,3,4..... $n-1$ )

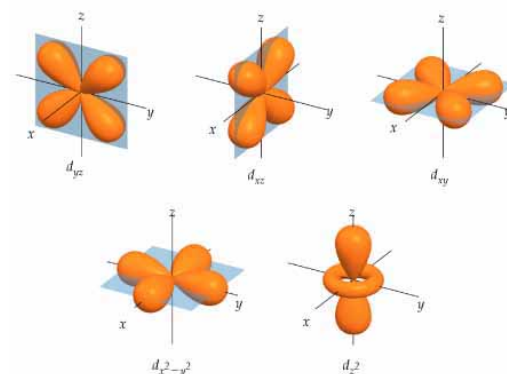
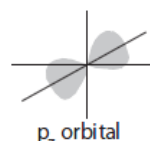
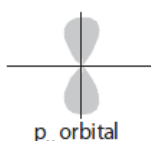
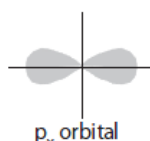
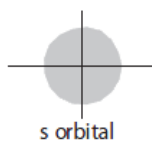
Energy level ( $n$ )	1	2	3	4
L value	0	0,1	0,1,2,	0,1,2,3,
Sub-shell	s	s,p	s,p,d	s,p,d,f

### #3 $m$ – magnetic quantum number

$m$ : orientation direction of 3D spaces (define the shape of the orbital) (- $l$ ,...0,... $l$ )

Energy level ( $n$ )	1	2	3
L value	0	0,1	0,1,2
M value	0	-1,0,1	-2,-1,0,1,2
Orbitals	S	$P_x, P_y, P_z$	$d_{xy}, d_{yz}, d^{zx}, d_{x^2-y^2}, d_{zz}$

s orbital – sphere shape



### #4 $s$ – spin quantum number

$s$ : how electrons move inside an orbital ( $\pm \frac{1}{2}$  clockwise and anticlockwise)

## Filling up electrons

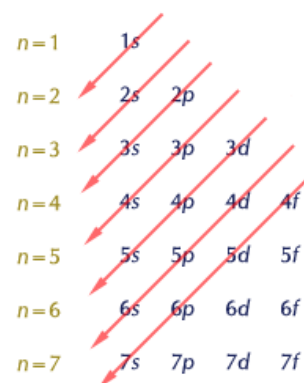
### Pauli's Exclusion Principle

No more than two electrons can occupy any one orbital and if two electrons are in the same orbital they must spin in opposite directions

(no two electrons can have the same  $n, l, m, s$  value)

### Aufbau Principle

Electrons are placed into orbitals of lowest energy first ( $n+l$  -- energy)

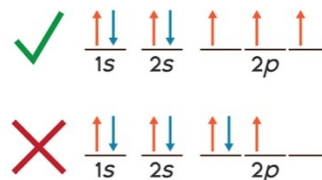


Lower n+l value orbital will be filled first

Same n+l value, lower n will be filled first

### Hund's Third Rule

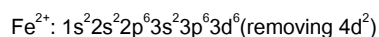
Sub-shell of more than one orbital, no pair of electrons will happen till all orbitals have 1 electron each



### Removing electrons

Removing electrons always is from outermost electrons.

For example: Fe:  $1s^2 2s^2 2p^6 3s^2 3p^6 4d^2 3d^6$  ( $4d^2$  is the outermost electrons)



There are two **exceptions**: (they will then have half filled (or full filled) 3d orbitals --- more stable)

1. Chromium:  $[\text{Ar}]3d^5 4s^1 [1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5]$
2. Copper:  $[\text{Ar}]3d^{10} 4s^1 [1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10}]$

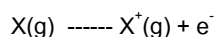
## Topic 12: Atomic structure (HL)

### 12.1 Electrons in atoms

U1	In an emission spectrum, the limit of convergence at higher frequency corresponds to the first ionization energy.
U2	Trends in first ionization energy across periods account for the existence of main energy levels and sub-levels in atoms.
U3	Successive ionization energy data for an element give information that shows relations to electron configurations.
A1	Solving problems using $E = h\nu$ . ( $\nu$ -- frequency)
A2	Calculation of the value of the first ionization energy from spectral data which gives the wavelength or frequency of the convergence limit..
A3	Deduction of the group of an element from its successive ionization energy data.
A4	Explanation of the trends and discontinuities in first ionization energy across a period.

### First Ionisation Energy

**Definition:** Amount of energy required to remove one mole of electrons from one mole of atom in its gaseous state.



### Shielding effect

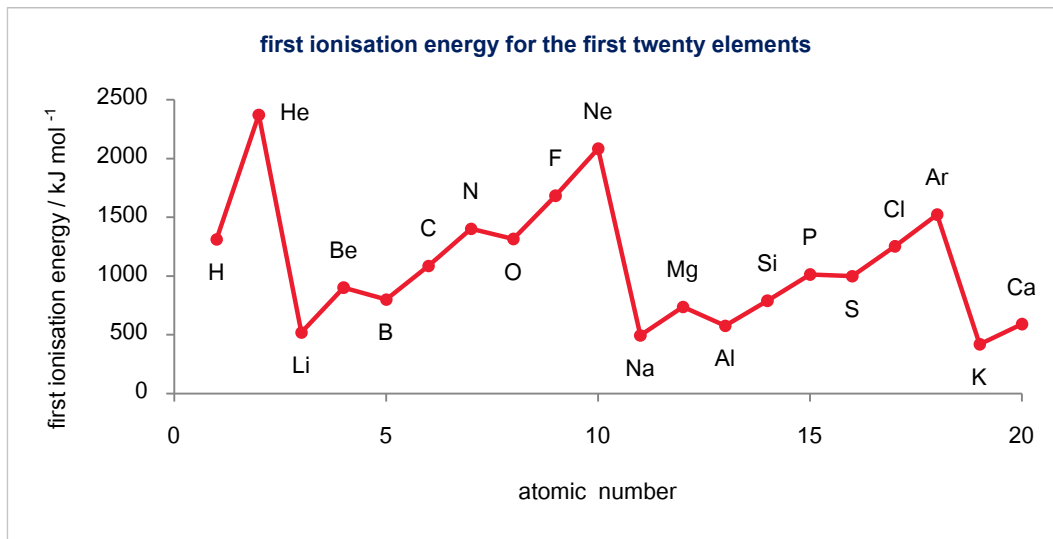
Inner electrons act as shield to block the charge from nucleus. So outermost electrons don't receive all the forces from the nucleus.

- Distances have more effect than charges, that why as we go down the group, first ionisation energy gets smaller

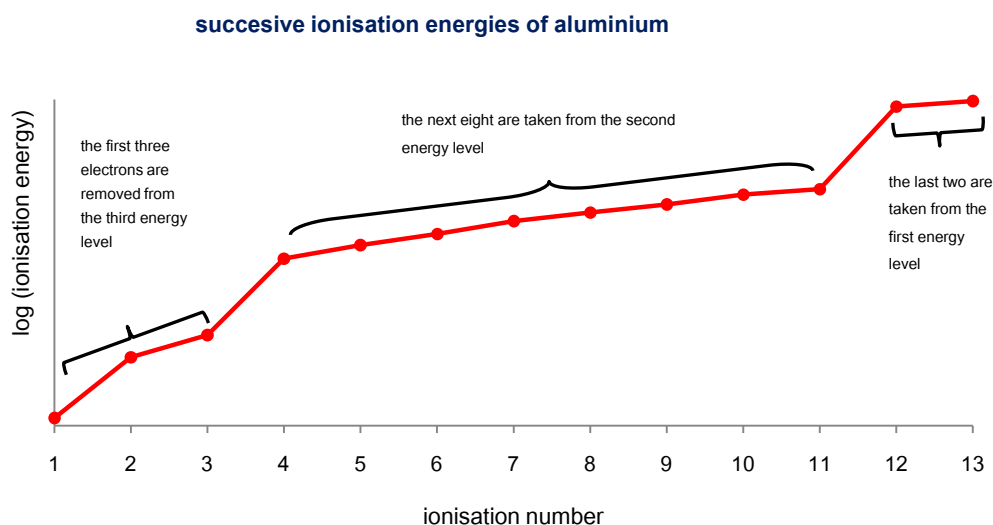
### Effective charges

Effective charges show the effective forces on the electrons. Larger  $Z_{\text{eff}}$  means stronger forces which the electrons experienced.

Effective charges ( $Z_{\text{eff}}$ ) are depended on numbers of protons and amount of shielding effects. More protons and weaker shielding effect will lead to large  $Z_{\text{eff}}$



- In a group: from top to bottom, first ionisation energy decreases (more shielding effect, electrons are further away from the nucleus –  $Z_{\text{eff}}$  decrease)
- In a period: generally increase in the period (more protons but same shielding effect –  $Z_{\text{eff}}$  increases)
- HOWEVER, there is a decrease from group 2 to group 3 (e.g. Boron has smaller 1<sup>st</sup> IE value than beryllium); that is because that electrons are taken from the p orbitals, which is further from nucleus than s orbitals (remember, distance always have most effect)
- Group 5 elements (e.g. nitrogen and phosphorus) have much higher 1<sup>st</sup> IE value because they have half-filled p-shell, half filled shell is more stable.



#### Use $E=h\nu$ to calculate first ionisation energy

First ionisation energy (in J) =  $h\nu$

First ionisation energy (in  $\text{kJ mol}^{-1}$ ) =  $h\nu N_A$  (Avogadro's constant)

Shortest wavelength – highest frequency and energy – always dextricate from  $n = \infty$  to  $n = 1$ ; limit of convergence at higher frequency corresponds to the first ionization energy (removing one electron)

#### Example

Question: Calculate the first ionisation energy in  $\text{KJ mol}^{-1}$ , for hydrogen given that its shortest-wavelength line in the Lyman series is 91.16nm.

$$\text{Solution: } IE = h\nu = \frac{hc}{\lambda} = \frac{6.626 \times 10^{-34} \times 2.998 \times 10^8}{91.16 \times 10^{-9}} = 2.719 \times 10^{-18} \text{ J}$$

$$\text{Converted in to } \text{KJ mol}^{-1} IE = 2.719 \times 10^{-18} \text{ J} \times 6.022 \times 10^{23} = 1.312 \times 10^6 \text{ J mol}^{-1} = \mathbf{1312 \text{ kJ mol}^{-1}}$$