Chapter 2: Atomic structure – fast facts

2.1 The nuclear atom

The mass of an atom is concentrated in its minute, positively charged nucleus.

- Protons and neutrons are known as nucleons and are present in the nucleus of an atom.
- Electrons have a negative charge, occupy space outside the nucleus and are responsible for an atom's volume.
- The relative masses and relative charges of the sub-atomic particles are:

	Relative mass	Relative charge
Proton	1	+1
Neutron	1	0
Electron	5×10^{-4}	–1

- The mass of the electron is generally considered to be negligible.
- **Atomic number (Z)** = number of protons. It is the fundamental characteristic of an element.
- **Mass number (A)** = number of (protons + neutrons).
- **Isotopes** are atoms with the same atomic number but with different mass numbers. They have the same number of protons but different numbers of neutrons.
- For a species ${}^{A}_{Z}X$:

  number of protons = Z

  number of electrons = Z

  number of neutrons = $A - Z$
- Isotopes differ in physical properties that depend on mass such as density, rate of diffusion, etc. This difference is very significant for the isotopes of hydrogen because deuterium, ${}^{2}_{1}H$, has twice the mass of the more abundant ${}^{1}_{1}H$. As isotopes have the same electron arrangement they have the same chemical properties.
- For an element, the mass spectrum gives two important pieces of information: the number of isotopes and the abundance of each isotope. This allows the relative average atomic mass, A_r to be calculated.
- **Relative atomic mass** (A_r) of an element is the average mass of an atom according to the relative abundances of its isotopes, on a scale where the mass of one atom of ${}^{12}_{6}C$ is 12 exactly.

  For example for Cl which has two isotopes ${}^{35}_{17}Cl$ (75 %) and ${}^{37}_{17}Cl$ (25 %):

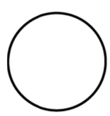
  $$A_r = \frac{(35 \times 75) + (37 \times 25)}{100} = 35.50$$
- For a molecule, the peak with largest mass represents the molecular (parent) ion and its mass gives the relative molecular mass (M_r) of the compound.

2.2 Electron configuration

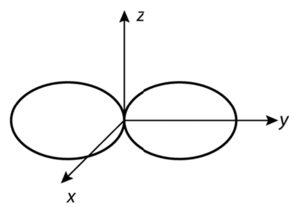
The electron configuration of an atom can be deduced from its atomic number.

- The electromagnetic spectrum includes waves in order of decreasing frequency/energy: γ rays, X-rays, ultraviolet radiation, visible light, IR radiation, microwaves, and radio waves (see section 3 of the IB data booklet).
- Frequency (ν) and wavelength (λ) are related by: c (speed of light) = ν λ.
- The energy of a photon (E_{photon}) is related to the frequency (ν) of the radiation by Planck's equation: $E_{photon} = h\nu$ (the equation is given in section 1 of the IB data booklet)

  h is Planck's constant (see section 2 of the IB data booklet).
- A **continuous spectrum** contains radiation of all wavelengths within a given range (e.g. the visible spectrum).
- A **line spectrum** consists of discrete lines of different wavelengths/frequencies.
- The emission spectrum of hydrogen atom consists of different series of lines in different regions of the electromagnetic spectrum.
- The lines in an emission spectrum are produced by excited electrons falling from higher to lower energy levels: $\Delta E_{atom} = h\nu = hc/\lambda$.
- As the energy levels of the hydrogen atom converge at higher energy as they are further from the nucleus, the lines in the spectrum also converge at higher energy/frequency.
- The main energy levels of electrons in atoms (in order of increasing energy) are identified by integers, $n = 1, 2, 3, 4$ …
- Each main energy level can hold a maximum of $2\,n^2$ electrons.
- Each main energy level contains n sub-levels and n^2 orbitals.
- The sub-levels in order of increasing energy are identified by letters: **s**, **p**, **d**, **f**, etc.
- The **electron configuration** of an atom describes the number of electrons in each energy sub-level.
- **Orbitals** are regions in space in which an electron may be found in an atom. Each orbital can hold two electrons of opposite spin.
- They have characteristic shapes. s orbitals are spherical and p orbitals are dumb-bell shaped. There are three p orbitals orientated along the *x*, *y* and *z* axis.



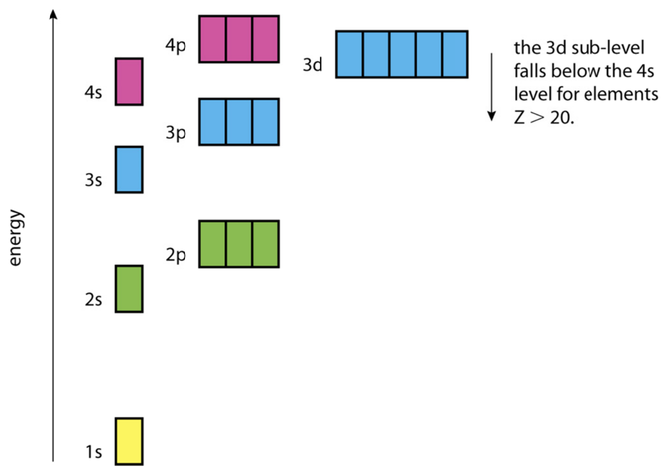
s orbital



p_y orbital

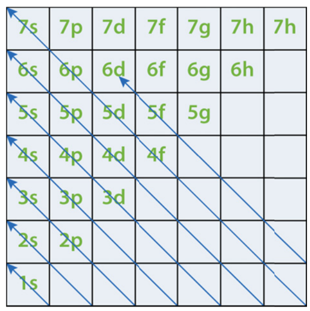
- The **Pauli exclusion principle** states that only electrons with opposite spin can occupy the same orbital.

- Orbital diagrams are used to describe the number of electrons in each orbital. Each orbital is represented by a box and each electron by a single-headed arrow which represents the direction of its spin.
- The relative energies of the sub-levels and their composition are summarized.



Level	Sub-level	Maximum no. of electrons in sub-level	Maximum no. of electrons in level
$n = 4$	4f	14 (seven f orbitals)	32
	4d	10 (five d orbitals)	
	4p	6 (three p orbitals)	
	4s	2 (one s orbital)	
$n = 3$	3d	10 (five d orbitals)	18
	3p	6 (three p orbitals)	
	3s	2 (one s orbital)	
$n = 2$	2p	6 (three p orbitals)	8
	2s	2 (one s orbital)	
$n = 1$	1s	2 (one s orbital)	2

Here is a useful mnemonic to the order of filling orbitals. Follow the arrows to see the order in which the sub-levels are filled.
1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4f, 5d, 6p, 7s …



- The **Aufbau principle** states that orbitals with lower energy are filled before those with higher energy.
- **Hund's rule** states that every orbital in a sub-level is singly occupied with electrons of the same spin before any one orbital is doubly occupied.
- The number of electrons in a sub-level is represented by a superscript number.
- Condensed electron configurations use square brackets to show the noble gas core.

Element	Electron configuration
H	$1s^1$
Li	$1s^2 2s^1$
B	$1s^2 2s^2 2p^1$
Na	$1s^2 2s^2 2p^6 3s^1$

Element	Electron configuration
Sr	[Ar] $3d^1 4s^2$
Cr	[Ar] $3d^5 4s^1$
Ni	[Ar] $3d^8 4s^2$
Cu	[Ar] $3d^{10} 4s^1$

- Note the exceptional configuration of copper and chromium, which can be accounted for the stability of the half- full (d5) and full (d10) d sub-shell.
- The block nature of the Periodic Table is determined by the highest energy occupied sub-level. Elements in the s block have valence electrons in s orbitals; elements in the p block have valence electrons in the p sub-level.
- Positive ions are formed by removing electrons from the neutral atom. The electron configuration of Na^+ for example is $1s^22s^22p^6$. Negative ions are formed by adding electrons to a neutral atom. The electron configuration of F^- $1s^22s^22p^6$.

12.1 Electron configuration

The quantized nature of energy transitions is related to the energy states of electrons in atoms and molecules.

- The ionization energy of hydrogen corresponds to the transition n = 1 to n = ∞(the convergence limit at higher energies).
- The **first ionization energy** is the minimum energy required to remove one mole of electrons from one mole of gaseous atoms to form one mole of univalent cations in the gaseous state. It is the enthalpy change for the reaction: $X(g) \rightarrow X^+(g) + e^-$.
- Ionization energy can be calculated from the equation $E_{photon} = hv$ (the equation is given in section 1 of the IB data booklet)
- Trends in first ionization energies across periods gives evidence for the existence of main energy levels and sub-levels.
- First ionization energy:
  - decreases down a group – due to increasing distance of outer electrons from the nucleus
  - increases in general along a period – due to increasing effective nuclear charge
  - shows regular discontinuities in the increase across a period – due to the existence of sub-shells.
- Successive ionization energies of the same element give evidence for electron configurations.
- Large increases in successive ionization energies of an atom occur when an electron is removed from a different energy level. Smaller increases occur when an electron is removed from a different sub-level. For example, a very small jump occurs when there is a change from a p^4 to a p^3 configuration as paired electrons are easier to remove than unpaired electrons as they are strongly repelled by their partner.