CHEM1101

Generic attributes

Significant figures and important equations

Which figures are significant?

- All non-zero digits are significant
- Zeros appearing between any two non-zero digits are significant
- Leading zeros are not significant
- Training zeros in a number after a decimal point are significant

Important equations:

$$n\ (number\ of\ moles) = \frac{m\ (mass)}{M\ (molecular\ mass)}$$

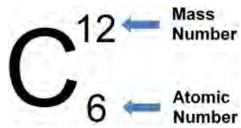
$$n\ (number\ of\ moles) = \frac{N\ (Number\ of\ particles)}{N_A\ (Avogadro's\ number)}$$

Avogadro's constant, $N_A = 6.022 \times 10^{23}$ moles
1 atomic mass unit (amu) = 1.66×10^{-27} kg

The nucleus

Nuclides and isotopes

The nucleus contains nucleons; protons, neutrons, electrons and positrons (positive electrons).



Nuclide – an atom with a particular mass and atomic number
Isotope – nuclides with the same atomic number but different mass numbers

Nuclear stability

Half-life – the amount of time taken for half of the sample to decay. Despite all radioactive nuclides having different rates of decay, this data forms an exponential decay curve.

The **rate of decay** depends on the number of nuclei present. For example, despite the percentage of the sample that will decay per time unit remaining constant (k), a smaller number of nuclei equals a smaller amount that decays.

Carbon dating

- C-14 exists in living organisms
- When an organism dies, C-14 -> N-14
- Ratio of C-14 to N-14 can then be used to estimate the time since death

The stability of a nucleus involves two opposing forces:

- **Electrostatic repulsion** between protons (long range force)
- Strong **nuclear attraction** between all nucleons (short range force)

Determining stability:

- As the **size of the nucleus** increases, the electrostatic repulsion becomes greater than the nuclear attraction forces and the atom becomes **unstable**, leading to nuclear decay.
- Composition of the nucleus – instability can also occur when there are too few or too many neutrons in the nucleus. If both forces act equally, the atom is stable.
- Anything larger than Lead-208 is unstable
- Smaller atomic numbers follow a 1:1 (neutron:proton) ratio

Nucleogenesis and the proton-proton chain

Nucleogenesis is the formation of new nuclei from existing nucleons. The proton-proton chain is the primary nucleogenesis reaction:

$$Overall\ hydrogen\ burning\ reaction{:}\ 4{}_{1}^{1}H \rightarrow {}_{2}^{4}He + 2{}_{1}^{0}e + \gamma$$

Activity – specific and molar

Activity (A) – the number of nuclei that disintegrate per second. Activity is measured in Becquerels (Bq). Activity is also proportional to the number of nuclei:

$$\boldsymbol{A = kN}\ (1)\ where\ k\ is\ decay\ constant$$
$$Using\ N = N_0 e^{-kt}\ and\ (1),$$
$$\therefore \boldsymbol{A = A_0 e^{-kt}}$$

These equations can be used to find the amount of sample remaining at various times and additionally the half-life at t = $t_{1/2}$ and N = $N_0/2$.
Key: A = activity, A_0 = initial activity, k = decay constant and t = time.

Low activity	High activity
Small decay constant (k)	Large decay constant (k)
Long half-life	Short half-life

Specific activity (activity per gram) and **molar activity** (activity per mole) can also be found.

$$\frac{activity\ (Bq)}{mass\ (g)} = specific\ activity\ (Bq/g)$$

$$\frac{activity\ (Bq)}{moles\ (n)} = molar\ activity\ (Bq/mol)$$

Biological damage by ionising radiation

The biological effect of radiation is measured in sieverts (sv). This measure takes into account the type, energy and activity of the source.

What makes radiation damaging?

The high energy of radiation causes the ionisation of matter – such as H20!

- Enzymes lose function as water is converted into products that alter the internal environment
- Causes DNA and cell membrane damage

Severity of radiation damage

The effects of radiation depend upon:

1. The type of radiation
   - Penetration varies with each type of radiation: α < β < γ
   - Biological damage also varies with each type: γ < β < α

2. The length of exposure
   - Short term/acute can lead to radiation poisoning
   - Long term/chronic can lead to radiation-induced cancer

3. The source of exposure
   - Internal i.e. ingestion/inhalation of α or β radiation
   - External i.e. penetration of skin by γ radiation

Radioactive isotopes: cancer therapy and imaging

Cancer therapy - radiation can kill cells!

- Ionising radiation can be focused onto the tumour (γ)
- Radiopharmaceuticals can be internally administrated and can target the tumour (α or β) e.g. iodine-131 targets thyroid cancer

Imaging

- Radio-imaging (γ)
- Can be used to create a 3D view of the body
- PET (Positron emission tomography) imaging
  - The positron reacts with an electron inside the body, producing two gamma rays which can be detected outside the body
  - E.g. fludeoxyglucose (FDG) can be used for parts of the body that use high levels of glucose such as the brain and tumours

Unstable nuclei decay modes

α decay – decay of a helium nucleus ${}^{4}_{2}He$

β decay – electron is ejected from the nucleus to balance the charge of the atom ${}^{1}_{0}n \rightarrow {}^{1}_{1}p + {}^{0}_{-1}e^{-}$

- Neutron: atomic number ratio decreases

β+ decay (positron decay) – positron is ejected from the nucleus to balance the charge of the atom ${}^{1}_{1}p \rightarrow {}^{1}_{0}n + {}^{0}_{1}e^{+}$

- Neutron: atomic number ratio increases

Electron capture – electron 'captured' from inner shell causing electrons from higher shells to fall to fill the gap, emitting x-rays

- Neutron: atomic number ratio increases

Neutron emission – emission of a neutron ${}^{1}_{0}n$
γ decay – often accompanies other decay forms

Wave Theory of Electrons and Atomic Energy Levels

Photons: energy and wavelength

Light – electromagnetic radiation that has **both wave and particle nature**
Photon – a discrete (quantised) bundle of light energy
The amount of energy in a photon is determined by its frequency and wavelength:
$\nu = \frac{c}{\lambda}$ (where ν 'nu' = the frequency of oscillation, c = the speed of light)

Quantum theory – developed to explain experimental observations that could not be understood using 'classical' theories of physics

Max **Planck** proposed that energy is quantised:
$E = h\nu$ (where h = Planck's constant)

The photoelectric effect demonstrates that light can eject electrons from a metal if it has a high enough frequency. This can be explained by the suggested that light has a particle nature, it is quantised as a photon.

Changes in electron energy levels

Atoms lose energy by **quantum jumps** between electron orbits, producing the discrete wavelengths seen in the visible atomic emission spectra.

One-electron atoms

Bohr's model does not work for atoms with more than one electron.

(**Bohr's atomic model suggests continuous loss of energy**, but this means that the electrons would eventually spiral into the nucleus. This model could also not explain why an electron could have discrete orbits/energies.)

Particles: wavelength and momentum

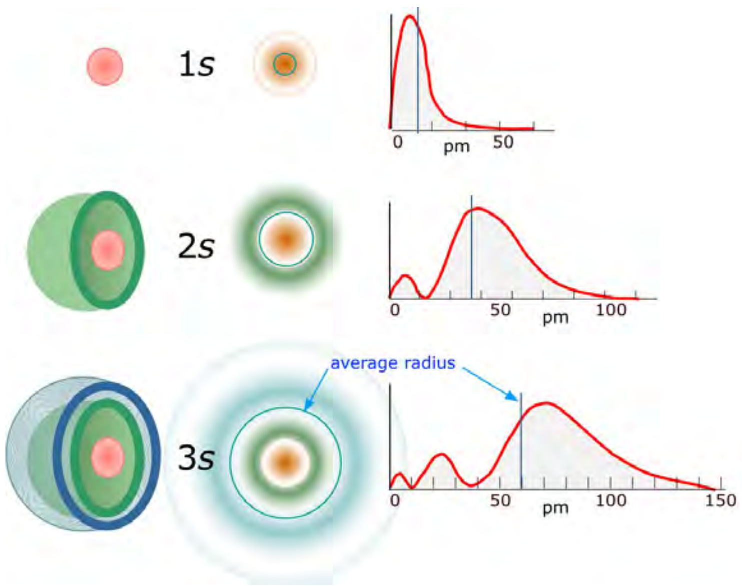
If light can behave both as a wave and a particle, **De Broglie** reasoned than an electron could also have these properties.
$\lambda = \frac{h}{p} = \frac{h}{mV}$ (where m = mass, h = Planck's constant, p = momentum, V = velocity)

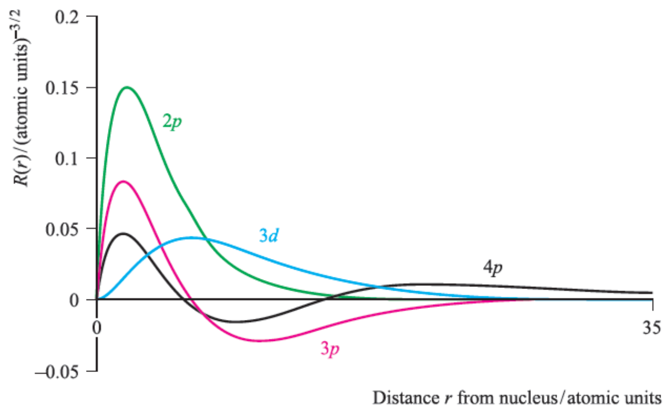
Shape of Atomic Orbitals and Quantum Numbers

Waves

Unlike Bohr's model, **electrons move in 3D waves** rather than circular orbits. The lowest energy level for a wave is called the fundamental. The energy of this fundamental is dependent upon the degree of confinement of the electron.

Wave representations





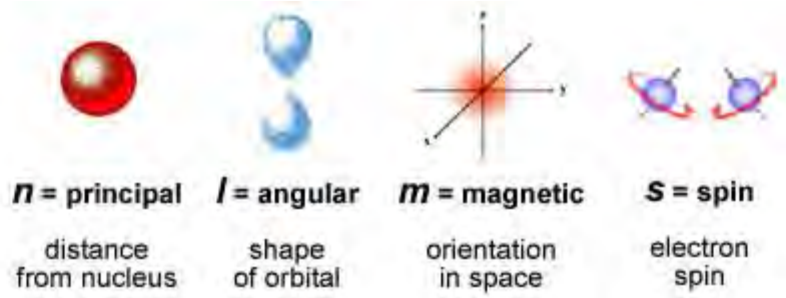
Born interpretation of the electron wave

Wavefunction (Ψ)

Electron density (Ψ^2)

Max **Born** stated that, the electron density at any given point is proportional to the probability of finding an electron at that certain point in space. Therefore, Ψ^2 is always > 0.

Quantum numbers and orbitals



name	symbol	orbital meaning	range of values	value example
principal quantum number	n	shell	$1 \le n$	$n = 1, 2, 3\ldots$
azimuthal quantum number (angular momentum)	ℓ	subshell	$0 \le \ell \le n-1$	for $n = 3$: $\ell = 0, 1, 2\,(s, p, d)$
magnetic quantum number, (projection of angular momentum)	m_ℓ	energy shift	$-\ell \le m_\ell \le \ell$	for $\ell = 2$: $m_\ell = -2, -1, 0, 1, 2$
spin projection quantum number	m_s	spin	$-\frac{1}{2}, \frac{1}{2}$	for an electron, either: $-\frac{1}{2}, \frac{1}{2}$

More nodes = more energy and a shorter wavelength.

Also, ℓ gives the number of planar nodes. Use (n-1) – ℓ to find the number of spherical nodes.