

INFORMATION ONLY

Atomic Structure

Early Atomic Theories

Dalton's Atomic Theory:

- Each element is composed of extremely small particles called atoms.
- All of the atoms of 1 element are identical to each other but are different from the atoms of another element.
- Atoms of one element cannot be changed into atoms of a different element by chemical reactions; atoms are neither created nor destroyed in chemical reactions.
- Compounds are formed when more than one elements combine.

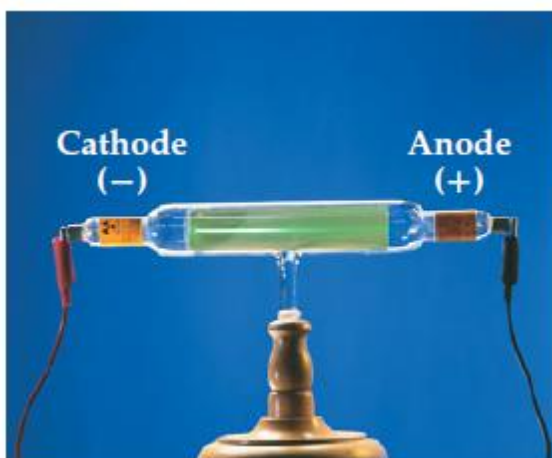
Therefore, based on Daltons' Theory atoms are considered to be the smallest particles of an element that retain the chemical identity of the element.

An element is composed of only one kind/ type of atom. A compound contains two or more elements.

- Cathode Rays and Electrons (J.J. Thomson's experiments)

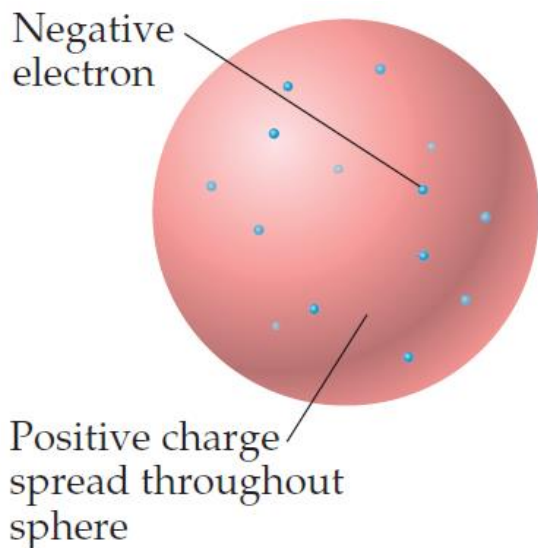
Scientists began studying electrical discharge through partially evacuated tubes (i.e. tubes with a partial vacuum) called cathode-ray tubes. When a high voltage was applied to the electrodes in the tube, radiation was produced. This radiation was called **cathode rays** and originated from the negative electrode or cathode. There were conflicting views about the nature of cathode rays. It was not initially clear whether the rays were an invisible stream of particles or a new form of radiation.

Experiments showed that these rays were deflected by electric or magnetic fields therefore, the rays were actually streams of negative electrical charge.



J.J. Thomson called these negatively-charged particles **electrons**. He used the cathode-ray tubes to study the electric and magnetic properties of this stream of electrons.

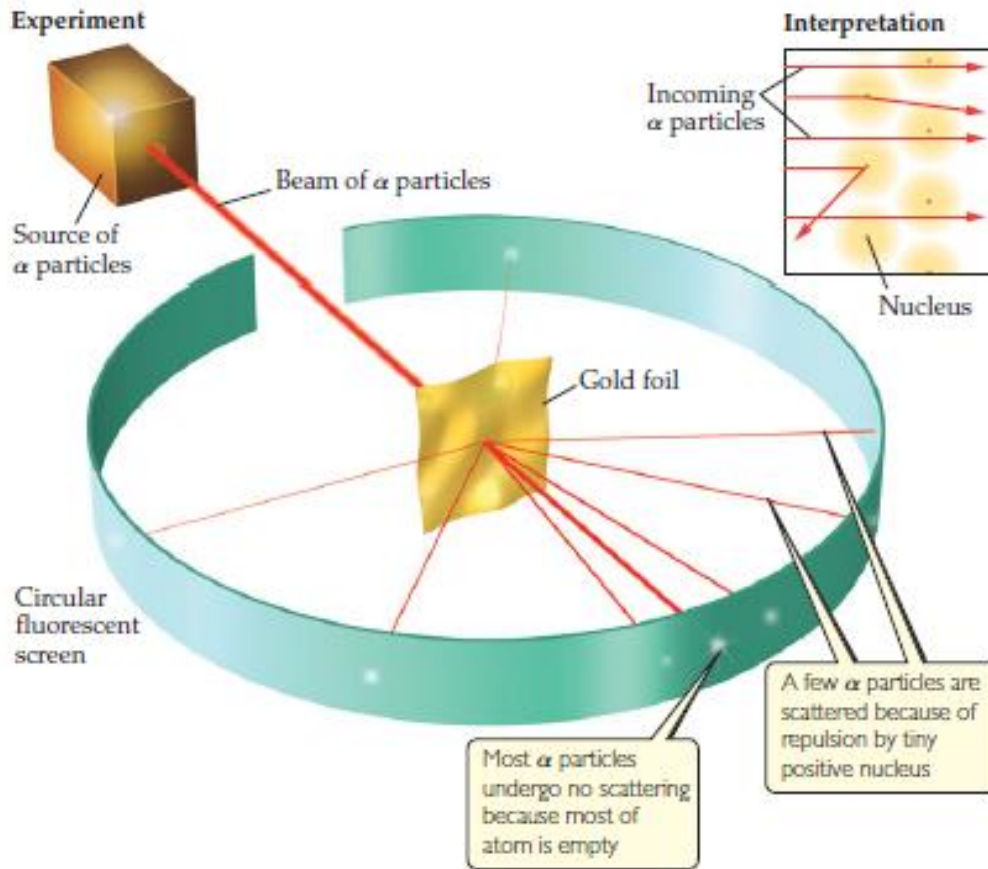
Thomson proposed that the atom consisted of a uniform positive sphere of matter in which electrons were embedded:



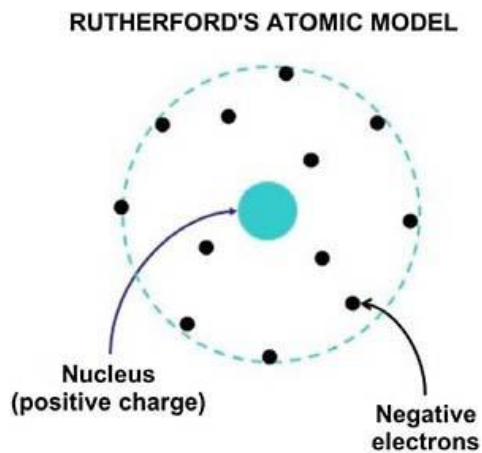
➤ Rutherford's experiments

Rutherford studied the angles at which alpha-particles (positively-charged particles) were scattered/ deflected as they passed through a thin gold foil. Almost all of the particles passed through the foil without deflection. It was therefore concluded that most of the mass of each gold atom in the foil and all of its positive charge resided in a very small, extremely dense region which he called the nucleus. He further postulated that most of the total volume of the atom was empty space in which electrons moved around the nucleus.

In the α -particle scattering experiment, most of the α -particles passed directly through the gold foil because they did not encounter the minute nucleus of any of the gold atoms; they merely passed through the empty space making up the greatest part of all the atoms in the foil. Occasionally however, an α -particle came close to a gold nucleus and there was repulsion between the two giving a strong deflection at a large angle.



Rutherford's discovery of the nuclear nature of the atom suggested that the atom can be thought of as a "microscopic solar system" in which **electrons orbit the nucleus**. He thereby disproved Thomson's atomic model.



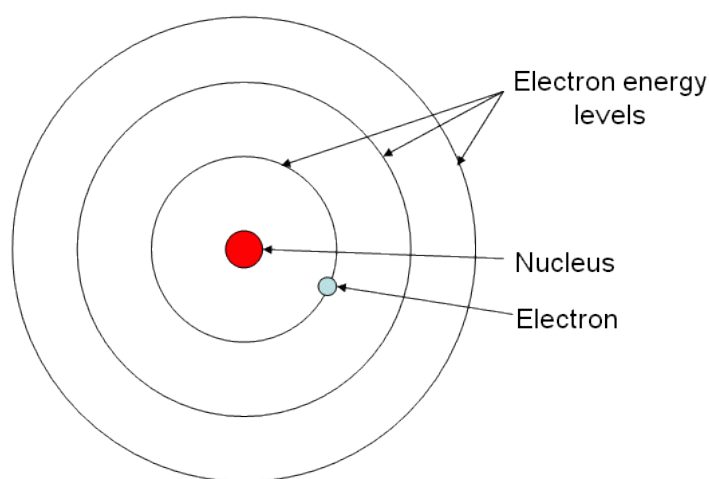
Rutherford also discovered the **proton**.

➤ Bohr's Atomic Theory

Bohr assumed that electrons move in circular orbits around the nucleus. He also adopted the idea that **energies in an atom are quantized**, i.e. electrons are found in orbits which exist at specific energy states/ levels. Energy is emitted or absorbed by the electrons only as the electron changes from one energy state to another. This energy is the energy emitted or absorbed by a photon (a particle of light). In other words, energy is required to move electrons from one state/ level to another.

[**Ground state** – refers to when an electron is in its lowest possible energy state.

Excited state – refers to when an electron is in any other energy state besides its ground state.]



➤ Modern Atomic Structure

An atom is more than just empty space and scattered electrons. **It is comprised of a small, dense, positively-charged centre called a nucleus which contains most of its mass. The nucleus contains protons and neutrons, while electrons can be found orbiting the nucleus.** Protons, neutrons and electrons are called **sub-atomic particles**.

Sub-atomic particle	Charge	Mass (amu)
Proton	+	1.0073 \approx 1
Neutron	0	1.0087 \approx 1
Electron	-	5.486 x 10 ⁻⁴ \approx 0

(amu = atomic mass unit)

Because they have opposite charges, an electrostatic force of attraction exists between protons on the nucleus and the orbiting electrons.

Atomic/ Proton number (Z) – number of protons in the nucleus

Mass number (A) – number of protons and neutrons in the nucleus

i.e. mass no. (A) = no. of protons + no. of neutrons

An atom is **neutral** therefore in any atom: **no. of protons = no. of electrons**

The number of neutrons in an atom can vary.

Isotopes are atoms of the same element with the same atomic/ proton number (Z) but different mass numbers (A). i.e. same no. of protons and electrons but different nos. of neutrons.

e.g. The isotopes of carbon are: ^{11}C , ^{12}C , ^{13}C & ^{14}C

[The number at the top (in superscript) represents the mass no. of the isotope/ element.]

Isotopes of an element are present in varying abundances/ amounts in nature.

Calculating the **Relative Atomic Mass (R.A.M.)** of an element using its isotopes:

R.A.M. = \sum (mass of each isotope x abundance of each isotope)

e.g. (1) Naturally-occurring chlorine is 75.78% ^{35}Cl (mass = 34.969) and 24.22% ^{37}Cl (mass = 36.966). Calculate the atomic mass of chlorine.

$$\begin{aligned}\text{R.A.M.} &= \sum (\text{mass of each isotope} \times \text{abundance of each isotope}) \\ &= (34.969 \times 0.7578) + (36.966 \times 0.2422) \\ &= 35.45\end{aligned}$$

N.B.: The total abundance of all the isotopes of an element is always 100% or 1.

To calculate the abundances if the R.A.M. is given, let one abundance value be x and the other abundance will be (1-x). Then substitute these terms in the above equation, solve for x and work out the abundance values of each isotope.

➤ Quantum mechanics

The Bohr model of the atom used only one quantum number, n to describe the orbits in an atom.

The quantum mechanical model of the atom however, uses **4 quantum numbers: n , l , m_l & m_s** to describe/ denote an orbital and the location of an electron in that orbital:

1) **Principal quantum no. (n)** also referred to as the **electron shell**.

The principal quantum number indicates the:

- Energy of the shell
- Size of the shell

The larger the value of n , the greater the size of the shell and the shell is further away from the nucleus. Consequently, the energy of the shell is higher and the electrons are less attracted to the nucleus.

n usually takes **positive integer values** e.g. 1,2,3,4.....

The value of n also indicates the **number of subshells** present in the electron shell. e.g. If $n = 2$, then we are in the second electron shell and there are 2 subshells present. Each subshell in turn contains a specific set of orbitals.



2) **Subsidiary quantum number/ Angular momentum quantum number (l)** also referred to as the **subshell**.

This indicates the shape of the subshell.

l usually takes **positive integer values** from **0** to **($n-1$)**.

Each specific value of l has its own distinct shape:

0 = s subshell; **1 = p** subshell; **2 = d** subshell; **3 = f** subshell

Atomic Orbital	Shape of Orbital	Diagram
s	Spherical	
p	Dumbbell-Shaped; has 2 lobes	
d	Double-Dumbbell	(Not required)

e.g. For $n = 3 \rightarrow l = 0, 1, 2$

s, p, d

Therefore, the third electron shell has three subshells: 3s, 3p, 3d.

3) **Magnetic quantum number (m_l)** also referred to as the **orbital**.

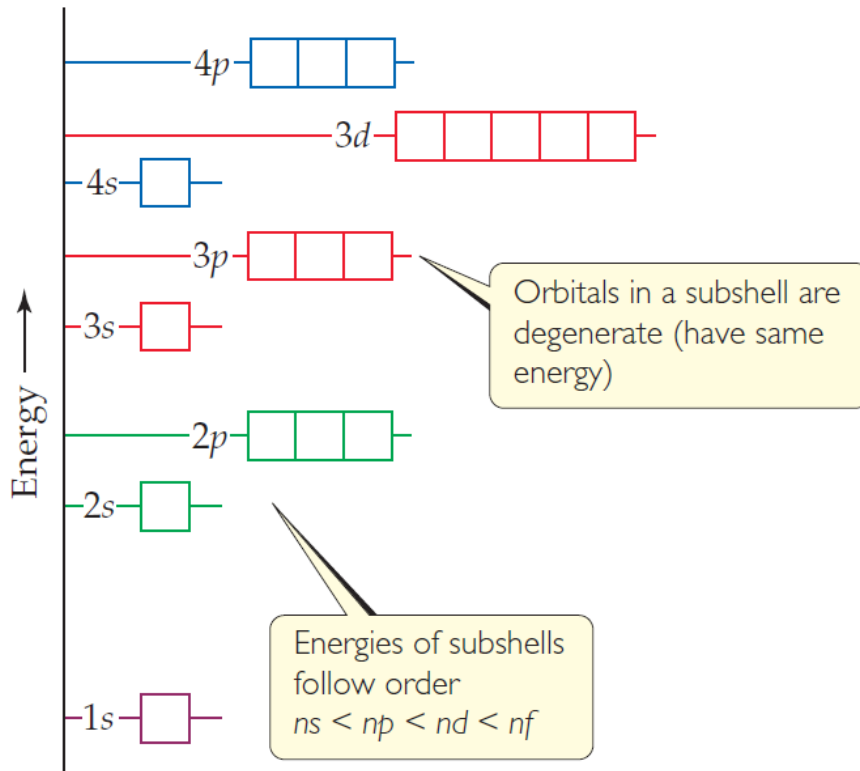
This depicts the orientation in space of the orbital. Each value of l will have a distinct set of values of m_l .

m_l usually takes **integer values** from **-l to l, including 0**.

e.g. If $l = 2 \rightarrow m_l = -2, -1, 0, 1, 2$

All the orbitals that make up a particular subshell are **degenerate** (i.e. have the **same energy**).

n	Possible Values of l	Subshell Designation	Possible Values of m_l	Number of Orbitals in Subshell	Total Number of Orbitals in Shell
1	0	1s	0	1	1
2	0	2s	0	1	
	1	2p	1, 0, -1	3	4
3	0	3s	0	1	
	1	3p	1, 0, -1	3	
	2	3d	2, 1, 0, -1, -2	5	9
4	0	4s	0	1	
	1	4p	1, 0, -1	3	
	2	4d	2, 1, 0, -1, -2	5	
	3	4f	3, 2, 1, 0, -1, -2, -3	7	16



- 4) **Spin magnetic quantum number (m_s)** – only 2 values :- either $+\frac{1}{2}$ (spin: **up**) or $-\frac{1}{2}$ (spin: **down**)

It was postulated that electrons have an intrinsic property called electron spin that causes each electron to behave as if it were a tiny magnet.

The values of m_s refer to the direction/ orientation of spin of the electron (either ‘up’ or ‘down’).

- Hybridisation – this involves the **mixing of atomic orbitals to form new (hybrid) orbitals**

e.g. mixing s and p orbitals can create new orbitals called sp orbitals.

➤ Electronic configuration

This refers to the distribution of electrons among the various orbitals in an atom.

Three sets of rules govern the placement/ distribution of electrons in an atom:

Aufbau principle – electrons will always occupy the **lowest energy orbitals** first.

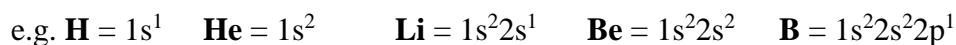
The orbitals in any atom can be arranged according to energetics (see energy diagram above).

Hund's rule of maximum multiplicity – electrons occupy the lowest energy orbitals singly and with parallel/ same spin, then they are each paired with an electron of opposite spin; this is done so as to minimize electron repulsion in the orbital

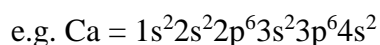


Pauli's Exclusion Principle – no 2 electrons in an atom can have the same 4 quantum numbers (n, l, m_l, m_s). Therefore an orbital can only hold a maximum of 2 electrons and they must have opposite spins.

Shell No. (n)	Subshell	Maximum no. of Electrons in each subshell
1	s	2 (Total)
2	s	2 } 6 } 8 (Total)
	p	
3	s	2 } 6 } 10 } 18 (Total)
	p	
	d	



order of filling in electrons: 1s 2s 2p 3s 3p 4s 3d (**fill 4s before 3d**; 4s has lower energy than 3d)



The electronic configuration of some elements:

Element	Total Electrons	Orbital Diagram				Electron Configuration
		1s	2s	2p	3s	
Li	3	$\uparrow\downarrow$	\uparrow	\square \square \square	\square	$1s^2 2s^1$
Be	4	$\uparrow\downarrow$	$\uparrow\downarrow$	\square \square \square	\square	$1s^2 2s^2$
B	5	$\uparrow\downarrow$	$\uparrow\downarrow$	\uparrow \square \square	\square	$1s^2 2s^2 2p^1$
C	6	$\uparrow\downarrow$	$\uparrow\downarrow$	\uparrow \uparrow \square	\square	$1s^2 2s^2 2p^2$
N	7	$\uparrow\downarrow$	$\uparrow\downarrow$	\uparrow \uparrow \uparrow	\square	$1s^2 2s^2 2p^3$
Ne	10	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$	\square	$1s^2 2s^2 2p^6$
Na	11	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$	\uparrow	$1s^2 2s^2 2p^6 3s^1$

➤ Condensed electronic configuration

Condensed electronic configuration abbreviates electronic configuration by using the **closest/nearest noble gas configuration** to the element. The noble gas chosen has a lower proton no.

e.g. $K = 1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$ becomes $K = [Ar]4s^1$

since $1s^2 2s^2 2p^6 3s^2 3p^6$ is the elec. config. of argon (Ar); i.e. use the closest noble gas configuration to figure out the condensed elec. config. of the element

➤ Electronic configuration of ions

e.g. $Na - e^- \rightarrow Na^+$

$1s^2 2s^2 2p^6 3s^1 \rightarrow 1s^2 2s^2 2p^6$ (or $1s^2 2s^2 2p^6 3s^0$)

Electronic structure of atoms and the energy changes in an atom

Relationship between frequency and wavelength:

$$c = \lambda \nu$$

where c = speed of light ($3.00 \times 10^8 \text{ m s}^{-1}$)

λ = wavelength (m)

ν = frequency (s^{-1})

e.g. (2) The yellow light given off by a sodium vapour lamp used for public lighting has a wavelength of 589 nm. What is the frequency of this radiation?

$$\lambda = 589 \text{ nm} = 589 \times 10^{-9} \text{ m}$$

$$[1 \text{ nm} = 10^{-9} \text{ m}]$$

$$c = \lambda \nu$$

$$3.00 \times 10^8 \text{ m s}^{-1} = (589 \times 10^{-9} \text{ m}) \nu$$

$$\nu = \frac{3.00 \times 10^8 \text{ m s}^{-1}}{589 \times 10^{-9} \text{ m}} = 5.09 \times 10^{14} \text{ s}^{-1}$$

Relationship between energy and frequency:

Recall: Energy in an atom is quantized. [Refer to note on Bohr's atomic model.]

Energy is absorbed or released in fixed amounts called 'quanta'.

Energy of a single quantum:

$$E = h\nu$$

where E = energy (J)

h = Planck's constant ($6.626 \times 10^{-34} \text{ J s}$)

ν = frequency (s^{-1})

The values of E are restricted to certain quantities. Matter is allowed to emit and absorb energy only in whole number multiples of $h\nu$. e.g. $h\nu$, $2h\nu$, $3h\nu$, etc.

Energy of a photon (a particle) of light:

$$E = h\nu$$

e.g. (3) Calculate the energy of a photon of yellow light with a wavelength of 589 nm.

$$c = \lambda \nu \quad \text{therefore: } \nu = c / \lambda$$

$$\text{And: } E = h\nu$$

$$\text{Therefore: } E = \frac{hc}{\lambda}$$

$$E = \frac{(6.626 \times 10^{-34} \text{ J s})(3.00 \times 10^8 \text{ m s}^{-1})}{589 \times 10^{-9} \text{ m}} = 3.37 \times 10^{-19} \text{ J}$$

e.g. (4) Calculate the energy of 1 mole of photons of yellow light with a wavelength of 589 nm.

$$\text{Energy of 1 photon} = 3.37 \times 10^{-19} \text{ J} \quad [\text{Refer to example (3) above.}]$$

$$\begin{aligned} \text{Energy of 1 mole of photons} &= (3.37 \times 10^{-19})(6.023 \times 10^{23}) = 203\,000 \text{ J mol}^{-1} \\ &\text{or } 203 \text{ kJ mol}^{-1} \end{aligned}$$

➤ Energy changes in an atom

When an electron in an atom moves from a **lower energy state** to a **higher energy state**, energy is **absorbed**.

When an electron in an atom moves from a **higher energy state** to a **lower energy state**, energy is **released**.

The amount of energy absorbed or released is determined using the **Rydberg equation**:

$$\Delta E = R_H \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \quad \begin{array}{l} \text{where } R_H = \text{Rydberg constant } (2.179 \times 10^{-18} \text{ J}) \\ n_i = \text{initial energy state} \\ n_f = \text{final energy state} \end{array}$$

e.g. (5) Calculate the energy, frequency and wavelength if an electron moves from $n = 1$ to $n = 3$:

$$\begin{aligned} \Delta E &= R_H \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \\ \Delta E &= 2.179 \times 10^{-18} \text{ J} \left(\frac{1}{(1)^2} - \frac{1}{(3)^2} \right) \\ &= 1.94 \times 10^{-18} \text{ J} \end{aligned}$$

$$E = h\nu$$

$$1.94 \times 10^{-18} \text{ J} = (6.626 \times 10^{-34} \text{ J s}) \nu$$

$$\nu = \frac{1.94 \times 10^{-18} \text{ J}}{6.626 \times 10^{-34} \text{ J s}} = 2.93 \times 10^{15} \text{ s}^{-1}$$

$$c = \lambda\nu$$

$$3.00 \times 10^8 \text{ m s}^{-1} = \lambda (2.93 \times 10^{15} \text{ s}^{-1})$$

$$\lambda = \frac{3.00 \times 10^8 \text{ m s}^{-1}}{2.93 \times 10^{15} \text{ s}^{-1}} = 1.02 \times 10^{-7} \text{ m}$$

Note:

If ΔE is **positive (+)**, energy is being **absorbed** as the electron goes from a lower energy state to a higher energy state. [Refer to example (5).]

If ΔE is **negative (-)**, energy is being **released** since the electron is going from a higher energy state to a lower energy state.

If ΔE is negative (-), use the positive (+) value to calculate ν and λ since they are positive values.

The wave behaviour of matter

➤ de Broglie's Wave equation

Bohr postulated that electrons existed only in certain discrete (fixed) energy levels described by the principal quantum no. (n). de Broglie suggested that as the electron moves about the nucleus, it is associated with a particular wavelength, which depends on the electron's mass and velocity. In other words, he proposed that **the electron can behave as a wave as well as a particle.**

de Broglie's wave equation:

$$\lambda = \frac{h}{m\nu}$$

where λ = de Broglie wavelength (m)

h = Planck's constant ($6.626 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1}$)

m = mass (kg)

ν = velocity (m s^{-1})

N.B.: The units of Planck's constant have been converted:

$$1 \text{ J} = 1 \text{ kg m}^2 \text{ s}^{-2}$$

$$\text{Therefore: } 6.626 \times 10^{-34} \text{ J s} = (6.626 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-2}) \text{ s} = 6.626 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1}$$

e.g. (6) What is the wavelength of an electron moving with a speed of $5.97 \times 10^6 \text{ m s}^{-1}$. The mass of an electron is $9.11 \times 10^{-31} \text{ kg}$.

$$\lambda = \frac{h}{mv}$$

$$\lambda = \frac{6.626 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1}}{(9.11 \times 10^{-31} \text{ kg})(5.97 \times 10^6 \text{ m s}^{-1})} = 1.22 \times 10^{-10} \text{ m}$$

➤ Heisenberg uncertainty principle (this was a major criticism of the Bohr Model)

Because of the proposed wave-like property of the electron, the Heisenberg uncertainty principle was developed.

The Heisenberg uncertainty principle states that it is impossible to know both the position and velocity of an electron at the same time. That is, if one knows the position, one cannot know the velocity and likewise if one knows the velocity, one cannot know the position.

This concept may be extended to the momentum of the electron since momentum is a direct function of velocity: therefore, one cannot know the position and momentum of an electron at the same time.

The exact location of an electron in an atom's space is unknown. Rather there is a probability of them existing in a given space at any point in time, not a certainty.

To calculate the uncertainty in the position of an electron:

$$\Delta x \geq \frac{h}{4\pi m \Delta v}$$

Where: x = distance (m)

h = Planck's constant ($\text{kg m}^2 \text{ s}^{-1}$)

m = mass (kg)

v = velocity (ms^{-1})

$$\text{or: } \Delta x \geq \frac{h}{4\pi \Delta p}$$

where p = momentum = mv

(this equation is less frequently

used)

[Δ means 'uncertainty' in these two equations e.g. Δx means uncertainty in distance]

e.g. (7) Find the position of uncertainty of an electron moving at a speed of $5 \times 10^6 \text{ m s}^{-1}$ if the uncertainty in its speed is known to 1%. The mass of an electron is $9.11 \times 10^{-31} \text{ kg}$.

$$\text{uncertainty in the speed} = 0.01 (5 \times 10^6 \text{ ms}^{-1}) = 5 \times 10^4 \text{ m s}^{-1}$$

$$\begin{aligned} \Delta x &\geq \frac{h}{4\pi m \Delta v} \\ &= \frac{6.626 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1}}{4\pi (9.11 \times 10^{-31} \text{ kg})(5 \times 10^4 \text{ m s}^{-1})} \\ &= 1 \times 10^{-9} \text{ m} \end{aligned}$$

Note:

Uncertainty can also be expressed as for e.g.:

$$(5 \pm 0.01) \times 10^6 \text{ m s}^{-1}$$

± 0.01 also means 1% uncertainty

➤ Effective nuclear charge

Recall: There are **electrostatic forces of attraction** between the positively-charged nucleus and the negatively-charged electrons in an atom.

But there is also **repulsion** taking place between the electrons of the atom.

Effective nuclear charge (Z_{eff}) is the **net nuclear charge/ net attraction** experienced by an electron to the nucleus taking electronic repulsions into account.

Outer electrons are screened/ shielded by inner electrons, therefore they experience **less effective nuclear charge**.

Inner shell electrons are called **core electrons** and are located **closer to the nucleus**.

Outer shell electrons are called **valence electrons** and are located in the **last/ outermost electron shell**.






















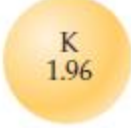


The effective nuclear charge in an atom can be approximated by using the equation:




$$Z_{\text{eff}} = Z - S \quad [Z = \text{proton no.}; \quad S = \text{screening constant (no. of core electrons)}]$$

$$\text{e.g. For Na:} \quad Z_{\text{eff}} = 11 - 10 = 1$$

Effective nuclear charge **increases** across a Period from (left to right) because **Z increases**.

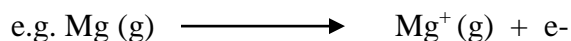
$$\text{e.g. Li (1s}^2\text{2s}^1\text{): } Z_{\text{eff}} = 3 - 2 = 1 \quad \text{Be (1s}^2\text{2s}^2\text{): } Z_{\text{eff}} = 4 - 2 = 2$$

Group 1	Group 2	Group 3	Group 6	Group 7
Li ⁺ 0.90   Li 1.34	Be ²⁺ 0.59   Be 0.90	B ³⁺ 0.41   B 0.82	 O ²⁻ 1.26  O 0.73	 F ⁻ 1.19  F 0.71
 Na ⁺ 1.16  Na 1.54	Mg ²⁺ 0.86   Mg 1.30	Al ³⁺ 0.68   Al 1.18	 S ²⁻ 1.70  S 1.02	 Cl ⁻ 1.67  Cl 0.99
 K ⁺ 1.52  K 1.96	Ca ²⁺ 1.14   Ca 1.24			

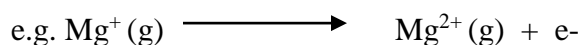
 = cation
  = anion
  = neutral atom

➤ Ionization energy (I.E.)

1st I.E. – the energy required to remove 1 electron from an atom in its gaseous state



2nd I.E. – the energy required to remove 1 electron from an ion in its gaseous state

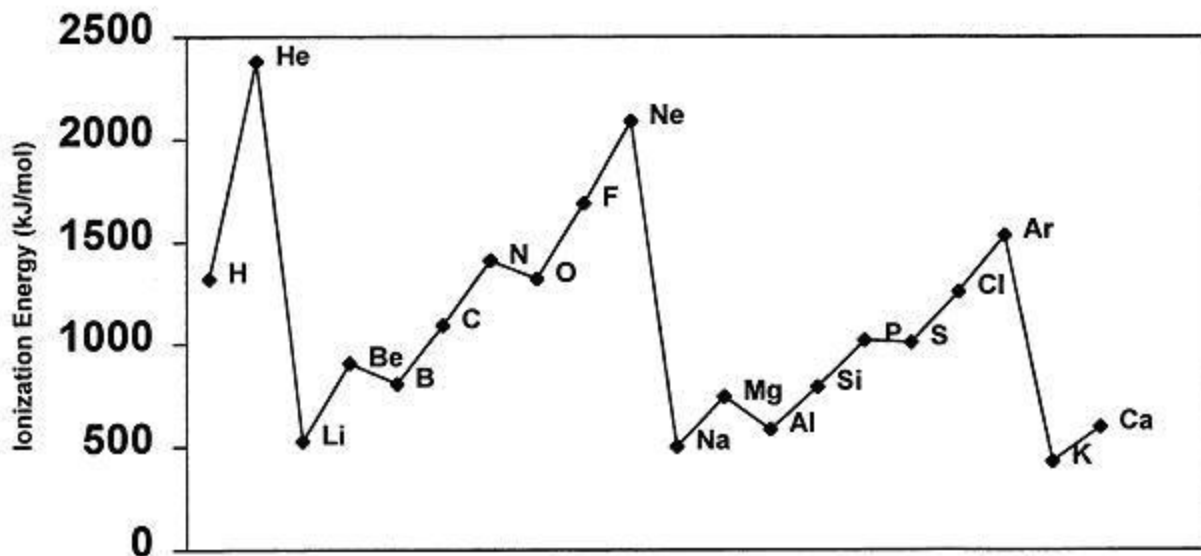


Successive I.E. values increase for a given element because it becomes increasingly difficult to remove electrons from ions, therefore **removing more electrons requires more energy**.

That is: $1^{\text{st}} \text{ I.E.} < 2^{\text{nd}} \text{ I.E.} < 3^{\text{rd}} \text{ I.E.}$

Down a Group, I.E. **decreases** due to an **increase in atomic radius** and **decrease in Z_{eff}** (since outer electrons are further away from the nucleus and effective nuclear charge is lower, electrons are easier/ require less energy to remove).

Ionization Energies of the First 20 Elements in the Periodic Table



General Trend in I.E. – **Increase across Period** [As seen in Graph above]

The anomalies are: **Be** and **B**; **N** and **O** for Period 2

Mg and **Al**; **P** and **S** for Period 3

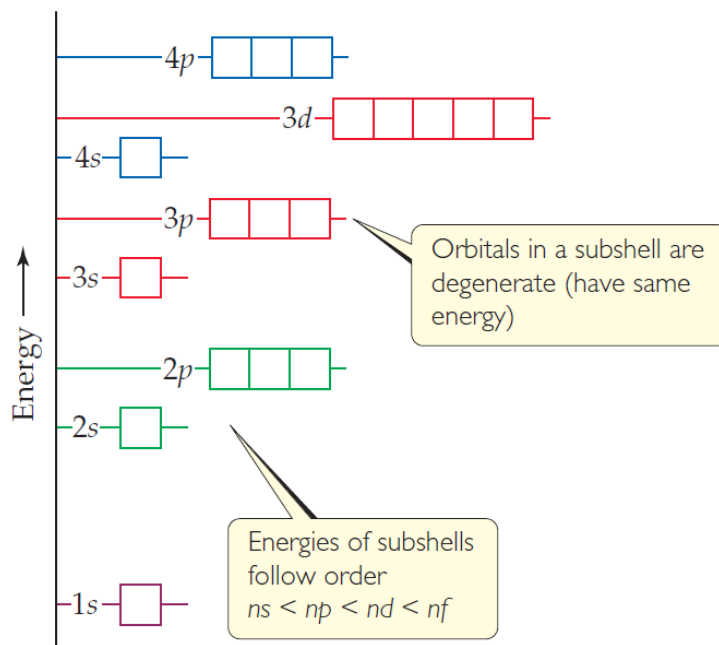
Across a Period, I.E. generally **increases** due to a **decrease in atomic radius** and **increase in Z_{eff}** (since outer electrons are closer to the nucleus and effective nuclear charge is higher, electrons are harder/ require more energy to remove).

However, there are some **important anomalies/ exceptions** to this trend:

Going from Be ($1s^2 2s^2$) to B ($1s^2 2s^2 2p^1$), I.E. actually **decreases**.

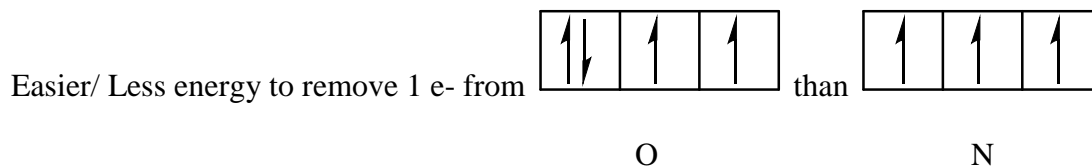
This is because the 2p subshell exists at a higher energy than the 2s subshell, therefore less energy is required to remove electrons from 2p than 2s.

Recall the energy level diagram:



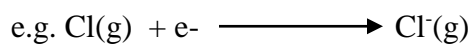
Going from N ($1s^2 2s^2 2p^3$) to O ($1s^2 2s^2 2p^4$), I.E. also **decreases**.

This is because less energy is required to remove the p electron of O which has an opposite spin than any of the 3 p electrons in N (which all have the same spin). Also, the electron pair in O experiences repulsion so to minimize this repulsion, it is preferable to lose one of the electrons in the pair.



➤ Electron affinity

In the same way that atoms can lose electrons to form cations, they can also gain electrons to form anions. The energy change that occurs when an atom gains an electron is called **electron affinity**. Electron affinity represents the attraction or affinity of an atom for additional electrons.



Halogens (Group VII) have the **highest electron affinities** of all the elements in the Periodic Table followed by those elements in Group VI e.g. O, S

e.g. Which element has the higher ionization energy: Mg or Be?

Consider the periodic table:

1 Hydrogen H							2 Helium He
3 Lithium Li	4 Beryllium Be	5 Boron B	6 Carbon C	7 Nitrogen N	8 Oxygen O	9 Fluorine F	10 Neon Ne
11 Sodium Na	12 Magnesium Mg	13 Aluminium Al	14 Silicon Si	15 Phosphorus P	16 Sulfur S	17 Chlorine Cl	18 Argon Ar
19 Potassium K	20 Calcium Ca						

Be has the higher ionization energy. Going up a Group, I.E. increases. Be has a smaller atomic radius than Mg therefore Z_{eff} is higher and it requires more energy to remove a valence electron.

e.g. Which element has the higher ionization energy: Cl or Al?

Cl has the higher ionization energy. Going across a Period, I.E. increases. Cl has a smaller atomic radius than Al therefore Z_{eff} is higher and it requires more energy to remove a valence electron.

Summary: Atomic radius and Z_{eff} are inversely related (i.e. as one increases the other decreases)

Both Atomic radius and Z_{eff} can be used to explain the general trend in Ionization Energies down a Group and across a Period.

Past Paper Questions:

July/ August 2016

(a) The wavelength of light required to dissociate a chlorine molecule is 493 nm. Calculate the energy needed to dissociate 2 moles of chlorine molecules into chlorine atoms. (6 marks)

$$E = \frac{hc}{\lambda} = \frac{(6.63 \times 10^{-34} \text{ J s})(3.00 \times 10^8 \text{ m s}^{-1})}{(493 \times 10^{-9} \text{ m})} = 4.03 \times 10^{-19} \text{ J}$$

$$E \text{ for 2 mols. of Cl}_2 = 4.03 \times 10^{-19} \text{ J} \times 2 \times 6.023 \times 10^{23} = 486 \text{ kJ}$$

(b) Calculate the energy required to excite an electron from the $n = 2$ to the $n = 4$ level in atomic hydrogen. What is the maximum wavelength of light that causes this excitation? (4 marks)

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

$$\Delta E = 2.179 \times 10^{-18} \text{ J} \left(\frac{1}{(2)^2} - \frac{1}{(4)^2} \right)$$

$$= 4.1 \times 10^{-19} \text{ J}$$

$$\lambda = \frac{hc}{E} = \frac{(6.63 \times 10^{-34} \text{ J s})(3.0 \times 10^8 \text{ m s}^{-1})}{(4.1 \times 10^{-19} \text{ J})} = 4.85 \times 10^{-7} \text{ m}$$

(c) The mass of a neutron is $1.67 \times 10^{-27} \text{ kg}$. What is the wavelength of a neutron moving at a speed of $4.21 \times 10^3 \text{ m s}^{-1}$? (6 marks)

$$h = 6.63 \times 10^{-34} \text{ J s} = 6.63 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1}$$

$$\lambda = \frac{h}{mv}$$

$$\lambda = \frac{6.63 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1}}{(1.67 \times 10^{-27} \text{ kg})(4.21 \times 10^3 \text{ m s}^{-1})} = 9.43 \times 10^{-11} \text{ m}$$

(d) Which if the following sets of four quantum numbers (n, l, m, s) are not allowed for an electron in an atom? Explain your answer.

(4, 2, 2, +1/2)

(4, 1, 0, -1/2)

(4, 2, 3, +1/2)

(4 marks)

(4, 2, 3, +1/2) – Not allowed

If n = 4 and l = 2: m = -2, -1, 0, 1, 2 therefore, m cannot be 3.

December 2015

(a) The energy needed to dissociate a chlorine molecule into chlorine atoms is 243 kJ mol⁻¹.

What is the wavelength of light that will initiate this reaction?

(6 marks)

$$E = 243 \text{ kJ mol}^{-1} = 243\,000 \text{ J mol}^{-1}$$

$$E \text{ (per molecule)} = 243\,000 \text{ J} \div 6.02 \times 10^{23} = 4.04 \times 10^{-19} \text{ J}$$

$$\lambda = \frac{hc}{E} = \frac{(6.63 \times 10^{-34} \text{ J s})(3.0 \times 10^8 \text{ m s}^{-1})}{(4.04 \times 10^{-19} \text{ J})} = 4.92 \times 10^{-7} \text{ m}$$

(b) One electron has the set of quantum numbers n = 3, l = 1, m_l = -1 and m_s = +1/2 ; another electron has the set n = 3, l = 1, m_l = 1 and m_s = +1/2.

(i) Could the electrons be in the same atom? Explain.

(2 marks)

(ii) Could they be in the same orbital? Explain.

(2 marks)

(i) Pauli's exclusion principle holds because the two electrons do not have the same set of four quantum numbers. Therefore, both electrons can be in the same atom.

(ii) The electrons are in the 'p' subshell of the 3rd electron shell. Therefore, they are each located in a 3p orbital of the atom. However, the m_l values for each electron are different (m_l = -1 and m_l = 1) so they are located in two different 3p orbitals.

Alternative answer: Both electrons have m_s values of +1/2, so according to Pauli's exclusion principle they cannot be in the same orbital if they have the same/parallel spins. They must have opposite spins.