

Sub-atomic Particles

Proton, neutron and electron are sub-atomic particles. Proton and neutron remains ~~on~~ in the nucleus of an atom while electron revolves round the nucleus.

Proton is positively charged particle having mass equal to an atom of hydrogen.

Neutron is chargeless particle having mass nearly equal to proton while electron is negatively charged particle whose mass is equal to $\frac{1}{1837}$ times of a hydrogen atom.

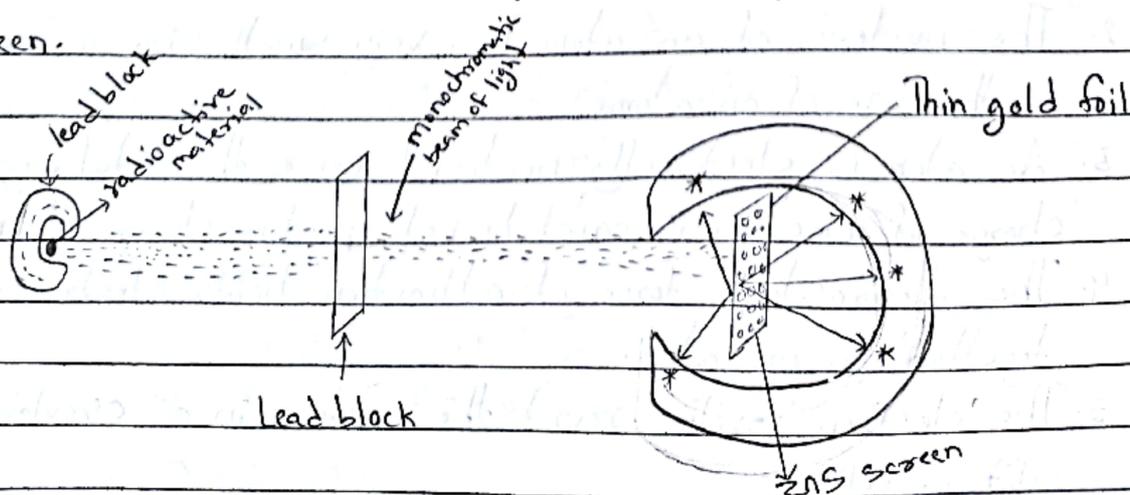
Mass of proton = 1.67×10^{-24} gm

Mass of electron = ~~9.09×10^{-28}~~ 9.09×10^{-28} gm

Rutherford's Atomic Model

Ernest Rutherford (1911) performed an experiment called α -particles scattering experiment. In this experiment, a thin gold foil was placed in the centre of circular, moveable zinc sulphide screen and a beam of α -particles (α -ray) emitted from the radioactive source ~~was~~ were directed at the gold foil.

After heating the foil, the scattering of alpha ~~or~~ α -particles were observed with the help of microscope on the zinc sulphide screen.



From the α -particles scattering experiment performed by Rutherford, following observations were obtained.

- a. Most of the α -particles passed straight line through the gold foil without deflection.
- b. Some of the α -particles deflected through small angle.
- c. Very few number of α -particles were reflected back.

On the basis of above observation, Rutherford made some conclusion which are;

- a. Most of the α -particle passed through the gold foil in straight path represents that, most of the space inside atom is empty.
- b. Some of the α -particles deflect through small angle shows that there is repulsion between α -particles and positively charged mass in the centre of atom.
- c. The deflection of α -particle through large angle or reflection back represents that there is a small rigid mass with positive charge at the centre of atom called nucleus.

On the basis of above conclusion, Rutherford put forward the following postulates, called ^{of} Rutherford atomic model

1. An atom consist of a small positively charged mass at the centre of it which is called nucleus.
2. The nucleus of an atom has very small size in comparison to the size of an atom.
3. An atom is electrically neutral because the total negative charge of electron is equal to net positive charge of nucleus.
4. The electrostatic force of attraction holds electron and proton together in an atom.
5. The electron revolve round the nucleus in a circular path called orbit or cell.

Limitation of Rutherford's Atomic Model

- i. This atomic model fails to explain the ~~act~~ actual reason for the ~~est~~ stability of an atom.
- ii. This theory is unable to explain the origin of line spectra of hydrogen atom in presence of electric field (Zeeman effect) and Magnetic field (Stark effect).
- iii. This model didn't specify the orbit and number of electron in each orbit.

Postulates of Bohr's Atomic Model

1. Electron revolve around the nucleus in a defined circular path called orbits. The electrostatic force^{of} attraction between the revolving electron and nucleus is equal to the centrifugal force acting on the electron.
2. As long as the atom remains in a particular orbit, it will ~~never~~ neither gain nor loose energy and hence the energy of the electron in a particular orbit remains constant. This means these orbits are non-radiating and thus stationary state of or energy level and designated K, L, M, N etc.
3. Only these orbits are permitted in an atom whose angular momentum of the electron is equal to the whole number multiple of $h/2\pi$ where h is Plank's constant.

$$\text{Angular momentum } (Mvr) = \frac{nh}{2\pi}$$

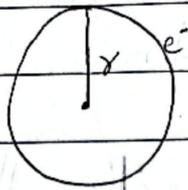
where, M = Mass of electron

v = Velocity of electron

r = Radius of orbit

$n = 1, 2, 3, \dots$

$h = \text{Plank's Constant } (6.67 \times 10^{-27} \text{ erg sec})$



4. Energy is emitted or absorbed by the electron in the form of a photon only when it jumps from one energy level to another. The quantum or photon of energy absorbed or emitted is the difference between the higher and lower energy level.

$$\Delta E = E_2 - E_1 = h\nu$$

$\Delta E = \text{Energy emitted or absorbed}$

$E_2 = \text{higher energy level}$

$E_1 = \text{Lower energy level}$

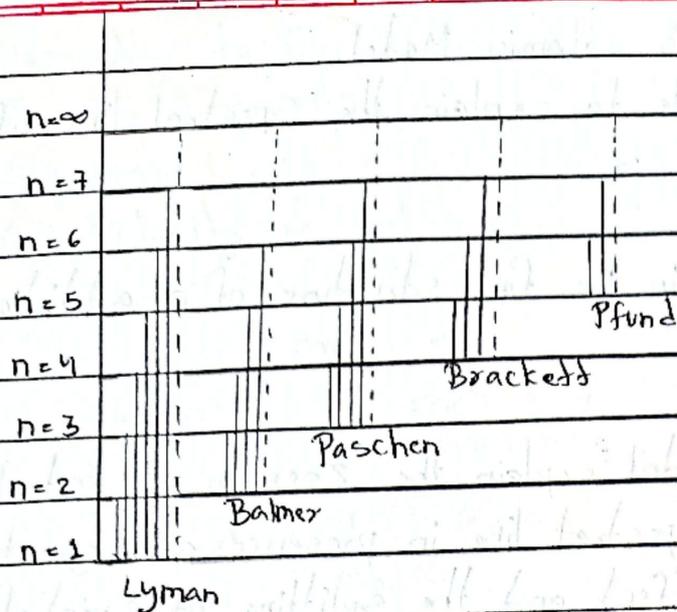
$h = \text{Plank's Constant}$

$\nu = \text{Frequency of radiation}$

Energy is absorbed when an electron jumps from lower to higher energy level and energy is emitted when an electron jumps from higher to lower energy level.

Origin of hydrogen Spectrum

When hydrogen gas is taken in discharge tube and high voltage is applied, then there is the dissociation of hydrogen molecule into hydrogen atom. Although hydrogen consists of only one electron, it produces different types of spectra. When energy is supplied, the electron of hydrogen atom absorb energy and jumps to a high energy level. The electron in high energy level (excited state) are unstable and jump to lower energy level with the emission of the electromagnetic radiation which gives rise to the line spectra called Spectral Series.



1. Lyman Series (92 - 120 nm)

It is observed when an atom jumps from a higher energy level to the first energy level. It lies in the ultraviolet region.

2. Balmer Series (400 - 650 nm)

It is observed when an atom electron jumps from a higher energy level to a second energy level. It lies in visible region.

3. Paschen Series (950 - 2875 nm)

It is observed when an electron jumps from a higher energy level to a third energy level. It lies in the infrared region.

4. Brackett Series (1945 - 4050 nm)

It is observed when an electron jumps from a higher energy level to the fourth energy level. It lies in the infrared region.

5. Pfund Series (above 4050 nm)

It is observed when an electron jumps from a higher energy level to a fifth energy level. It lies in the infrared region.

Limitations of Bohr's Atomic Model

1. Bohr's theory is unable to explain the spectral lines of multi-electron system.

2. This theory cannot explain the fine structure of an additional quantum number.

3. Bohr's atomic model didn't explain the Zeeman and Stark effect.

Note: The splitting of spectral lines in the presence of a magnetic field is called the Zeeman effect and the splitting of spectral lines in the presence of an electric field is called the Stark effect.

4. No explanation for the dual nature of electron.

Dual Nature of Matter (de-Broglie equation)

In 1905, Einstein suggested the dual nature of light. According to this, light possesses a wave and particle nature. In 1924, de-Broglie advanced the idea that not only photons of light but also matter like electrons show the dual nature. The wave associated with matter is the matter wave or de-Broglie wave. So, the electron is a subatomic particle that can behave sometimes as a particle and sometimes as a wave.

The wave-particle duality of matter led de-Broglie to derive the equation $\lambda = h/p$ which indicates the wave and particle nature of the matter in motion.

Derivation;

According to Planck's quantum theory,

$$E = h\nu \quad \text{--- (i)}$$

where, E = energy of photon,

h = Planck's constant

ν = frequency

According to Einstein equation,

$$E = mc^2 \text{ --- (ii)}$$

m = mass

c = Velocity of light

Combining (i) and (ii),

$$h\nu = mc^2$$

$$\text{or, } \frac{h c}{\lambda} = mc^2 \quad (v = c/\lambda \text{ and } \lambda = \text{wavelength})$$

$$\text{or, } \lambda = \frac{h}{mv}$$

$$\text{or, } \lambda = \frac{h}{P} \quad (P \text{ is momentum and } P = mv)$$

It is de - Broglie wave equation. It shows that the momentum of a particle in motion is inversely proportional to its wavelength.

Heisenberg Uncertainty Principle

It states that "It is impossible to determine the position and momentum of microscopic particles like an electron simultaneously and accurately."

Mathematically,

$$\Delta x \cdot \Delta y \geq \frac{h}{2\pi}$$

Δx = Uncertainty in position

Δy = Uncertainty in momentum

Uncertainty means,

- i. If we measure the position more accurately, then the uncertainty in momentum occurs.
- ii. If we measure the momentum more accurately then the uncertainty in position, occurs.

Concept of Probability

Bohr's atomic model is defective according to Heisenberg uncertainty principle because in Bohr's atomic model, the position and momentum of an electron can be measured simultaneously which is impossible according to uncertainty principle.

Concept of Probability

The space around the nucleus where the probability of finding the electron is maximum is called orbital / probability.

Differences between orbit and orbitals.

Orbit	Orbitals
i. It is the well defined circular path where the electron revolves around the nucleus	i. It is the space around the nucleus where the probability of finding the electron is maximum
ii. Orbits are circular in shape	ii. Orbitals are three-dimensional concept.
iii. Orbits don't have directional characteristics.	iii. Orbitals have directional characteristics except for s-orbitals.
iv. One orbit can accommodate a maximum of $2n^2$ number of electron where n is the principal quantum number.	iv. One orbital can accommodate a maximum of two electrons.
v. Orbit Concept can't explain the geometry of a molecule.	v. The orbital concept explains the geometry of a molecules.
vi. It is developed by Bohr's atomic model.	vi. It is developed by the Heisenberg uncertainty principle.

Shape of s and p orbital

s-orbitals are spherical in shape and p-orbitals are dumb-bell shape.

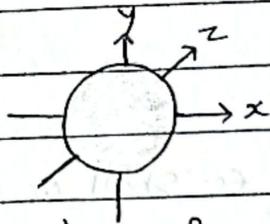


Fig: Shape of s-orbital

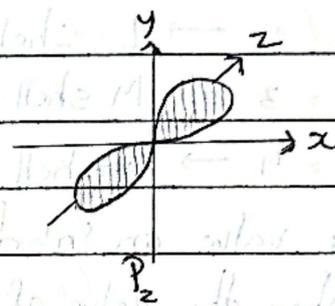
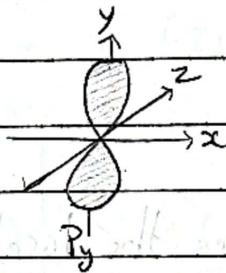
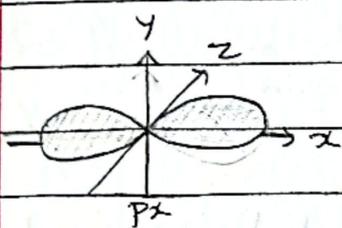


Fig: Shape of P-orbital

s-orbitals are non-directional in nature due to spherical shape. The $2s$ orbital is greater than $1s$ both in size and energy. Similarly, $3s$ orbital has more energy than $2s$ orbital.

p-orbitals are directional in nature. p_x orbitals are directed to x-axis, p_y orbital towards y-axis and p_z orbital towards z-axis. Each lobe of p-orbital contains an electron, so a p orbital contain 2 electron which are located in opposite spin.

Quantum Numbers

The quantum mechanical parameters which tells us about the location and motion of an electron in an atom are called quantum numbers. It gives complete information of a particular electron relating to its energy level, shape and orientation of orbital with its spin. The quantum number are as follows:

1. Principal quantum number (n)
2. Azimuthal quantum number (l)
3. Magnetic quantum number (m)
4. Spin quantum number (s)

1. Principal quantum number (n)

Principal quantum number represents major shell or energy level, which are denoted by K, L, M, N.

$n = 1 \rightarrow$ K shell

$n = 2 \rightarrow$ L shell

$n = 3 \rightarrow$ M shell

$n = 4 \rightarrow$ N shell

The value of ' n ' determines the location of electron in a shell.

Higher the value of ' n ' more far is the electron from the nucleus and size of the shell is also greater.

The value of ' n ' also determines the energy of electron in a given shell.

This quantum number gives the maximum number of electron that can hold by s-shell. It is given by $2n^2$.

2. Azimuthal quantum number (l)

It describes the sub-shell or sub energy level. Its value lies from 0 to $(n-1)$ for the value of ' n '. It is also called a subsidiary quantum number.

n	l	number of sub-shells
1	0 (s-sub shell)	1
2	0 (s-sub shell)	2
	1 (p-sub shell)	
3	0 (s-sub shell)	3
	1 (p-sub shell)	
	2 (d-sub shell)	

Here,

l represent sub-shells namely sharp (s); Principal (p), diffuse (d)

and fundamental (f). The value of 'l' helps to calculate the total number of electron hold by a sub-shell using the formula $2(2l + 1)$.

The value of 'l' helps to determine the angular momentum of an electron moving round the nucleus. So, that this quantum number is also called angular momentum quantum number;

3. Magnetic quantum number (m)

It gives information about the number of orbitals in a sub-shell. For the value of l, there are $(2l + 1)$ number of orbitals with the value of m from $-l$ to $+l$.

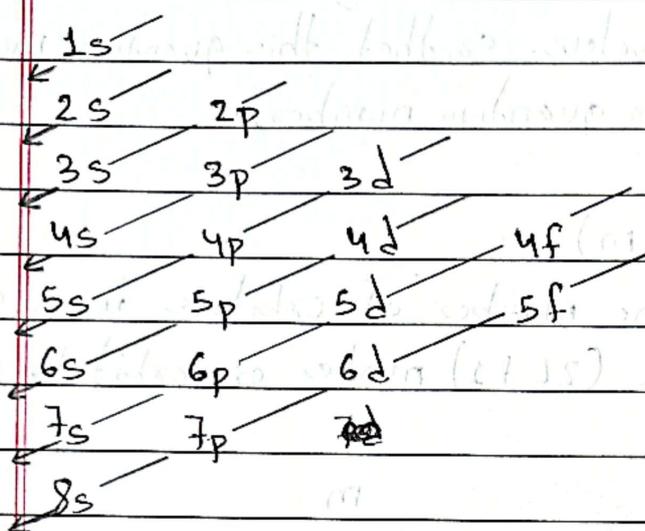
n	l	m
1	0 (s-subshell)	0 (s-orbital)
2	0 (s-subshell)	0 (s-orbital)
	1 (p-subshell)	-1 (p _x -orbital)
	1 (p)	0 (p _y -orbital)
		+1 (p _z -orbital)
3	0 (s-subshell)	0 (s-orbital)
	1 (p-subshell)	-1 (p _x -orbital)
		0 (p _y -orbital)
		+1 (p _z -orbital)
	2 (d-subshell)	-2 (d _{xy} -orbital)
		-1 (d _{yz} -orbital)
		0 (d _{xz} -orbital)
		+1 (d _{x²-y²} -orbital)
		+2 (d _{z²} -orbital)

4. Spin quantum number (s)

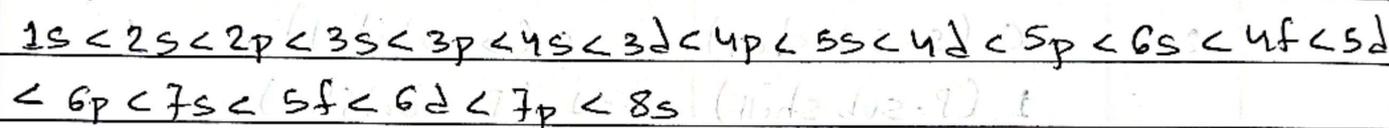
It denotes the spin of an electron on its own axis. for clockwise spin, $+1/2$ (\uparrow) and for an anti-clockwise spin $-1/2$ (\downarrow) is assigned.

Aufbau Principle

It states that "The orbitals are filled up with electrons in the increasing order of their energy".



Here,



Limitation of Aufbau principle

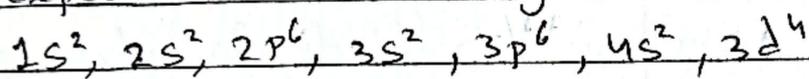
Exactly half filled and full filled orbitals have greater stability than other due to following reasons.

1. **Symmetry:** Half filled and full filled orbitals are more symmetrical than any other and symmetry lead to stability.
2. **Exchange energy:** The electrons present in different orbits of the same subshell can exchange their position. Each such exchange leads to decrease in energy known as exchange energy. Greater the number of exchanges the greater the exchange energy and the greater the stability.

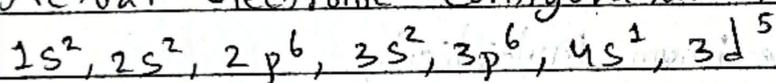
Electronic Configuration of Elements in ground State

Name	Symbol	Electronic Configuration
Hydrogen	H	$1s^1$
Oxygen	O	$1s^2, 2s^2, 2p^4$
Sodium	Na	$1s^2, 2s^2, 2p^6, 3s^1$
Magnesium	Mg	$1s^2, 2s^2, 2p^6, 3s^2$
Potassium	K	$1s^2, 2s^2, 2p^6, 4s^1, 3s^2, 3p^6, 4s^1$
Calcium	Ca	$1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2$
Chromium	Cr	$1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^1, 3d^5$
Copper	Cu	$1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^1, 3d^{10}$

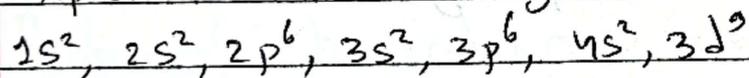
29. Expected Electronic Configuration of Chromium (Cr)



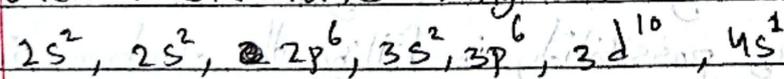
Actual Electronic Configuration of Chromium (Cr)



Expected Electronic Configuration of Copper (Cu)



Actual Electronic Configuration of Copper (Cu)



Reason:

The abnormal electronic configuration of Chromium and Copper can be explained on the basis of Aufbau principle that, the half filled and full-filled orbitals have greater stability and lower energy so that in Chromium and Copper one of electron from 4s sub-shell transfer to 3d sub-shell is result both 4s and 3d are half filled in Chromium and in case of Copper and 4s become half filled and 3d become full-filled due to which both sub-shell are more stable than expected electronic configuration.

Pauli's Exclusion principle

It states that "No two electrons in an atom can have identical set of four quantum numbers."

	n	l	m	s
K-shell	1	0	0	$+\frac{1}{2}$
	1	0	0	$-\frac{1}{2}$
	2	0	0	$+\frac{1}{2}$
	2	0	0	$-\frac{1}{2}$
L-shell	2	1	-1	$+\frac{1}{2}$
	2	1	-1	$-\frac{1}{2}$
	2	1	0	$+\frac{1}{2}$
	2	1	0	$-\frac{1}{2}$
	2	1	+1	$+\frac{1}{2}$
	2	1	+1	$-\frac{1}{2}$

Hund's rule for maximum Multiplicity

It states that "In an orbital of the same sub-shell, electrons are filled singly first before pairing starts."

Illustration:

Let us take an example of the filling electrons in a nitrogen atom. The electronic configuration of nitrogen is $1s, 2s, 2p$.

There are the following possibility in filling the electrons in $2p$

1↓	1		one paired electron (incorrect)
1	1	1	Three unpaired electron (correct)