- de Broglie's concept of matter waves :→ (Dual nature of Matter or electron / Wave-particle nature of matter):→ (द्रव्य तंरगो की डी-ब्रोग्ली संकल्पना)
- According to Max Planck's quantum theory of radiation, some phenomena like photoelectric effect (प्रकाश विद्युत प्रभाव) and black body radiation (कृष्णिका विकिरण) can be explained on the basis of particle nature of light.
- According to Maxwell's theory of radiation, other phenomena like, diffraction (विवर्तन), interference (व्यतिकरण) and polarisation (ध्रुवण) can be explained on the basis of wave nature of light.
- Thus we can say light behave both as particle and as a wave.
- In 1924, a French physicist, Lonius de Broglie extended the ideal of dual character of light to matter particle and suggested that all matter particle in motion (e.g. e^-, proton, neutron, atoms or molecules etc) have a dual character, i.e. all matter particles particles possess characterstics of both a material particle and a wave.
- The wave associated with matter particle is called de Broglie matter wave.
- The idea of de Broglie is called Dual nature of matter.
- According to de Broglie an e^- behave both as material particle and as a wave.

→ de Broglie's equation:→

- According to de Broglie, the momentum of a moving electron or particle is inversely proportional to its wavelength

$$\boxed{\lambda \propto \frac{1}{P}}$$

here

h = Planck's constant ($6 \cdot 626\ 10^{-34}$ J s)

λ = wavelength of wave

m = mass of e−

V = Velocity of electron

or $$\boxed{\lambda = \frac{h}{P}}$$

or $$\boxed{\lambda = \frac{h}{mv}} \quad \because P = mv$$

or $$\boxed{\text{de Broglie's wavelength}(\lambda) = \frac{\text{Planck's constant }(h)}{\text{Momentum of the } e^- (mv)}}$$

- Derivation of de Broglie equation:→

According to Planck, energy of photon is given by

$$E = h\nu \text{ ——— ① (Planck's equation)}$$

According to Einstein, energy of photon is given by

$$E = mc^2 \text{ ——— ② (Einstein equation)}$$

from eq. ① and ②

$$h\nu = mc^2$$

or $h \cdot \frac{c}{\lambda} = mc^2 \quad \left[\because \nu = \frac{c}{\lambda} \right]$ ν = frequency

or $\frac{h}{\lambda} = mc$

or $\boxed{\lambda = \frac{h}{mc}}$ — ③ c = velocity of light

If eq. ③ is applied to a moving e⁻ of mass m and velocity v then the above eq. reduces to

$$\boxed{\lambda = \frac{h}{mv}} \text{ — } ④$$

eq. ④ is de Broglie equation wich gives the value of wavelength of a moving e⁻ in terms of its mass and velocity

- Limitations of de Broglie equation:→

- de Broglie equation is applicable only for small particle (microscopic particles) like electrons, proton, neutrons etc. and has no significant for large particles (macroscopic particles).

- Proof of limilation:-

ⓐ Wavelength of large particle:→

mass of stone → 1×10^{-3} kg or 1gm

Velocity = 1m/sec

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34}}{(1 \times 10^{-3})(1)} \, m$$

$$\lambda = 6.626 \times 10^{-31} \, m$$

Value of wavelength is not in range of electromagnetic radiation

ⓑ Wave length of small particle:→

mass of e^- in H-atom → 9.108×10^{-31} kg

Velocity → 2.188×10^{6} m/s

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34}}{(9.108 \times 10^{-31})(2.88 \times 10^{6})}$$

$$\lambda = 0.3323 \times 10^{-9} \, m$$

Value of wavelength is within the range of electromagnetic radiation

→ Heisenberg's uncertainty principle :→

- Bohr's theory considered e⁻ as material particle. so position and momentum of an e⁻ can be determined with great accurancy.
- de Broglie considered e⁻ as wave. so it is not possible to measure simultaneously its exact position and velocity at a given time. because a wave is extending throughout a region of space.
- Thus if we measure exact position of an e⁻, the exact measurment of its velocity becomes uncertain and vice-versa.
- In 1927, Werner Heisenberg explained about the uncertainty in simultaneous measurment of position and momomentum of an e⁻ in his principle. This principle is known as Heisenberg's uncertainty principle.
- According to this principle, " It is impossible to measure simultaneously the exact position and exact velocity (or momentum) of sub atomic particles like electron and neutron

→ Mathematical expression for the principle :→

- According to Heisenberg, the relationship b/w uncertainty in measurment of position and uncertainty in measurement of momentum of sub-atomic particles like e- and neutron is

$$\boxed{\Delta x \cdot \Delta p \geq \frac{h}{4\pi}} \quad \text{— ①}$$

or

$$\boxed{\Delta x \cdot \Delta p \geq \frac{\hbar}{2}} \quad \text{— ②}$$

here Δx = uncertainty in measurement of position
Δp = uncertainty in measurement of momentum
h = Planck's constant ($6 \cdot 626 \times 10^{-34}$ Js)
$\hbar$ = Reduced Planck's constant $\left[\hbar = \frac{h}{2\pi}\right]$

- The relation given above is called uncertainty relation.
- From the eq. ①, it is evident that if Δx is small (measured accurately) then Δp will be large (measured less accurately) and vice versa.
- In other words, certain determination of one quantity introduces uncertainty in determination of other quantity.
- If position of particle is measured accurately then Δx should be zero and hence

$$\Delta p = \frac{h}{4\pi \times \Delta x} \quad \text{or} \quad \Delta p = \frac{h}{4\pi \times 0} \quad \text{or} \quad \Delta p = \infty$$

i.e. error in determination of momentum.

- If m is the mass of the particle and ΔV is the uncertainty in the measurement of its velocity, then

$$\boxed{\Delta P = m . \Delta V}$$

- On putting value of ΔP in eq. ①

$$\Delta x . m . \Delta V \geq \frac{h}{2\pi}$$

or $$\boxed{\Delta x . \Delta V \geq \frac{h}{4\pi m}} \quad — ③$$

- Limitations of Heisenberg uncertainty principle :→
- The uncertainty principle is applicable only for small particles (microscopic particles) like e^-, neutrons etc and has no significance for large particles (macroscopic particles).
- **Proof**:- if we calculate Δv for large particle (ball) using eq. ③, then value of ΔV is very small and hence is negligible to the usual velocity of ball. The value of Δv for e^- is quite large and hence meaningful.

→ Atomic orbitals :→

- The three dimentional region or space (i.e. volume) round the nucleus of an atom where probability of finding e- having a certain energy is maximum (90-95%.) is called atomic orbital.

OR

- An atomic orbital represents the space round the nucleus in an atom where the e- spends most of its time while in constant motion.

OR

- The thin, shell-like, region in space surroundings the nucleus for which e- probability has a high value is known as atomic orbital.
- The energy of e- in an atomic orbital is always the same.
- The e- is free to found anywhere in the atomic orbital at any given time.

fig:- represention of probability of finding an e- in 1s orbital of hydrogen atom

- Difference b/w orbit and Orbital :→

Orbit	*Orbital*
(*i*) As postulated by Bohr, an orbit is a definite circular path at a definite distance from the nucleus in which the electron revolves round the nucleus. Orbits are numbered as 1, 2, 3, 4...... from the nucleus and are designated by the capital letters K, L, M, N......etc.	(*i*) As postulated by wave nature of an electron, an orbital is defined as a three-dimensional region or space around the nucleus within which the probability of finding an electron with a certain energy is maximum.
(*ii*) An orbit indicates an exact position or location of an electron in an atom. For example, according to Bohr's theory, an electron of hydrogen is found at a distance of 0.53Å from the nucleus.	(*ii*) An orbital does not specify the definite or exact position of an electron in an atom, since the electron, due to its wave-nature, can not be found at a fixed distance from the nucleus.
(*iii*) There is a certainty about the movement of an electron in an orbit.	(*iii*) Due to uncertainty principle, there is no certainty about the movement of an electron in an orbital.
(*iv*) It represents the planar motion of the electron.	(*iv*) It represents the three-dimensional motion of the electron round the nucleus.
(*v*) The maximum number of electrons in an orbit is equal to $2n^2$ where n is the number of the orbit.	(*v*) An orbital cannot accommodate more than two electrons. These two electrons must have opposite spins.
(*vi*) Orbits are circular in shape.	(*vi*) Orbitals have different shapes, *e.g.*, *s*-orbital is spherically symmetrical, *p* orbitals are dumb-bell shaped etc.

→ Schrodinger's Wave equation :→

- The model which refered e- as particle and wave is called wave mechanical model of the atom.
- In 1926, an Austrian physicist, Erwin Schrodinger, developed a wave mechanical model of the atom. In his model he suggested than an atom contains positively charged nucleus and nucleus is surrounded by standing or stationary e- wave which extends in Bohr's circular orbits.
- Thus this model described the e- as three dimensional wave in the electric field of a positively charged nucleus.
- Schrodinger proposed that if e- behaves as wave, then it should obey the same equation of motion followed by known waves.
- on the basis of this idea, he derived a equation which describes the wave motion of an electron along any of three axis viz. x, y and z. This eq. is called Schrodinger wave equation.
- Schrodinger wave equation is a differential eq. of second order.

- Schrodinger wave equation of a wave moving in one direction (x) (one dimension)

$$\boxed{\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0} \quad -①$$

- Schrodinger wave equation of a wave moving in three directions (x,y,z) (3 dimension)

$$\boxed{\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0} \quad -②$$

here x, y, z = three space coordinates

E = Total energy of electron

m = mass of electron

h = Planck's constant (6.626×10^{-34} Js)

V = Potential energy of e^-

ψ = wave function.

- Equation ② can also be written as

$$\boxed{\nabla^2\psi + \frac{8\pi^2 m}{h}(E-V)\psi = 0} \quad -③$$

here $\nabla^2 = \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}$

Called laplacian operator

- Schrodinger eqution can also be written as

$$\boxed{H\Psi = E\Psi} \quad - ④$$

here H = Hamiltonian operator

$$\boxed{H = -\frac{h^2}{8\pi^2 m}\nabla^2 + V}$$

or

$$\boxed{H = -\frac{\hbar^2}{2m}\nabla^2 + V}$$

here $\hbar$ = Reduced Planck's constant

$$\boxed{\hbar = \frac{h}{2\pi}}$$

→ Significance of ψ and ψ^2 :→

- In Schrodinger's wave equation the wave function, ψ represents the amplitude of the wave. The wave function, ψ by itself has no physical significance. The value of ψ may +ve or -ve.
- The square of wave function (ψ^2) is used to find out the e⁻ density around nucleus in an atom.

$$\psi^2 \propto e^- \text{ density around nucleus}$$

- The probability of finding an e⁻ around the nucleus is called electron probability function (D)

$$\boxed{D = 4\pi r^2 . dr . \psi^2} \quad -①$$

or D = volume of sphericall shell of radius r and thickness $dr \times \psi^2$

- Eq. ① shows that value of D depends on r.

Example :- for 1s e⁻ of H-atom

Ⓐ if $r = 0$ the $D = 0$

(b) if $r = 0.529 Å$ (radius of Bohr's first orbit) then probability of finding e⁻ is maximum (95%)

→ Quantum Numbers :→

- The term quantum number is used to various energy levels available for an electron in atom.
- The quantum numbers are used to completely define the electron in an atom. i.e. position or location of e^-, Energy of e^-, angular momentum of e^-, direction of spin etc. Each quantum no. refers to a particular character of an e^- in an atom.
- The Schrodinger wave equation for H-atom which explain the energy of e in H-atom, contain three constants called Principal quantum number (n), azimuthal quantum number (l), and magnetic quantum number (m).
- Fourth quantum number called spin quantum number (s) was given by Goud-smith and Uhlenbeck in 1925.

① Principal quantum number (n) :→

- n represents energy levels or shell in which e^- revolves around nucleus in an atom

Value of n (whole no.) →	1	2	3	4	......
Designation of shells →	K (1st shell)	L (2nd shell)	M (3rd shell)	N (4rt shell)	....

✱ Desigation of shell named on the basis of x-ray spectrum. x-ray spectrum consist of discrete spectral line which grouped into K-series, L-sereis, M-series etc.

- n value determines the location of e^- in a shell

$$n \text{ value} \rightarrow 1 < 2 < 3 < 4 \ldots$$

$$r \text{ value} \rightarrow r_1 < r_2 < r_3 < r_4 \ldots$$

Thus n value represents size of the electron orbit.

- n determines the energy of an e^- in given orbit

$$\boxed{E_n = -\frac{2\pi^2 m e^4}{n^2 h^2}}$$

here E_n = energy of e^- in nth orbit
m = mass of e^-
e = charge of e^-
n = shell
h = Planck's constant

- n gives the maximun no. of e- in a shell

max. no. of e- in a shell = $2n^2$

Shell	n	no. of e-
K	1	$2 \times 1^2 = 2$
L	2	$2 \times 2^2 = 8$
M	3	$2 \times 3^2 = 18$
N	4	$2 \times 4^2 = 32$

② Azimuthal or subsidiary quantum number (l):→

- l represents sub-shell of the shell
- The value of l depends on value of n. For a given value of n, l have the values from 0 to (n-1) i.e

$$l = 0, 1, 2, 3 \ldots\ldots (n-2)(n-1)$$

Thus l have n values.

- Different values of l represent different sub shells which are designated by small letters s, p, d, f ... . These letters stand for sharp, principal, diffuse and fundamental which are spectral terms used to describe the series of line observed in spectrum.

Value of l →	0	1	2	3	----
Designations of Sub shell →	s	p	d	f	------

- The order of energies of sub shell is $s < p < d < f$
- The sequence of filling is $s < p < d < f$
- l also explain about shapes of sub shells

$l = 0$ → spherical shape

$l = 1$ → dumb-bell

$l = 2$ → double dumb-bell

higher l values have complex shape.

- The number of e- a sub shell is given by $2(2l + 1)$.

Subshell	l	no. of e-
s	0	$2(2\times0+1)=2$
p	1	$2(2\times1+1)=6$
d	2	$2(2\times2+1)=10$
f	3	$2(2\times3+1)=14$

- l value used to calculate no of subshells in a given shell

Shell	n	l (0 to $n-1$)	Designation of sub shell
K	1	0	1s
L	2	0,1	2s
M	3	0,1,2	3s,3p,3d
N	4	0,1,2,3	4s,4p,4d,4f

- l values is a measure of orbital angular momentum of an e⁻. so it is also called angular momentum quantum number or orbital quantum no.
- sub shell having equal l values have similar shape but their size increases with increase in Value of n

1s and 2s have same size but 2s is larger in size as compare to 1s.

③ Magnetic quantum number (m):→

- m represents the orbitals present is sub-shell.
- Value of m depends on the value of l. m can have integral values ranging from $-l, 0, +l$

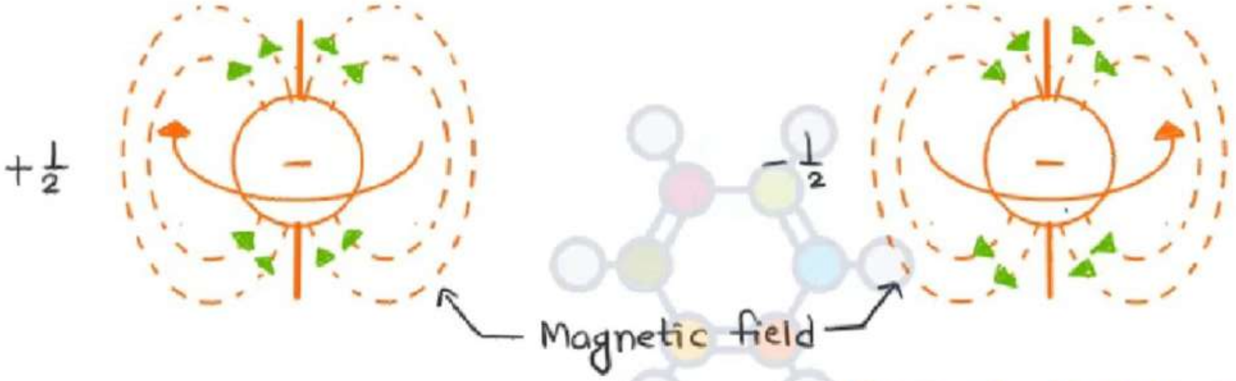
$$m = 0, \pm 1, \pm 2, \pm 3, \ldots \pm l$$

- total no. of orbital (or m) is given by $(2l+1)$
- Different value of m gives the total no. of orbitals in a given sub-shell or total no. of different ways in which sub shell can be arranged in the presence of magnetic field.

Value of l	Sub-shell	Value of m	no. of orbitals
0	s	0	1
1	p	−1, 0, +1	3
2	d	−2, −1, 0, +1, +2	5
3	f	−3, −2, −1, 0, +1, +2, +3	7

④ spin quantum number (s):->

- In 1925, Goudsmit and Uhlenback suggested that an e^- while moving in an orbit around the nucleus, also rotates or spin about its own axis.



clockwise spin of e^- Anti clockwise spin of e^-

- spin of e^- on own axis generates magnetic moment.
- The spinning of the e^- in clock wise and anti clock wise directions produces opposite magnetic fields.

spin	value of s	representation of e^-
clockwise	$+\frac{1}{2}$	↑
Anticlockwise	$-\frac{1}{2}$	↓

n	l	Designation of sub-shell (nl)	m	Designation of orbital (nm)	No. of electrons in each orbital = 2	s for two electrons	No. of sub-shells in a main shell = n	No. of orbitals in a sub-shell = $(2l+1)$	No. of orbitals in a main shell = n^2	No. of electrons in a main shell = $2n^2$	No. of electrons in a sub-shell = $2(2l+1)$
1	0	1s	0	1s	2(↑↓)	+1/2, −1/2	1	2×0+1 = 1	1^2 = 1 (1s)	$2\times1^2 = 2$	2×1 = 2
(1st shell or K-shell)							(1s)				
2	0	2s	0	2s	2(↑↓)	+1/2, −1/2	2	2×0+1 = 1	$2^2 = 4$	$2\times2^2 = 8$	2×1 = 2
(2nd shell							(2s,		or		
or L-shell)							2p)				
	1	2p	−1	$2p_z$	2(↑↓)	+1/2, −1/2			1+3 = 4(2s,		
			+1	$2p_y$	2(↑↓)	+1/2, −1/2			$2p_z$, $2p_y$, $2p_x$		2×3 = 6
			0	$2p_x$	2(↑↓)	+1/2, −1/2		2×1+1 = 3			
	0	3s	0	3s	2(↑↓)	+1/2, −1/2	3	2×0+1 = 1	$3^2 = 9$	$2\times3^2 = 18$	2×1 = 2
3	1	3p	−1	$3p_z$	2(↑↓)	+1/2, −1/2	(3s,		or		
(3rd shell			+1	$3p_y$	2(↑↓)	+1/2, −1/2	3p,	2×1+1 = 3	1+3+5 = 9		2×3 = 6
or M-shell)			0	$3p_x$	2(↑↓)	+1/2, −1/2	3d)		(3s, $3p_z$, $3p_y$,		
	2	3d	0	$3d_{z^2}$	2(↑↓)	+1/2, −1/2			$3p_x$, $3d_{z^2}$,		
			+1	$3d_{xz}$	2(↑↓)	+1/2, −1/2			$3d_{xz}$, $3d_{yz}$,		
			−1	$3d_{yz}$	2(↑↓)	+1/2, −1/2		2×2+1 = 5	$3d_{x^2-y^2}$,		
			+2	$3d_{x^2-y^2}$	2(↑↓)	+1/2, −1/2			$3d_{xy}$)		2×5 = 10
			−2	$3d_{xy}$	2(↑↓)	+1/2, −1/2					

Example:- Write the quantum number values for last e- of Na.

$Na = 1s^2\ 2s^2\ 2p^6\ 3s^1$

$n = 3\ ,\ l = 0\ ,\ m = 0\ ,\ s = +\frac{1}{2}$

Example :- Arrange the orbitals with the following quantum numbers in the increasing order of their energy.

(i) $n = 3,\ l = 0,\ m = 0,\ s = +\frac{1}{2}$

(ii) $n = 3,\ l = 1,\ m = 1,\ s = +\frac{1}{2}$

(iii) $n = 3,\ l = 2,\ m = 1,\ s = +\frac{1}{2}$

(iv) $n = 4,\ l = 0,\ m = 0,\ s = +\frac{1}{2}$

Answer orbitals are (i) 3s (ii) 3p (iii) 3d (iv) 4s

order $3s < 3p < 4s < 3d$

→ Radial and Angular wave functions and Probability distribution curve :→

- The solution of schrodinger wave equation for H-atom is

$$\boxed{\psi = R(r) \cdot \Theta(\theta) \cdot \Phi(\phi)} \quad \text{— ①}$$

r, θ and ϕ = polar coordinates

$R(r)$ = A function that depends on the distance from the nucleus, which depends on quantum no. n and l.

$\Theta(\theta)$ = A function of θ, which depends on the quantum no. l and m

$\Phi(\phi)$ = A function of ϕ, which depends only on quantum no. m

- Eq. ① may be written as

$$\boxed{\psi = R(r)_{nl} A_{ml}} \text{— ②} \qquad \because A_{ml} = \Theta(\theta), \Phi(\phi)$$

eq. ② splits wave function into two parts -

① $R(r)_{nl}$ the radial wave function, which depends on quantum no. n and l

② A_{ml} the total angular wave function, which depends on quantum no. m and l

- The radial wave functions for the first three orbitals in the hydrogen atom are -

$n = 1, l = 0, m = 0$ $\boxed{R = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}}$ 1s orbital — ③

$n = 2, l = 0, m = 0$ $\boxed{R = \left(\frac{1}{2\sqrt{2}}\right)\left(\frac{Z}{a_0}\right)^{3/2}\left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}}$ 2s orbital — ④

$n = 2, l = 1, m = 0$ $\boxed{R = \left(\frac{1}{2\sqrt{6}}\right)\left(\frac{Z}{a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0}}$ 2p orbital — ⑤

here Z = nuclear charge e = base of natural logarithms

a_0 = Borh's orbit = $\frac{h^2}{4\pi^2 m e^2}$

here h = Planck's constant (6.626×10^{-34} Js)

m = mass of e-

e - charge of e-

- For a given atom z will be constant and may be combined with other constants. so eq. ③, ④ and ⑤ can be simplified as

$$\boxed{R = K_{1s} e^{-Zr/a_0}} \quad - ⑥ \qquad \therefore \boxed{K_{1s} = \left(2 \frac{Z}{a_0}\right)^{3/2}} \quad 1s\text{-orbital}$$

$$\boxed{R = K_{2s}\left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}} \quad - ⑦ \qquad \therefore \boxed{K_{2s} = \left(\frac{1}{2\sqrt{2}}\right)\left(\frac{Z}{a_0}\right)^{3/2}} \quad 2s\text{-orbital}$$

$$\boxed{R = K_{2p}\, r e^{-Zr/2a_0}} \quad - ⑧ \qquad \therefore \boxed{K_{2p} = \left(\frac{1}{2\sqrt{6}}\right)\left(\frac{Z}{a_0}\right)^{3/2} \frac{Z}{a_0}} \quad 2p \text{ orbital}$$

- The radial function R has no physical significance, but R^2 gives the probability of finiding the e^- in small volume dv near the point at which R is measured.
- For a given value of r small volume is $4\pi r^2$
- The probability of e^- at r from the nucleus is called radial distribution function which is $4\pi r^2 R^2$.

- A Radial distribution function gives the probability of finding e⁻ at a given distance from the nucleus, regardless of the direction.
- Graph of the radial distribution function for hydrogen plotted against r are shown in figure.
- These diagrams show that probability is zero at the nucleus (r = 0)
- By examining the plots for 1s, 2s and 3s that the most probable distance increases as the principal quantum number (n) increases.
- By comparining the plots for 2s and 2p or 3s, 3p and 3d it can be seen that most probable radius decreases slightly as the azimuthal quantum number(l) increases.
- All s-orbitals except 1s have shell like structure, rather like onion or hailstone. Similarly all but the first p orbital (2p) and the first d orbital (3d) have shell like structure

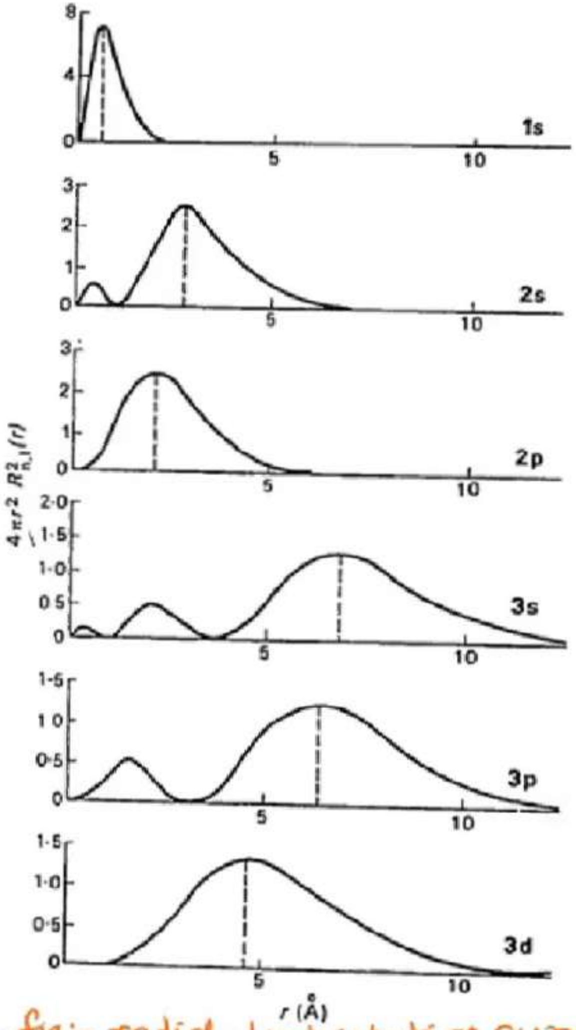


fig:- radial distriubution curve for H- atom

- The spherical surface where the probability of finding e^- is zero is called Radial node.

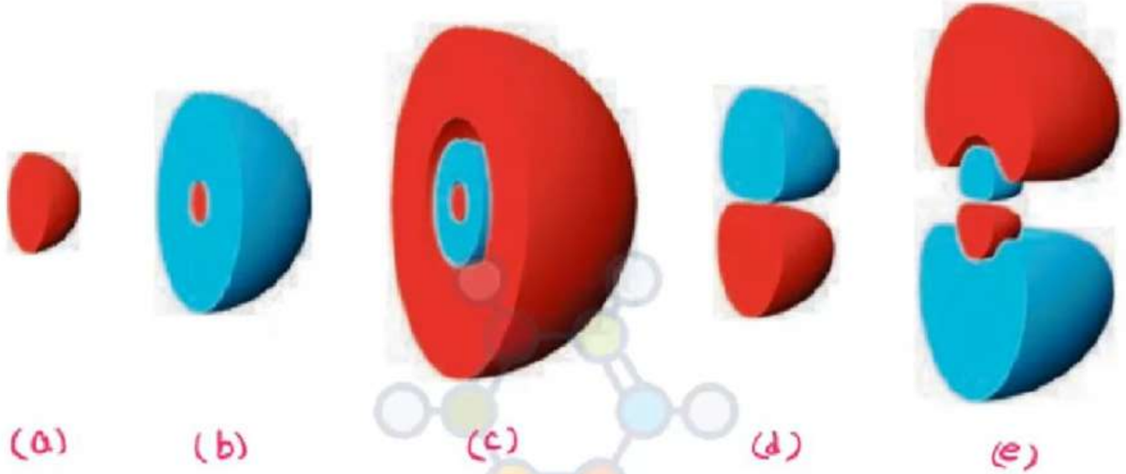


fig:- cross section of orbitals (a) 1s (no radial nodes) (b) 2s (one radial nodes) (c) 3s (two radial nodes) (d) 2p (no radial nodes) (e) 3p (one radial nodes)

- Number of radial nodes:-

for ns orbitals → n-1
for np orbitals → n-2
for nd orbitals → n-3
for nf orbitals → n-4

- The angular wave function A depends only on the direction and is independent of the distance from nucleus(r).
- Thus A^2 is the probability of finding an e- at a given direction θ, ϕ at any direction nucleus to infinity.
- The orbital is normally represented by a spherical surface with the nucleus at its center. The surface is called boundary surface of the orbital and represent high (90-95%) probability of finding e-
- The plane at angular wave function is zero is called angular node or nodal plane. e- density is zero at angular node
- No. of angular node in any orbital is equal to azimuthal quantum number (l)

s ($l=0$) has no angular node

p ($l=1$) has 1 angular node

d ($l=2$) has 2 angular nodes

f ($l=3$) has 3 angular nodes

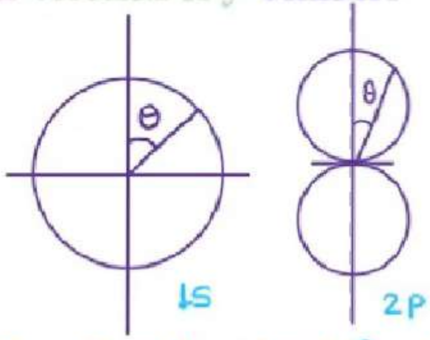


fig:- Angular wave function for H-atom

-Angular wave function depends on orbital and orientation

s orbital $\Theta\phi = (1/4\pi)^{1/2}$

P_z orbital $\Theta\phi = (3/4\pi)^{1/2} \cos\theta$

dz^2 orbital $\Theta\phi = (5/16\pi)^{1/2}(3\cos^2\theta - 1)$

- The angular wave funct. A are plotted as polar diagrams in figure ⓐ

- These polar diagram do not represent total wave function ψ, but only angular part of the wave function.

- These polar diagram are commonly used to illustrate overlap of orbitals giving bonding between atoms.

- sign + and − relating to symmetry of wave function

- For bonding like signs must overlap.

- The probability of finding an e⁻ simultaneously at a distance r and in a given direction θ, ϕ is

$$\boxed{\psi^2_{r,\theta,\phi} = R^2(r) \cdot A^2(\theta,\phi)}$$

- A full represention of probability of finding an e⁻ is given by 3d diagrams as shown in fig. ⓑ

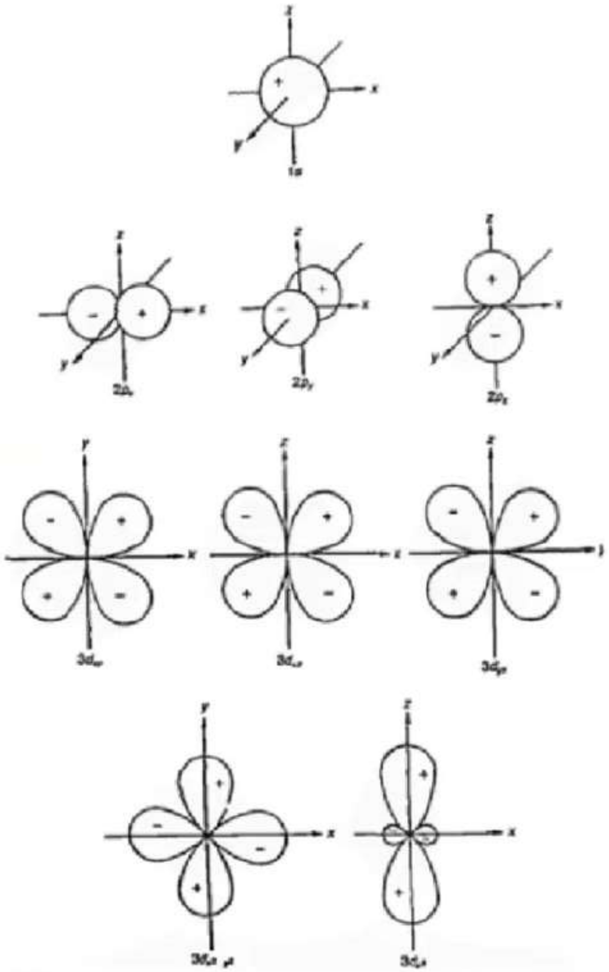
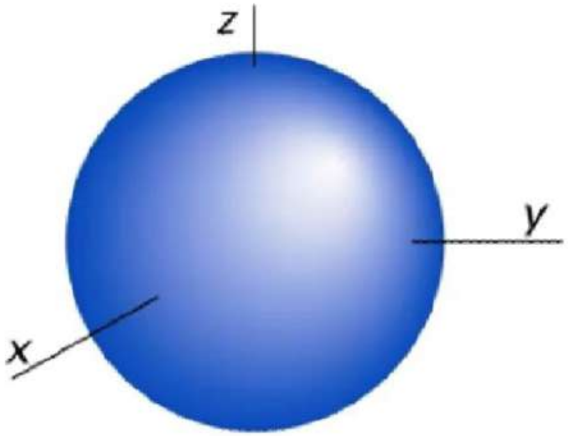


fig :ⓐ Boundary surface for the angular part of wave function A (polar diagram for H-atom)



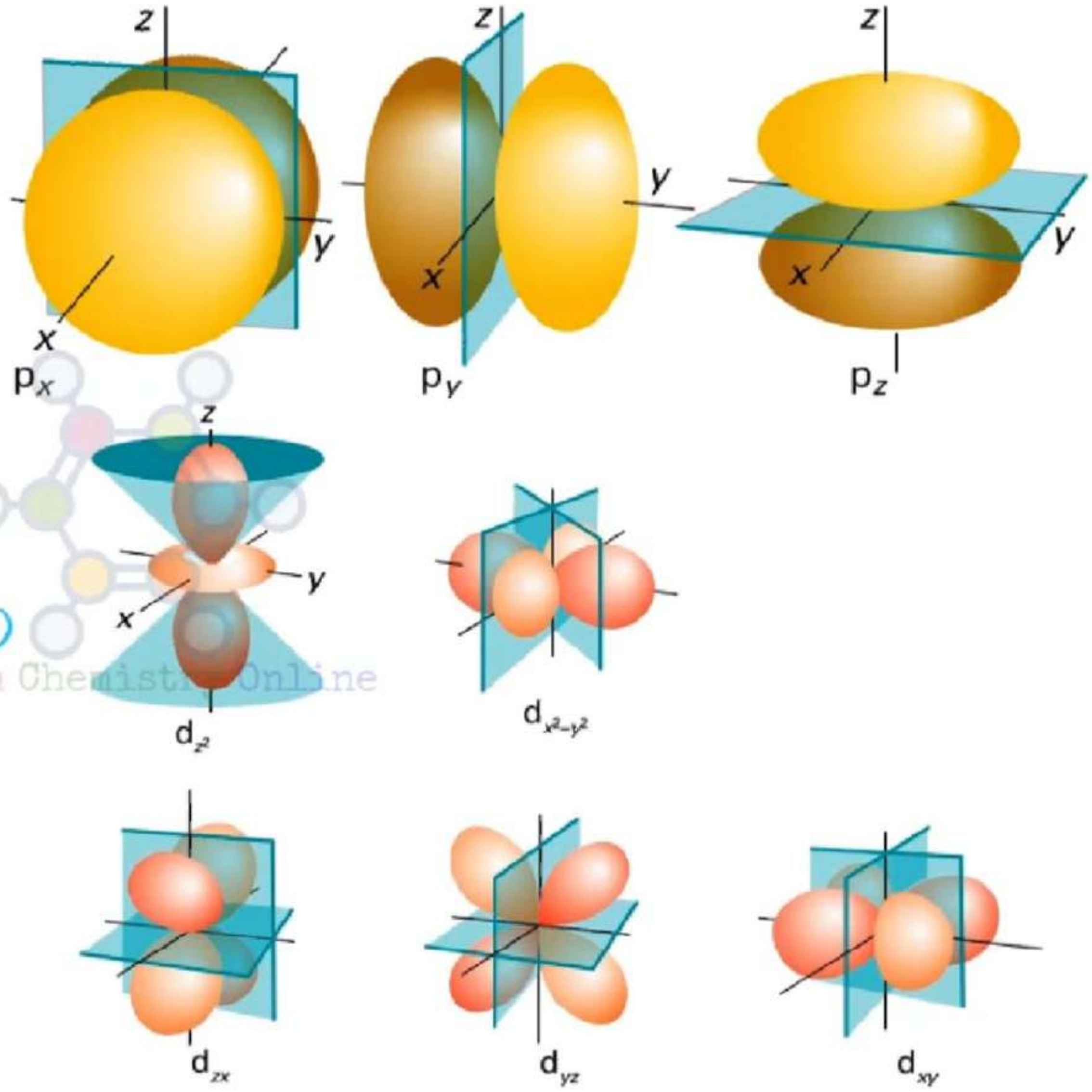


Fig ⓑ :- Total wave function (orbitals) for H-atom

→ Shapes of orbitals :→

① s - Orbital :-

- s- orbital is spherical in shape and hence e⁻ density is not concentrated along any particular direction,
- For s-orbital $l = 0$ and hence $m = 0$
- As the value of principal quantum no. (n) increases the size of s-orbital is increases. for example 2s orbital is larger than 1s orbital.
- An e⁻ in 2s orbital is farther away from the nucleus and has greater energy than in 1s orbital.
- Order of energy is $1s < 2s < 3s$
- The spherical shell b/w 1s and 2s orbitals where probability of finding e⁻ is zero, called nodal plane or nodal surface.
- No. of nodal surface for s orbital $= n - 1$

example   for $1s = (1-1) = 0$

for $2s = (2-1) = 1$

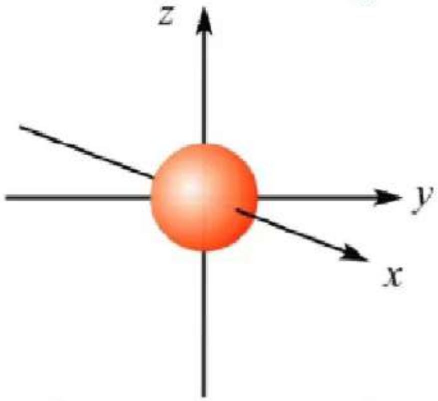


fig:- s-orbital

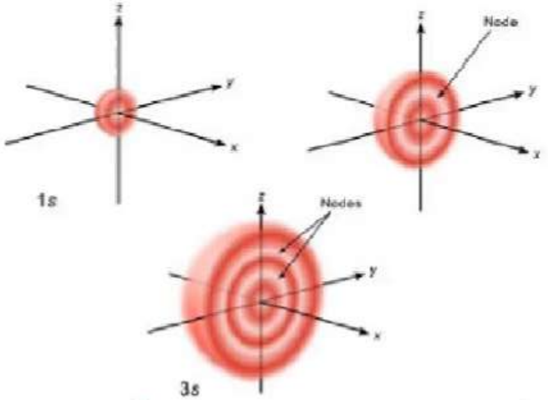


fig:- nodal surface

② p-orbital :>

- For p-orbital, $l = 1$ and $m = -1, 0, +1$
- Three values of m show that p-orbitals have three orientations i.e. there are three p-orbitals, P_x, P_y and P_z. (x, y, z represent coordinate axes).
- In the absence of magnetic field these three orbitals are equivalent in energy and are called three-fold degenerate or triply degenerate.
- In the presence of magnetic field the energies of these orbitals change and depends on magnetic quantum number.
- The p-orbitals are dumb-bell shape.
- Three p-orbitals are perpendicular to each other.
- The two lobes of dumb-bell of p-orbital is contains the nucleus and perpendicular to corresponding axis. Such plane is called nodal plane. There is no probability of finding the e^- density on this plane. i.e such plane has zero e^- density.
- Each p-orbital has one nodal plane.

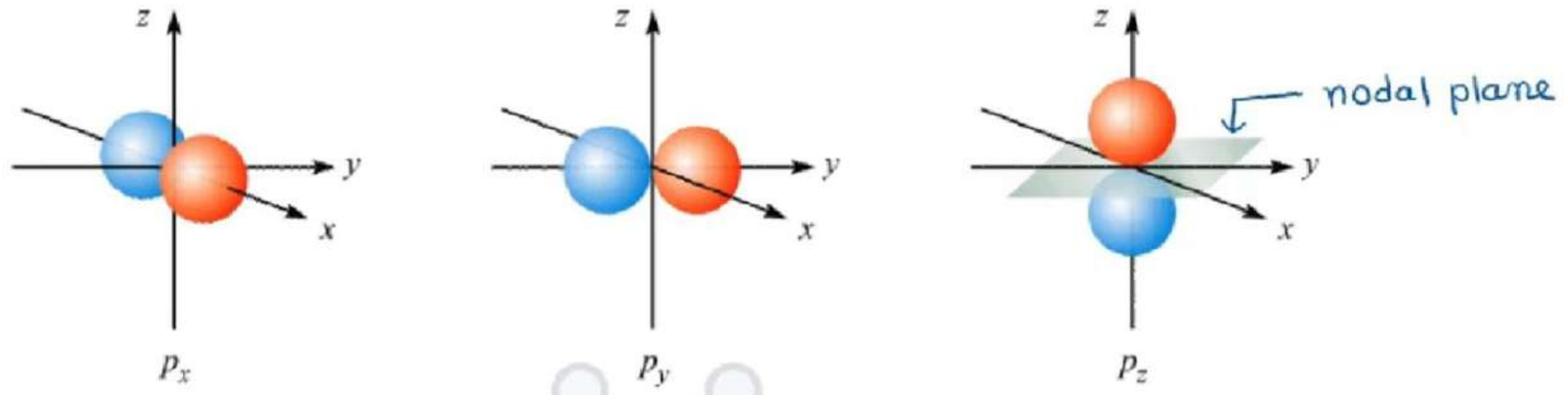


fig:- Three p-orbitals

③ d- orbitals :→

- These orbitals started with 3rd main energy level ($n = 3$, M-shell).
- $l = 2$ and $m = -2, -1, 0, +1, +2$.
- Values of m show that d orbitals have five orientations. i.e. there are five orbitals - d_{xy}, d_{yz}, d_{xz}, $d_{x^2-y^2}$, d_{z^2}.
- In the absence of magnetic field, these five orbitals have same energy and are called five fold degenerate.
- d-orbital contain double dumb-bell

- d-orbitals are divided into two sets -

t_{2g} set (Triply degenerate)

- d_{xy}, d_{yz}, d_{xz}
- lobes lying b/w the axes
- non-axial set

e_g set (Doubly degenerate)

- $d_{x^2-y^2}$, d_{z^2}
- lobes lying along the axes
- axial set

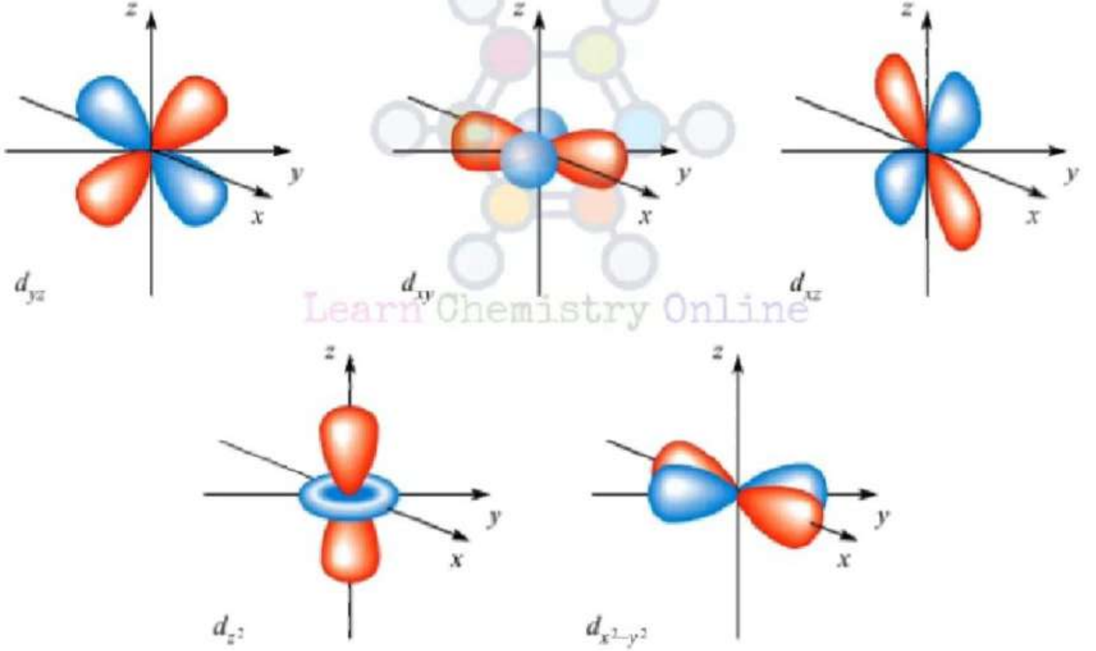


fig:- d-orbitals

→ Aufbau Principle :→

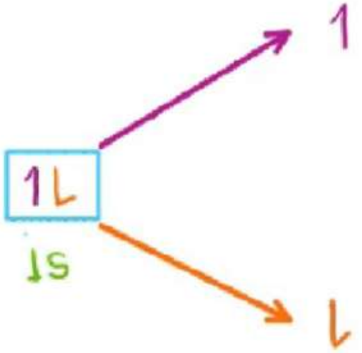
- The filling of electrons into orbitals of different orbitals of different atoms takes place according to the Aufbau principle which is based on the following principles.
  ① Pauli's Exclusion principle
  ② Hund's rule of maximum multiplicity
  ③ Relative energies of the orbitals or $n+\ell$ Rule.
- The word "Aufbau" in German means "building up".
- The building up of orbital means the filling up of electrons in orbitals.
- According to aufbau principle, electrons first occupy the lowest energy orbitals and then enter into higher energy orbitals.

① Pauli's Exclusion principle :→

- This principle was given by Wolfgang Pauli in 1925.
- According to this principle, there are some restrictions on the assignment of the values of quantum numbers of e^- in same orbital of an atom and hence the name exclusion principle.

- This principle states that, "it is impossible for two electrons in a given atom to have all the four quantum numbers identical."
- In other words, in an atom, two e⁻ can have maximum three quantum numbers (n,l,m) same and fourth (s) will definitely be having a different value. Thus If $s = +\frac{1}{2}$ for one electron, s should be equal to $-\frac{1}{2}$ for the other e⁻. i.e. the two e⁻ in the same orbital should have opposite spin (↿⇂).

- **Example** :- 1s orbital



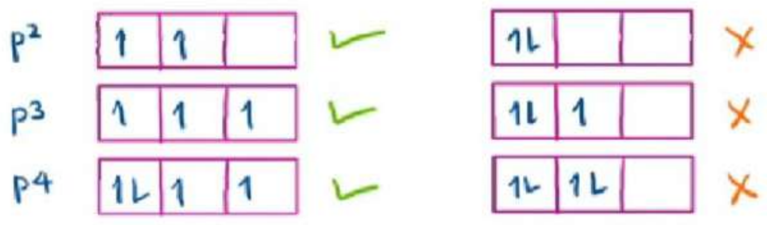
$n = 1,\ l = 0,\ m = 0,\ s = +\frac{1}{2}$

$n = 1;\ l = 0,\ m = 0,\ s = -\frac{1}{2}$

② Hund's rule of maximum multiplicity :→

- On the basis of magnetic measurements which are helpful in determining the electronic configuration of elements, Hund gave an empirical rule known as Hund's rule of maximum multiplicity.
- According to this rule, pairing of electrons in the orbitals belonging to the same subshell does not take place until each orbital belonging the that shell has got one e^- each i.e. it is singly occupied.
- The entering of e^- in orbitals in this manner minimises the inter-electron repulsion energy (e^-–e^- replusion) and hence stability of system increases. Thus this rule is also called rule of minimum energy.

Example :-



③ $n+l$ Rule :→

- The relative energy of different orbitals or the sequence of filling e^- in orbitals can also be determined with help of $n+l$ Rule.
- According to this rule, The orbital having lowest value of $n+l$ has the lowest energy and hence is filled up first with electrons. when two or more orbitals have the same value of $n+l$, the orbital with lower value of n is lower in energy and hence is filled up first with electrons.
-

Orbital →	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f
Principal q. no. (n)	1	2	2	3	3	3	4	4	4	4
Azimuthal q. no. (l)	0	0	1	0	1	2	0	1	2	3
(n+l)	1	2	3	3	4	5	4	5	6	7

- Relative order of energy of different orbitals or sequence of filling orbital → $1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s < 5f < 6d < 7p$ ...

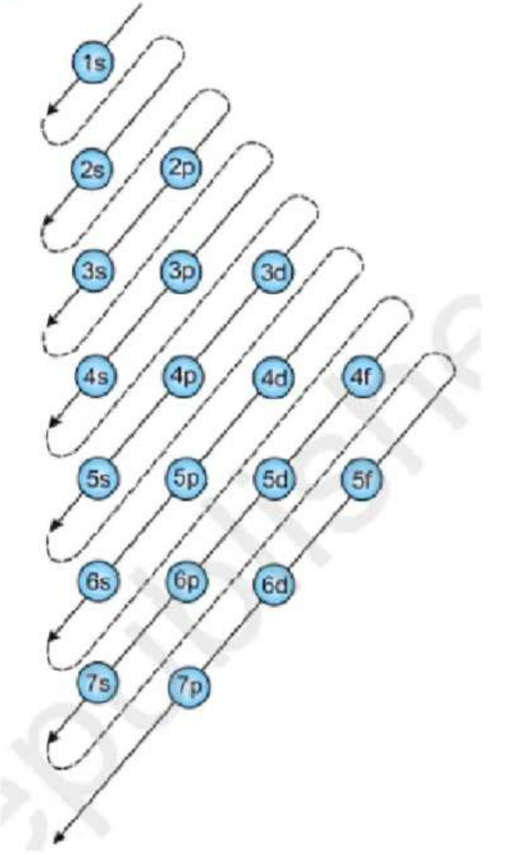


fig:- sequence of filling orbitals.

→ Electronic configuration of the elements :→

- The distribution of e⁻ in various shells, sub-shells and orbitals of an atom is called its electronic configuration.

- Valence shell configuration:→

- The distribution of e⁻ in various sub-shells and orbitals of the valence shell is called valence-shell configuration.

- Representation of electronic configuration:→

- The electronic configuration of an atom is written in terms of

$$n\,l^{x}$$

Shell number ⟶ n

x ⟵ no. of electrons

sub-shell → l

- **Example** if $n = 3$, $l = 1$, $x = 2$ → $3p^2$

- Rules for writing electronic configuration:→

① Maximum no. of e⁻ in shell :→

K-shell or 1st shell $(n = 1) = 2$
L-shell or 2nd shell $(n = 2) = 8$
M-shell or 3rd shell $(n = 3) = 18$
N-shell or 4th shell $(n = 4) = 32$

② Maximun no. of e^- in sub-shell :→

Value of l →	0	1	2	3
sub shell →	s	p	d	f
max. no. of e^- →	2	6	10	14

③ Aufbau principle :-

ⓐ Pauli's Exclusion principle

ⓑ Hund's rule of maximum multiplicity

ⓒ Relative enenrg of orbitals or $n+l$ Rule

④ Rule of half-filled or completely filled orbitals

- stability order of orbitals is

Completely filled > Half-filled > Imcompletely filled

1	H	$1s^1$	↑				
2	He	$1s^2$	↑↓				
3	Li	$1s^2 2s^1$	↑↓	↑			
4	Be	$1s^2 2s^2$	↑↓	↑↓			
5	B	$1s^2 2s^2 2p^1$	↑↓	↑↓	↑ | |		
6	C	$1s^2 2s^2 2p^2$	↑↓	↑↓	↑ | ↑ |		
7	N	$1s^2 2s^2 2p^3$	↑↓	↑↓	↑ | ↑ | ↑		
8	O	$1s^2 2s^2 2p^4$	↑↓	↑↓	↑↓ | ↑ | ↑		
9	F	$1s^2 2s^2 2p^5$	↑↓	↑↓	↑↓ | ↑↓ | ↑		
10	Ne	$1s^2 2s^2 2p^6$	↑↓	↑↓	↑↓ | ↑↓ | ↑↓		
11	Na	$1s^2 2s^2 2p^6 3s^1$	↑↓	↑↓	↑↓ | ↑↓ | ↑↓	↑	
12	Mg	$1s^2 2s^2 2p^6 3s^2$	↑↓	↑↓	↑↓ | ↑↓ | ↑↓	↑↓	
13	Al	$1s^2 2s^2 2p^6 3s^2 3p^1$	↑↓	↑↓	↑↓ | ↑↓ | ↑↓	↑↓	↑ | |
14	Si	$1s^2 2s^2 2p^6 3s^2 3p^2$	↑↓	↑↓	↑↓ | ↑↓ | ↑↓	↑↓	↑ | ↑ |
15	P	$1s^2 2s^2 2p^6 3s^2 3p^3$	↑↓	↑↓	↑↓ | ↑↓ | ↑↓	↑↓	↑ | ↑ | ↑

16	S	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][↑][↑]		
17	Cl	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][↑]		
18	Ar	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][⇅]		
19	K	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^0\ 4s^1$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][⇅]	[ ][ ][ ][ ][ ]	[↑]
20	Ca	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^0\ 4s^2$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][⇅]	[ ][ ][ ][ ][ ]	[⇅]
21	Sc	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^1\ 4s^2$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][⇅]	[↑][ ][ ][ ][ ]	[⇅]
22	Ti	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^2\ 4s^2$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][⇅]	[↑][↑][ ][ ][ ]	[⇅]
23	V	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^3\ 4s^2$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][⇅]	[↑][↑][↑][ ][ ]	[⇅]
㉔	Cr	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^5\ 4s^1$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][⇅]	[↑][↑][↑][↑][↑]	[↑]
25	Mn	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^5\ 4s^2$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][⇅]	[↑][↑][↑][↑][↑]	[⇅]
26	Fe	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^6\ 4s^2$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][⇅]	[⇅][↑][↑][↑][↑]	[⇅]
27	Co	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^7\ 4s^2$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][⇅]	[⇅][⇅][↑][↑][↑]	[⇅]
28	Ni	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^8\ 4s^2$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][⇅]	[⇅][⇅][⇅][↑][↑]	[⇅]
㉙	Cu	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^1$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][⇅]	[⇅][⇅][⇅][⇅][⇅]	[↑]
30	Zn	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2$	[⇅]	[⇅]	[⇅][⇅][⇅]	[⇅]	[⇅][⇅][⇅]	[⇅][⇅][⇅][⇅][⇅]	[⇅]

1	H	$1s^1$
2	He	$1s^2$
3	Li	$[He]2s^1$
4	Be	$[He]2s^2$
5	B	$[He]2s^22p^1$
6	C	$[He]2s^22p^2$
7	N	$[He]2s^22p^3$
8	O	$[He]2s^22p^4$
9	F	$[He]2s^22p^5$
10	Ne	$[He]2s^22p^6$
11	Na	$[Ne]3s^1$
12	Mg	$[Ne]3s^2$
13	Al	$[Ne]3s^23p^1$
14	Si	$[Ne]3s^23p^2$
15	P	$[Ne]3s^23p^3$
16	S	$[Ne]3s^23p^4$
17	Cl	$[Ne]3s^23p^5$
18	Ar	$[Ne]3s^23p^6$
19	K	$[Ar]4s^1$
20	Ca	$[Ar]4s^2$

	21	Sc	$[Ar]3d^14s^2$
	22	Ti	$[Ar]3d^24s^2$
	23	V	$[Ar]3d^34s^2$
●	24	Cr	$[Ar]3d^54s^1$
	25	Mn	$[Ar]3d^54s^2$
	26	Fe	$[Ar]3d^64s^2$
	27	Co	$[Ar]3d^74s^2$
	28	Ni	$[Ar]3d^84s^2$
●	29	Cu	$[Ar]3d^{10}4s^1$
	30	Zn	$[Ar]3d^{10}4s^2$
	31	Ga	$[Ar]3d^{10}4s^24p^1$
	32	Ge	$[Ar]3d^{10}4s^24p^2$
	33	As	$[Ar]3d^{10}4s^24p^3$
	34	Se	$[Ar]3d^{10}4s^24p^4$
	35	Br	$[Ar]3d^{10}4s^24p^5$
	36	Kr	$[Ar]3d^{10}4s^24p^6$
	37	Rb	$[Kr]5s^1$
	38	Sr	$[Kr]5s^2$
	39	Y	$[Kr]4d^15s^2$
	40	Zr	$[Kr]4d^15s^2$

- Exceptions

●	41	Nb	$[Kr]4d^4 5s^1$	
●	42	Mo	$[Kr]4d^5 5s^1$	
●	43	Tc	$[Kr]4d^5 5s^2$	or $[Kr]4d^6 5s^1$
●	44	Ru	$[Kr]4d^7 5s^1$	
●	45	Rh	$[Kr]4d^8 5s^1$	
●	46	Pd	$[Kr]4d^{10}$	
●	47	Ag	$[Kr]4d^{10} 5s^1$	
	48	Cd	$[Kr]4d^{10} 5s^2$	
	49	In	$[Kr]4d^{10} 5s^2 5p^1$	
	50	Sn	$[Kr]4d^{10} 5s^2 5p^2$	
	51	Sb	$[Kr]4d^{10} 5s^2 5p^3$	
	52	Te	$[Kr]4d^{10} 5s^2 5p^4$	
	53	I	$[Kr]4d^{10} 5s^2 5p^5$	
	54	Xe	$[Kr]4d^{10} 5s^2 5p^6$	
	55	Cs	$[Xe]6s^1$	
	56	Ba	$[Xe]6s^2$	
●	57	La	$[Xe]5d^1 6s^2$	
●	58	Ce	$[Xe]4f^1 5d^1 6s^2$	
	59	Pr	$[Xe]4f^3 6s^2$	
	60	Nd	$[Xe]4f^4 6s^2$	
	61	Pm	$[Xe]4f^5 6s^2$	
	62	Sm	$[Xe]4f^6 6s^2$	
	63	Eu	$[Xe]4f^7 6s^2$	
●	64	Gd	$[Xe]4f^7 5d^1 6s^2$	
	65	Tb	$[Xe]4f^9 6s^2$	
	66	Dy	$[Xe]4f^{10} 6s^2$	
	67	Ho	$[Xe]4f^{11} 6s^2$	
	68	Er	$[Xe]4f^{12} 6s^2$	
	69	Tm	$[Xe]4f^{13} 6s^2$	
	70	Yb	$[Xe]4f^{14} 6s^2$	
	71	Lu	$[Xe]4f^{14} 5d^1 6s^2$	
	72	Hf	$[Xe]4f^{14} 5d^2 6s^2$	

	73	Ta	$[Xe]4f^{14} 5d^3 6s^2$	
	74	W	$[Xe]4f^{14} 5d^4 6s^2$	
	75	Re	$[Xe]4f^{14} 5d^5 6s^2$	
	76	Os	$[Xe]4f^{14} 5d^6 6s^2$	
	77	Ir	$[Xe]4f^{14} 5d^7 6s^2$	
●	78	Pt	$[Xe]4f^{14} 5d^9 6s^1$	
●	79	Au	$[Xe]4f^{14} 5d^{10} 6s^1$	
	80	Hg	$[Xe]4f^{14} 5d^{10} 6s^2$	
	81	Tl	$[Xe]4f^{14} 5d^{10} 6s^2 6p^1$	
	82	Pb	$[Xe]4f^{14} 5d^{10} 6s^2 6p^2$	
	83	Bi	$[Xe]4f^{14} 5d^{10} 6s^2 6p^3$	
	84	Po	$[Xe]4f^{14} 5d^{10} 6s^2 6p^4$	
	85	At	$[Xe]4f^{14} 5d^{10} 6s^2 6p^5$	
	86	Rn	$[Xe]4f^{14} 5d^{10} 6s^2 6p^6$	
	87	Fr	$[Rn]7s^1$	
	88	Ra	$[Rn]7s^2$	
●	89	Ac	$[Rn]6d^1 7s^2$	
●	90	Th	$[Rn]6d^2 7s^2$	
●	91	Pa	$[Rn]5f^2 6d^1 7s^2$	
●	92	U	$[Rn]5f^3 6d^1 7s^2$	
●	93	Np	$[Rn]5f^4 6d^1 7s^2$	
	94	Pu	$[Rn]5f^6 7s^2$	
	95	Am	$[Rn]5f^7 7s^2$	
●	96	Cm	$[Rn]5f^7 6d^1 7s^2$	
	97	Bk	$[Rn]5f^9 7s^2$	or $[Rn]\ 5f^8 6d^1 7s^2$
	98	Cf	$[Rn]5f^{10} 7s^2$	
	99	Es	$[Rn]5f^{11} 7s^2$	
	100	Fm	$[Rn]5f^{12} 7s^2$	
	101	Md	$[Rn]5f^{13} 7s^2$	
	102	No	$[Rn]5f^{14} 7s^2$	
●	103	Lr	$[Rn]5f^{14} 6d^1 7s^2$	

● Exceptions

- Stability of completely filled and half filled subshells :→

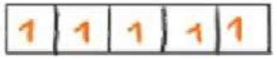
- The stability of completely filled and half filled subshells is due to following reasons.

① symmtrical distribution of electrons:→

- The completely filled and half filled subshell have symmtrical distribution of of electrons i.e these are symmtrical and hence are more stable

symmetry $\propto$ stability

- **Example:-**

	p-subshell			d-subshell	
p^2		unsymmetrical → less stable	d^4		unsymmetrical → less stable
p^3		symmetrical → more stable	d^5		symmetrical → more stable
p^5		unsymmetrical → less stable	d^9		unsymmetrical → less stable
p^6		symmetrical → more stable	d^{10}		symmetrical → more stable

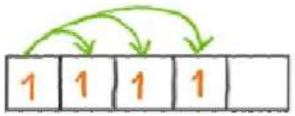
② Exchange energy:→

- The two or more electrons with the same spin in the degenerate orbitals of a subshell tend to exchange their position and the energy released due to this exchange is called exchange energy.

No. of exchange ∝ exchange energy ∝ stability of subshell

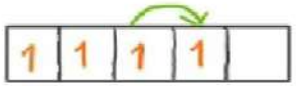
- Half filled and completely filled subshells have more no. of exchange. As a the exchange energy is maximum and so is the stability.

- Example:- d^4 Configuration



3 exchange by e^- 1

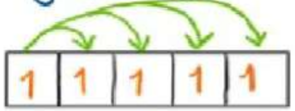
2 exchange by e^- 2



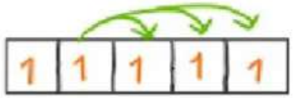
1 exchange by e^- 3

Total exchange = 3 + 2 + 1 = 6

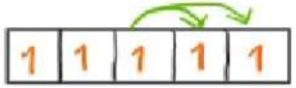
- d^5 configuration



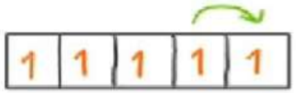
4 exchange by e^- 1



3 exchange by e^- 2



2 exchange by e^- 3



1 exchange by 4 e^-

Total exchange = 4 + 3 + 2 + 1 = 10

– The exchange energy in terms of K can be calculated by the following formula –
(Value of K depends on the atom or ion)

$$\boxed{\text{Exchange energy} = \sum \frac{N(N-1)}{2} K}$$

here N = no. of electrons with parallel spin

– <u>Example</u>:–

$d^9 \rightarrow \boxed{\uparrow\downarrow \mid \uparrow\downarrow \mid \uparrow\downarrow \mid \uparrow\downarrow \mid \uparrow\ }$

for clockewise e^- N = 5

for anticlockwise e^- = N = 4

$$E.E. = \frac{N(N-1)}{2} + \frac{N(N-1)}{2}$$

$$= \frac{5(5-1)}{2} + \frac{4(4-1)}{2}$$

$$= 10 + 6$$

$$E.E. = 16K$$

$d^{10} \rightarrow \boxed{\uparrow\downarrow \mid \uparrow\downarrow \mid \uparrow\downarrow \mid \uparrow\downarrow \mid \uparrow\downarrow}$

for clockwise e^- N = 5

for anticlockwise e^- N = 5

$$E.E. = \frac{N(N-1)}{2} + \frac{N(N-1)}{2}$$

$$= \frac{5(5-1)}{2} + \frac{5(5-1)}{2}$$

$$= 10 + 10$$

$$E.E. = 20K$$

Example $_{24}Cr = [Ar]\,3d^5\,4s^1$

$3d^4\,4s^2$

3d	1	1	1	1	

– unsymmetrical

$N = 4$

$$E.E. = \frac{N(N-1)}{2}K$$

$$= \frac{4(4-1)}{2}$$

$$= 6K$$

$3d^5\;4s^1$

3d	1	1	1	1	1

– symmetrical

$N = 5$

$$E.E. = \frac{N(N-1)}{2}K$$

$$= \frac{5(5-1)}{2}$$

$$= 10K$$

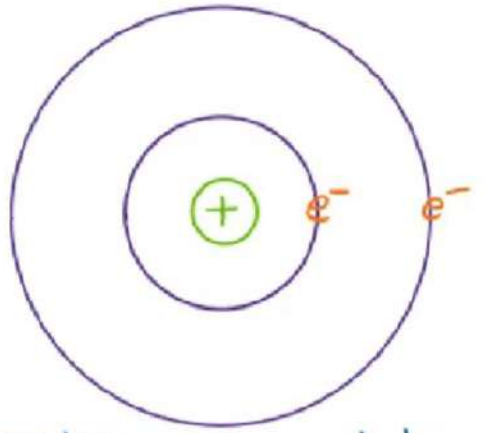
→ Effective Nuclear charge (Z_{eff}):→

- Nuclear charge (z):→

- The charge present on nucleus of an atom is called nuclear charge. it is due to presence of protons.
- Nuclear charge is equal to atomic no. of an atom.

- Shielding effect or screening effect:→

- The valence shell e^- experience less attraction from the Nucleus due to the presence of inner shell electrons. This effect is called shielding or screening effect



- Effective Nuclear charge (Z_{eff}):→

- Valence electrons experience less attraction from nucleus (nucleus charge) due to shielding effect of inner electrons. This decreased nuclear charge is called effective nuclear charge and is represented by Z_{eff}.
- It is given by the relation -

$$\boxed{Z_{eff} = Z - \sigma}$$

here Z = nuclear charge

σ = screening constant

- Screening constant is measure of screening effect or shielding effect.
- Effective nuclear charge is defined as the actual nuclear charge, Z minus the screening effect caused by the electrons (called intervening e-) lie between nucleus and outer electrons.
- No. of intervening e- $\propto$ magnitude of σ $\propto$ $\frac{1}{\text{magnitude of } Z_{eff}}$

- Calculation of σ and Z_{eff} by Slater's Rule :→

- Rules :-

① Write down the comple electronic configuration of the element and divide the e- into the following orbital groups starting from inside of the atom.
(1s); (2s,2p); (3s,3p); (3d); (4s,4p); (4d); (4f); (5s,5p); (6s,6p) etc.

② Now select the electron for which value of σ is to be calculated. for this calculation, add up the contributions to σ for other electrons according to following rules.

	Type of e^-	Contribution to σ for each e^-
1	All e^- in groups out side the e^- selected	0
2.	All e^- belong to same group of selected e^-	0.35 (0.30 for 1s e^-)
3.	All e^- in shell immediately inside	0.85
4	All e^- further inside	1.00

Example :- Calculate the Z_{eff} experienced by the 4s e^- in potassium atom.

Electronic confi. of $K = 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$

$K = (1s^2);(2s^2\ 2p^6);(3s^2\ 3p^6);(4s^1) \rightarrow$ total 4 shells

$\sigma = [(0.85 \times \text{no. of } e^- \text{ in 3rd shell}) + (1.00 \times \text{no. of } e^- \text{ in inner shell})]$

$\sigma = [(0.85 \times 8) + (1.00 \times 10)]$

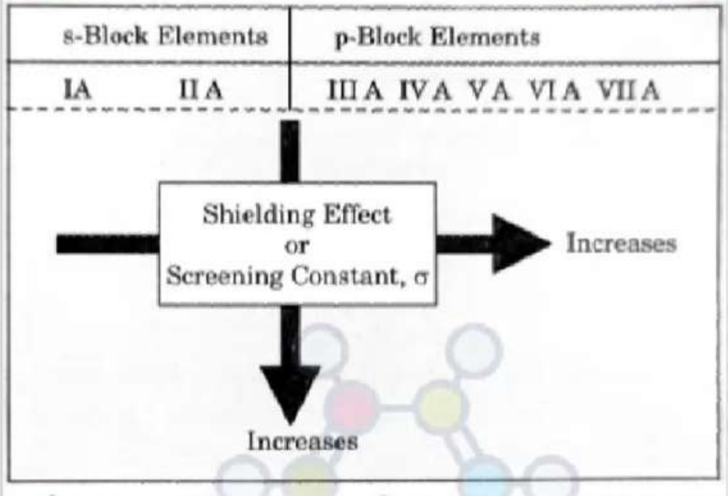
$\sigma = 16.8$

$Z_{eff} = Z - \sigma$

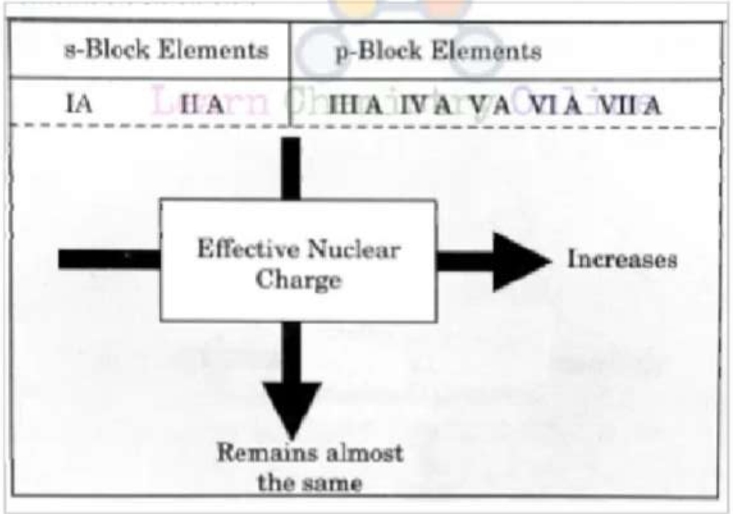
$= 19 - 16.8$

$Z_{eff} = 2.2$

→ Variation of screening effect or σ in the periodic table :→



→ Variation of Effective nuclear charge in the periodic table :→



→ Applications of Effective Nuclear charge :→

① 4s orbital is filled before 3d orbitals :-

- e^- in 4s experienced more Z_{eff} than in 3d.

② 4s e^- are removed before 3d e^- in the conversion of 3d transition metal in to cation:-

- Z_{eff} acting on one of the 4s e^- is less than one of the 3d e^-

③ The succesive ionisation potential of an atom.

$$I.P._1 < I.P._2 < I.P._3 \cdots$$

④ Decrease in atomic and ionic radius of s and p-block elements from left to right in a period.

⑤ A cation is smaller than its parent atom.

⑥ An anion is larger than its parent atom.