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MDCAT

ATOMIC STRUCTURE

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- 1) Atom discovery:- Democritus suggested that there is no other particle smaller than atom that can not be further divided.
- 2) Postulates of John Dalton :-
 - 1) Atom is smallest, indivisible particle.
 - 2) It can not be created nor destroyed but can change its form.
 - 3) Atoms undergo chemical combination to form molecules ; but as a whole, molecule is smallest identity that exists independently.
 - 4) Atoms have same mass, size, properties etc if they're of element.
- 3) Electron discovery:- JJ Thomson discovered electron.
 - 1) It was discovered due to discharge tube experiment based on cathod ray.
 - 2) The glass tube had 2 electrodes (+ve) and (-ve). The particle emitted from electron gun deflected and bent toward (+ve) side.
 - 3) This means that electrons have negative nature and so are attracted towards +ve anode.
- 4) Postulates of JJ Thomson :-
 - 1) Atom is divisible in sub-atomic particles.
 - 2) Atoms do differ in mass in case of isotopes, and do have different properties.
- 5) Neil Bohr discovery:- Neil Bohr's atomic model further classified the atomic picture.
- 6) Postulates of Neil Bohr :-
 - 1) His model was first approach to quantized energy levels or electronic shells with fixed energy.

(Point 5-7) Or 2(i). ∴ Quanta = Packets of energy

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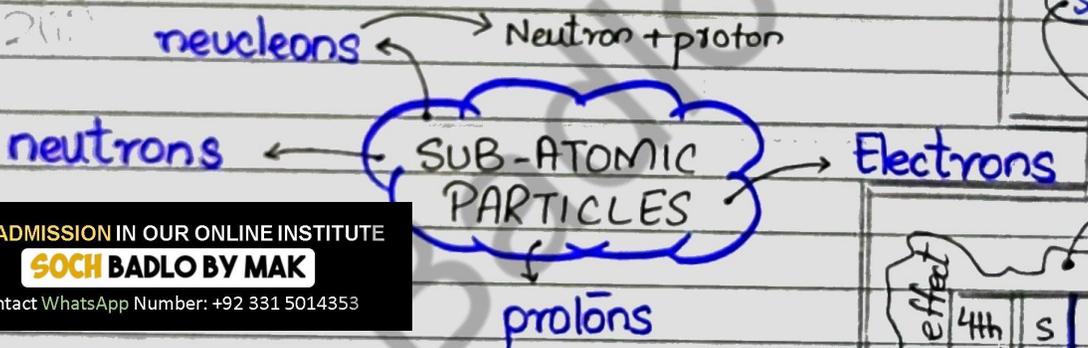
- 2) He calculated the radius of H-atom. (roughly 10^{-10})
- 3) energy of electrons in H-atoms.
- 4) The emission of spectrum was explained.
- 5) Defects of Bohr's theory:-

When high resolution spectrophotometer were made, fine spectrum originated with splitted spectral lines. These lines were splitting in electric/magnetic field giving Stark & Zemen effect.

1) Contribution of Heisenberg:-

- 1) He described or formulated the principle of uncertainty; "It is not possible to know certain properties of sub-atomic particles like position & speed simultaneously."
- 2) He gave rise to concepts of subshells/orbitals.

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Splitting in Elec. F
Stark effect

Splitting in magnt. f
Zemen effect

Zemen effect	4 th	s	p	d	f
	3 rd	s	p	d	
	2 nd	s	p		
	1 st	s	p		

1} ELECTRONS :-

- Discovery :- JJ Thomson
- Nature :- Negative
- Charge :- $-1.6022 \times 10^{-19} C$
- Location :- Shells of atom
- Deflection in Ef :- Deflect towards +ve pole.
- Mass :- $9.1095 \times 10^{-31} kg$.

Relative Charge :- -1

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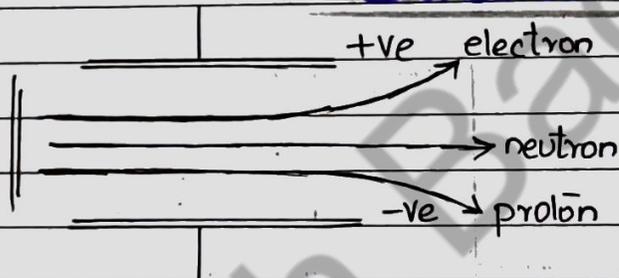
PROTON:-

- Discovery Goldstein
- Nature Positive
- Charge $+1.6622 \times 10^{-19} \text{ C}$ → Relative charge. +1.
- Location In nucleus
- Deflection Towards -ve pole.
- Mass $1.6727 \times 10^{-27} \text{ kg}$ (1836x more than e^-).

NEUTRON:-

- Discovery Chadwick
- Nature Neutral
- Charge No charge
- Mass $1.6750 \times 10^{-27} \text{ kg}$.
- Location In nucleus
- Deflection No deflection
- Relative charge No charge

→ Behaviour in electric field



- -ve electron → +ve pole
- +ve proton → -ve pole
- (±) neutron → No deflection
- Share same velocity
- Divergence depend on velocity

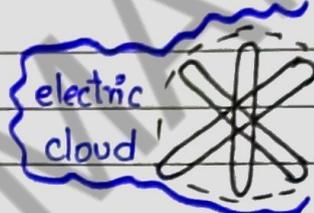
→ Atomic CHARACTERISTICS

- Atomic no.
 - No. of protons
 - (Z) proton = electrons
 - $N^+ = 7$ atomic no.
- Mass no.
 - No. of nucleons (neutrons + protons)
 - (A) → $P + N = A$
- anion = -ve = gain e^-
 - $e^- \text{ no.} = \text{atomic no.} + \text{charge}$
 - $\text{Cl}^- = 17 + 1 = 18$
- cation = + = lose e^-
 - exp :- Ca^{+2}
 - $e^- \text{ no.} = \text{Atomic no.} - \text{charge}$
 - $20 - 2 = 18$

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ATOMIC RADIUS

Definition :- The average distance of nucleus from outermost valence electron is radius of an atom.

TREND	REASON (Main group)	Diagram
Periodic Trend L → R	{Decrease} It decreases as the nuclear charge increases; thus; No. of electrons in valence shell increase which results in increase force of attraction by nucleus on valence e ⁻ causing size to shrink.	electric cloud 

Group Trend ↓ B	{Increases} It increases as the no. of shells increases and increase in shielding effect.
-----------------------	---

TRANSITIONAL METALS :-

TREND	REASON	Atomic S	Period	Group
Periodic Trend L → R	Decrease to {Increase} electrons are in d-group. Initial behaviour of elements shows decrease in atomic radii. Then it becomes constant for few. Eg in last it increases. Decrease → Greater force of attraction b/w nucleus & e ^s . Increase → electrons repel each other.	Main G.	Dec	Inc.
Group Trend ↓ B	In group trend it {Increase} as no. of shells increases and shielding effect increases.	Transition	Dec → Inc	Inc.

Group Trend ↓ B	In group trend it {Increase} as no. of shells increases and shielding effect increases.
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IONIC RADIUS :- Ion \rightarrow Gain/Lose of electrons.

- 1) Cation: (+ve) Lose electrons and is of smaller size than parent.
- 2) Anion: (-ve) Gain electron and is greater size than parent atom.
 \rightarrow Trends are same as of main group elements. Qs 2(v)

QUANTUM NUMBERS -

[Short / Long imp]

Qs 2(vii) (Q 3)

1) Brief Introduction :-

- Set of 4 numbers to explain behaviour of electrons are Q.N.
- By :- Schrodinger equation of wave.
- To :- Used to determine location, shell, sub-shell, energy, rotation, size, distance from nucleus, shape, of electron of atom.
- Numbers = 4.

PRINCIPLE QUANTUM NUMBERS :- (n)

1) Importance :-

- \rightarrow It express Bohr's shells in quantum form.
- \rightarrow Depicts period no. in periodic table.
- \rightarrow Atomic size (Greater the value of "n" greater the size).
- \rightarrow Nature of shell (K, L, M, N ...)
- \rightarrow Energy of shell ($E = n + 1$).
- $\rightarrow n \neq 0$ $\rightarrow n = 1, 2, 3, \dots$
- \rightarrow To predict no. of $e^- \rightarrow 2n^2$.
- $\rightarrow n$ is always +ve.
- \rightarrow Maximum no. of sub shells in $n \rightarrow n^2$.

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n	Energy level	Shell	Sub Shell	No. of $e^- = 2n^2$
1	1st E.L	K	s	$2(1)^2 = 2e^-$
2	2 nd E.L	L	s p	$2(2)^2 = 8e^-$
3	3 rd E.L	M	s p d	$2(3)^2 = 18e^-$
4	4 th E.L	N	s p d f	$2(4)^2 = 32e^-$

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AZIMUTHAL QUANTUM NUMBERS :-

Denoted by 'l'

1) Importance :-

- Tells us about e^- 's subshell.
- Shape of orbital (place where max e^- can be found)
- One shell may have more than one sub-shells.
- It determine angular momentum of e^- .
- $l = 0, 1, 2, 3 \dots$
- $l = n - 1$.
- To find no. of e^- in sub-shell $\rightarrow 2(2l + 1)$.
- Sub-shells cause fine spectral lines in spectrum.
- position of e^- (s, p, d, f) blocks in table.

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$l = n - 1$	Subshell	Shape of Subshell	e^- in subshell
$l = 1 - 1 = 0$	s (sharp)	spherical 	$2(2l + 1)s \rightarrow 2e^-$
$l = 2 - 1 = 1$	p (principle)	dumbbell  <small>psiclon</small>	$2(2(1) + 1) \rightarrow 6e^-$
$l = 3 - 1 = 2$	d (diffused)	double dumbbell 	$2(2(2) + 1) \rightarrow 10e^-$
$l = 4 - 1 = 3$	f (fundamental)	Complex 3D	$2(2 \times 3 + 1) \rightarrow 14e^-$

MAGNETIC QUANTUM NO. :- (m)

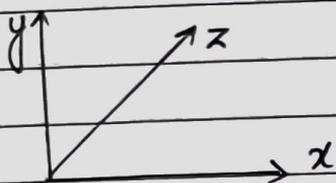
$s = 0 \quad p = 1$
 $d = 2 \quad f = 3$

1) Importance :-

- Zeeman effect (fine spectral lines into influence of magnetic field) can be explained by MQN.
- It is orientation quantum no.
- m could be from negative integers to "0" to positive integers.
- It shows deflection of e^- in subshells in different directional axis.
- Direction in degenerate orbit = Orb having space.
- Deflection in different direction with same energy.

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l	Subshell	Degenerate Orbit $2l + 1 = m$	m values	Degenerate Orbit detail directions.
0	s	$2(0) + 1 = 1$	0	s
1	p	$2(1) + 1 = 3$	-1 0 1	$P_x P_z P_y$
2	d	$2(2) + 1 = 5$	-2 -1 0 1 2	$d_{xy}, d_{xz}, d_{yz}, d_{x^2-y^2}, d_{z^2}$
3	f	$2(3) + 1 = 7$	-3 -2 -1 0 1 2 3	-



$P_x = -1$ $P_z = 0$ $P_y = 1$
 $d_{xy} = -2$ $d_{xz} = -1$ $d_{yz} = 0$ $d_{x^2-y^2} = 1$ $d_{z^2} = 2$
 $s = 0$

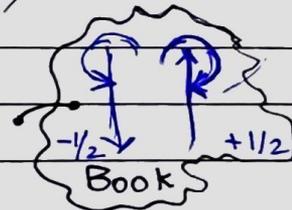
SPIN QUANTUM NUMBERS:- (s)

1) Importance:- (GoudSmith)

- Indicates angular momentum of e^- .
- Possible values of $s = +1/2, -1/2$.
- Spin of e^- in magnetic field.
- Always oppose in direction thus;

(↑) anticlockwise → $-1/2$

(↓) clockwise = $+1/2$

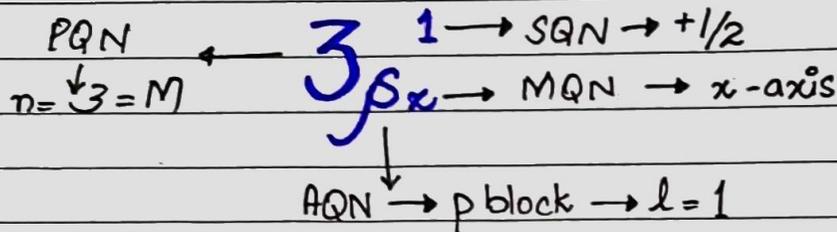


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- e^- s in one orbitals (d_{xy}, P_z, P_x etc...) have opposite spins.
- Called as Self-rotation.

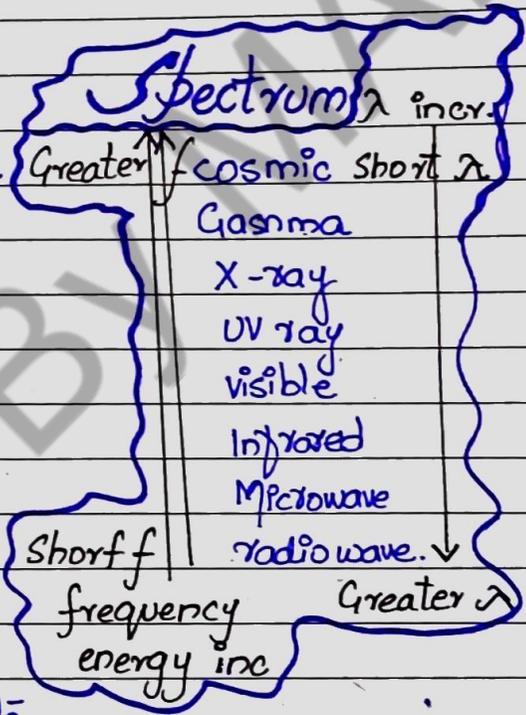
Shell	Subshell	SON	No. of e^- in SHELL
K	s	$+1/2 \quad -1/2$	$2e^-$
L	s	$+1/2 \quad -1/2$	$2e^-$
	p	$P_x = +1/2 \quad P_y = +1/2 \quad P_z = +1/2$	$6e^-$
M	s	$+1/2 \quad -1/2$	$2e^-$
	p	$P_x = +1/2 \quad P_y = +1/2 \quad P_z = +1/2$	$6e^-$
	d	$d_{xy} = +1/2 \quad d_{xz} = +1/2 \quad d_{yz} = +1/2 \quad d_{z^2} = +1/2$ $d_{x^2-y^2} = +1/2$	$10e^-$

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Spectrum :- Range of diff $\lambda/f/E$.

- From higher to lower shell → e^- emits energy.
- From lower to higher shell → e^- absorbs.
- No. of spectral lines \propto shell numbers.
- e^- occupy quantized energy levels.



Visible Spectrum

Continuous

- No marks
- No boundaries
- Colors are mixed
- Can't be distinguish

Line

- Marks
- Boundaries
- Colors are separate
- Can be distinguish

Atomic emission
(emission spectrum)

Atomic absorption.
(Absorption spectrum).

Line Spectrum Analysis.

→ each element has its own emission spectrum (E_{conf} is ^{also} specific).

E. Configuration Deduction.

→ No. of lines on spectrum determines no. of shells.

Spectral Series :- {LBPBP}

- 1) Lyman
- 2) Balmer
- 3) Paschen
- 4) Brackett
- 5) P. fund

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	UV Rays	UV Rays	Infra Red	Bracket IR	Infra Red
$n=7$	-----				
$n=6$	-----				
$n=5$	-----				
$n=4$	-----				
$n=3$	-----				
$n=2$	-----				
$n=1$	-----				
	Lyman	Balmer	Paschen	Bracket	Pfund

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"Rules for E. configurations" (Q 5)

E. Configuration: - Arrangements of electrons around the nucleus.

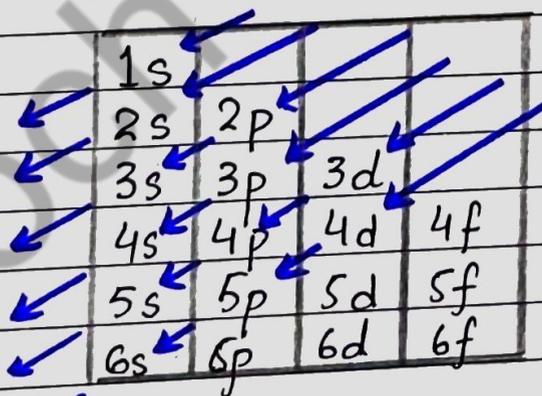
1) Rule Auf Bau Principle -

"The electrons are filled in

Arrangement
↓
increasing energy

the orbitals of lowest energy sequence OR

Electrons are distributed in sub-shells in order of increasing energy. firstly, low energy orbitals are filled then higher ones.



→ Auf Bau Rule :-

∴ 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s.

s=2 p=6
d=10 f=14

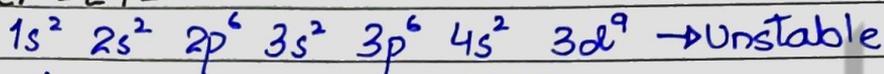
→ Example :-

Mg = 12 $1s^2, 2s^2, 2p^6, 3s^2$.

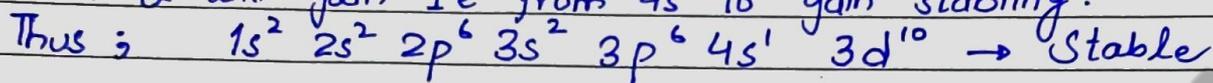
Exceptional 3 elements They are stable (fully filled) > half filled
& unstable at partial fillings. (1 2 3 4 6 7 8 9)

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Usual conf of Copper = $29 =$



Now d will gain $1e^-$ from 4s to gain stability.



2) Rule for energy = $n+l$ Or 2 (ix)

"It states higher the value of $n+l$ the higher the energy will be."

OR
"Orbital having least value of $n+l$ will be filled first."

example :- 1) $5s \rightarrow n=5 \quad l=0$

$$E = 5 = n+l = 5+0$$

2) $4p \rightarrow n=4 \quad p=1 \rightarrow n+l = 4+1 = 5 \rightarrow E=5$

3) $2p \rightarrow n=2 \quad p=1 \rightarrow n+l = 2+1 = 3 \rightarrow E=3$

NOTE: In case of some energy like $5s$ & $4p = 5$ then lower "n" will be filled first like "4p".

3) Pauli Exclusion Rule :-

It states :- that in an atom no two electrons can have same set of quantum no. at least / must be their spin no. will be different.



$e_1 = n=1 \quad \longleftrightarrow \quad e_2 = n=1$

$l=s=0 \quad \longleftrightarrow \quad l=s=0$

$m=0 \quad \longleftrightarrow \quad m=0$

$s = +1/2 \quad \leftarrow \text{Different} \rightarrow \quad s = -1/2$

spinning / opposite

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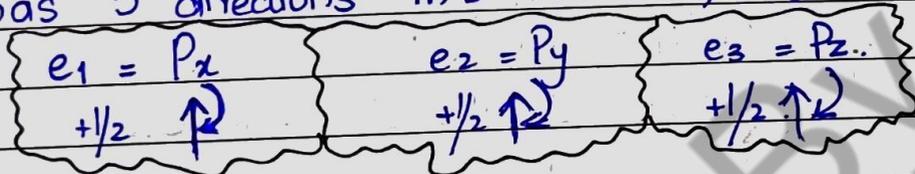
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4) Hund's Rule :-

Statements :- If the orbitals are available to be filled then e^- will occupy each orbital single rather than pairing up with any other e^- . Thus, their spin will be same as paired e^- have opposite spin but single electrons may have same directional spin.

example :- $1s^2 2s^2 2p^3 = p = 3e^-$.

→ P has 3 directions $m = -1, 0, 1$; thus P_x, P_y, P_z .



DETERMINATIONS

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- E.C of neutral atom = Atomic No. $Z(N) \rightarrow 1s^2 2s^2 2p^3$.
- E.C of positive anion = Atomic no. $Z(N) \rightarrow (N)^{-3} \rightarrow (1s^2 2s^2 2p^6)^+$
(Add in valence shell)
- E.C of cation = Atomic no. $Z(N) \rightarrow (Na)^{+1} \rightarrow (1s^2 2s^2 2p^6)^+$
(Remove from valence shell).

- Repulsion force of e^- :- e^- will exert force of repulsion as are of same charges placed in same orbital. When their orbitals will be changed then repulsion will be minimum.
- Orbital energy :- orbitals of low energy are filled first.
The nucleus exerts more energy on e^- near/close to it.
- Spin repulsion :- e^- having same spin, will repel each other. overcome this either Hund's rule is used or e^- of opposite are placed together.

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SHAPE OF ORBITALS :-

Orbital :- The region in space where the probability of finding an electron is maximum.

Node / Nodal plane :- The region in space where the probability of finding electron is minimum / zero.

1) S-orbital :-

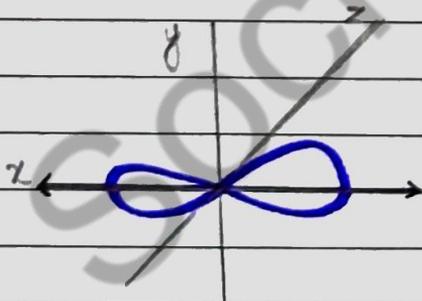
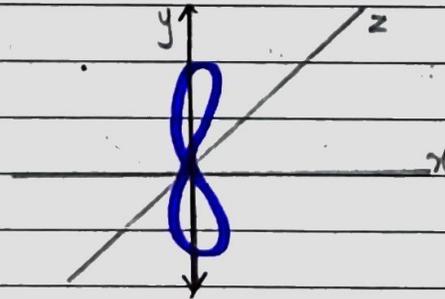
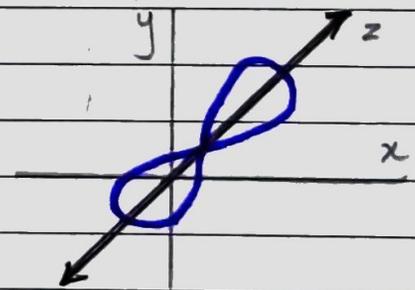


- Maximum electrons = $2e^-$.
- It has 3D spherical shape (tennis ball).
- The size of s-orbital increases as value of n increases.
 $1s < 2s < 3s < \dots n$.
- It doesn't deflect in magnetic field as $m = 2(l) + 1 = 1$.
- Thus $m=0$ only (value of $m=0$) (directional $m=1$).

2) P-orbital :-

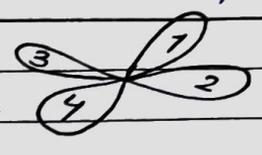


- It can have maximum $6e^-$.
- It has 2 lobes.
- Its shape is dumbbell like.
- It shows 3 directional deflection in magnetic field.
 $m = 2(1) + 1 = 3 \rightarrow +1, 0, -1$ (P_x, P_y, P_z)
- The dumbbell of axis will be drawn on its own axis.

 P_x  P_y  P_z

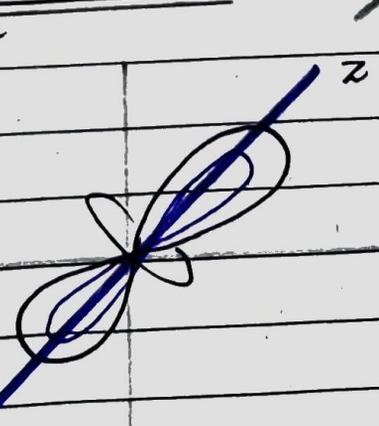
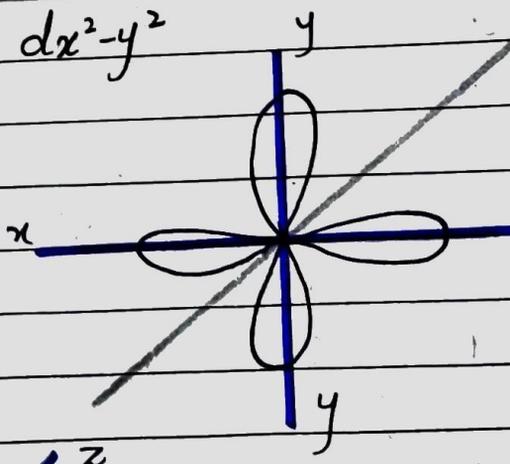
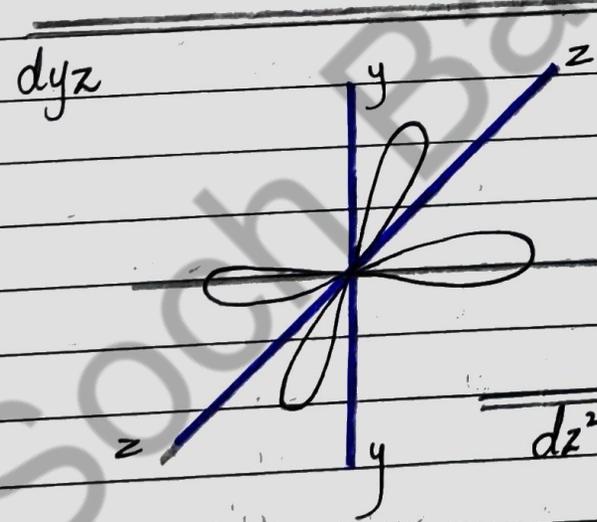
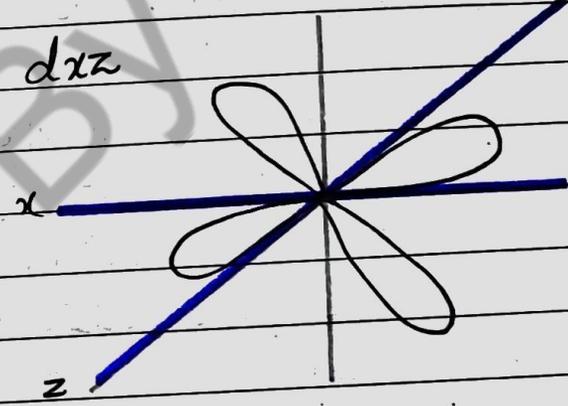
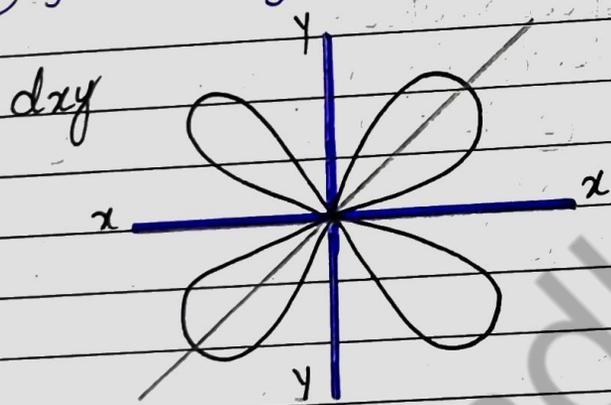
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3) d-Orbital:-

- ① It can have $10e^-$.
- ② It's shape is like double dumbbell, sausage, session, clover leaf.
- ③ It has 4 lobes.
- ④ It's deflection is in 5 different direction ;
 $m = 2(2) + 1 = 5 = -2, -1, 0, 1, 2$; $d_{xy}, d_{xz}, d_{yz}, d_{x^2-y^2}, d_{z^2}$
- ⑤ The shape will be drawn in blw of 2-axis (at inter)
- ⑥ If there is n^2 then shape will be drawn twice on
- ⑦ for $d_{x^2-y^2}$ the shape will be on the axis.



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4) f-Orbital :-

- ① It can have maximum $14e^-$
- ② It can deflect into 7 directions,
 $m = 2(3) + 1 = 7$.
- ③ It has complicated complex shape.

④) ⇒ MASS SPECTROMETRY

Mass Spectrometer :- Instrument used to measure exact mass isotopes and their relative abundance is mass spectrometer.

Technique mass spectrometry :- Technique in which mass spectrometer is used to determine, ① Isotopes ② Abundance of Isotopes %
③ Relative atomic mass ④ Molecular mass. ⑤ Molecular structure

Types :- ① Aston ② Dempster (solid).

Principle :- To find m/e ratio ;

Sample → Vapour → Ion → EF → MF → m/e .

Isotopes of an element are separated on the basis of their mass to charge m/e ratio & record in form of peaks on graph.

WORKING :-

a) Vapourization :- Substance to analyze is converted into vapour state by application of $10^{-6} - 10^{-7}$ torr pressure.

b) Ionization :- High energy electrons (EI) at ionizing source will change gaseous vapours into +ve gaseous ions.

c) Electric field effect :- High voltages are applied to +ve gaseous ions (500-2000 V) which will accelerate them.

d) Magnetic field effect :- The accelerated ions are directed mass analyzer by deflection due to magnetic field effect.

- It separates ions based on m/e ratio.

- $m/e = \frac{H^2 r}{E}$ $r = \text{radius}$ $E = \text{Strength of EF.}$
 $H = \text{Strength of MF}$

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e) Detection:- Ion collector / electrometer / detector ; records the time taken by each ion to reach for calculation of m/e .

→ Ion having definite m/e are collected in ion collector.

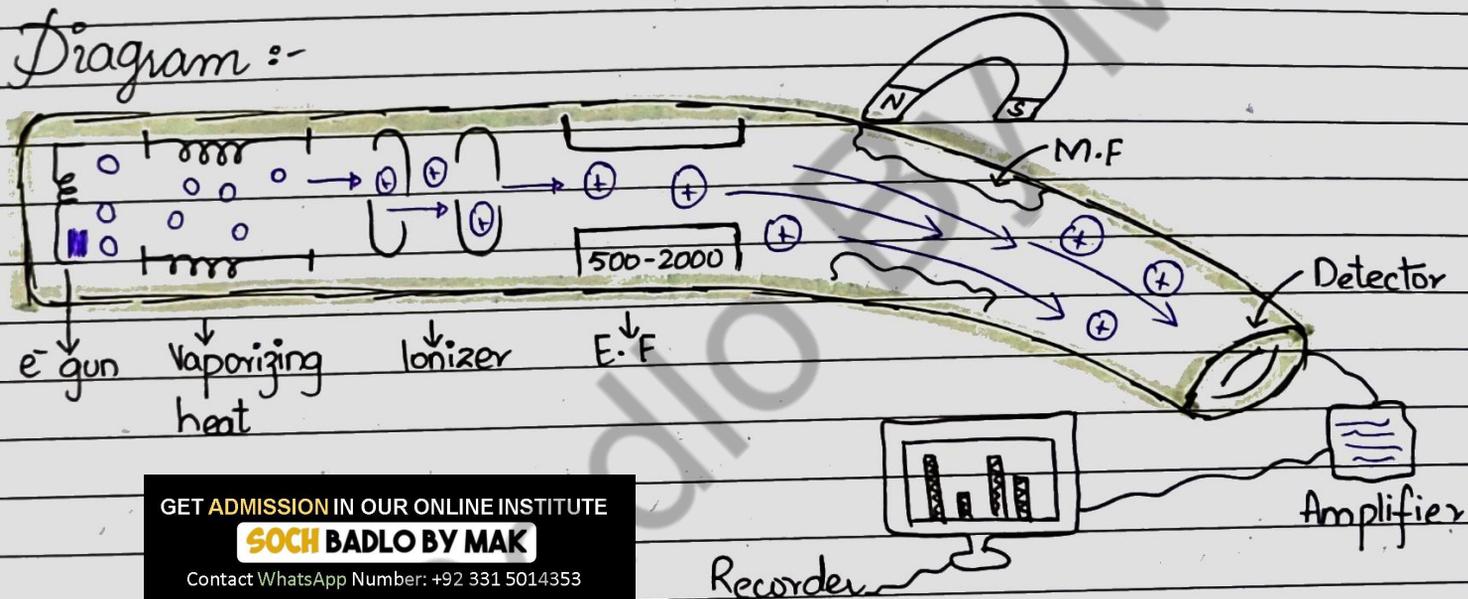
→ It produces different values of current.

→ Heavy ions have more current value & high peak.

f) Amplifier:- It increases current to put it in graph and record it.

g) Recorder:- It record & illustrate graph.

Diagram :-



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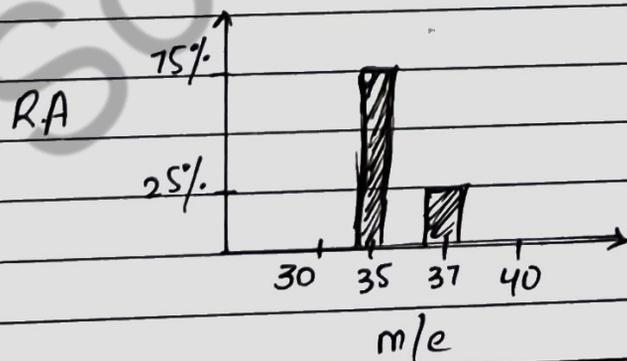
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GRAPH :-

The graph is plotted between m/e at x -axis (abscissa) and relative abundance at y -axis (ordinate).

for chlorine :-



Info :

Isotopes = 2

Iso 1 = 35 - 75%

Iso 2 = 37 - 25%

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Formula for numericals:-

$$\text{Avg. atomic mass} = \frac{(\text{Mass no.} \times \text{Na}) + (\text{Mass no.} \times \text{Na})}{100}$$

Na = natural abundance.

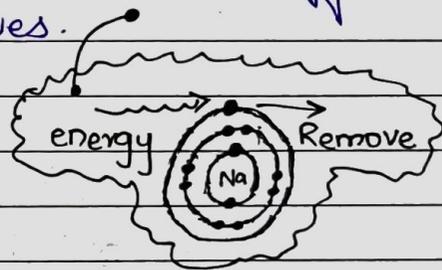
$$\begin{aligned} \text{Avg A of Cl}^- &= (35 \times 75) + (37 \times 25) / 100 \\ &= 35.5 \text{ amu.} \end{aligned}$$

→ IONIZATION ENERGY (Qs 6)

Definition:-

The minimum energy needed to remove the outermost electron from gaseous isolated atom.

Gaseous Compulsion:- Gaseous state compulsion is due to nature of solid & liquid of transfer of energy. Thus, when the energy will given they will distribute among themselves.



TRENDS

REASON

Group ↓ decrease; Along group it decreases due to increase in shielding effect as it becomes difficult for nucleus to hold on valence electrons, and less energy is needed.

Period. ↑ increases; Along period it increases as the nuclear charge increases and force effect increase that holds electrons tightly. Atomic size decrease Thus more energy is needed to remove electrons.

Dated: _____

Exception in periodic trend:- As the group 3A along period occupy energy of (np^1) and losing one electron is easier thus ionization energy decreases.

(2) As the group VA along period occupy more electrons which is half sub-shell occupation thus it is stable and ionization increases to remove them. (np^3)

→ fully filled > half filled > Partial filled
Most stable stable Unstable.

• $p = 6$
• $d = 10$

$p = 3$
 $d = 5$

$p = 1, 2, 4, 5$
 $d = 1, 2, 3, 4, 6, 7, 8, 9$

FACTORS :-

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(1) Nuclear Charge:- $\propto 2(x^2)$

• As nuclear charge increase force of attraction by nucleus increases thus ionization energy increases.

• As nuclear charge is described by

$$C = k q_1 q_2 / r^2$$

P
-- N.C \propto IE
-- A.R \propto $1/IE$
-- S.E \propto $1/IE$
-- S.R \propto $1/IE$

(2) Atomic radii:-

(1) Atomic radii decreases along period thus ionization also increases due to increase in charge.

(2) Atomic radii increases along group thus ionization decreases.

(3) Shielding effect:-

(1) Increase in shielding effect along group decreases ionization energy as nuclear attraction becomes weak.

(2) It remains constant along period thus no effect on

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④ Spin Repulsion :-

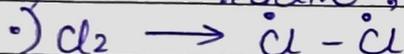
① When p is half filled, e^- repel each other which excites or increase their energy, made easy to remove thus, ionization decreases.

② / \rightarrow Big gap shows inner e^- are removed thus more energy is needed.

FREE RADICALS :-

① A free radical is an atom that bears unpaired or lone electrons in valance shell.

② It is reactive, activated, bearing dot in structure



① Deduction of position based on periodic table :-
(ionization energy)

① Trends :-

\rightarrow Group: IE decreases.

\rightarrow Period: IE increases except of few exception.

② Periodic table Organization :-

\rightarrow Some IE elements are grouped in same column. Eg chemical properties can also be determined.

MODERN MATERIALS :-

"Semi-conductors" are materials that possesses character like metal as well as non-metal.

• Valance-band :- Describes energy level of e^- in a valance shell excites and move out of atom.

• Conduction-band :- Area where excited e^- went. Elect need energy to go to conduction band.

Dated: _____

-) Metals :- No energy is needed for e^- to move to conduction band from valence band.
-) Non metals :- Need so much energy to move to electrical conducting band from valence band, that's why they usually don't conduct electricity.
-) Semi-conductor :- Energy is provided to move from valence band to conduction band through a hole-pair by process 'excitation'.

•) Types of Semi-conductor :

- 1) Intrinsic :- Pure semi conductor, Si , Ge .
- 2) Extrinsic :- They are made intentionally to enhance conductivity.
→ Trivalent or tetravalent electrons are used to for silicon enhancement.

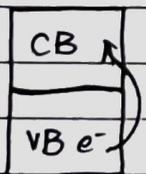
→ In 10^6 atoms of Si , 1 atom of either Boron or P is added. This process is "doping". And impurity is "dopant".

Application : Transistors, gates etc..

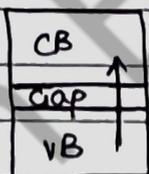
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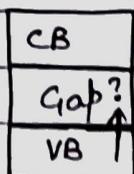
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Conductor



Semi-C



Insulator

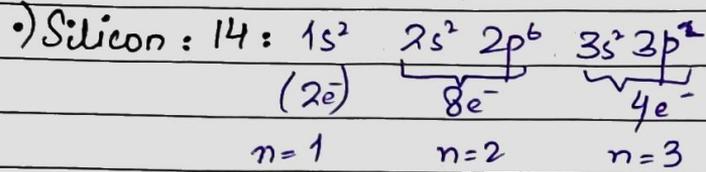
•) Semi-C will absorb energy and then it moves to CB from VB after covering Gap of band.

•) Insulators have gap and high amount of energy is needed to cover it by excited e^- . Thus, insulators can not conduct it.

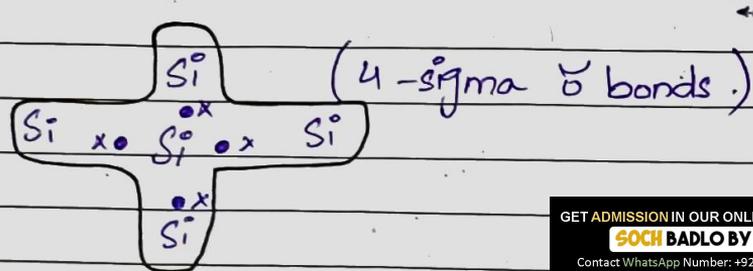
•) Band Gap $\propto \frac{1}{\text{conductivity}}$.

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Semiconductor elect activity can be controlled by increasing or decreasing temperature.



S-subshell bond = sigma bond.



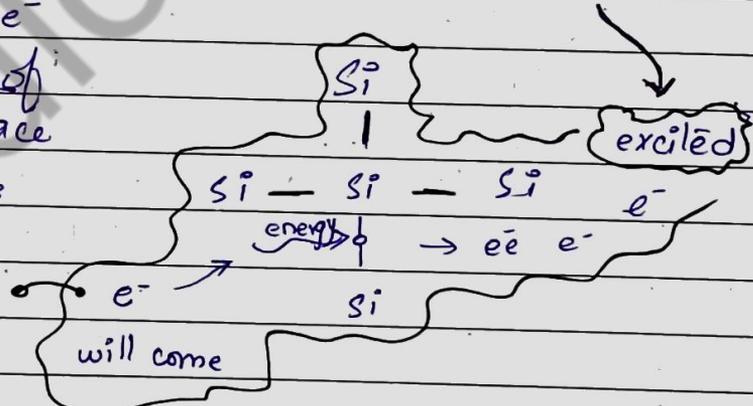
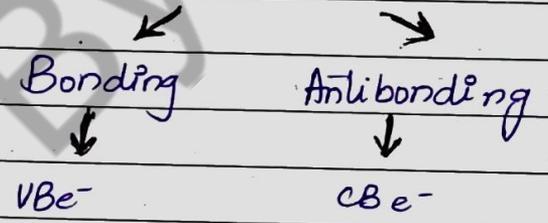
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→ Valence bond e⁻ = 4e⁻

→ energy is given to Si-bonds, e⁻ excites and move to region of excited e⁻ leaving a hole-space at behind. Another e⁻ will come to take place.

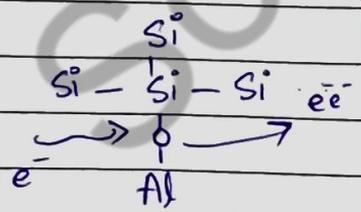
→ Thus e⁻ movement indicates start of conduction.

Molecular orbital theory



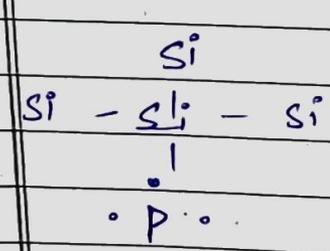
Dopant (Al, P)

P-type



creates hole & conductivity

n-type



extra e⁻ & general conduction.

junction PN
 controls amount of e⁻ passing.